



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:40 PM UTC

PDB ID : 5EBZ / pdb_00005ebz
Title : Crystal structure of human IKK1
Authors : Polley, S.; Passos, D.; Huang, D.; Biswas, T.; Verma, I.; Lyumkis, D.; Ghosh, G.
Deposited on : 2015-10-20
Resolution : 4.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

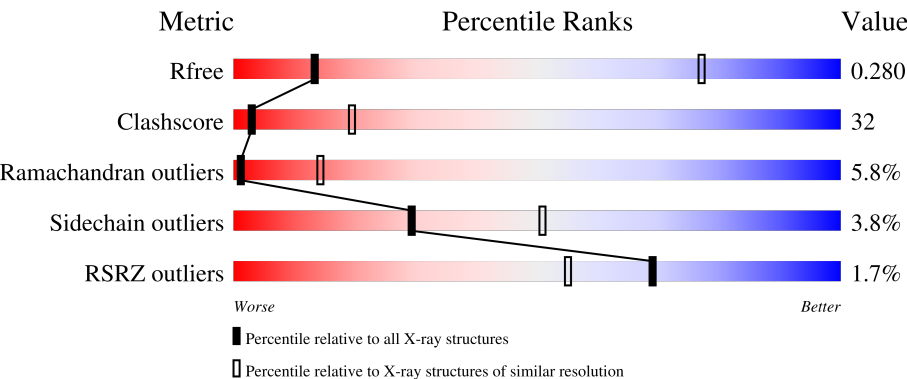
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	655	2% 44% 50% 6%
1	B	655	2% 43% 51% 6%
1	C	655	2% 43% 52% 5%
1	D	655	3% 42% 54% .
1	E	655	2% 41% 53% 5% .

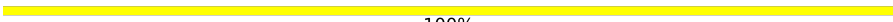
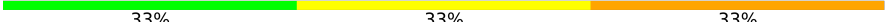
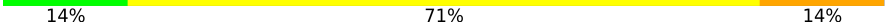
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Mol	Chain	Length	Quality of chain
1	F	655	
1	G	655	
1	H	655	
1	I	655	
1	J	655	
1	K	655	
1	L	655	
2	M	3	
2	N	3	
2	P	3	
2	Q	3	
2	R	3	
2	S	3	
2	U	3	
2	V	3	
2	W	3	
2	X	3	
2	Y	3	
2	Z	3	
2	a	3	
2	b	3	
2	d	3	
2	e	3	
2	f	3	
2	g	3	

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Mol	Chain	Length	Quality of chain
2	h	3	 100%
2	j	3	 100%
2	k	3	 33% 67%
2	l	3	 33% 33% 33%
2	m	3	 67% 33%
2	n	3	 100%
3	O	7	 14% 71% 14%
3	T	7	 43% 57%
3	c	7	 14% 86%
3	i	7	 14% 86%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	j	2	-	-	X	-
4	5TL	A	701	-	X	-	-
4	5TL	B	701	-	X	-	-
4	5TL	C	701	-	X	-	-
4	5TL	D	701	-	X	-	-
4	5TL	E	701	-	X	-	-
4	5TL	F	701	-	X	-	-
4	5TL	G	701	-	X	-	-
4	5TL	H	701	-	X	-	-
4	5TL	I	701	-	X	-	-
4	5TL	J	701	-	X	-	-
4	5TL	K	701	-	X	-	-
4	5TL	L	701	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 65132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inhibitor of nuclear factor kappa-B kinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	B	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	C	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	D	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	E	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	F	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	G	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	H	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	I	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	J	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	K	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			
1	L	655	Total	C	N	O	S	0	0	0
			5263	3348	905	971	39			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASP	-	expression tag	UNP O15111
A	7	PRO	-	expression tag	UNP O15111
A	8	GLU	-	expression tag	UNP O15111
A	9	PHE	-	expression tag	UNP O15111
A	176	GLU	SER	engineered mutation	UNP O15111

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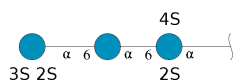
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLU	SER	engineered mutation	UNP O15111
A	268	ILE	VAL	variant	UNP O15111
B	6	ASP	-	expression tag	UNP O15111
B	7	PRO	-	expression tag	UNP O15111
B	8	GLU	-	expression tag	UNP O15111
B	9	PHE	-	expression tag	UNP O15111
B	176	GLU	SER	engineered mutation	UNP O15111
B	180	GLU	SER	engineered mutation	UNP O15111
B	268	ILE	VAL	variant	UNP O15111
C	6	ASP	-	expression tag	UNP O15111
C	7	PRO	-	expression tag	UNP O15111
C	8	GLU	-	expression tag	UNP O15111
C	9	PHE	-	expression tag	UNP O15111
C	176	GLU	SER	engineered mutation	UNP O15111
C	180	GLU	SER	engineered mutation	UNP O15111
C	268	ILE	VAL	variant	UNP O15111
D	6	ASP	-	expression tag	UNP O15111
D	7	PRO	-	expression tag	UNP O15111
D	8	GLU	-	expression tag	UNP O15111
D	9	PHE	-	expression tag	UNP O15111
D	176	GLU	SER	engineered mutation	UNP O15111
D	180	GLU	SER	engineered mutation	UNP O15111
D	268	ILE	VAL	variant	UNP O15111
E	6	ASP	-	expression tag	UNP O15111
E	7	PRO	-	expression tag	UNP O15111
E	8	GLU	-	expression tag	UNP O15111
E	9	PHE	-	expression tag	UNP O15111
E	176	GLU	SER	engineered mutation	UNP O15111
E	180	GLU	SER	engineered mutation	UNP O15111
E	268	ILE	VAL	variant	UNP O15111
F	6	ASP	-	expression tag	UNP O15111
F	7	PRO	-	expression tag	UNP O15111
F	8	GLU	-	expression tag	UNP O15111
F	9	PHE	-	expression tag	UNP O15111
F	176	GLU	SER	engineered mutation	UNP O15111
F	180	GLU	SER	engineered mutation	UNP O15111
F	268	ILE	VAL	variant	UNP O15111
G	6	ASP	-	expression tag	UNP O15111
G	7	PRO	-	expression tag	UNP O15111
G	8	GLU	-	expression tag	UNP O15111
G	9	PHE	-	expression tag	UNP O15111
G	176	GLU	SER	engineered mutation	UNP O15111

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Chain	Residue	Modelled	Actual	Comment	Reference
G	180	GLU	SER	engineered mutation	UNP O15111
G	268	ILE	VAL	variant	UNP O15111
H	6	ASP	-	expression tag	UNP O15111
H	7	PRO	-	expression tag	UNP O15111
H	8	GLU	-	expression tag	UNP O15111
H	9	PHE	-	expression tag	UNP O15111
H	176	GLU	SER	engineered mutation	UNP O15111
H	180	GLU	SER	engineered mutation	UNP O15111
H	268	ILE	VAL	variant	UNP O15111
I	6	ASP	-	expression tag	UNP O15111
I	7	PRO	-	expression tag	UNP O15111
I	8	GLU	-	expression tag	UNP O15111
I	9	PHE	-	expression tag	UNP O15111
I	176	GLU	SER	engineered mutation	UNP O15111
I	180	GLU	SER	engineered mutation	UNP O15111
I	268	ILE	VAL	variant	UNP O15111
J	6	ASP	-	expression tag	UNP O15111
J	7	PRO	-	expression tag	UNP O15111
J	8	GLU	-	expression tag	UNP O15111
J	9	PHE	-	expression tag	UNP O15111
J	176	GLU	SER	engineered mutation	UNP O15111
J	180	GLU	SER	engineered mutation	UNP O15111
J	268	ILE	VAL	variant	UNP O15111
K	6	ASP	-	expression tag	UNP O15111
K	7	PRO	-	expression tag	UNP O15111
K	8	GLU	-	expression tag	UNP O15111
K	9	PHE	-	expression tag	UNP O15111
K	176	GLU	SER	engineered mutation	UNP O15111
K	180	GLU	SER	engineered mutation	UNP O15111
K	268	ILE	VAL	variant	UNP O15111
L	6	ASP	-	expression tag	UNP O15111
L	7	PRO	-	expression tag	UNP O15111
L	8	GLU	-	expression tag	UNP O15111
L	9	PHE	-	expression tag	UNP O15111
L	176	GLU	SER	engineered mutation	UNP O15111
L	180	GLU	SER	engineered mutation	UNP O15111
L	268	ILE	VAL	variant	UNP O15111

- Molecule 2 is an oligosaccharide called 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	N	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	P	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	Q	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	R	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	S	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	U	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	V	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	W	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	X	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	Y	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	Z	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	a	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	b	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	d	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	e	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	f	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	g	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	h	3	Total	C	O	S	0	0	0
			50	18	28	4			

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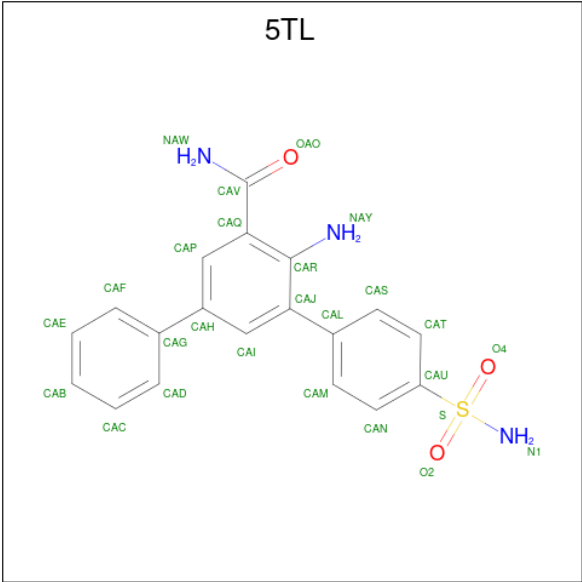
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	j	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	k	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	l	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	m	3	Total	C	O	S	0	0	0
			50	18	28	4			
2	n	3	Total	C	O	S	0	0	0
			50	18	28	4			

- Molecule 3 is an oligosaccharide called [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	O	7	Total	C	O	S	0	0	0
			116	42	62	12			
3	T	7	Total	C	O	S	0	0	0
			116	42	62	12			
3	c	7	Total	C	O	S	0	0	0
			116	42	62	12			
3	i	7	Total	C	O	S	0	0	0
			116	42	62	12			

- Molecule 4 is 2-azanyl-5-phenyl-3-(4-sulfamoylphenyl)benzamide (CCD ID: 5TL) (formula: C₁₉H₁₇N₃O₃S).

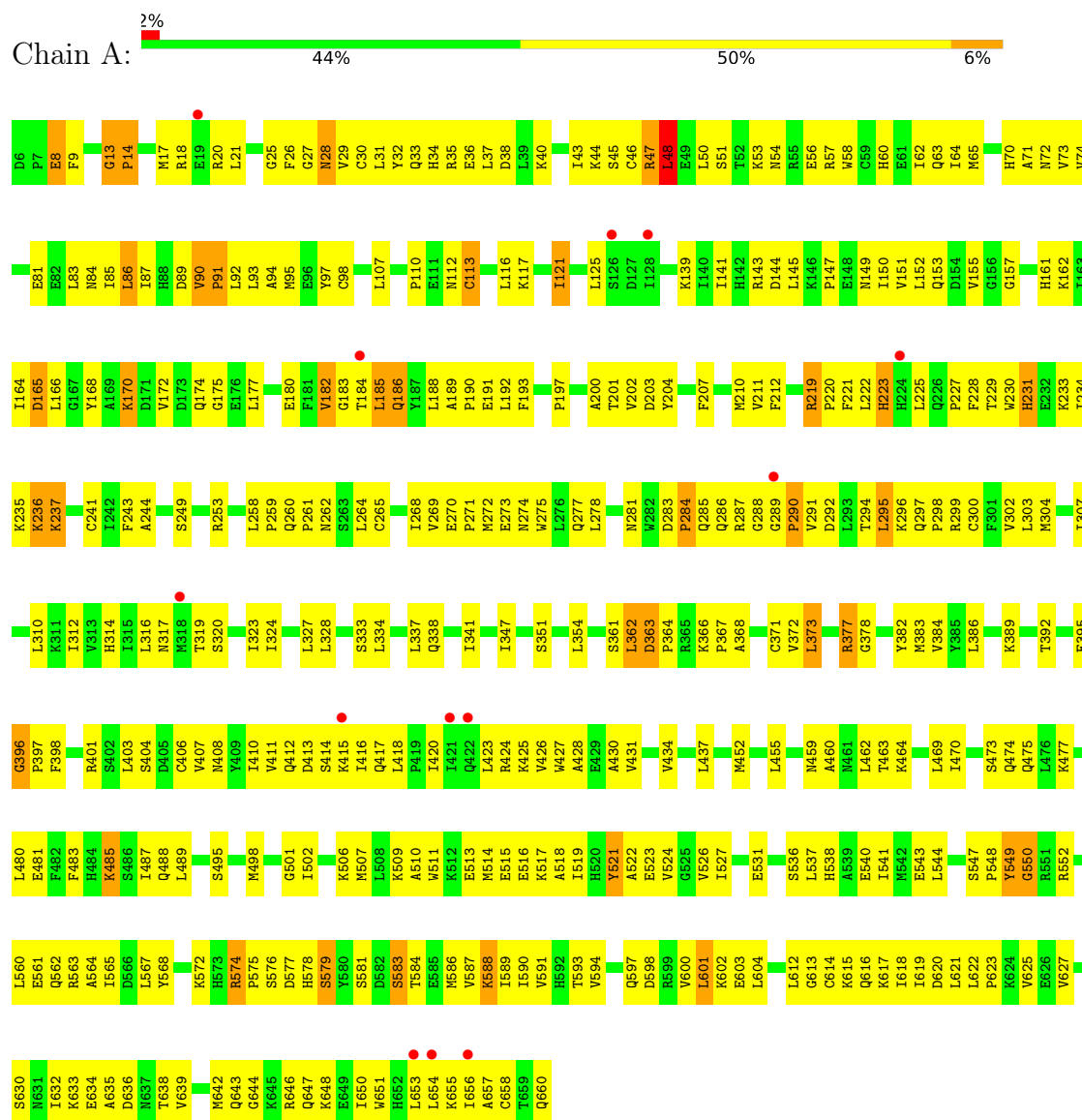


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	B	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	C	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	D	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	E	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	F	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	G	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	H	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	I	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	J	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	K	1	Total	C	N	O	S	0	0
			26	19	3	3	1		
4	L	1	Total	C	N	O	S	0	0
			26	19	3	3	1		

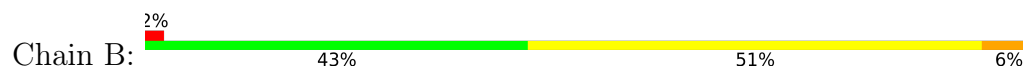
3 Residue-property plots

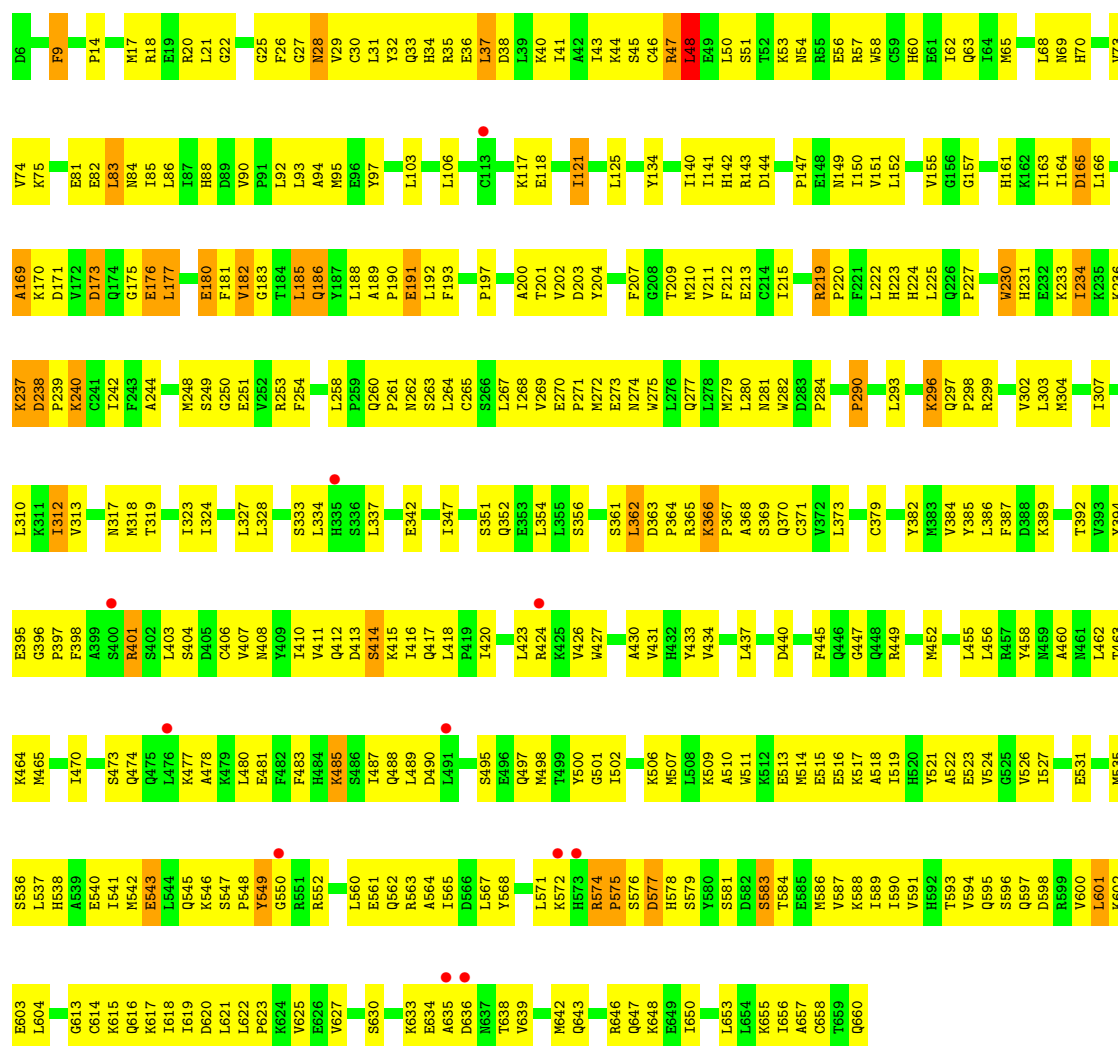
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

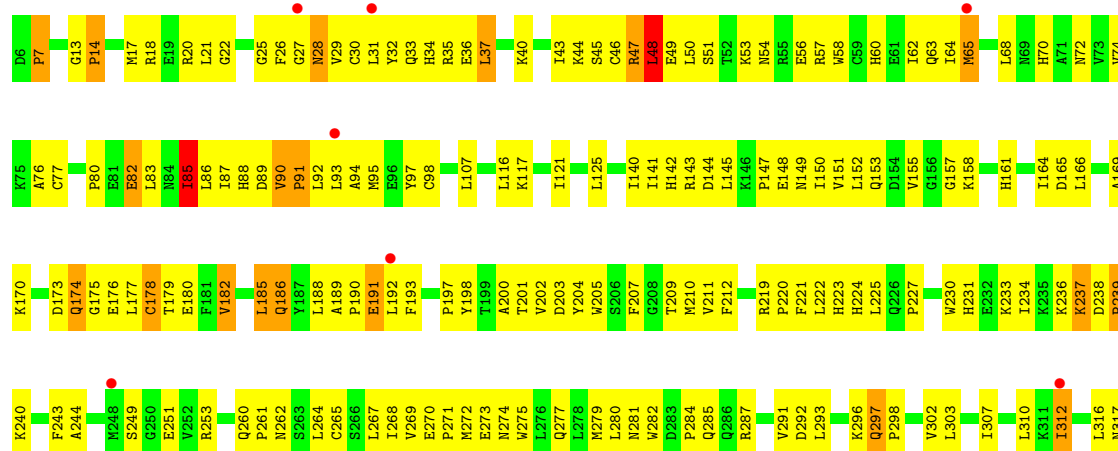


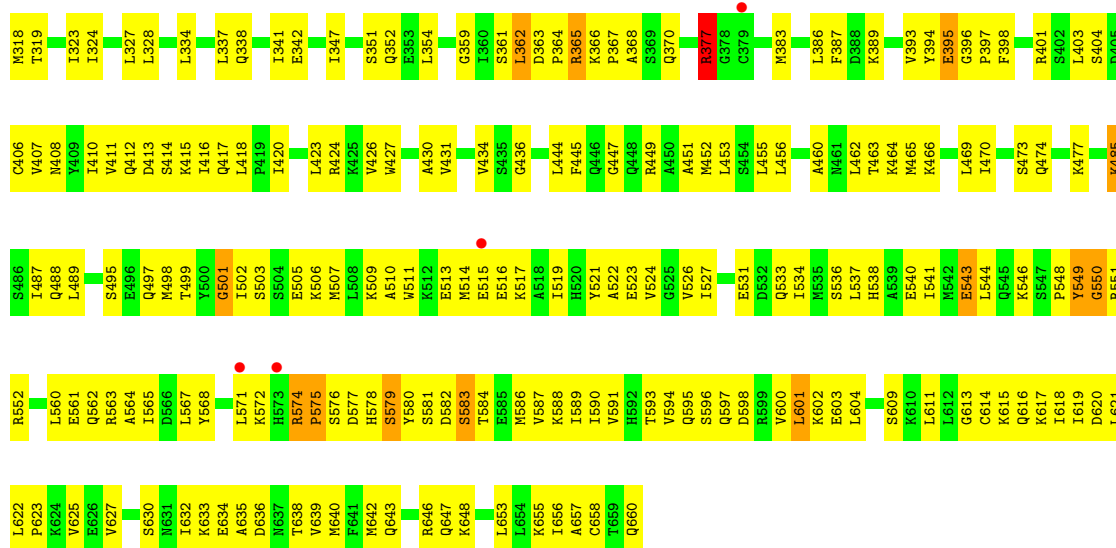
- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



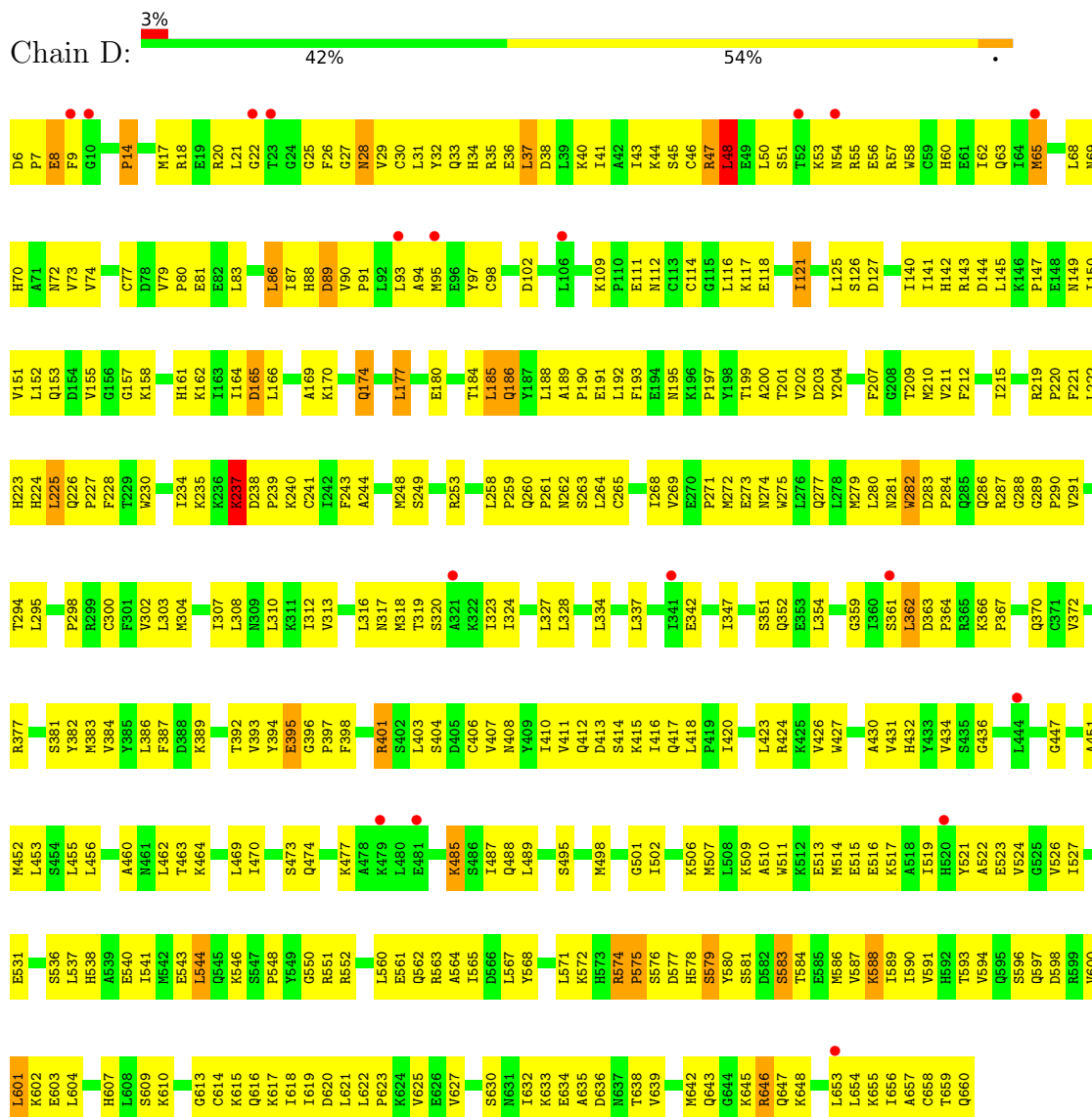


● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

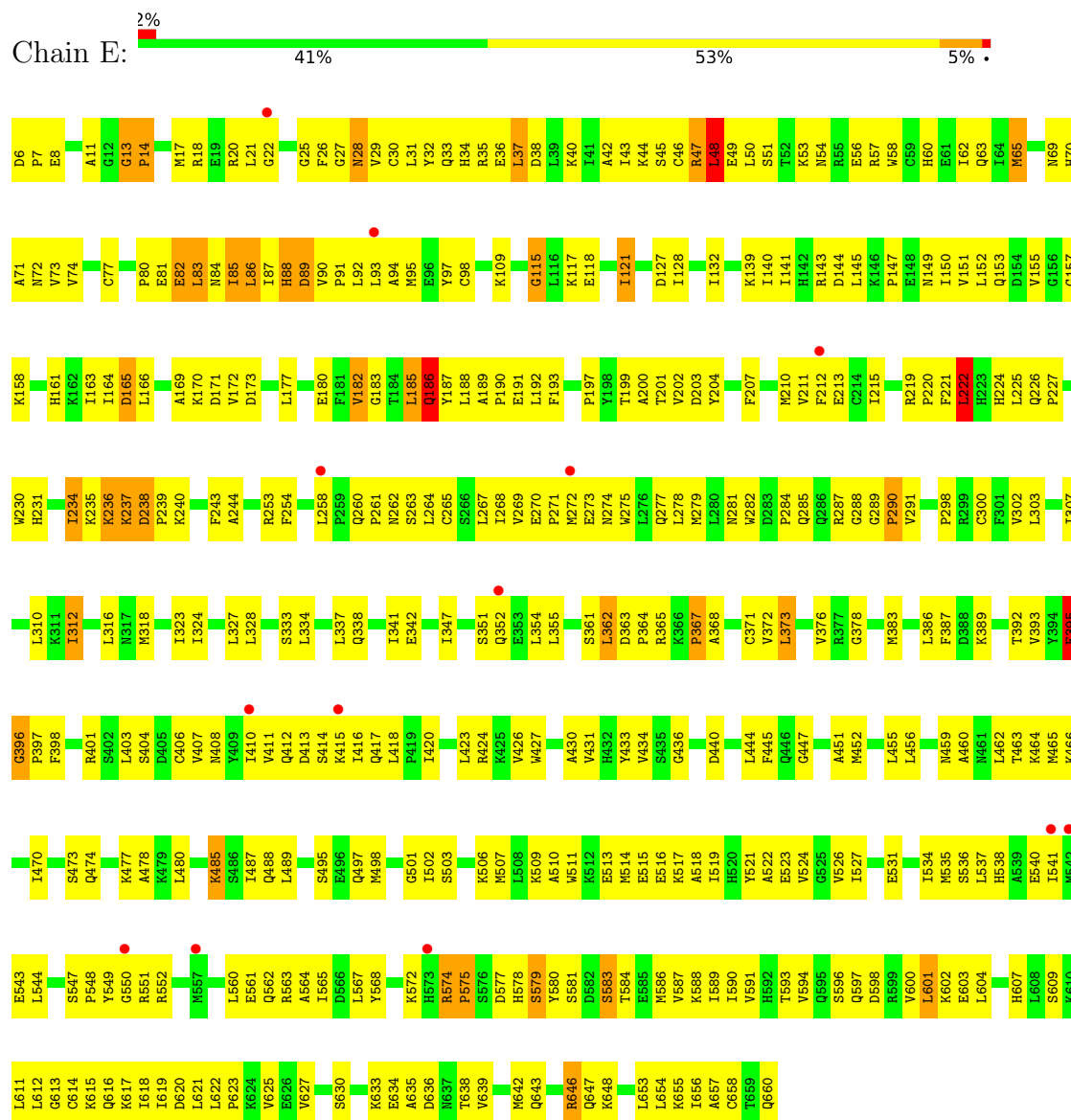




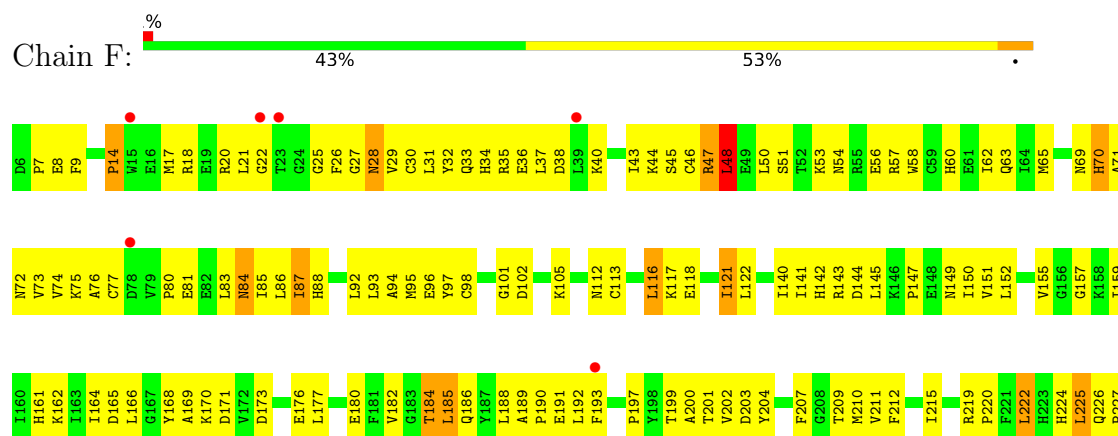
● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

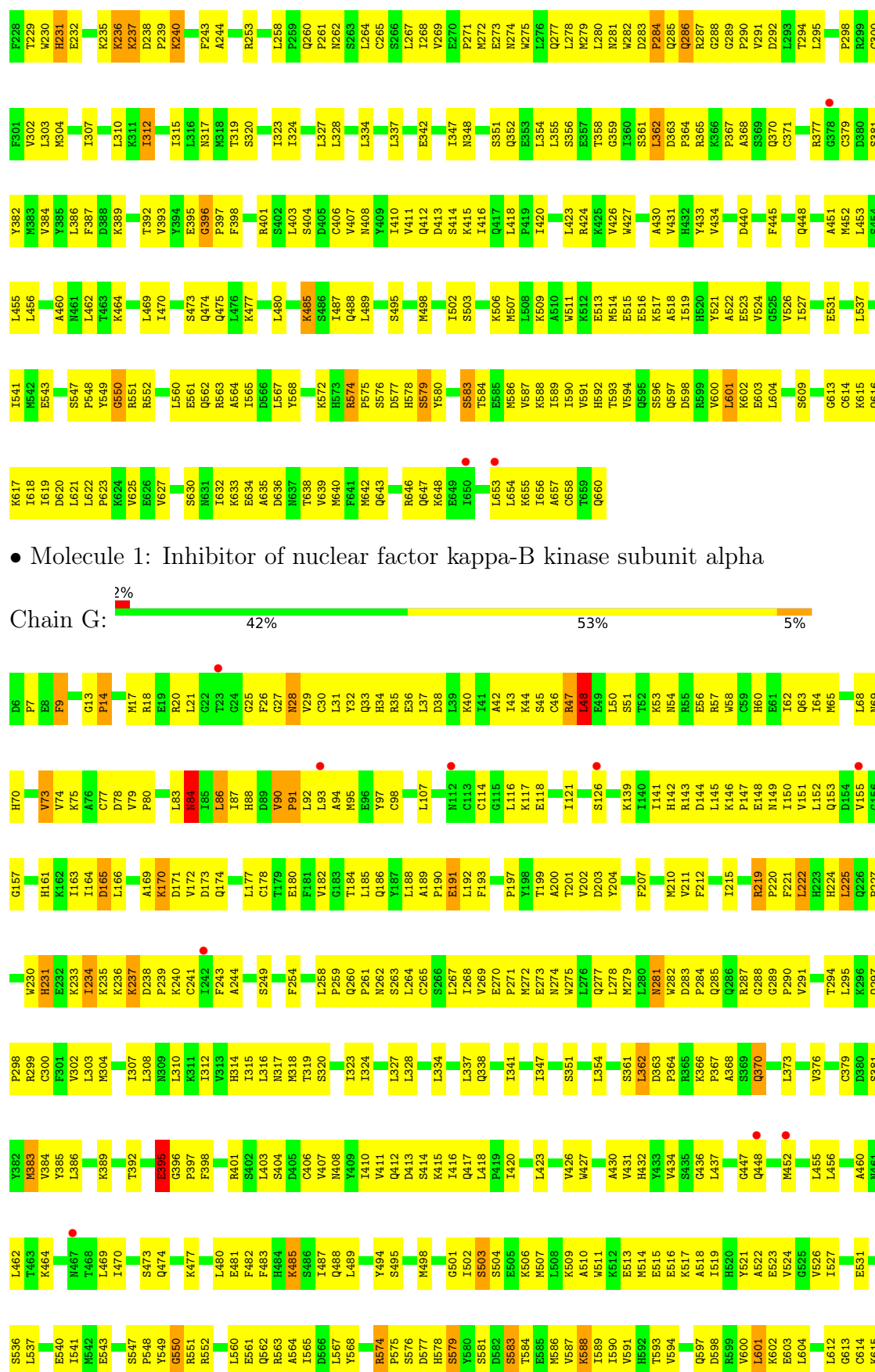


• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



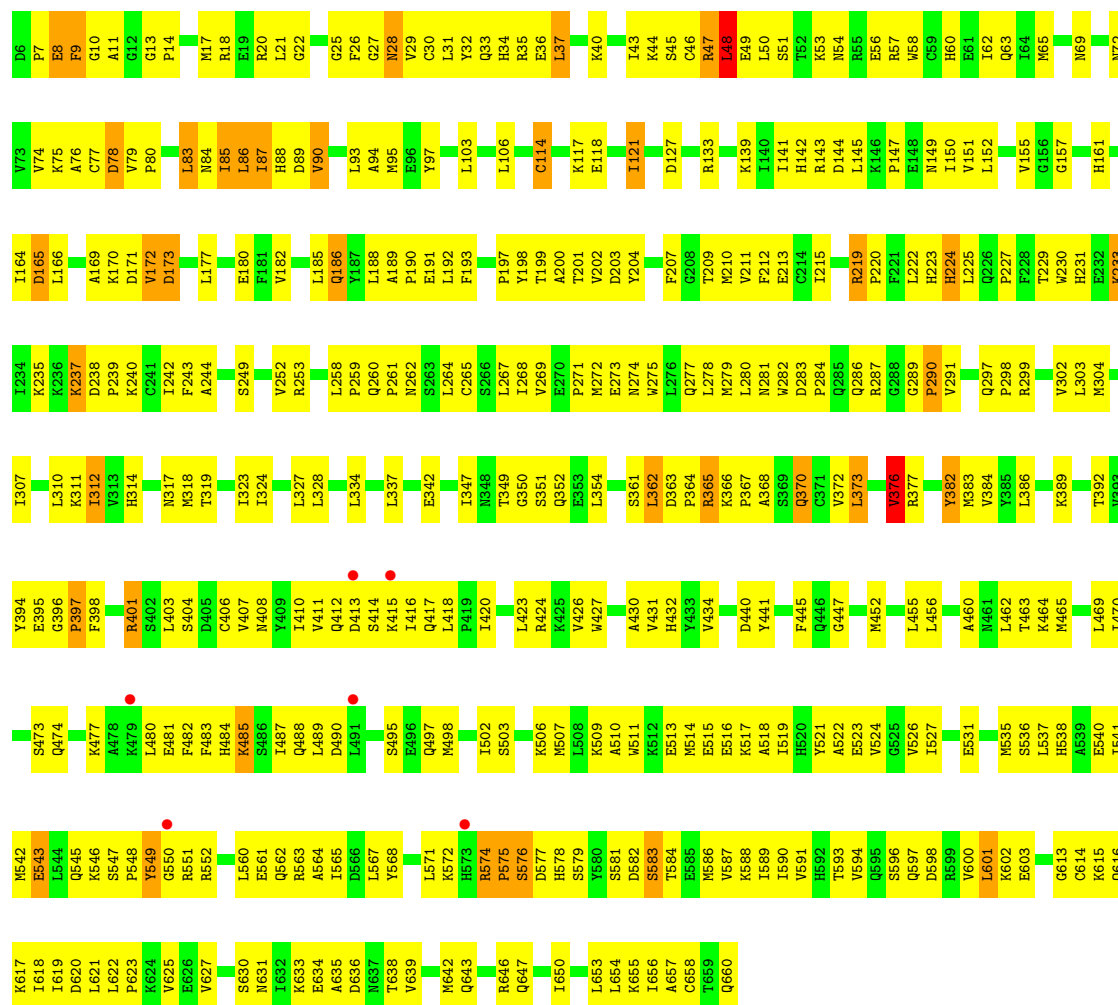
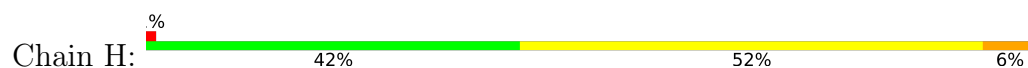
• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



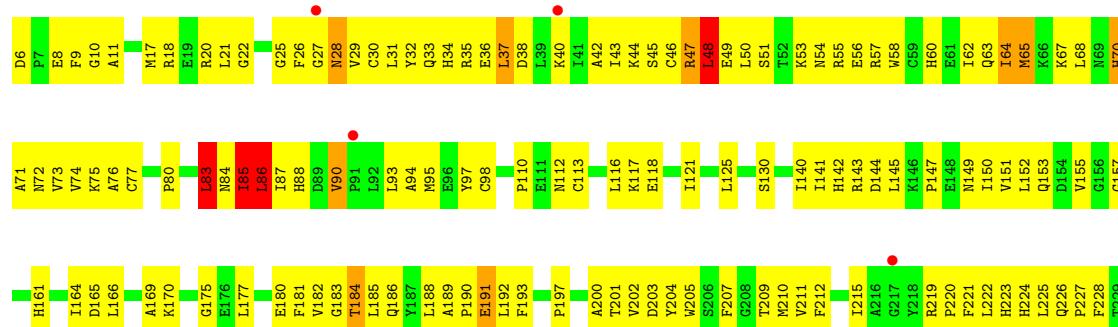


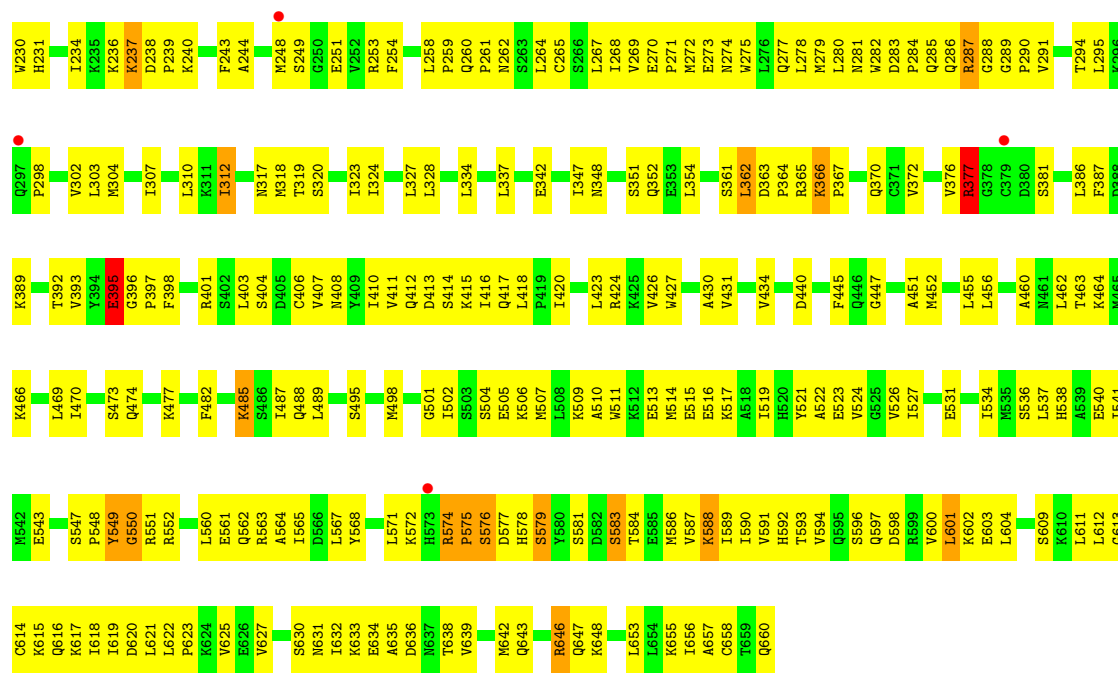


● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



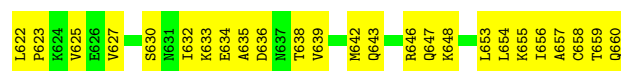
● Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



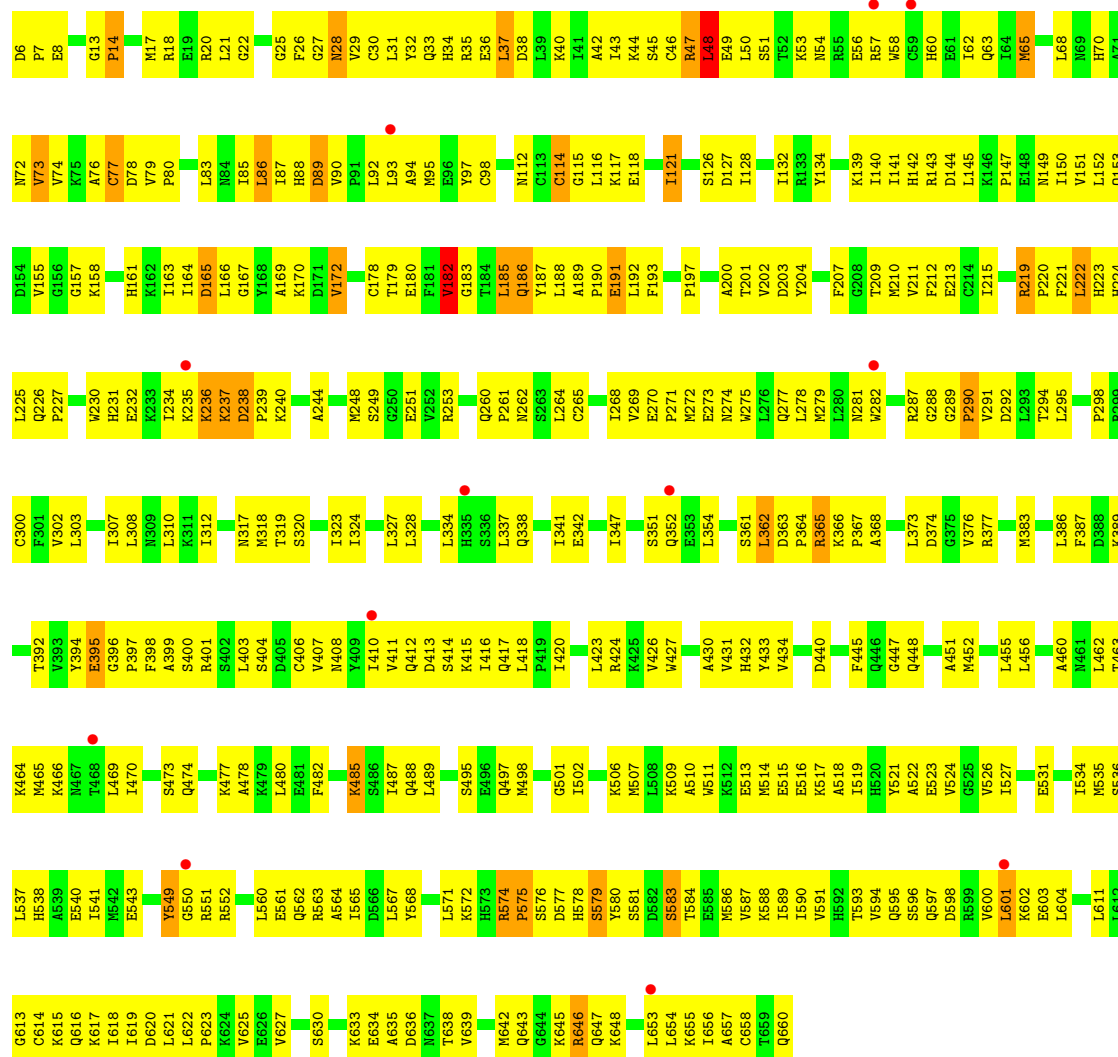


- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha

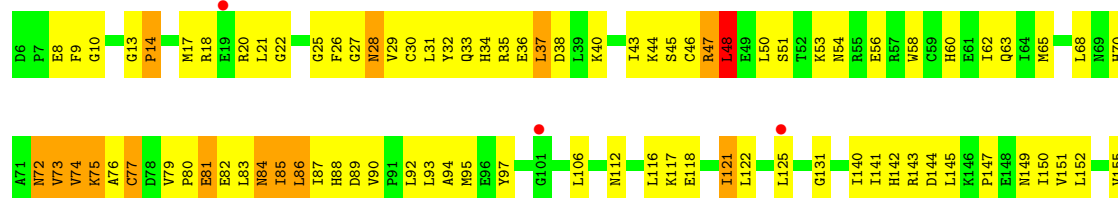


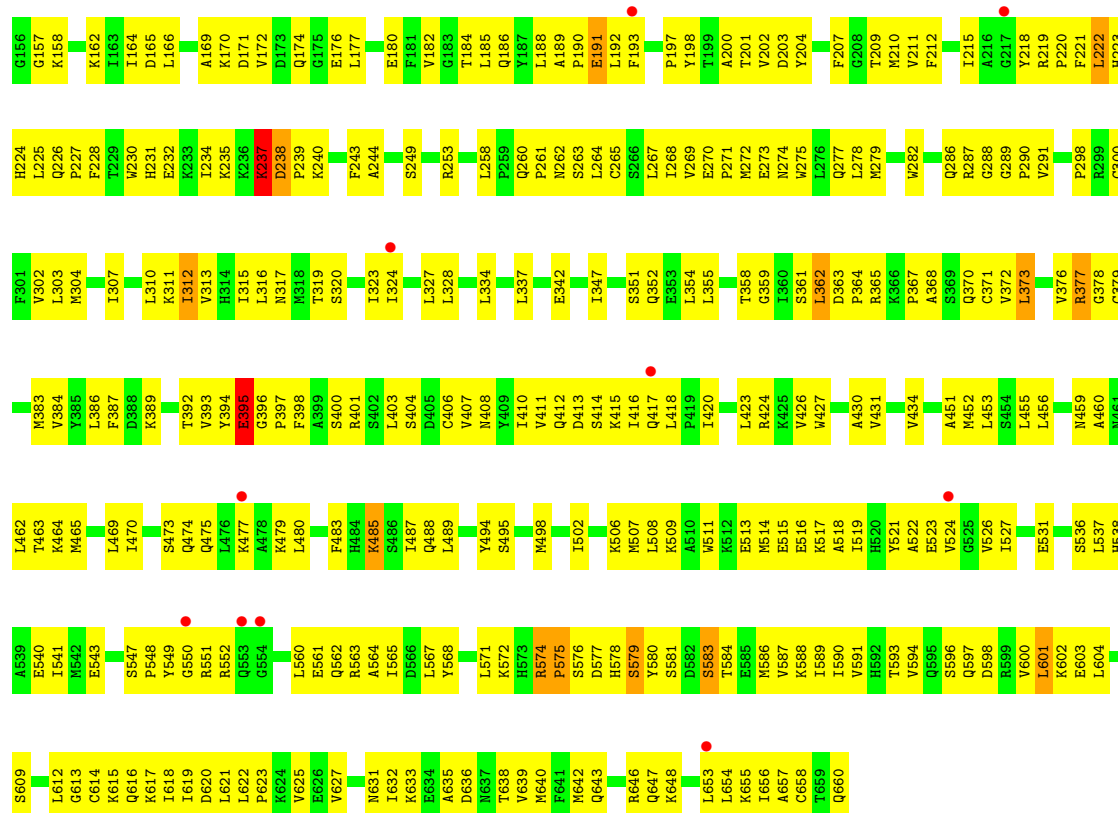


• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit alpha





- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain M: 33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain N: 33% 67%

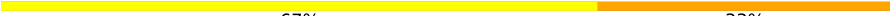


- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain P: 33% 33% 33%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain Q:  67% 33%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain R:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain S:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain U:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain V:  33% 33% 33%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain W:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain X:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain Y:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain Z:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain a:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain b:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain d:  100%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain e:  33% 67%

5LS1
GLC2
PDX3

- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain f:  33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain g: 33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain h: 100%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain j: 100%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain k: 33% 67%



- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain l: 33% 33% 33%

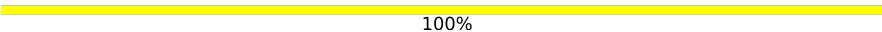


- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain m: 67% 33%

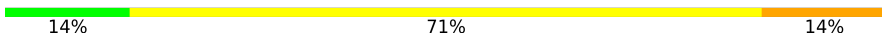


- Molecule 2: 2,3-di-O-sulfo-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain n:  100%

5LS1
GLC2
PDX3

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain O:  14% 71% 14%

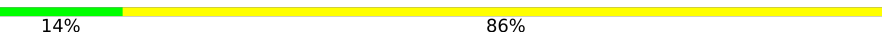
5LS1
5TJ2
5TM3
5TJ4
24K5
5TK6
5TH7

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain T:  43% 57%

5LS1
5TJ2
5TM3
5TJ4
24K5
5TK6
5TH7

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain c:  14% 86%

5LS1
5TJ2
5TM3
5TJ4
24K5
5TK6
5TH7

- Molecule 3: [(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-2,4-bis(oxidanyl)-5-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-(2S,3R,4R,5S,6R)-6-(hydroxymethyl)-5-oxidanylsulfanyloxy-oxane-2,3,4-triol-(1-6)-2-O-sulfo-alpha-D-glucopyranose-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-b

is(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-[(2S,3R,4S,5R,6R)-6-(hydroxymethyl)-2,5-bis(oxidanyl)-4-oxidanylsulfanyloxy-oxan-3-yl] hydrogen sulfate-(1-6)-[(2R,3R,4R,5R,6S)-2-(hydroxymethyl)-5,6-bis(oxidanyl)-3-oxidanylsulfanyloxy-oxan-4-yl] hydrogen sulfate-(1-6)-2,4-di-O-sulfo-alpha-D-glucopyranose

Chain i:

14%

86%

5LS1	5LJ2	5TH3	5TJ4	24K5	5TH6	5TH7
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	174.51Å 186.94Å 275.83Å 90.00° 98.84° 90.00°	Depositor
Resolution (Å)	29.94 – 4.50 29.94 – 4.50	Depositor EDS
% Data completeness (in resolution range)	68.1 (29.94-4.50) 82.6 (29.94-4.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 4.45Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.238 , 0.276 0.241 , 0.280	Depositor DCC
R_{free} test set	4167 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	178.9	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 444.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	65132	wwPDB-VP
Average B, all atoms (Å ²)	267.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5998e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 5TJ, Z4K, 5TK, PDX, 5TH, 5TM, 5LS, 5TL, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/5370	0.73	2/7239 (0.0%)
1	B	0.30	0/5370	0.73	0/7239
1	C	0.31	0/5370	0.72	0/7239
1	D	0.30	0/5370	0.74	0/7239
1	E	0.33	0/5370	0.72	1/7239 (0.0%)
1	F	0.30	0/5370	0.74	1/7239 (0.0%)
1	G	0.35	0/5370	0.72	0/7239
1	H	0.30	0/5370	0.72	0/7239
1	I	0.31	0/5370	0.73	1/7239 (0.0%)
1	J	0.30	0/5370	0.73	1/7239 (0.0%)
1	K	0.32	0/5370	0.72	1/7239 (0.0%)
1	L	0.30	0/5370	0.72	0/7239
All	All	0.31	0/64440	0.73	7/86868 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	ASP	CA-C-N	6.10	125.58	119.24
1	A	363	ASP	C-N-CA	6.10	125.58	119.24
1	E	8	GLU	CB-CA-C	-5.85	109.85	116.63
1	I	86	LEU	CB-CA-C	-5.61	109.12	115.79
1	J	234	ILE	N-CA-C	-5.29	107.56	112.43
1	F	84	ASN	CB-CA-C	-5.17	109.06	115.89
1	K	86	LEU	CB-CA-C	-5.15	109.66	115.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5263	0	5320	370	0
1	B	5263	0	5320	371	0
1	C	5263	0	5320	350	0
1	D	5263	0	5320	360	0
1	E	5263	0	5320	359	0
1	F	5263	0	5320	337	0
1	G	5263	0	5320	389	0
1	H	5263	0	5320	345	0
1	I	5263	0	5320	341	0
1	J	5263	0	5320	343	0
1	K	5263	0	5320	364	0
1	L	5263	0	5320	363	0
2	M	50	0	19	0	0
2	N	50	0	19	1	0
2	P	50	0	19	1	0
2	Q	50	0	19	4	0
2	R	50	0	19	1	0
2	S	50	0	19	3	0
2	U	50	0	19	0	0
2	V	50	0	19	1	0
2	W	50	0	19	1	0
2	X	50	0	19	1	0
2	Y	50	0	19	2	0
2	Z	50	0	19	1	0
2	a	50	0	19	0	0
2	b	50	0	19	1	0
2	d	50	0	19	1	0
2	e	50	0	19	1	0
2	f	50	0	19	0	0
2	g	50	0	19	0	0
2	h	50	0	19	4	0
2	j	50	0	19	6	0
2	k	50	0	19	0	0
2	l	50	0	19	1	0
2	m	50	0	19	2	0
2	n	50	0	19	2	0
3	O	116	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	116	0	0	5	0
3	c	116	0	0	0	0
3	i	116	0	0	0	0
4	A	26	0	0	3	0
4	B	26	0	0	2	0
4	C	26	0	0	4	0
4	D	26	0	0	2	0
4	E	26	0	0	3	0
4	F	26	0	0	6	0
4	G	26	0	0	4	0
4	H	26	0	0	2	0
4	I	26	0	0	6	0
4	J	26	0	0	2	0
4	K	26	0	0	3	0
4	L	26	0	0	2	0
All	All	65132	0	64296	4141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (4141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:701:5TL:NAY	4:J:701:5TL:CAS	1.99	1.20
4:G:701:5TL:NAY	4:G:701:5TL:CAS	2.00	1.18
4:D:701:5TL:NAY	4:D:701:5TL:CAS	1.99	1.17
4:K:701:5TL:CAS	4:K:701:5TL:NAY	2.00	1.17
4:A:701:5TL:NAY	4:A:701:5TL:CAS	2.00	1.16
4:B:701:5TL:NAY	4:B:701:5TL:CAS	2.00	1.16
4:F:701:5TL:CAS	4:F:701:5TL:NAY	1.98	1.15
4:E:701:5TL:NAY	4:E:701:5TL:CAS	1.99	1.14
4:I:701:5TL:NAY	4:I:701:5TL:CAS	1.99	1.14
4:C:701:5TL:CAS	4:C:701:5TL:NAY	1.99	1.12
4:H:701:5TL:NAY	4:H:701:5TL:CAS	2.00	1.13
4:L:701:5TL:NAY	4:L:701:5TL:CAS	1.99	1.12
1:I:185:LEU:HD11	1:I:188:LEU:HB3	1.38	1.03
1:C:477:LYS:HB2	1:C:524:VAL:HG21	1.43	1.01
1:J:227:PRO:HA	1:J:230:TRP:HB2	1.44	1.00
1:L:185:LEU:HD11	1:L:188:LEU:HB3	1.42	1.00
1:A:227:PRO:HA	1:A:230:TRP:HB3	1.42	0.99
1:L:563:ARG:HH12	2:n:2:GLC:H2	1.27	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:HG21	1:C:95:MET:HE3	1.41	0.98
1:L:222:LEU:HB3	1:L:225:LEU:HD12	1.42	0.98
1:J:13:GLY:H	1:J:14:PRO:HD3	1.26	0.96
1:F:434:VAL:HG13	1:F:593:THR:HG21	1.46	0.96
1:H:142:HIS:ND1	1:H:169:ALA:HB2	1.81	0.96
1:A:13:GLY:H	1:A:14:PRO:HD3	1.30	0.95
1:L:434:VAL:HG13	1:L:593:THR:HG21	1.46	0.95
1:C:434:VAL:HG13	1:C:593:THR:HG21	1.47	0.95
1:F:260:GLN:HE21	1:F:261:PRO:HA	1.32	0.95
1:B:185:LEU:HD11	1:B:188:LEU:HB3	1.47	0.94
1:A:185:LEU:HD11	1:A:188:LEU:HB3	1.47	0.94
1:C:260:GLN:HE21	1:C:261:PRO:HA	1.33	0.94
1:K:260:GLN:HE21	1:K:261:PRO:HA	1.32	0.94
1:L:477:LYS:HB2	1:L:524:VAL:HG21	1.50	0.94
1:I:260:GLN:HE21	1:I:261:PRO:HA	1.33	0.94
1:A:396:GLY:H	1:A:397:PRO:HD3	1.29	0.94
1:E:260:GLN:HE21	1:E:261:PRO:HA	1.33	0.94
1:G:260:GLN:HE21	1:G:261:PRO:HA	1.32	0.94
1:L:260:GLN:HE21	1:L:261:PRO:HA	1.33	0.93
1:C:227:PRO:HA	1:C:230:TRP:HB3	1.49	0.93
1:I:477:LYS:HB2	1:I:524:VAL:HG21	1.48	0.93
1:J:477:LYS:HB2	1:J:524:VAL:HG21	1.50	0.93
1:E:328:LEU:HD13	1:E:368:ALA:HB1	1.48	0.93
1:A:260:GLN:HE21	1:A:261:PRO:HA	1.34	0.92
1:G:328:LEU:HD13	1:G:368:ALA:HB1	1.51	0.92
1:B:577:ASP:H	1:F:579:SER:HB3	1.32	0.92
1:H:260:GLN:HE21	1:H:261:PRO:HA	1.34	0.92
1:B:260:GLN:HE21	1:B:261:PRO:HA	1.35	0.92
1:B:434:VAL:HG13	1:B:593:THR:HG21	1.52	0.91
1:A:462:LEU:HD22	1:A:618:ILE:HG23	1.52	0.91
1:H:50:LEU:HD22	1:H:90:VAL:HG11	1.51	0.91
1:D:185:LEU:HD11	1:D:188:LEU:HB3	1.53	0.91
1:D:260:GLN:HE21	1:D:261:PRO:HA	1.34	0.91
1:K:185:LEU:HD11	1:K:188:LEU:HB3	1.53	0.90
1:J:260:GLN:HE21	1:J:261:PRO:HA	1.34	0.90
1:B:290:PRO:HB2	1:B:299:ARG:HB2	1.53	0.90
1:E:74:VAL:HG21	1:E:95:MET:HE3	1.53	0.90
1:F:462:LEU:HD22	1:F:618:ILE:HG23	1.52	0.90
1:F:477:LYS:HB2	1:F:524:VAL:HG21	1.53	0.89
1:C:395:GLU:HG2	1:C:397:PRO:HD3	1.52	0.89
1:I:278:LEU:HD23	1:I:288:GLY:HA2	1.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:434:VAL:HG13	1:H:593:THR:HG21	1.55	0.89
1:E:316:LEU:HB2	1:E:383:MET:HE2	1.53	0.89
1:E:373:LEU:HB2	1:E:378:GLY:HA3	1.56	0.88
1:F:186:GLN:HE22	1:F:227:PRO:HD3	1.38	0.88
1:I:366:LYS:HD2	1:I:367:PRO:HD2	1.54	0.88
1:E:477:LYS:HB2	1:E:524:VAL:HG21	1.55	0.88
1:H:373:LEU:HD21	1:H:382:TYR:HB2	1.55	0.87
1:D:219:ARG:HD3	1:D:224:HIS:H	1.39	0.87
1:D:395:GLU:HG3	1:D:397:PRO:HD3	1.57	0.87
1:K:477:LYS:HB2	1:K:524:VAL:HG21	1.57	0.86
2:m:2:GLC:H62	2:m:3:PDX:H5	1.57	0.86
1:B:363:ASP:HB3	1:B:370:GLN:HE22	1.39	0.86
1:F:278:LEU:HD23	1:F:288:GLY:HA2	1.57	0.86
1:L:462:LEU:HD22	1:L:618:ILE:HG23	1.56	0.86
1:A:112:ASN:HD22	1:A:116:LEU:HA	1.40	0.86
1:B:227:PRO:HA	1:B:230:TRP:HB2	1.58	0.86
1:I:434:VAL:HG13	1:I:593:THR:HG21	1.54	0.86
1:E:396:GLY:H	1:E:397:PRO:HD3	1.40	0.85
1:F:219:ARG:HE	1:F:224:HIS:H	1.23	0.85
1:B:73:VAL:HG23	1:B:163:ILE:HB	1.55	0.85
1:J:222:LEU:HD23	1:J:234:ILE:HD11	1.59	0.85
1:K:595:GLN:HE21	2:l:3:PDX:H6C1	1.42	0.84
1:E:434:VAL:HG13	1:E:593:THR:HG21	1.59	0.84
1:F:237:LYS:HG3	1:F:282:TRP:HB2	1.57	0.84
1:C:185:LEU:HD11	1:C:188:LEU:HB3	1.57	0.84
1:H:477:LYS:HB2	1:H:524:VAL:HG21	1.60	0.84
1:F:227:PRO:HA	1:F:230:TRP:HB3	1.60	0.84
1:C:219:ARG:HH21	1:C:223:HIS:HB2	1.43	0.84
1:D:434:VAL:HG13	1:D:593:THR:HG21	1.60	0.83
1:H:577:ASP:H	1:L:579:SER:HB3	1.43	0.83
1:K:434:VAL:HG13	1:K:593:THR:HG21	1.58	0.83
1:A:434:VAL:HG13	1:A:593:THR:HG21	1.59	0.83
1:D:477:LYS:HB2	1:D:524:VAL:HG21	1.60	0.83
1:K:654:LEU:HD12	1:L:654:LEU:HD12	1.61	0.83
1:C:219:ARG:HE	1:C:223:HIS:HA	1.44	0.82
1:K:502:ILE:HD12	1:L:654:LEU:HD11	1.59	0.82
1:C:86:LEU:HD23	1:C:92:LEU:HD11	1.61	0.82
1:I:502:ILE:HD11	1:J:654:LEU:HD11	1.61	0.82
1:A:477:LYS:HB2	1:A:524:VAL:HG21	1.61	0.82
1:J:462:LEU:HD22	1:J:618:ILE:HG23	1.62	0.82
1:L:65:MET:HB3	1:L:76:ALA:HB2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LEU:H	1:G:230:TRP:HE1	1.25	0.81
1:C:577:ASP:H	1:E:579:SER:HB3	1.46	0.81
1:K:48:LEU:HD13	1:K:48:LEU:H	1.45	0.81
1:B:396:GLY:H	1:B:397:PRO:HD3	1.46	0.81
1:K:185:LEU:HD13	1:K:186:GLN:H	1.45	0.81
1:J:408:ASN:HD21	1:L:26:PHE:HD1	1.27	0.81
1:G:199:THR:HG21	1:G:285:GLN:HE22	1.45	0.81
1:J:74:VAL:HG21	1:J:95:MET:HE3	1.62	0.81
1:E:13:GLY:H	1:E:14:PRO:HD3	1.45	0.81
1:A:395:GLU:HG3	1:A:397:PRO:HD3	1.62	0.81
1:G:220:PRO:O	1:G:243:PHE:HA	1.80	0.81
1:B:48:LEU:H	1:B:48:LEU:HD13	1.46	0.81
1:G:434:VAL:HG13	1:G:593:THR:HG21	1.62	0.80
1:B:477:LYS:HB2	1:B:524:VAL:HG21	1.62	0.80
1:E:654:LEU:HD12	1:F:654:LEU:HD12	1.64	0.80
1:I:48:LEU:HD13	1:I:48:LEU:H	1.47	0.80
1:C:48:LEU:HD13	1:C:48:LEU:H	1.47	0.80
1:C:297:GLN:HG3	1:C:298:PRO:HD2	1.63	0.80
1:G:48:LEU:H	1:G:48:LEU:HD13	1.47	0.80
1:J:434:VAL:HG13	1:J:593:THR:HG21	1.64	0.80
1:K:86:LEU:HD13	1:K:92:LEU:HD11	1.63	0.80
1:H:86:LEU:HD23	1:H:87:ILE:HG13	1.63	0.80
1:D:142:HIS:ND1	1:D:169:ALA:HB2	1.96	0.80
1:G:222:LEU:HB2	1:G:230:TRP:CD1	2.16	0.80
1:L:50:LEU:HD22	1:L:90:VAL:HG11	1.63	0.80
1:G:501:GLY:HA3	1:H:655:LYS:HE2	1.64	0.80
1:G:91:PRO:C	1:G:92:LEU:HD12	2.08	0.79
1:G:290:PRO:HB2	1:G:299:ARG:HB2	1.64	0.79
1:J:431:VAL:HG21	1:J:568:TYR:HB2	1.63	0.79
1:A:236:LYS:H	1:A:236:LYS:HD3	1.46	0.79
1:E:48:LEU:H	1:E:48:LEU:HD13	1.47	0.79
1:H:48:LEU:HD13	1:H:48:LEU:H	1.48	0.79
1:H:238:ASP:HB3	1:H:239:PRO:HD2	1.65	0.79
1:A:48:LEU:HD13	1:A:48:LEU:H	1.48	0.79
1:K:240:LYS:HD2	1:K:277:GLN:HB3	1.63	0.79
1:L:227:PRO:HA	1:L:230:TRP:HB3	1.63	0.79
1:I:577:ASP:H	1:K:579:SER:HB3	1.48	0.78
1:E:318:MET:HE2	1:E:447:GLY:HA3	1.65	0.78
1:A:222:LEU:HB2	1:A:230:TRP:HD1	1.46	0.78
1:C:462:LEU:HD22	1:C:618:ILE:HG23	1.63	0.78
1:D:589:ILE:H	1:D:589:ILE:HD12	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:477:LYS:HB2	1:G:524:VAL:HG21	1.63	0.78
1:J:395:GLU:HG3	1:J:397:PRO:HD3	1.65	0.78
1:L:13:GLY:H	1:L:14:PRO:HD3	1.48	0.78
1:L:237:LYS:HD2	1:L:238:ASP:H	1.47	0.78
1:K:73:VAL:HG23	1:K:163:ILE:HB	1.64	0.78
1:F:395:GLU:HG2	1:F:396:GLY:H	1.49	0.78
1:J:48:LEU:H	1:J:48:LEU:HD13	1.48	0.78
1:G:502:ILE:HD12	1:H:654:LEU:HD11	1.64	0.78
1:I:219:ARG:HE	1:I:223:HIS:HA	1.49	0.78
1:L:328:LEU:HD21	1:L:337:LEU:HD13	1.66	0.78
1:A:320:SER:HA	1:A:398:PHE:HB3	1.66	0.77
1:D:48:LEU:HD13	1:D:48:LEU:H	1.48	0.77
1:K:46:CYS:H	1:K:86:LEU:HD23	1.48	0.77
1:L:311:LYS:HD2	1:L:372:VAL:HG21	1.65	0.77
1:F:48:LEU:HD13	1:F:48:LEU:H	1.48	0.77
1:F:420:ILE:HB	1:F:580:TYR:HB3	1.65	0.77
1:H:142:HIS:HA	1:H:169:ALA:HB1	1.64	0.77
1:D:408:ASN:HD21	1:F:26:PHE:HD1	1.32	0.77
1:I:221:PHE:HB2	1:I:230:TRP:HE1	1.50	0.77
1:J:589:ILE:HD12	1:J:589:ILE:H	1.50	0.77
1:E:401:ARG:HH21	1:E:436:GLY:C	1.93	0.77
1:L:219:ARG:HH21	1:L:224:HIS:H	1.28	0.77
1:B:589:ILE:HD12	1:B:589:ILE:H	1.49	0.77
1:G:185:LEU:HD13	1:G:186:GLN:N	1.99	0.77
1:H:589:ILE:H	1:H:589:ILE:HD12	1.49	0.77
1:F:328:LEU:HD21	1:F:337:LEU:HD13	1.67	0.77
1:A:579:SER:HB3	1:E:577:ASP:H	1.49	0.76
1:E:288:GLY:HA3	1:E:300:CYS:SG	2.25	0.76
1:L:48:LEU:HD13	1:L:48:LEU:H	1.49	0.76
1:C:237:LYS:HD3	1:C:282:TRP:HB2	1.65	0.76
1:D:412:GLN:HE22	1:F:7:PRO:HB3	1.50	0.76
1:H:227:PRO:HA	1:H:230:TRP:HB3	1.67	0.76
1:K:589:ILE:H	1:K:589:ILE:HD12	1.51	0.76
1:G:73:VAL:HG22	1:G:74:VAL:H	1.49	0.76
1:L:33:GLN:HG3	1:L:40:LYS:HG2	1.67	0.76
1:C:328:LEU:HD21	1:C:337:LEU:HD13	1.68	0.76
1:C:589:ILE:H	1:C:589:ILE:HD12	1.51	0.76
1:G:33:GLN:HG3	1:G:40:LYS:HG2	1.68	0.76
1:L:589:ILE:H	1:L:589:ILE:HD12	1.50	0.76
1:F:33:GLN:HG3	1:F:40:LYS:HG2	1.67	0.75
1:G:46:CYS:H	1:G:86:LEU:HG	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:HG3	1:A:40:LYS:HG2	1.68	0.75
1:A:473:SER:HB2	1:A:524:VAL:HA	1.68	0.75
1:I:33:GLN:HG3	1:I:40:LYS:HG2	1.66	0.75
1:D:83:LEU:HG	1:D:86:LEU:HD11	1.67	0.75
1:G:462:LEU:HD22	1:G:618:ILE:HG23	1.66	0.75
1:A:91:PRO:C	1:A:92:LEU:HD12	2.11	0.75
1:B:33:GLN:HG3	1:B:40:LYS:HG2	1.69	0.75
1:G:185:LEU:HD11	1:G:188:LEU:HB3	1.69	0.75
1:G:589:ILE:H	1:G:589:ILE:HD12	1.50	0.75
1:H:33:GLN:HG3	1:H:40:LYS:HG2	1.69	0.75
1:B:417:GLN:HB3	1:B:581:SER:HB3	1.68	0.75
1:I:589:ILE:H	1:I:589:ILE:HD12	1.51	0.75
1:K:231:HIS:HB3	1:K:282:TRP:HH2	1.51	0.75
1:A:487:ILE:HG12	1:A:515:GLU:HB2	1.68	0.75
1:I:284:PRO:HA	1:I:287:ARG:HH21	1.52	0.75
1:F:589:ILE:H	1:F:589:ILE:HD12	1.51	0.74
1:K:79:VAL:HG11	1:K:83:LEU:HD13	1.68	0.74
1:K:224:HIS:O	1:K:225:LEU:HD22	1.86	0.74
1:A:589:ILE:H	1:A:589:ILE:HD12	1.51	0.74
1:K:403:LEU:HD23	1:K:403:LEU:H	1.52	0.74
1:D:328:LEU:HD21	1:D:337:LEU:HD13	1.68	0.74
1:D:420:ILE:HG21	1:D:578:HIS:H	1.50	0.74
1:E:563:ARG:HH12	2:Y:2:GLC:H2	1.51	0.74
1:J:328:LEU:HD21	1:J:337:LEU:HD13	1.69	0.74
1:E:237:LYS:HE2	1:E:282:TRP:H	1.52	0.74
1:G:73:VAL:HG23	1:G:163:ILE:HB	1.70	0.74
1:C:33:GLN:HG3	1:C:40:LYS:HG2	1.67	0.74
1:H:328:LEU:HD21	1:H:337:LEU:HD13	1.70	0.74
1:J:33:GLN:HG3	1:J:40:LYS:HG2	1.68	0.74
1:D:33:GLN:HG3	1:D:40:LYS:HG2	1.68	0.74
1:E:589:ILE:H	1:E:589:ILE:HD12	1.53	0.74
1:F:65:MET:HB3	1:F:76:ALA:HB3	1.70	0.74
1:H:170:LYS:HG2	1:H:177:LEU:HG	1.68	0.74
1:G:222:LEU:HD22	1:G:230:TRP:HD1	1.52	0.74
1:H:240:LYS:HD2	1:H:277:GLN:HB3	1.69	0.74
1:H:564:ALA:HB2	1:H:589:ILE:HG21	1.69	0.74
1:I:328:LEU:HD21	1:I:337:LEU:HD13	1.69	0.74
1:I:423:LEU:HA	1:I:426:VAL:HG22	1.70	0.74
1:A:328:LEU:HD21	1:A:337:LEU:HD13	1.70	0.73
1:B:328:LEU:HD21	1:B:337:LEU:HD13	1.69	0.73
1:J:13:GLY:H	1:J:14:PRO:CD	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:18:ARG:HH21	1:J:33:GLN:HE22	1.36	0.73
1:L:18:ARG:HH21	1:L:33:GLN:HE22	1.36	0.73
1:B:334:LEU:HD22	1:B:366:LYS:O	1.88	0.73
1:E:564:ALA:HB2	1:E:589:ILE:HG21	1.70	0.73
1:G:328:LEU:HD21	1:G:337:LEU:HD13	1.70	0.73
1:H:424:ARG:NH1	1:H:572:LYS:HG2	2.03	0.73
1:D:63:GLN:HE22	1:D:174:GLN:HE22	1.33	0.73
1:G:231:HIS:HB3	1:G:282:TRP:HH2	1.53	0.73
1:A:517:LYS:HD2	1:A:642:MET:HE1	1.71	0.73
1:B:415:LYS:HA	1:B:584:THR:HB	1.70	0.73
1:D:462:LEU:HD22	1:D:618:ILE:HG23	1.70	0.73
1:G:395:GLU:HG3	1:G:397:PRO:HD3	1.69	0.73
1:K:33:GLN:HG3	1:K:40:LYS:HG2	1.69	0.73
1:D:18:ARG:HH21	1:D:33:GLN:HE22	1.37	0.73
1:F:431:VAL:HG21	1:F:568:TYR:HB2	1.71	0.73
1:K:423:LEU:HA	1:K:426:VAL:HG22	1.70	0.73
1:C:501:GLY:HA3	1:D:655:LYS:HE2	1.69	0.73
1:I:462:LEU:HD22	1:I:618:ILE:HG23	1.68	0.73
1:E:517:LYS:HD2	1:E:642:MET:HE1	1.71	0.73
1:G:18:ARG:HH21	1:G:33:GLN:HE22	1.37	0.73
2:j:2:GLC:H61	2:j:3:PDX:H3	1.71	0.73
1:G:502:ILE:HD13	1:G:656:ILE:HD12	1.70	0.73
1:K:328:LEU:HD21	1:K:337:LEU:HD13	1.71	0.73
1:B:564:ALA:HB2	1:B:589:ILE:HG21	1.70	0.73
1:E:423:LEU:HA	1:E:426:VAL:HG22	1.71	0.73
1:C:185:LEU:HD13	1:C:186:GLN:H	1.53	0.72
1:D:238:ASP:HB3	1:D:239:PRO:HD2	1.72	0.72
1:F:18:ARG:HH21	1:F:33:GLN:HE22	1.37	0.72
1:D:564:ALA:HB2	1:D:589:ILE:HG21	1.70	0.72
1:E:328:LEU:HD21	1:E:337:LEU:HD13	1.71	0.72
1:G:517:LYS:HD2	1:G:642:MET:HE1	1.71	0.72
1:I:112:ASN:HB3	1:I:116:LEU:HD23	1.70	0.72
1:C:18:ARG:HH21	1:C:33:GLN:HE22	1.38	0.72
1:E:392:THR:HG22	1:E:616:GLN:HE22	1.54	0.72
1:G:221:PHE:HB2	1:G:230:TRP:HE1	1.55	0.72
1:G:579:SER:HB3	1:K:577:ASP:H	1.55	0.72
1:K:564:ALA:HB2	1:K:589:ILE:HG21	1.71	0.72
1:C:527:ILE:HG22	1:C:531:GLU:HG3	1.72	0.72
1:C:564:ALA:HB2	1:C:589:ILE:HG21	1.72	0.72
1:E:33:GLN:HG3	1:E:40:LYS:HG2	1.70	0.72
1:G:487:ILE:HG12	1:G:515:GLU:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:564:ALA:HB2	1:J:589:ILE:HG21	1.71	0.72
1:B:363:ASP:HB3	1:B:370:GLN:NE2	2.04	0.72
1:I:18:ARG:HH21	1:I:33:GLN:HE22	1.38	0.72
1:J:118:GLU:HB2	1:J:263:SER:O	1.90	0.72
1:L:564:ALA:HB2	1:L:589:ILE:HG21	1.70	0.72
1:A:564:ALA:HB2	1:A:589:ILE:HG21	1.72	0.71
1:D:310:LEU:HD22	1:D:327:LEU:HD21	1.72	0.71
1:G:396:GLY:H	1:G:397:PRO:HD3	1.54	0.71
1:H:290:PRO:HB2	1:H:299:ARG:HB2	1.72	0.71
1:A:523:GLU:HB2	1:A:632:ILE:HG12	1.73	0.71
1:C:423:LEU:HA	1:C:426:VAL:HG22	1.72	0.71
1:E:527:ILE:HG22	1:E:531:GLU:HG3	1.72	0.71
1:J:240:LYS:HD2	1:J:277:GLN:HB3	1.71	0.71
1:D:209:THR:HG22	1:D:220:PRO:HG3	1.70	0.71
1:E:73:VAL:HG23	1:E:163:ILE:HB	1.71	0.71
1:K:18:ARG:HH21	1:K:33:GLN:HE22	1.38	0.71
1:L:310:LEU:HD22	1:L:327:LEU:HD21	1.71	0.71
1:G:47:ARG:O	1:G:87:ILE:HD12	1.91	0.71
1:J:238:ASP:HB3	1:J:239:PRO:HD2	1.72	0.71
1:K:328:LEU:HD13	1:K:368:ALA:HB1	1.72	0.71
1:A:18:ARG:HH21	1:A:33:GLN:HE22	1.38	0.71
1:B:240:LYS:HB3	1:B:277:GLN:HB3	1.71	0.71
1:F:237:LYS:HE2	1:F:281:ASN:HA	1.72	0.71
1:F:396:GLY:H	1:F:397:PRO:HD3	1.55	0.71
1:L:13:GLY:N	1:L:14:PRO:HD3	2.05	0.71
1:F:310:LEU:HD22	1:F:327:LEU:HD21	1.71	0.71
1:F:564:ALA:HB2	1:F:589:ILE:HG21	1.70	0.71
1:L:141:ILE:HG23	1:L:170:LYS:HB2	1.72	0.71
1:B:18:ARG:HH21	1:B:33:GLN:HE22	1.38	0.71
1:F:83:LEU:HA	1:F:86:LEU:HD12	1.72	0.71
1:H:142:HIS:HA	1:H:169:ALA:CB	2.21	0.71
1:E:18:ARG:HH21	1:E:33:GLN:HE22	1.38	0.71
1:G:170:LYS:HG2	1:G:177:LEU:HG	1.72	0.71
1:H:18:ARG:HH21	1:H:33:GLN:HE22	1.38	0.71
1:J:473:SER:HB2	1:J:524:VAL:HA	1.73	0.71
1:L:403:LEU:HD23	1:L:403:LEU:H	1.56	0.71
1:L:516:GLU:HA	1:L:519:ILE:HD12	1.73	0.71
1:C:48:LEU:HA	1:C:87:ILE:HG21	1.73	0.71
1:F:423:LEU:HA	1:F:426:VAL:HG22	1.72	0.71
1:F:516:GLU:HA	1:F:519:ILE:HD12	1.73	0.71
1:J:412:GLN:CD	1:L:27:GLY:HA2	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:219:ARG:HH12	1:K:224:HIS:H	1.36	0.71
1:E:310:LEU:HD22	1:E:327:LEU:HD21	1.73	0.70
1:E:551:ARG:HB3	1:E:552:ARG:HH21	1.54	0.70
1:I:395:GLU:H	1:I:395:GLU:CD	1.98	0.70
1:B:74:VAL:HG21	1:B:95:MET:HE3	1.72	0.70
1:D:579:SER:HB3	1:F:577:ASP:H	1.55	0.70
1:F:328:LEU:HD13	1:F:368:ALA:HB1	1.73	0.70
1:K:310:LEU:HD22	1:K:327:LEU:HD21	1.73	0.70
1:B:392:THR:HG22	1:B:616:GLN:HE22	1.56	0.70
1:I:527:ILE:HG22	1:I:531:GLU:HG3	1.73	0.70
1:J:310:LEU:HD22	1:J:327:LEU:HD21	1.73	0.70
1:J:424:ARG:NH1	1:J:572:LYS:HG2	2.06	0.70
1:J:502:ILE:HD13	1:J:656:ILE:HD12	1.73	0.70
1:K:527:ILE:HG22	1:K:531:GLU:HG3	1.74	0.70
1:C:403:LEU:HD23	1:C:403:LEU:H	1.55	0.70
1:D:423:LEU:HA	1:D:426:VAL:HG22	1.72	0.70
1:E:550:GLY:HA3	1:E:604:LEU:HD13	1.74	0.70
1:G:231:HIS:HB3	1:G:282:TRP:CH2	2.26	0.70
1:D:431:VAL:HG21	1:D:568:TYR:HB2	1.72	0.70
1:B:403:LEU:HD23	1:B:403:LEU:H	1.56	0.70
1:E:403:LEU:H	1:E:403:LEU:HD23	1.57	0.70
1:G:564:ALA:HB2	1:G:589:ILE:HG21	1.73	0.70
1:I:564:ALA:HB2	1:I:589:ILE:HG21	1.74	0.70
1:G:516:GLU:HA	1:G:519:ILE:HD12	1.74	0.70
1:I:144:ASP:OD1	1:I:182:VAL:HG11	1.92	0.70
1:K:238:ASP:CG	1:K:239:PRO:HD2	2.17	0.70
1:L:423:LEU:HA	1:L:426:VAL:HG22	1.73	0.70
1:A:112:ASN:ND2	1:A:116:LEU:HA	2.06	0.69
1:C:310:LEU:HD22	1:C:327:LEU:HD21	1.72	0.69
1:A:185:LEU:HD13	1:A:186:GLN:N	2.07	0.69
1:A:298:PRO:O	1:A:302:VAL:HG23	1.91	0.69
1:B:516:GLU:HA	1:B:519:ILE:HD12	1.74	0.69
1:E:417:GLN:HB3	1:E:581:SER:HB3	1.74	0.69
1:B:420:ILE:HD12	1:B:423:LEU:HB2	1.74	0.69
1:F:403:LEU:HD23	1:F:403:LEU:H	1.56	0.69
1:G:186:GLN:HG2	1:G:219:ARG:HD2	1.74	0.69
1:G:310:LEU:HD22	1:G:327:LEU:HD21	1.74	0.69
1:H:310:LEU:HD22	1:H:327:LEU:HD21	1.74	0.69
1:A:562:GLN:HA	1:A:565:ILE:HD12	1.74	0.69
1:D:29:VAL:HA	1:D:44:LYS:HA	1.75	0.69
1:K:72:ASN:HD21	1:K:127:ASP:HA	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD22	1:B:327:LEU:HD21	1.74	0.69
1:F:560:LEU:HD13	1:F:593:THR:HA	1.74	0.69
1:H:502:ILE:HG21	1:H:656:ILE:HG21	1.75	0.69
1:J:423:LEU:HA	1:J:426:VAL:HG22	1.73	0.69
1:K:448:GLN:OE1	1:K:549:TYR:HB3	1.92	0.69
1:A:527:ILE:HG22	1:A:531:GLU:HG3	1.74	0.69
1:E:278:LEU:HD23	1:E:288:GLY:HA2	1.73	0.69
1:G:527:ILE:HG22	1:G:531:GLU:HG3	1.74	0.69
1:H:516:GLU:HA	1:H:519:ILE:HD12	1.74	0.69
1:L:186:GLN:NE2	1:L:227:PRO:HD3	2.08	0.69
1:A:420:ILE:HD12	1:A:423:LEU:HB2	1.73	0.69
1:B:423:LEU:HA	1:B:426:VAL:HG22	1.73	0.69
1:G:396:GLY:N	1:G:397:PRO:HD3	2.06	0.69
1:L:230:TRP:O	1:L:234:ILE:HG12	1.93	0.69
1:C:550:GLY:HA3	1:C:604:LEU:HD13	1.74	0.69
1:D:420:ILE:HG21	1:D:577:ASP:HB3	1.74	0.69
1:H:29:VAL:HA	1:H:44:LYS:HA	1.75	0.69
1:J:46:CYS:SG	1:J:86:LEU:HD12	2.33	0.69
1:J:516:GLU:HA	1:J:519:ILE:HD12	1.75	0.69
1:A:501:GLY:HA3	1:B:655:LYS:HE2	1.74	0.69
1:D:74:VAL:HG21	1:D:95:MET:HE3	1.75	0.69
1:D:527:ILE:HG22	1:D:531:GLU:HG3	1.75	0.69
1:A:577:ASP:H	1:C:579:SER:HB2	1.58	0.69
1:A:516:GLU:HA	1:A:519:ILE:HD12	1.75	0.68
1:B:328:LEU:HD13	1:B:368:ALA:HB1	1.75	0.68
1:B:427:TRP:HZ3	1:B:567:LEU:HB3	1.59	0.68
1:G:577:ASP:H	1:I:579:SER:HB3	1.58	0.68
1:K:29:VAL:HA	1:K:44:LYS:HA	1.75	0.68
1:L:420:ILE:HD12	1:L:423:LEU:HB2	1.73	0.68
1:L:527:ILE:HG22	1:L:531:GLU:HG3	1.75	0.68
1:H:420:ILE:HD12	1:H:423:LEU:HB2	1.75	0.68
1:H:527:ILE:HG22	1:H:531:GLU:HG3	1.74	0.68
1:A:221:PHE:HB2	1:A:230:TRP:HE1	1.59	0.68
1:C:516:GLU:HA	1:C:519:ILE:HD12	1.74	0.68
1:G:420:ILE:HD12	1:G:423:LEU:HB2	1.74	0.68
1:I:185:LEU:HD11	1:I:188:LEU:CB	2.20	0.68
1:I:403:LEU:HD23	1:I:403:LEU:H	1.57	0.68
1:I:516:GLU:HA	1:I:519:ILE:HD12	1.74	0.68
1:K:288:GLY:HA3	1:K:300:CYS:SG	2.33	0.68
1:A:288:GLY:HA3	1:A:300:CYS:SG	2.32	0.68
1:G:221:PHE:HB2	1:G:230:TRP:NE1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:423:LEU:HA	1:G:426:VAL:HG22	1.73	0.68
1:I:424:ARG:NH1	1:I:572:LYS:HG2	2.08	0.68
1:L:359:GLY:HA3	1:L:453:LEU:HB2	1.74	0.68
1:A:310:LEU:HD22	1:A:327:LEU:HD21	1.75	0.68
1:D:516:GLU:HA	1:D:519:ILE:HD12	1.75	0.68
1:E:540:GLU:O	1:E:544:LEU:HG	1.94	0.68
1:H:328:LEU:HD13	1:H:368:ALA:HB1	1.75	0.68
1:I:395:GLU:HG2	1:I:397:PRO:HD3	1.75	0.68
1:D:420:ILE:HD12	1:D:423:LEU:HB2	1.75	0.68
1:G:180:GLU:HB3	1:G:192:LEU:HD23	1.74	0.68
1:H:427:TRP:HZ3	1:H:567:LEU:HB3	1.59	0.68
1:L:185:LEU:HD13	1:L:186:GLN:N	2.07	0.68
1:J:46:CYS:H	1:J:86:LEU:HD12	1.59	0.68
1:L:560:LEU:HD13	1:L:593:THR:HA	1.75	0.68
1:L:562:GLN:HA	1:L:565:ILE:HD12	1.76	0.68
1:A:110:PRO:O	1:A:113:CYS:HB3	1.94	0.68
1:B:527:ILE:HG22	1:B:531:GLU:HG3	1.75	0.68
1:H:423:LEU:HA	1:H:426:VAL:HG22	1.73	0.68
1:I:575:PRO:HB3	1:K:574:ARG:NH1	2.08	0.68
1:J:420:ILE:HD12	1:J:423:LEU:HB2	1.75	0.68
1:B:29:VAL:HA	1:B:44:LYS:HA	1.76	0.68
1:D:189:ALA:HB3	1:D:202:VAL:HG13	1.76	0.68
1:J:222:LEU:HD22	1:J:244:ALA:O	1.94	0.68
1:L:186:GLN:HE21	1:L:227:PRO:HD3	1.58	0.68
1:L:288:GLY:HA3	1:L:300:CYS:SG	2.34	0.68
1:L:420:ILE:HB	1:L:580:TYR:HB3	1.74	0.68
1:J:29:VAL:HA	1:J:44:LYS:HA	1.76	0.68
1:A:473:SER:HB3	1:A:632:ILE:HD13	1.76	0.67
1:B:401:ARG:HH22	1:B:440:ASP:HB2	1.59	0.67
1:D:415:LYS:HA	1:D:584:THR:HB	1.76	0.67
1:H:560:LEU:HD13	1:H:593:THR:HA	1.76	0.67
1:L:431:VAL:HG21	1:L:568:TYR:HB2	1.75	0.67
1:A:201:THR:HB	1:A:287:ARG:HH12	1.58	0.67
1:A:403:LEU:HD23	1:A:403:LEU:H	1.59	0.67
1:A:423:LEU:HA	1:A:426:VAL:HG22	1.75	0.67
1:A:480:LEU:HD22	1:A:518:ALA:HB1	1.77	0.67
1:D:396:GLY:N	1:D:397:PRO:HD3	2.10	0.67
1:G:316:LEU:HB2	1:G:383:MET:HE2	1.76	0.67
1:I:267:LEU:HD12	1:I:312:ILE:HG23	1.76	0.67
1:J:527:ILE:HG22	1:J:531:GLU:HG3	1.76	0.67
1:D:334:LEU:HD11	1:D:364:PRO:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:ASP:OD1	1:H:286:GLN:HG2	1.95	0.67
1:I:310:LEU:HD22	1:I:327:LEU:HD21	1.75	0.67
1:L:48:LEU:HA	1:L:87:ILE:HD12	1.75	0.67
1:B:267:LEU:HD12	1:B:312:ILE:HG23	1.76	0.67
1:B:463:THR:HG21	1:B:538:HIS:HD2	1.60	0.67
1:C:551:ARG:HB3	1:C:552:ARG:HH21	1.58	0.67
1:D:424:ARG:NH1	1:D:572:LYS:HG2	2.08	0.67
1:D:560:LEU:HD13	1:D:593:THR:HA	1.75	0.67
1:F:527:ILE:HG22	1:F:531:GLU:HG3	1.77	0.67
1:A:29:VAL:HA	1:A:44:LYS:HA	1.76	0.67
1:G:143:ARG:NH1	1:G:180:GLU:HA	2.08	0.67
1:G:562:GLN:HA	1:G:565:ILE:HD12	1.76	0.67
1:H:74:VAL:HG11	1:H:164:ILE:HA	1.77	0.67
1:H:249:SER:HB3	1:J:185:LEU:H	1.59	0.67
1:H:311:LYS:HD2	1:H:372:VAL:HG11	1.77	0.67
1:J:189:ALA:HB3	1:J:202:VAL:HG13	1.77	0.67
1:E:29:VAL:HA	1:E:44:LYS:HA	1.77	0.67
1:F:74:VAL:HG21	1:F:164:ILE:HG13	1.76	0.67
1:L:377:ARG:HA	1:L:377:ARG:HE	1.58	0.67
1:C:420:ILE:HD12	1:C:423:LEU:HB2	1.76	0.67
1:F:29:VAL:HA	1:F:44:LYS:HA	1.77	0.67
1:F:141:ILE:HD12	1:F:200:ALA:HA	1.76	0.67
1:K:516:GLU:HA	1:K:519:ILE:HD12	1.75	0.67
1:B:396:GLY:N	1:B:397:PRO:HD3	2.10	0.67
1:B:643:GLN:HE21	1:B:647:GLN:HG3	1.59	0.67
1:C:185:LEU:HD13	1:C:186:GLN:N	2.09	0.67
1:D:427:TRP:HZ3	1:D:567:LEU:HB3	1.59	0.67
1:E:487:ILE:HA	1:E:646:ARG:HD2	1.77	0.67
1:E:498:MET:HA	1:E:503:SER:HB3	1.75	0.67
1:G:116:LEU:HD12	1:G:116:LEU:H	1.58	0.67
1:G:560:LEU:HD13	1:G:593:THR:HA	1.77	0.67
1:C:265:CYS:SG	1:C:268:ILE:HG13	2.35	0.67
1:C:395:GLU:H	1:C:395:GLU:CD	2.03	0.67
1:D:463:THR:HG21	1:D:538:HIS:HD2	1.60	0.67
1:H:514:MET:HA	1:H:517:LYS:HD2	1.77	0.67
1:I:74:VAL:HG11	1:I:164:ILE:HG13	1.76	0.67
1:J:396:GLY:N	1:J:397:PRO:HD3	2.10	0.67
1:K:209:THR:HG22	1:K:220:PRO:HG3	1.77	0.67
1:D:141:ILE:HD12	1:D:200:ALA:HA	1.77	0.67
1:G:29:VAL:HA	1:G:44:LYS:HA	1.76	0.67
1:J:212:PHE:CD2	1:J:220:PRO:HA	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:643:GLN:HE21	1:K:647:GLN:HG3	1.60	0.67
1:A:395:GLU:HG3	1:A:396:GLY:H	1.60	0.66
1:B:189:ALA:HB3	1:B:202:VAL:HG13	1.77	0.66
1:D:227:PRO:HA	1:D:230:TRP:HB3	1.77	0.66
1:G:473:SER:HB2	1:G:524:VAL:HA	1.77	0.66
1:G:473:SER:HB3	1:G:632:ILE:HD13	1.77	0.66
1:A:182:VAL:HG12	1:A:183:GLY:H	1.59	0.66
1:A:514:MET:HA	1:A:517:LYS:HD2	1.77	0.66
1:E:516:GLU:HA	1:E:519:ILE:HD12	1.76	0.66
1:J:403:LEU:HD23	1:J:403:LEU:H	1.60	0.66
1:L:29:VAL:HA	1:L:44:LYS:HA	1.77	0.66
1:B:449:ARG:HH22	3:O:1:5LS:C3	2.08	0.66
1:B:560:LEU:HD13	1:B:593:THR:HA	1.77	0.66
1:C:562:GLN:HA	1:C:565:ILE:HD12	1.78	0.66
1:D:70:HIS:HB3	1:D:73:VAL:HG22	1.76	0.66
1:E:643:GLN:HE21	1:E:647:GLN:HG3	1.61	0.66
1:G:91:PRO:O	1:G:92:LEU:HD12	1.96	0.66
1:G:219:ARG:NH2	1:G:224:HIS:H	1.93	0.66
1:D:249:SER:HB3	1:F:184:THR:HA	1.77	0.66
1:J:560:LEU:HD13	1:J:593:THR:HA	1.76	0.66
1:L:141:ILE:HD12	1:L:200:ALA:HA	1.76	0.66
1:A:473:SER:OG	1:A:524:VAL:HG13	1.95	0.66
1:F:514:MET:HA	1:F:517:LYS:HD2	1.78	0.66
1:J:410:ILE:HG23	1:J:583:SER:OG	1.95	0.66
1:K:142:HIS:ND1	1:K:169:ALA:HB2	2.11	0.66
1:A:265:CYS:SG	1:A:268:ILE:HG13	2.34	0.66
1:D:562:GLN:HA	1:D:565:ILE:HD12	1.77	0.66
1:F:420:ILE:HD12	1:F:423:LEU:HB2	1.75	0.66
1:J:579:SER:HB3	1:L:577:ASP:H	1.61	0.66
1:A:560:LEU:HD13	1:A:593:THR:HA	1.78	0.66
1:D:260:GLN:NE2	1:D:261:PRO:HA	2.11	0.66
1:F:238:ASP:HB3	1:F:239:PRO:HD2	1.78	0.66
1:G:219:ARG:NH1	1:G:224:HIS:H	1.94	0.66
1:H:417:GLN:HB3	1:H:581:SER:HB3	1.78	0.66
1:J:417:GLN:HB3	1:J:581:SER:HB3	1.76	0.66
1:J:562:GLN:HA	1:J:565:ILE:HD12	1.77	0.66
1:K:560:LEU:HD13	1:K:593:THR:HA	1.76	0.66
1:A:549:TYR:H	1:A:552:ARG:HD2	1.61	0.66
1:C:189:ALA:HB3	1:C:202:VAL:HG13	1.78	0.66
1:G:514:MET:HA	1:G:517:LYS:HD2	1.78	0.66
1:I:562:GLN:HA	1:I:565:ILE:HD12	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:514:MET:HA	1:L:517:LYS:HD2	1.78	0.66
1:B:141:ILE:HD12	1:B:200:ALA:HA	1.77	0.65
1:C:396:GLY:N	1:C:397:PRO:HD3	2.10	0.65
1:E:227:PRO:HA	1:E:230:TRP:CB	2.26	0.65
1:E:560:LEU:HD13	1:E:593:THR:HA	1.76	0.65
1:H:396:GLY:N	1:H:397:PRO:HD3	2.11	0.65
1:J:209:THR:HG22	1:J:220:PRO:HG3	1.77	0.65
1:C:514:MET:HA	1:C:517:LYS:HD2	1.79	0.65
1:D:212:PHE:CD2	1:D:220:PRO:HA	2.31	0.65
1:J:141:ILE:HD12	1:J:200:ALA:HA	1.78	0.65
1:C:560:LEU:HD13	1:C:593:THR:HA	1.78	0.65
1:E:141:ILE:HD12	1:E:200:ALA:HA	1.78	0.65
1:F:562:GLN:HA	1:F:565:ILE:HD12	1.79	0.65
1:H:396:GLY:H	1:H:397:PRO:HD3	1.61	0.65
1:I:420:ILE:HD12	1:I:423:LEU:HB2	1.77	0.65
1:K:141:ILE:HD12	1:K:200:ALA:HA	1.78	0.65
1:K:189:ALA:HB3	1:K:202:VAL:HG13	1.79	0.65
1:C:517:LYS:HD2	1:C:642:MET:HE1	1.79	0.65
1:F:209:THR:HG22	1:F:220:PRO:HG3	1.77	0.65
1:H:141:ILE:HD12	1:H:200:ALA:HA	1.77	0.65
1:H:643:GLN:HE21	1:H:647:GLN:HG3	1.61	0.65
1:C:29:VAL:HA	1:C:44:LYS:HA	1.76	0.65
1:F:189:ALA:HB3	1:F:202:VAL:HG13	1.79	0.65
1:H:562:GLN:HA	1:H:565:ILE:HD12	1.76	0.65
1:I:396:GLY:N	1:I:397:PRO:HD3	2.10	0.65
1:J:328:LEU:HD13	1:J:368:ALA:HB1	1.78	0.65
1:G:227:PRO:HA	1:G:230:TRP:HB2	1.78	0.65
1:H:267:LEU:HD12	1:H:312:ILE:HG23	1.77	0.65
1:I:514:MET:HA	1:I:517:LYS:HD2	1.79	0.65
1:I:560:LEU:HD13	1:I:593:THR:HA	1.78	0.65
1:J:46:CYS:H	1:J:86:LEU:CD1	2.09	0.65
1:K:420:ILE:HD12	1:K:423:LEU:HB2	1.77	0.65
1:C:595:GLN:HB3	2:S:2:GLC:H3	1.79	0.65
1:I:141:ILE:HD12	1:I:200:ALA:HA	1.77	0.65
1:J:290:PRO:HB2	1:J:299:ARG:HB2	1.79	0.65
1:C:260:GLN:NE2	1:C:261:PRO:HA	2.09	0.65
1:C:420:ILE:HB	1:C:580:TYR:HB3	1.76	0.65
1:C:424:ARG:NH1	1:C:572:LYS:HG2	2.12	0.65
1:D:551:ARG:HB3	1:D:552:ARG:HH21	1.62	0.65
1:G:219:ARG:CZ	1:G:224:HIS:H	2.08	0.65
1:A:189:ALA:HB3	1:A:202:VAL:HG13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ASN:HB3	1:F:116:LEU:HD22	1.79	0.65
1:L:74:VAL:HG12	1:L:75:LYS:H	1.61	0.65
1:A:643:GLN:HE21	1:A:647:GLN:HG3	1.61	0.65
1:F:643:GLN:HE21	1:F:647:GLN:HG3	1.62	0.65
1:G:265:CYS:SG	1:G:268:ILE:HG13	2.36	0.65
1:H:403:LEU:HD23	1:H:403:LEU:H	1.61	0.65
1:I:260:GLN:NE2	1:I:261:PRO:HA	2.09	0.65
1:K:139:LYS:HD2	1:K:172:VAL:HG11	1.77	0.65
1:A:48:LEU:HA	1:A:87:ILE:HG21	1.79	0.64
1:C:477:LYS:HE3	1:C:524:VAL:HG11	1.77	0.64
1:E:222:LEU:HD22	1:E:222:LEU:H	1.61	0.64
1:I:29:VAL:HA	1:I:44:LYS:HA	1.76	0.64
1:B:227:PRO:HA	1:B:230:TRP:CB	2.26	0.64
1:B:514:MET:HA	1:B:517:LYS:HD2	1.80	0.64
1:E:463:THR:HG21	1:E:538:HIS:HD2	1.61	0.64
1:F:469:LEU:HD12	1:F:625:VAL:HG13	1.78	0.64
1:H:265:CYS:SG	1:H:268:ILE:HG13	2.38	0.64
1:I:324:ILE:H	1:I:324:ILE:HD12	1.63	0.64
1:J:366:LYS:HE3	1:J:367:PRO:HD2	1.80	0.64
1:J:424:ARG:HH11	1:J:572:LYS:HG2	1.62	0.64
1:L:209:THR:HG22	1:L:220:PRO:HG3	1.79	0.64
1:L:415:LYS:HA	1:L:584:THR:HB	1.79	0.64
1:A:185:LEU:HD13	1:A:186:GLN:H	1.62	0.64
1:F:359:GLY:HA3	1:F:453:LEU:HB2	1.78	0.64
1:I:643:GLN:HE21	1:I:647:GLN:HG3	1.60	0.64
1:J:215:ILE:HD13	1:J:264:LEU:HD11	1.79	0.64
1:A:324:ILE:H	1:A:324:ILE:HD12	1.63	0.64
1:A:401:ARG:HH21	1:A:437:LEU:HD23	1.63	0.64
1:G:643:GLN:HE21	1:G:647:GLN:HG3	1.61	0.64
1:H:26:PHE:HD1	1:L:408:ASN:HD21	1.46	0.64
1:J:514:MET:HA	1:J:517:LYS:HD2	1.78	0.64
1:K:489:LEU:HD21	1:L:648:LYS:HG3	1.78	0.64
1:A:84:ASN:CG	1:A:85:ILE:H	2.06	0.64
1:A:502:ILE:HG13	1:B:658:CYS:SG	2.37	0.64
1:B:209:THR:HG22	1:B:220:PRO:HG3	1.80	0.64
1:C:351:SER:HA	1:C:389:LYS:HD2	1.80	0.64
1:E:420:ILE:HD12	1:E:423:LEU:HB2	1.77	0.64
1:H:141:ILE:HG23	1:H:170:LYS:HB2	1.78	0.64
1:I:351:SER:HA	1:I:389:LYS:HD2	1.80	0.64
1:I:477:LYS:HE3	1:I:524:VAL:HG11	1.78	0.64
1:K:562:GLN:HA	1:K:565:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:CYS:SG	1:B:268:ILE:HG13	2.38	0.64
1:B:324:ILE:H	1:B:324:ILE:HD12	1.62	0.64
1:D:291:VAL:HA	1:D:298:PRO:HA	1.79	0.64
1:D:324:ILE:H	1:D:324:ILE:HD12	1.63	0.64
1:D:643:GLN:HE21	1:D:647:GLN:HG3	1.62	0.64
1:E:562:GLN:HA	1:E:565:ILE:HD12	1.80	0.64
1:F:395:GLU:H	1:F:395:GLU:CD	2.05	0.64
1:G:237:LYS:HE2	1:G:282:TRP:H	1.61	0.64
1:K:424:ARG:NH1	1:K:572:LYS:HG2	2.12	0.64
1:D:265:CYS:SG	1:D:268:ILE:HG13	2.38	0.64
1:D:514:MET:HA	1:D:517:LYS:HD2	1.78	0.64
1:H:498:MET:HA	1:H:503:SER:HB3	1.77	0.64
1:B:351:SER:HA	1:B:389:LYS:HD2	1.79	0.64
1:G:648:LYS:HG3	1:H:489:LEU:HD21	1.78	0.64
1:H:420:ILE:HG21	1:H:578:HIS:H	1.63	0.64
1:I:517:LYS:HD2	1:I:642:MET:HE1	1.80	0.64
1:L:189:ALA:HB3	1:L:202:VAL:HG13	1.80	0.64
1:B:236:LYS:HG3	1:B:237:LYS:H	1.61	0.64
1:E:351:SER:HA	1:E:389:LYS:HD2	1.80	0.64
1:F:86:LEU:HD23	1:F:87:ILE:HD12	1.79	0.64
1:J:643:GLN:HE21	1:J:647:GLN:HG3	1.63	0.64
1:K:514:MET:HA	1:K:517:LYS:HD2	1.79	0.64
1:L:185:LEU:HD12	1:L:193:PHE:HZ	1.63	0.64
1:A:13:GLY:H	1:A:14:PRO:CD	2.07	0.64
1:B:410:ILE:O	1:B:587:VAL:HG22	1.98	0.64
1:G:288:GLY:HA3	1:G:300:CYS:SG	2.38	0.64
1:H:114:CYS:SG	1:H:432:HIS:HB2	2.38	0.64
1:H:260:GLN:NE2	1:H:261:PRO:HA	2.11	0.64
1:I:265:CYS:SG	1:I:268:ILE:HG13	2.37	0.64
1:L:643:GLN:HE21	1:L:647:GLN:HG3	1.63	0.64
1:A:234:ILE:O	1:A:237:LYS:HB2	1.97	0.63
1:B:29:VAL:HG22	1:B:44:LYS:HB2	1.80	0.63
1:B:170:LYS:HA	1:B:177:LEU:HA	1.79	0.63
1:B:260:GLN:NE2	1:B:261:PRO:HA	2.11	0.63
1:C:324:ILE:HD12	1:C:324:ILE:H	1.63	0.63
1:F:25:GLY:H	1:F:28:ASN:HD22	1.46	0.63
1:J:265:CYS:SG	1:J:268:ILE:HG13	2.38	0.63
1:L:551:ARG:HB3	1:L:552:ARG:HH21	1.63	0.63
1:H:408:ASN:ND2	1:J:26:PHE:HA	2.13	0.63
1:H:463:THR:HG21	1:H:538:HIS:HD2	1.64	0.63
1:L:13:GLY:H	1:L:14:PRO:CD	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:200:ALA:HA	1.79	0.63
1:A:289:GLY:O	1:A:291:VAL:HG23	1.98	0.63
1:C:141:ILE:HD12	1:C:200:ALA:HA	1.79	0.63
1:E:189:ALA:HB3	1:E:202:VAL:HG13	1.81	0.63
1:G:324:ILE:H	1:G:324:ILE:HD12	1.63	0.63
1:J:351:SER:HA	1:J:389:LYS:HD2	1.81	0.63
1:J:354:LEU:HB3	1:J:384:VAL:HG12	1.81	0.63
1:K:351:SER:HA	1:K:389:LYS:HD2	1.81	0.63
1:C:643:GLN:HE21	1:C:647:GLN:HG3	1.61	0.63
1:G:222:LEU:HB2	1:G:230:TRP:HD1	1.61	0.63
1:I:189:ALA:HB3	1:I:202:VAL:HG13	1.81	0.63
1:J:88:HIS:CG	1:J:89:ASP:H	2.16	0.63
1:K:114:CYS:SG	1:K:432:HIS:HB2	2.37	0.63
1:K:318:MET:HE2	1:K:447:GLY:HA3	1.79	0.63
1:B:74:VAL:HB	1:B:164:ILE:HG13	1.79	0.63
1:E:372:VAL:O	1:E:373:LEU:HD13	1.99	0.63
1:E:514:MET:HA	1:E:517:LYS:HD2	1.79	0.63
1:H:29:VAL:HG22	1:H:44:LYS:HB2	1.81	0.63
1:J:324:ILE:H	1:J:324:ILE:HD12	1.64	0.63
1:E:420:ILE:HG21	1:E:578:HIS:H	1.63	0.63
1:H:209:THR:HG22	1:H:220:PRO:HG3	1.81	0.63
1:B:562:GLN:HA	1:B:565:ILE:HD12	1.79	0.63
1:D:351:SER:HA	1:D:389:LYS:HD2	1.81	0.63
1:E:227:PRO:HA	1:E:230:TRP:HB2	1.80	0.63
1:G:29:VAL:HG21	4:G:701:5TL:CAE	2.28	0.63
1:H:189:ALA:HB3	1:H:202:VAL:HG13	1.81	0.63
1:J:463:THR:HG21	1:J:538:HIS:HD2	1.64	0.63
1:L:427:TRP:HZ3	1:L:567:LEU:HB3	1.63	0.63
1:G:189:ALA:HB3	1:G:202:VAL:HG13	1.80	0.63
1:H:431:VAL:HG21	1:H:568:TYR:HB2	1.81	0.63
1:A:139:LYS:HD2	1:A:172:VAL:HG21	1.80	0.63
1:C:502:ILE:HD12	1:D:654:LEU:HD11	1.78	0.63
1:D:412:GLN:CD	1:F:27:GLY:HA2	2.24	0.63
1:H:48:LEU:HA	1:H:87:ILE:HD12	1.80	0.63
1:K:401:ARG:HH22	1:K:440:ASP:HB2	1.64	0.63
1:K:487:ILE:HA	1:K:646:ARG:HD2	1.79	0.63
1:A:469:LEU:HD12	1:A:625:VAL:HG13	1.80	0.62
1:B:237:LYS:HZ1	1:B:281:ASN:HA	1.63	0.62
1:D:25:GLY:H	1:D:28:ASN:HD22	1.47	0.62
1:E:222:LEU:HB2	1:E:230:TRP:HD1	1.64	0.62
1:F:77:CYS:HB2	1:F:94:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:351:SER:HA	1:L:389:LYS:HD2	1.81	0.62
1:A:396:GLY:N	1:A:397:PRO:HD3	2.10	0.62
1:G:25:GLY:H	1:G:28:ASN:HD22	1.46	0.62
1:G:143:ARG:NH2	1:G:144:ASP:HB2	2.15	0.62
1:H:473:SER:HB2	1:H:524:VAL:HA	1.80	0.62
1:I:185:LEU:HD13	1:I:186:GLN:N	2.13	0.62
1:K:25:GLY:H	1:K:28:ASN:HD22	1.48	0.62
1:K:281:ASN:O	1:K:287:ARG:HD3	1.99	0.62
1:L:143:ARG:NH2	1:L:144:ASP:HB2	2.14	0.62
1:L:170:LYS:HG2	1:L:177:LEU:HD23	1.81	0.62
1:A:351:SER:HA	1:A:389:LYS:HD2	1.80	0.62
1:C:212:PHE:CD2	1:C:220:PRO:HA	2.35	0.62
1:G:186:GLN:HE21	1:G:219:ARG:NH1	1.98	0.62
1:G:514:MET:HA	1:G:642:MET:HE1	1.81	0.62
1:H:351:SER:HA	1:H:389:LYS:HD2	1.81	0.62
1:H:547:SER:HB3	1:H:548:PRO:HD2	1.80	0.62
1:K:13:GLY:N	1:K:14:PRO:HD3	2.14	0.62
1:K:29:VAL:HG22	1:K:44:LYS:HB2	1.81	0.62
1:D:170:LYS:HB3	1:D:177:LEU:HA	1.80	0.62
1:E:220:PRO:O	1:E:243:PHE:HA	2.00	0.62
1:G:141:ILE:HD12	1:G:200:ALA:HA	1.80	0.62
1:I:70:HIS:HB3	1:I:73:VAL:HG12	1.81	0.62
1:K:260:GLN:NE2	1:K:261:PRO:HA	2.09	0.62
1:A:220:PRO:O	1:A:243:PHE:HA	1.99	0.62
1:D:158:LYS:HZ1	1:D:377:ARG:HH21	1.46	0.62
1:E:29:VAL:HG22	1:E:44:LYS:HB2	1.81	0.62
1:E:260:GLN:NE2	1:E:261:PRO:HA	2.10	0.62
1:E:324:ILE:H	1:E:324:ILE:HD12	1.65	0.62
1:E:501:GLY:HA2	1:F:658:CYS:HB3	1.81	0.62
1:H:420:ILE:HG21	1:H:578:HIS:N	2.14	0.62
1:I:220:PRO:O	1:I:243:PHE:HA	2.00	0.62
1:K:324:ILE:HD12	1:K:324:ILE:H	1.65	0.62
1:A:143:ARG:NH2	1:A:144:ASP:HB2	2.15	0.62
1:D:98:CYS:HB3	1:D:152:LEU:O	1.99	0.62
1:D:298:PRO:O	1:D:302:VAL:HG23	2.00	0.62
1:F:143:ARG:NH2	1:F:144:ASP:HB2	2.14	0.62
1:J:25:GLY:H	1:J:28:ASN:HD22	1.47	0.62
1:L:73:VAL:HG12	1:L:74:VAL:HG23	1.80	0.62
1:E:25:GLY:H	1:E:28:ASN:HD22	1.48	0.62
1:F:21:LEU:HD12	4:F:701:5TL:CAG	2.29	0.62
1:H:298:PRO:O	1:H:302:VAL:HG23	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:334:LEU:HD11	1:I:364:PRO:HA	1.80	0.62
1:B:212:PHE:CD2	1:B:220:PRO:HA	2.35	0.62
1:G:351:SER:HA	1:G:389:LYS:HD2	1.80	0.62
1:E:291:VAL:HA	1:E:298:PRO:HA	1.82	0.62
1:F:71:ALA:C	1:F:73:VAL:H	2.07	0.62
1:G:260:GLN:NE2	1:G:261:PRO:HA	2.09	0.62
1:H:25:GLY:H	1:H:28:ASN:HD22	1.47	0.62
1:J:85:ILE:HB	1:J:88:HIS:O	2.00	0.62
1:K:112:ASN:HB3	1:K:116:LEU:HD23	1.80	0.62
1:D:29:VAL:HG22	1:D:44:LYS:HB2	1.81	0.62
1:I:20:ARG:HG3	1:I:30:CYS:SG	2.40	0.62
1:J:29:VAL:HG22	1:J:44:LYS:HB2	1.81	0.62
1:C:595:GLN:CB	2:S:2:GLC:H3	2.30	0.61
1:G:185:LEU:HD12	1:G:193:PHE:HZ	1.65	0.61
1:H:324:ILE:HD12	1:H:324:ILE:H	1.64	0.61
1:K:221:PHE:HB2	1:K:230:TRP:CZ2	2.35	0.61
1:L:29:VAL:HG22	1:L:44:LYS:HB2	1.82	0.61
1:L:410:ILE:O	1:L:587:VAL:HG22	2.00	0.61
1:B:473:SER:HB2	1:B:524:VAL:HA	1.81	0.61
1:C:25:GLY:H	1:C:28:ASN:HD22	1.48	0.61
1:E:281:ASN:H	1:E:287:ARG:HD3	1.64	0.61
1:H:65:MET:HB3	1:H:76:ALA:HB2	1.80	0.61
1:E:48:LEU:HA	1:E:87:ILE:HG21	1.81	0.61
1:F:260:GLN:NE2	1:F:261:PRO:HA	2.09	0.61
1:K:224:HIS:HE2	1:K:424:ARG:HD2	1.64	0.61
1:K:298:PRO:O	1:K:302:VAL:HG23	1.99	0.61
1:L:320:SER:C	1:L:398:PHE:HB3	2.25	0.61
1:L:563:ARG:NH1	2:n:2:GLC:H2	2.08	0.61
1:B:143:ARG:NH2	1:B:144:ASP:HB2	2.14	0.61
1:C:29:VAL:HG22	1:C:44:LYS:HB2	1.82	0.61
1:D:215:ILE:HD13	1:D:264:LEU:HD11	1.83	0.61
1:I:25:GLY:H	1:I:28:ASN:HD22	1.49	0.61
1:L:316:LEU:HB2	1:L:383:MET:HE1	1.81	0.61
1:A:25:GLY:H	1:A:28:ASN:HD22	1.47	0.61
1:E:265:CYS:SG	1:E:268:ILE:HG13	2.40	0.61
1:F:324:ILE:H	1:F:324:ILE:HD12	1.64	0.61
1:F:351:SER:HA	1:F:389:LYS:HD2	1.83	0.61
1:F:415:LYS:HA	1:F:584:THR:HB	1.83	0.61
1:I:29:VAL:HG22	1:I:44:LYS:HB2	1.81	0.61
1:A:431:VAL:HG21	1:A:568:TYR:HB2	1.83	0.61
1:E:392:THR:O	1:E:612:LEU:HD23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:PHE:CD2	1:F:220:PRO:HA	2.35	0.61
1:I:227:PRO:HA	1:I:230:TRP:HB3	1.82	0.61
1:K:227:PRO:HA	1:K:230:TRP:CB	2.30	0.61
1:L:265:CYS:SG	1:L:268:ILE:HG13	2.40	0.61
1:L:324:ILE:H	1:L:324:ILE:HD12	1.64	0.61
1:L:328:LEU:HD13	1:L:368:ALA:HB1	1.83	0.61
1:L:469:LEU:HD12	1:L:625:VAL:HG13	1.81	0.61
1:A:236:LYS:HG2	1:A:237:LYS:N	2.16	0.61
1:H:415:LYS:HA	1:H:584:THR:HB	1.83	0.61
1:I:427:TRP:HZ3	1:I:567:LEU:HB3	1.66	0.61
1:A:648:LYS:HG3	1:B:489:LEU:HD21	1.83	0.61
1:C:463:THR:HG21	1:C:538:HIS:HD2	1.66	0.61
1:K:396:GLY:N	1:K:397:PRO:HD3	2.16	0.61
1:K:427:TRP:HZ3	1:K:567:LEU:HB3	1.66	0.61
1:B:141:ILE:HG23	1:B:170:LYS:HB2	1.83	0.61
1:C:427:TRP:HZ3	1:C:567:LEU:HB3	1.66	0.61
1:F:265:CYS:SG	1:F:268:ILE:HG13	2.40	0.61
1:J:517:LYS:HD2	1:J:642:MET:HE1	1.83	0.61
1:K:98:CYS:HB3	1:K:152:LEU:O	2.00	0.61
1:K:289:GLY:O	1:K:291:VAL:HG23	2.00	0.61
1:K:403:LEU:HB2	1:K:407:VAL:HB	1.83	0.61
1:L:222:LEU:HD22	1:L:244:ALA:O	2.00	0.61
1:D:294:THR:HG22	1:D:295:LEU:HD22	1.83	0.61
1:F:29:VAL:HG22	1:F:44:LYS:HB2	1.83	0.61
1:F:144:ASP:OD2	1:F:185:LEU:HD21	2.01	0.61
1:H:143:ARG:NH2	1:H:144:ASP:HB2	2.14	0.61
1:L:25:GLY:H	1:L:28:ASN:HD22	1.48	0.61
1:A:550:GLY:HA3	1:A:604:LEU:HD13	1.82	0.60
1:H:186:GLN:NE2	1:H:227:PRO:HD3	2.16	0.60
1:J:13:GLY:N	1:J:14:PRO:HD3	2.08	0.60
1:K:204:TYR:HB2	1:K:287:ARG:NH1	2.16	0.60
1:K:219:ARG:NH1	1:K:224:HIS:H	1.98	0.60
1:K:237:LYS:HE2	1:K:282:TRP:H	1.66	0.60
1:K:478:ALA:CB	1:L:475:GLN:HA	2.31	0.60
1:A:29:VAL:HG22	1:A:44:LYS:HB2	1.83	0.60
1:D:20:ARG:HG3	1:D:30:CYS:SG	2.42	0.60
1:D:230:TRP:O	1:D:234:ILE:HG12	2.01	0.60
1:E:234:ILE:HG22	1:E:254:PHE:HE1	1.66	0.60
1:E:392:THR:HG22	1:E:616:GLN:NE2	2.16	0.60
1:F:298:PRO:O	1:F:302:VAL:HG23	2.00	0.60
1:K:143:ARG:NH2	1:K:144:ASP:HB2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:260:GLN:NE2	1:L:261:PRO:HA	2.10	0.60
1:A:291:VAL:HA	1:A:298:PRO:HA	1.84	0.60
1:B:265:CYS:O	1:B:269:VAL:HG23	2.01	0.60
1:F:275:TRP:CZ2	1:F:304:MET:HE2	2.36	0.60
1:L:72:ASN:HB2	1:L:131:GLY:CA	2.31	0.60
1:B:25:GLY:H	1:B:28:ASN:HD22	1.49	0.60
1:B:318:MET:HE2	1:B:447:GLY:HA3	1.84	0.60
1:B:354:LEU:HB2	1:B:362:LEU:HD13	1.84	0.60
1:C:143:ARG:NH2	1:C:144:ASP:HB2	2.15	0.60
1:D:143:ARG:NH2	1:D:144:ASP:HB2	2.15	0.60
1:E:143:ARG:NH2	1:E:144:ASP:HB2	2.16	0.60
1:E:43:ILE:HG13	1:E:94:ALA:HA	1.84	0.60
1:H:289:GLY:O	1:H:291:VAL:HG23	2.01	0.60
1:K:77:CYS:H	1:K:95:MET:HA	1.65	0.60
1:B:142:HIS:HA	1:B:169:ALA:CB	2.31	0.60
1:C:347:ILE:HD12	1:C:386:LEU:HD21	1.84	0.60
1:D:401:ARG:HH22	1:D:436:GLY:C	2.09	0.60
1:D:473:SER:HB2	1:D:524:VAL:HA	1.84	0.60
1:F:265:CYS:O	1:F:269:VAL:HG23	2.01	0.60
1:I:289:GLY:O	1:I:291:VAL:HG23	2.01	0.60
1:I:347:ILE:HD12	1:I:386:LEU:HD21	1.84	0.60
1:A:483:PHE:HZ	1:A:514:MET:HB3	1.65	0.60
1:B:319:THR:O	1:B:397:PRO:HD2	2.02	0.60
1:E:502:ILE:HD12	1:F:654:LEU:HD11	1.83	0.60
1:G:29:VAL:HG22	1:G:44:LYS:HB2	1.84	0.60
1:G:489:LEU:HD22	1:H:647:GLN:OE1	2.01	0.60
1:H:507:MET:HE1	1:H:653:LEU:HD13	1.83	0.60
1:B:249:SER:HB3	1:D:185:LEU:H	1.67	0.60
1:H:576:SER:OG	1:L:577:ASP:HA	2.01	0.60
1:I:403:LEU:HB2	1:I:407:VAL:HB	1.84	0.60
1:J:7:PRO:HG3	1:J:17:MET:SD	2.42	0.60
1:J:550:GLY:HA3	1:J:604:LEU:HD13	1.83	0.60
1:L:298:PRO:O	1:L:302:VAL:HG23	2.01	0.60
1:L:473:SER:HB2	1:L:524:VAL:HA	1.84	0.60
1:B:86:LEU:HG	1:B:92:LEU:HD11	1.84	0.60
1:E:431:VAL:HG21	1:E:568:TYR:HB2	1.84	0.60
1:I:219:ARG:NH2	1:I:224:HIS:H	2.00	0.60
1:J:126:SER:HB2	1:J:308:LEU:CD1	2.32	0.60
1:B:543:GLU:HA	1:B:546:LYS:HE3	1.84	0.60
1:C:238:ASP:HB3	1:C:239:PRO:HD2	1.84	0.60
1:D:63:GLN:NE2	1:D:174:GLN:HE22	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:LEU:HD11	1:E:188:LEU:HB3	1.84	0.60
1:F:240:LYS:HZ2	1:F:240:LYS:HA	1.67	0.60
1:I:43:ILE:HG13	1:I:94:ALA:HA	1.83	0.60
1:J:219:ARG:HH22	1:J:224:HIS:H	1.50	0.60
1:L:354:LEU:HB3	1:L:384:VAL:CG1	2.31	0.60
1:B:356:SER:HB2	1:B:382:TYR:HE1	1.67	0.59
1:B:547:SER:HB3	1:B:548:PRO:HD2	1.82	0.59
1:C:265:CYS:O	1:C:269:VAL:HG23	2.02	0.59
1:C:431:VAL:HG21	1:C:568:TYR:HB2	1.83	0.59
1:F:396:GLY:N	1:F:397:PRO:HD3	2.16	0.59
1:G:495:SER:HA	1:G:498:MET:HE2	1.84	0.59
1:I:143:ARG:NH2	1:I:144:ASP:HB2	2.16	0.59
1:I:265:CYS:O	1:I:269:VAL:HG23	2.02	0.59
1:J:240:LYS:HB3	1:J:277:GLN:HB3	1.83	0.59
1:K:265:CYS:SG	1:K:268:ILE:HG13	2.41	0.59
1:A:201:THR:HB	1:A:287:ARG:NH1	2.16	0.59
1:E:185:LEU:HD13	1:E:186:GLN:H	1.67	0.59
1:E:473:SER:HB2	1:E:524:VAL:HA	1.84	0.59
1:L:424:ARG:NH1	1:L:572:LYS:HG2	2.16	0.59
1:A:260:GLN:NE2	1:A:261:PRO:HA	2.10	0.59
1:B:74:VAL:CG2	1:B:95:MET:HE3	2.32	0.59
1:C:142:HIS:ND1	1:C:169:ALA:HB2	2.17	0.59
1:D:6:ASP:N	1:D:7:PRO:HD2	2.17	0.59
1:D:46:CYS:SG	1:D:90:VAL:HG23	2.42	0.59
1:G:551:ARG:HB3	1:G:552:ARG:HH21	1.68	0.59
1:K:43:ILE:HG13	1:K:94:ALA:HA	1.84	0.59
1:K:463:THR:HG21	1:K:538:HIS:HD2	1.67	0.59
1:A:473:SER:HA	1:A:632:ILE:HG21	1.83	0.59
1:E:289:GLY:O	1:E:291:VAL:HG23	2.03	0.59
1:G:186:GLN:NE2	1:G:219:ARG:NH1	2.50	0.59
1:G:415:LYS:HA	1:G:584:THR:HB	1.83	0.59
1:H:265:CYS:O	1:H:269:VAL:HG23	2.02	0.59
1:B:595:GLN:HG3	2:Q:2:GLC:H62	1.84	0.59
1:C:191:GLU:CD	1:C:284:PRO:HB3	2.26	0.59
1:E:222:LEU:HB2	1:E:230:TRP:CD1	2.37	0.59
1:F:7:PRO:HG3	1:F:17:MET:HE1	1.83	0.59
1:F:410:ILE:HG23	1:F:583:SER:OG	2.03	0.59
1:I:392:THR:HG22	1:I:616:GLN:HE22	1.66	0.59
1:K:334:LEU:HD11	1:K:364:PRO:HA	1.82	0.59
1:B:69:ASN:HA	1:B:75:LYS:HE3	1.84	0.59
1:B:576:SER:OG	1:F:577:ASP:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASP:H	1:F:579:SER:CB	2.13	0.59
1:D:347:ILE:HD12	1:D:386:LEU:HD21	1.84	0.59
1:E:20:ARG:HG3	1:E:30:CYS:SG	2.43	0.59
1:G:275:TRP:CZ2	1:G:304:MET:HE2	2.37	0.59
1:J:142:HIS:ND1	1:J:169:ALA:HB2	2.18	0.59
1:A:98:CYS:HA	1:A:153:GLN:NE2	2.17	0.59
1:A:347:ILE:HD12	1:A:386:LEU:HD21	1.85	0.59
1:C:403:LEU:HB2	1:C:407:VAL:HB	1.85	0.59
1:D:502:ILE:HG21	1:D:656:ILE:HD13	1.85	0.59
1:E:403:LEU:HB2	1:E:407:VAL:HB	1.85	0.59
1:G:284:PRO:HA	1:G:287:ARG:NH1	2.17	0.59
1:K:462:LEU:HD22	1:K:618:ILE:HG23	1.85	0.59
1:K:465:MET:HB3	1:K:625:VAL:HG11	1.85	0.59
1:C:548:PRO:HB2	1:C:552:ARG:HG3	1.84	0.59
1:D:265:CYS:O	1:D:269:VAL:HG23	2.02	0.59
1:D:289:GLY:O	1:D:291:VAL:HG23	2.01	0.59
1:F:141:ILE:HG23	1:F:170:LYS:HB2	1.84	0.59
1:G:212:PHE:CE2	1:G:220:PRO:HA	2.38	0.59
1:L:220:PRO:O	1:L:243:PHE:HA	2.03	0.59
1:C:489:LEU:HD11	1:D:648:LYS:HE3	1.85	0.59
1:E:393:VAL:HG13	1:E:609:SER:OG	2.03	0.59
1:E:401:ARG:HH22	1:E:440:ASP:HB2	1.66	0.59
1:E:495:SER:HA	1:E:498:MET:HE2	1.85	0.59
1:G:347:ILE:HD12	1:G:386:LEU:HD21	1.85	0.59
1:G:473:SER:HA	1:G:632:ILE:HG21	1.83	0.59
1:J:347:ILE:HD12	1:J:386:LEU:HD21	1.84	0.59
1:K:495:SER:HA	1:K:498:MET:HE2	1.84	0.59
1:L:171:ASP:O	1:L:176:GLU:HA	2.03	0.59
1:L:265:CYS:O	1:L:269:VAL:HG23	2.02	0.59
1:A:265:CYS:O	1:A:269:VAL:HG23	2.02	0.59
1:A:334:LEU:HD22	1:A:366:LYS:O	2.01	0.59
1:A:495:SER:HA	1:A:498:MET:HE2	1.85	0.59
1:B:403:LEU:HB2	1:B:407:VAL:HB	1.85	0.59
1:C:424:ARG:HH11	1:C:572:LYS:HG2	1.68	0.59
1:D:403:LEU:HD23	1:D:403:LEU:H	1.67	0.59
1:H:427:TRP:O	1:H:431:VAL:HG23	2.03	0.59
1:I:240:LYS:HD2	1:I:277:GLN:HB3	1.84	0.59
1:I:658:CYS:HB3	1:J:501:GLY:HA2	1.85	0.59
1:J:143:ARG:NH2	1:J:144:ASP:HB2	2.17	0.59
1:J:334:LEU:HD11	1:J:364:PRO:HA	1.85	0.59
1:K:417:GLN:HB3	1:K:581:SER:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:427:TRP:O	1:L:431:VAL:HG23	2.03	0.59
1:L:480:LEU:HD22	1:L:518:ALA:HB1	1.84	0.59
1:B:495:SER:HA	1:B:498:MET:HE2	1.85	0.58
1:C:469:LEU:HD12	1:C:625:VAL:HG13	1.84	0.58
1:D:424:ARG:HH11	1:D:572:LYS:HG2	1.68	0.58
1:E:70:HIS:CD2	1:E:71:ALA:H	2.21	0.58
1:J:43:ILE:HG13	1:J:94:ALA:HA	1.85	0.58
1:J:427:TRP:HZ3	1:J:567:LEU:HB3	1.68	0.58
1:B:427:TRP:O	1:B:431:VAL:HG23	2.04	0.58
1:C:498:MET:HA	1:C:503:SER:HB3	1.84	0.58
1:H:314:HIS:HB2	1:H:383:MET:HG2	1.85	0.58
1:B:207:PHE:O	1:B:211:VAL:HG23	2.02	0.58
1:E:410:ILE:HG23	1:E:583:SER:OG	2.02	0.58
1:F:410:ILE:O	1:F:587:VAL:HG22	2.03	0.58
1:H:622:LEU:N	1:H:623:PRO:HD2	2.18	0.58
1:I:186:GLN:HG2	1:I:219:ARG:HD3	1.85	0.58
1:K:265:CYS:O	1:K:269:VAL:HG23	2.04	0.58
1:A:223:HIS:O	1:A:225:LEU:HD23	2.02	0.58
1:A:406:CYS:SG	1:A:407:VAL:HG23	2.44	0.58
1:A:577:ASP:N	1:C:579:SER:HB2	2.18	0.58
1:B:281:ASN:HD22	1:B:282:TRP:N	2.02	0.58
1:B:424:ARG:NH1	1:B:572:LYS:HG2	2.18	0.58
1:G:207:PHE:O	1:G:211:VAL:HG23	2.02	0.58
1:H:74:VAL:CG1	1:H:164:ILE:HA	2.33	0.58
1:H:401:ARG:HE	1:H:401:ARG:H	1.49	0.58
1:I:219:ARG:HH21	1:I:224:HIS:H	1.50	0.58
1:F:219:ARG:HE	1:F:224:HIS:N	1.98	0.58
1:F:289:GLY:O	1:F:291:VAL:HG23	2.03	0.58
1:G:265:CYS:O	1:G:269:VAL:HG23	2.02	0.58
1:H:354:LEU:HB2	1:H:362:LEU:HD13	1.86	0.58
1:D:288:GLY:HA3	1:D:300:CYS:SG	2.43	0.58
1:D:410:ILE:HG23	1:D:583:SER:OG	2.03	0.58
1:I:424:ARG:HH11	1:I:572:LYS:HG2	1.67	0.58
1:J:265:CYS:O	1:J:269:VAL:HG23	2.03	0.58
1:L:495:SER:HA	1:L:498:MET:HE2	1.86	0.58
1:A:98:CYS:HB3	1:A:152:LEU:O	2.02	0.58
1:A:547:SER:HB2	1:A:548:PRO:HD2	1.86	0.58
1:B:234:ILE:HG23	1:B:254:PHE:HE1	1.68	0.58
1:E:354:LEU:HB2	1:E:362:LEU:HD13	1.86	0.58
1:F:201:THR:C	1:F:287:ARG:HH21	2.11	0.58
1:F:347:ILE:HD12	1:F:386:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:590:ILE:O	1:G:594:VAL:HG23	2.04	0.58
1:H:186:GLN:HE22	1:H:227:PRO:HD3	1.69	0.58
1:I:648:LYS:HE3	1:J:489:LEU:HD11	1.86	0.58
1:J:20:ARG:HG3	1:J:30:CYS:SG	2.44	0.58
1:K:70:HIS:O	1:K:73:VAL:HG12	2.04	0.58
1:D:43:ILE:HG13	1:D:94:ALA:HA	1.85	0.58
1:E:298:PRO:O	1:E:302:VAL:HG23	2.03	0.58
1:G:170:LYS:HG3	1:G:177:LEU:HA	1.86	0.58
1:H:74:VAL:HG11	1:H:164:ILE:HG13	1.85	0.58
1:I:495:SER:HA	1:I:498:MET:HE2	1.86	0.58
1:J:46:CYS:SG	1:J:90:VAL:HG23	2.44	0.58
1:L:358:THR:O	1:L:453:LEU:HD13	2.03	0.58
1:L:424:ARG:HH11	1:L:572:LYS:HG2	1.68	0.58
1:L:590:ILE:O	1:L:594:VAL:HG23	2.03	0.58
1:D:237:LYS:HG2	1:D:241:CYS:HB3	1.85	0.58
1:G:403:LEU:HB2	1:G:407:VAL:HB	1.85	0.58
1:H:495:SER:HA	1:H:498:MET:HE2	1.85	0.58
1:L:72:ASN:HB2	1:L:131:GLY:HA3	1.85	0.58
1:B:595:GLN:HE21	2:Q:3:PDX:C1	2.16	0.58
1:C:495:SER:HA	1:C:498:MET:HE2	1.86	0.58
1:C:552:ARG:HE	1:C:552:ARG:N	2.02	0.58
1:C:590:ILE:O	1:C:594:VAL:HG23	2.03	0.58
1:D:506:LYS:H	1:D:506:LYS:HD3	1.69	0.58
1:G:473:SER:OG	1:G:524:VAL:HG13	2.03	0.58
1:H:597:GLN:O	1:H:601:LEU:HB2	2.04	0.58
1:I:396:GLY:HA2	1:I:398:PHE:CZ	2.39	0.58
1:J:506:LYS:H	1:J:506:LYS:HD3	1.69	0.58
1:K:497:GLN:HE22	1:L:654:LEU:CD2	2.17	0.58
1:L:373:LEU:HD23	1:L:373:LEU:H	1.69	0.58
1:B:191:GLU:OE2	1:B:284:PRO:HB3	2.03	0.57
1:B:236:LYS:HG3	1:B:237:LYS:N	2.19	0.57
1:E:77:CYS:H	1:E:95:MET:HA	1.68	0.57
1:F:427:TRP:O	1:F:431:VAL:HG23	2.04	0.57
1:F:495:SER:HA	1:F:498:MET:HE2	1.86	0.57
1:G:622:LEU:N	1:G:623:PRO:HD2	2.19	0.57
1:H:237:LYS:HE2	1:H:282:TRP:H	1.69	0.57
1:I:112:ASN:CB	1:I:116:LEU:HD23	2.34	0.57
1:I:431:VAL:HG21	1:I:568:TYR:HB2	1.85	0.57
1:L:354:LEU:HB3	1:L:384:VAL:HG12	1.86	0.57
1:B:143:ARG:HG3	1:B:192:LEU:HD21	1.87	0.57
1:B:597:GLN:O	1:B:601:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:HG3	1:C:30:CYS:SG	2.44	0.57
1:F:43:ILE:HG13	1:F:94:ALA:HA	1.86	0.57
1:F:622:LEU:N	1:F:623:PRO:HD2	2.20	0.57
1:I:420:ILE:HG21	1:I:578:HIS:N	2.19	0.57
1:J:122:LEU:HD11	1:J:268:ILE:HD13	1.85	0.57
1:J:237:LYS:HD2	1:J:238:ASP:O	2.04	0.57
1:J:495:SER:HA	1:J:498:MET:HE2	1.86	0.57
1:K:212:PHE:CD2	1:K:220:PRO:HA	2.39	0.57
1:K:431:VAL:HG21	1:K:568:TYR:HB2	1.87	0.57
1:A:373:LEU:HB2	1:A:378:GLY:CA	2.34	0.57
1:A:403:LEU:HB2	1:A:407:VAL:HB	1.86	0.57
1:B:142:HIS:ND1	1:B:169:ALA:HB2	2.19	0.57
1:C:219:ARG:NH2	1:C:223:HIS:HB2	2.15	0.57
1:D:417:GLN:HB3	1:D:581:SER:HB2	1.86	0.57
1:F:358:THR:O	1:F:453:LEU:HD13	2.04	0.57
1:H:403:LEU:HB2	1:H:407:VAL:HB	1.86	0.57
1:J:260:GLN:NE2	1:J:261:PRO:HA	2.11	0.57
1:J:403:LEU:HB2	1:J:407:VAL:HB	1.86	0.57
1:K:227:PRO:HA	1:K:230:TRP:HB3	1.84	0.57
1:L:347:ILE:HD12	1:L:386:LEU:HD21	1.86	0.57
1:L:403:LEU:HB2	1:L:407:VAL:HB	1.87	0.57
1:A:74:VAL:CG1	1:A:164:ILE:HA	2.34	0.57
1:A:622:LEU:N	1:A:623:PRO:HD2	2.19	0.57
1:D:313:VAL:HG22	1:D:372:VAL:HG12	1.87	0.57
1:D:403:LEU:HB2	1:D:407:VAL:HB	1.86	0.57
1:G:68:LEU:C	1:G:69:ASN:HD22	2.12	0.57
1:J:509:LYS:O	1:J:513:GLU:HG2	2.05	0.57
1:L:79:VAL:HG21	1:L:83:LEU:HD13	1.86	0.57
1:A:275:TRP:CZ2	1:A:304:MET:HE2	2.40	0.57
1:A:590:ILE:O	1:A:594:VAL:HG23	2.05	0.57
1:C:230:TRP:O	1:C:234:ILE:HG12	2.04	0.57
1:D:102:ASP:HB3	4:D:701:5TL:CAN	2.34	0.57
1:F:590:ILE:O	1:F:594:VAL:HG23	2.04	0.57
1:G:43:ILE:HG13	1:G:94:ALA:HA	1.85	0.57
1:H:224:HIS:O	1:H:225:LEU:HD22	2.04	0.57
1:J:7:PRO:O	1:J:8:GLU:HB3	2.05	0.57
1:J:333:SER:HA	1:J:368:ALA:H	1.69	0.57
1:A:13:GLY:N	1:A:14:PRO:HD3	2.11	0.57
1:A:412:GLN:CD	1:E:27:GLY:HA2	2.29	0.57
1:B:20:ARG:HG3	1:B:30:CYS:SG	2.44	0.57
1:B:319:THR:HG22	1:B:394:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ARG:HH21	1:C:223:HIS:CB	2.15	0.57
1:C:237:LYS:HZ2	1:C:281:ASN:HA	1.68	0.57
1:C:509:LYS:O	1:C:513:GLU:HG2	2.05	0.57
1:D:507:MET:HE1	1:D:653:LEU:HD13	1.87	0.57
1:D:597:GLN:O	1:D:601:LEU:HB2	2.03	0.57
1:E:506:LYS:H	1:E:506:LYS:HD3	1.70	0.57
1:F:118:GLU:HG2	1:F:379:CYS:SG	2.45	0.57
1:G:222:LEU:H	1:G:230:TRP:NE1	1.99	0.57
1:G:648:LYS:HE3	1:H:489:LEU:HD11	1.87	0.57
1:H:207:PHE:O	1:H:211:VAL:HG23	2.04	0.57
1:H:424:ARG:HH11	1:H:572:LYS:HG2	1.67	0.57
1:J:597:GLN:O	1:J:601:LEU:HB2	2.03	0.57
1:K:354:LEU:HB2	1:K:362:LEU:HD13	1.87	0.57
1:K:427:TRP:O	1:K:431:VAL:HG23	2.04	0.57
1:L:506:LYS:H	1:L:506:LYS:HD3	1.70	0.57
1:A:117:LYS:O	1:A:121:ILE:HG13	2.05	0.57
1:B:465:MET:HE3	1:B:625:VAL:HG21	1.86	0.57
1:C:209:THR:HG22	1:C:220:PRO:HG3	1.85	0.57
1:E:139:LYS:HD2	1:E:172:VAL:HG11	1.87	0.57
1:H:509:LYS:O	1:H:513:GLU:HG2	2.05	0.57
1:I:110:PRO:O	1:I:113:CYS:HB3	2.04	0.57
1:K:501:GLY:HA2	1:L:658:CYS:HB3	1.87	0.57
1:B:542:MET:HA	1:B:545:GLN:HE21	1.68	0.57
1:B:622:LEU:N	1:B:623:PRO:HD2	2.20	0.57
1:D:495:SER:HA	1:D:498:MET:HE2	1.86	0.57
1:E:265:CYS:O	1:E:269:VAL:HG23	2.05	0.57
1:F:403:LEU:HB2	1:F:407:VAL:HB	1.87	0.57
1:F:410:ILE:HD12	1:F:583:SER:OG	2.04	0.57
1:G:552:ARG:N	1:G:552:ARG:HE	2.02	0.57
1:I:231:HIS:HB3	1:I:282:TRP:HH2	1.68	0.57
1:J:143:ARG:HG3	1:J:192:LEU:HD21	1.87	0.57
1:K:551:ARG:HB3	1:K:552:ARG:HH21	1.70	0.57
1:L:622:LEU:N	1:L:623:PRO:HD2	2.20	0.57
1:B:401:ARG:H	1:B:401:ARG:HD2	1.68	0.57
1:D:427:TRP:O	1:D:431:VAL:HG23	2.04	0.57
1:D:552:ARG:HE	1:D:552:ARG:N	2.03	0.57
1:E:143:ARG:HG3	1:E:192:LEU:HD21	1.86	0.57
1:F:275:TRP:HZ2	1:F:304:MET:HE2	1.70	0.57
1:G:86:LEU:HD12	1:G:87:ILE:HG13	1.86	0.57
1:I:509:LYS:O	1:I:513:GLU:HG2	2.05	0.57
1:J:267:LEU:HD12	1:J:312:ILE:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:354:LEU:HB2	1:L:362:LEU:HD13	1.87	0.57
1:L:410:ILE:HD12	1:L:583:SER:OG	2.05	0.57
1:C:43:ILE:HG13	1:C:94:ALA:HA	1.86	0.57
1:E:427:TRP:O	1:E:431:VAL:HG23	2.05	0.57
1:G:483:PHE:HZ	1:G:514:MET:HB3	1.69	0.57
1:G:506:LYS:H	1:G:506:LYS:HD3	1.70	0.57
1:G:655:LYS:HE3	1:H:497:GLN:OE1	2.05	0.57
1:H:143:ARG:HG3	1:H:192:LEU:HD21	1.87	0.57
1:H:543:GLU:HA	1:H:546:LYS:NZ	2.20	0.57
1:K:485:LYS:HG2	1:L:640:MET:HE1	1.87	0.57
2:m:2:GLC:H62	2:m:3:PDX:C5	2.34	0.57
1:C:221:PHE:HB2	1:C:230:TRP:HE1	1.70	0.56
1:C:222:LEU:HB2	1:C:230:TRP:CD1	2.40	0.56
1:D:86:LEU:HD23	1:D:91:PRO:HA	1.87	0.56
1:D:235:LYS:HA	1:D:282:TRP:CH2	2.40	0.56
1:F:506:LYS:HD3	1:F:506:LYS:H	1.70	0.56
1:G:403:LEU:HD23	1:G:403:LEU:H	1.70	0.56
1:H:303:LEU:O	1:H:307:ILE:HG13	2.05	0.56
1:J:552:ARG:HE	1:J:552:ARG:N	2.04	0.56
2:N:1:5LS:C6	2:N:2:GLC:H5	2.35	0.56
1:A:354:LEU:HB2	1:A:362:LEU:HD13	1.86	0.56
1:A:502:ILE:HD13	1:A:656:ILE:HD12	1.87	0.56
1:C:427:TRP:O	1:C:431:VAL:HG23	2.05	0.56
1:F:320:SER:HA	1:F:398:PHE:HB3	1.86	0.56
1:G:227:PRO:HA	1:G:230:TRP:CB	2.36	0.56
1:J:622:LEU:N	1:J:623:PRO:HD2	2.21	0.56
1:K:506:LYS:HD3	1:K:506:LYS:H	1.70	0.56
1:K:622:LEU:N	1:K:623:PRO:HD2	2.19	0.56
1:A:91:PRO:O	1:A:92:LEU:HD12	2.05	0.56
1:A:427:TRP:HZ3	1:A:567:LEU:HB3	1.71	0.56
1:B:84:ASN:CG	1:B:85:ILE:H	2.14	0.56
1:B:250:GLY:HA3	1:D:226:GLN:HG2	1.87	0.56
1:C:303:LEU:O	1:C:307:ILE:HG13	2.06	0.56
1:D:143:ARG:HG3	1:D:192:LEU:HD21	1.87	0.56
1:D:207:PHE:O	1:D:211:VAL:HG23	2.05	0.56
1:D:226:GLN:O	1:D:230:TRP:HB2	2.05	0.56
1:D:622:LEU:N	1:D:623:PRO:HD2	2.21	0.56
1:E:347:ILE:HD12	1:E:386:LEU:HD21	1.86	0.56
1:E:395:GLU:HG3	1:E:397:PRO:HD3	1.87	0.56
1:E:401:ARG:HG3	1:E:433:TYR:CE1	2.41	0.56
1:E:480:LEU:HD22	1:E:518:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:LYS:HD2	2:W:2:GLC:H61	1.88	0.56
1:F:159:ILE:HG12	1:F:377:ARG:HH12	1.69	0.56
1:G:392:THR:HG22	1:G:616:GLN:HE22	1.70	0.56
1:G:406:CYS:SG	1:G:407:VAL:HG23	2.46	0.56
1:G:427:TRP:HZ3	1:G:567:LEU:HB3	1.70	0.56
1:G:427:TRP:O	1:G:431:VAL:HG23	2.05	0.56
1:G:597:GLN:O	1:G:601:LEU:HB2	2.05	0.56
1:J:87:ILE:O	1:J:88:HIS:HB2	2.05	0.56
1:J:207:PHE:O	1:J:211:VAL:HG23	2.05	0.56
1:J:354:LEU:HB2	1:J:362:LEU:HD13	1.88	0.56
1:K:207:PHE:O	1:K:211:VAL:HG23	2.05	0.56
1:K:347:ILE:HD12	1:K:386:LEU:HD21	1.87	0.56
1:K:509:LYS:O	1:K:513:GLU:HG2	2.05	0.56
1:L:20:ARG:HG3	1:L:30:CYS:SG	2.45	0.56
1:L:237:LYS:HE2	1:L:282:TRP:H	1.69	0.56
1:A:141:ILE:HG13	1:A:203:ASP:OD1	2.06	0.56
1:A:506:LYS:HD3	1:A:506:LYS:H	1.70	0.56
1:C:142:HIS:HA	1:C:169:ALA:CB	2.35	0.56
1:D:237:LYS:HE3	1:D:281:ASN:HA	1.88	0.56
1:H:427:TRP:CZ3	1:H:567:LEU:HB3	2.40	0.56
1:J:79:VAL:HG11	1:J:83:LEU:HD22	1.88	0.56
1:A:415:LYS:HA	1:A:584:THR:HB	1.86	0.56
1:D:509:LYS:O	1:D:513:GLU:HG2	2.06	0.56
1:D:589:ILE:H	1:D:589:ILE:CD1	2.19	0.56
1:E:84:ASN:ND2	1:E:85:ILE:H	2.04	0.56
1:F:74:VAL:HA	1:F:96:GLU:OE1	2.05	0.56
1:F:240:LYS:HD3	1:F:277:GLN:HB3	1.86	0.56
1:G:222:LEU:N	1:G:230:TRP:HE1	2.01	0.56
1:H:43:ILE:HG13	1:H:94:ALA:HA	1.86	0.56
1:I:502:ILE:HG23	1:J:658:CYS:SG	2.46	0.56
1:I:590:ILE:O	1:I:594:VAL:HG23	2.04	0.56
1:K:396:GLY:H	1:K:397:PRO:HD3	1.70	0.56
1:E:278:LEU:O	1:E:287:ARG:HG3	2.06	0.56
1:E:318:MET:CE	1:E:447:GLY:HA3	2.35	0.56
1:E:445:PHE:CE2	1:E:551:ARG:HD2	2.41	0.56
1:H:275:TRP:CZ2	1:H:304:MET:HE2	2.41	0.56
1:K:517:LYS:HD2	1:K:642:MET:HE1	1.86	0.56
1:A:427:TRP:O	1:A:431:VAL:HG23	2.05	0.56
1:B:509:LYS:O	1:B:513:GLU:HG2	2.06	0.56
1:B:590:ILE:O	1:B:594:VAL:HG23	2.06	0.56
1:C:212:PHE:CE2	1:C:220:PRO:HA	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:LEU:HD12	1:E:312:ILE:HG23	1.86	0.56
1:F:354:LEU:HB2	1:F:362:LEU:HD13	1.88	0.56
1:G:77:CYS:O	1:G:94:ALA:HB3	2.06	0.56
1:G:480:LEU:HD22	1:G:518:ALA:HB1	1.87	0.56
1:G:498:MET:HA	1:G:503:SER:HB3	1.86	0.56
1:H:412:GLN:NE2	1:J:20:ARG:HG2	2.20	0.56
1:L:43:ILE:HG13	1:L:94:ALA:HA	1.87	0.56
1:L:289:GLY:O	1:L:291:VAL:HG23	2.06	0.56
1:L:334:LEU:HD11	1:L:364:PRO:HA	1.86	0.56
1:L:552:ARG:HE	1:L:552:ARG:N	2.02	0.56
1:A:20:ARG:C	1:A:21:LEU:HD22	2.30	0.56
1:A:212:PHE:CE2	1:A:220:PRO:HA	2.41	0.56
1:C:415:LYS:HA	1:C:584:THR:HB	1.88	0.56
1:E:552:ARG:HE	1:E:552:ARG:N	2.02	0.56
1:G:97:TYR:HA	4:G:701:5TL:NAW	2.20	0.56
1:H:639:VAL:HA	1:H:642:MET:HG3	1.87	0.56
1:J:298:PRO:O	1:J:302:VAL:HG23	2.06	0.56
1:C:318:MET:HE2	1:C:447:GLY:HA3	1.88	0.56
1:D:544:LEU:HD11	1:D:610:LYS:HB3	1.88	0.56
1:E:478:ALA:CB	1:F:475:GLN:HA	2.36	0.56
1:G:231:HIS:N	1:G:231:HIS:ND1	2.53	0.56
1:G:262:ASN:ND2	1:G:264:LEU:H	2.04	0.56
1:H:623:PRO:O	1:H:627:VAL:HG23	2.05	0.56
1:I:143:ARG:HG3	1:I:192:LEU:HD21	1.88	0.56
1:I:552:ARG:HE	1:I:552:ARG:N	2.03	0.56
1:K:143:ARG:HG3	1:K:192:LEU:HD21	1.88	0.56
1:A:262:ASN:ND2	1:A:264:LEU:H	2.04	0.56
1:B:43:ILE:HG13	1:B:94:ALA:HA	1.86	0.56
1:D:410:ILE:O	1:D:587:VAL:HG22	2.06	0.56
1:D:546:LYS:HA	3:T:2:5TJ:S4	2.45	0.56
1:F:480:LEU:HD22	1:F:518:ALA:HB1	1.88	0.56
1:F:639:VAL:HA	1:F:642:MET:HG3	1.88	0.56
1:G:222:LEU:HD22	1:G:230:TRP:CD1	2.38	0.56
1:I:506:LYS:HD3	1:I:506:LYS:H	1.69	0.56
1:I:575:PRO:HB3	1:K:574:ARG:HH12	1.69	0.56
1:I:622:LEU:N	1:I:623:PRO:HD2	2.21	0.56
1:J:227:PRO:HA	1:J:230:TRP:CB	2.29	0.56
1:K:20:ARG:HG3	1:K:30:CYS:SG	2.46	0.56
1:L:143:ARG:HG3	1:L:192:LEU:HD21	1.86	0.56
1:A:597:GLN:O	1:A:601:LEU:HB2	2.06	0.55
1:B:303:LEU:O	1:B:307:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:622:LEU:N	1:C:623:PRO:HD2	2.20	0.55
1:D:354:LEU:HB2	1:D:362:LEU:HD13	1.89	0.55
1:D:411:VAL:HG12	1:D:590:ILE:HG21	1.88	0.55
1:E:98:CYS:HB3	1:E:152:LEU:O	2.05	0.55
1:E:396:GLY:N	1:E:397:PRO:HD3	2.16	0.55
1:F:143:ARG:HG3	1:F:192:LEU:HD21	1.87	0.55
1:F:597:GLN:O	1:F:601:LEU:HB2	2.06	0.55
1:G:20:ARG:C	1:G:21:LEU:HD22	2.31	0.55
1:G:170:LYS:CG	1:G:177:LEU:HG	2.36	0.55
1:G:354:LEU:HB2	1:G:362:LEU:HD13	1.88	0.55
1:G:551:ARG:HG3	1:G:551:ARG:O	2.06	0.55
1:H:20:ARG:HG3	1:H:30:CYS:SG	2.46	0.55
1:I:354:LEU:HB2	1:I:362:LEU:HD13	1.88	0.55
1:J:284:PRO:HG2	1:J:285:GLN:H	1.70	0.55
1:J:363:ASP:HB3	1:J:370:GLN:HE22	1.70	0.55
1:J:427:TRP:O	1:J:431:VAL:HG23	2.05	0.55
1:K:262:ASN:ND2	1:K:264:LEU:H	2.04	0.55
1:K:320:SER:C	1:K:398:PHE:HB3	2.31	0.55
1:L:396:GLY:N	1:L:397:PRO:HD3	2.21	0.55
1:A:70:HIS:CD2	1:A:72:ASN:HB3	2.42	0.55
1:B:298:PRO:O	1:B:302:VAL:HG23	2.06	0.55
1:C:354:LEU:HB2	1:C:362:LEU:HD13	1.88	0.55
1:C:507:MET:HE1	1:C:653:LEU:HD13	1.88	0.55
1:E:462:LEU:HD22	1:E:618:ILE:HG23	1.88	0.55
1:F:509:LYS:O	1:F:513:GLU:HG2	2.06	0.55
1:G:46:CYS:HA	1:G:58:TRP:CH2	2.41	0.55
1:H:347:ILE:HD12	1:H:386:LEU:HD21	1.86	0.55
1:L:509:LYS:O	1:L:513:GLU:HG2	2.06	0.55
1:A:552:ARG:HE	1:A:552:ARG:N	2.04	0.55
1:B:249:SER:O	1:D:227:PRO:HG2	2.06	0.55
1:C:98:CYS:HA	1:C:153:GLN:NE2	2.21	0.55
1:E:303:LEU:O	1:E:307:ILE:HG13	2.07	0.55
1:G:21:LEU:HD12	4:G:701:5TL:CAJ	2.37	0.55
1:H:27:GLY:HA2	1:L:412:GLN:CD	2.31	0.55
1:H:69:ASN:ND2	1:H:75:LYS:HE2	2.21	0.55
1:I:20:ARG:C	1:I:21:LEU:HD22	2.31	0.55
1:J:188:LEU:HD21	1:J:192:LEU:HD22	1.88	0.55
1:K:303:LEU:O	1:K:307:ILE:HG13	2.07	0.55
1:L:223:HIS:O	1:L:225:LEU:HG	2.07	0.55
1:A:185:LEU:O	1:A:186:GLN:HG2	2.06	0.55
1:A:207:PHE:O	1:A:211:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ARG:NH1	1:E:575:PRO:HB3	2.20	0.55
1:B:219:ARG:HH11	1:B:219:ARG:H	1.53	0.55
1:C:396:GLY:HA2	1:C:398:PHE:CE2	2.42	0.55
1:E:406:CYS:SG	1:E:407:VAL:HG23	2.47	0.55
1:E:489:LEU:HD21	1:F:648:LYS:HG3	1.88	0.55
1:E:622:LEU:N	1:E:623:PRO:HD2	2.20	0.55
1:G:98:CYS:HA	1:G:153:GLN:NE2	2.20	0.55
1:H:141:ILE:HG13	1:H:203:ASP:OD1	2.06	0.55
1:H:410:ILE:HG23	1:H:583:SER:OG	2.07	0.55
1:I:294:THR:HG22	1:I:295:LEU:HD12	1.89	0.55
1:J:589:ILE:H	1:J:589:ILE:CD1	2.20	0.55
1:K:410:ILE:HG23	1:K:583:SER:OG	2.05	0.55
1:A:236:LYS:HZ2	1:A:237:LYS:H	1.55	0.55
1:B:240:LYS:O	1:B:277:GLN:HG2	2.06	0.55
1:B:577:ASP:HA	1:D:576:SER:OG	2.06	0.55
1:C:506:LYS:HD3	1:C:506:LYS:H	1.70	0.55
1:D:427:TRP:CZ3	1:D:567:LEU:HB3	2.39	0.55
1:E:639:VAL:HA	1:E:642:MET:HG3	1.88	0.55
1:G:141:ILE:HG13	1:G:203:ASP:OD1	2.07	0.55
1:G:509:LYS:O	1:G:513:GLU:HG2	2.06	0.55
1:H:46:CYS:SG	1:H:90:VAL:HB	2.47	0.55
1:J:469:LEU:HD12	1:J:625:VAL:HG13	1.88	0.55
1:L:315:ILE:HD12	1:L:384:VAL:HB	1.89	0.55
1:L:502:ILE:HD13	1:L:656:ILE:HD12	1.89	0.55
1:A:43:ILE:HG13	1:A:94:ALA:HA	1.87	0.55
1:B:347:ILE:HD12	1:B:386:LEU:HD21	1.86	0.55
1:C:143:ARG:HG3	1:C:192:LEU:HD21	1.88	0.55
1:E:46:CYS:HA	1:E:58:TRP:CH2	2.41	0.55
1:G:289:GLY:O	1:G:291:VAL:HG23	2.06	0.55
1:J:123:SER:HB2	1:J:377:ARG:HD3	1.88	0.55
1:J:507:MET:HE1	1:J:653:LEU:HD13	1.88	0.55
1:A:17:MET:HB3	1:A:32:TYR:CE1	2.42	0.55
1:C:13:GLY:N	1:C:14:PRO:HD3	2.21	0.55
1:F:20:ARG:HG3	1:F:30:CYS:SG	2.47	0.55
1:G:278:LEU:HD23	1:G:288:GLY:HA2	1.88	0.55
1:G:303:LEU:O	1:G:307:ILE:HG13	2.06	0.55
1:J:212:PHE:CE2	1:J:220:PRO:HA	2.40	0.55
1:L:589:ILE:HD12	1:L:589:ILE:N	2.20	0.55
1:L:639:VAL:HA	1:L:642:MET:HG3	1.89	0.55
1:A:70:HIS:NE2	1:A:72:ASN:HB3	2.22	0.55
1:A:143:ARG:HG3	1:A:192:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:VAL:HG23	1:B:427:TRP:HD1	1.71	0.55
1:C:77:CYS:O	1:C:94:ALA:HB3	2.07	0.55
1:C:141:ILE:HG13	1:C:203:ASP:OD1	2.07	0.55
1:D:186:GLN:HE21	1:D:219:ARG:HE	1.54	0.55
1:D:589:ILE:HD12	1:D:589:ILE:N	2.20	0.55
1:E:502:ILE:HG13	1:F:658:CYS:SG	2.47	0.55
1:F:362:LEU:HG	1:F:363:ASP:H	1.72	0.55
1:G:222:LEU:HB3	1:G:225:LEU:HB2	1.89	0.55
1:L:238:ASP:HB3	1:L:239:PRO:HD2	1.89	0.55
1:L:362:LEU:HG	1:L:363:ASP:H	1.72	0.55
1:L:597:GLN:O	1:L:601:LEU:HB2	2.06	0.55
1:D:550:GLY:HA3	1:D:604:LEU:HD13	1.89	0.55
1:E:20:ARG:C	1:E:21:LEU:HD22	2.32	0.55
1:I:49:GLU:HA	1:I:88:HIS:HB2	1.88	0.55
1:I:417:GLN:HB3	1:I:581:SER:HB3	1.88	0.55
1:I:639:VAL:HA	1:I:642:MET:HG3	1.89	0.55
1:J:116:LEU:HD12	1:J:116:LEU:H	1.72	0.55
1:K:117:LYS:O	1:K:121:ILE:HG13	2.07	0.55
1:K:141:ILE:HG13	1:K:203:ASP:OD1	2.06	0.55
1:L:75:LYS:O	1:L:95:MET:HA	2.07	0.55
1:B:506:LYS:H	1:B:506:LYS:HD3	1.70	0.55
1:E:470:ILE:O	1:E:474:GLN:HG2	2.07	0.55
1:F:18:ARG:HH21	1:F:33:GLN:NE2	2.05	0.55
1:J:46:CYS:HA	1:J:58:TRP:CH2	2.42	0.55
1:J:590:ILE:O	1:J:594:VAL:HG23	2.06	0.55
1:L:473:SER:OG	1:L:524:VAL:HG13	2.07	0.55
1:A:47:ARG:O	1:A:87:ILE:HB	2.07	0.54
1:B:401:ARG:HG2	1:B:433:TYR:HE1	1.72	0.54
1:C:207:PHE:O	1:C:211:VAL:HG23	2.06	0.54
1:D:240:LYS:HB3	1:D:277:GLN:HB3	1.88	0.54
1:E:424:ARG:NH1	1:E:572:LYS:HG2	2.22	0.54
1:E:509:LYS:O	1:E:513:GLU:HG2	2.06	0.54
1:F:101:GLY:HA2	4:F:701:5TL:CAQ	2.37	0.54
1:I:227:PRO:HG2	1:K:249:SER:O	2.07	0.54
1:I:320:SER:C	1:I:398:PHE:HB3	2.33	0.54
1:A:46:CYS:HA	1:A:58:TRP:CH2	2.42	0.54
1:A:303:LEU:O	1:A:307:ILE:HG13	2.07	0.54
1:C:363:ASP:HB3	1:C:370:GLN:HE22	1.71	0.54
1:E:401:ARG:HG3	1:E:433:TYR:HE1	1.73	0.54
1:E:597:GLN:O	1:E:601:LEU:HB2	2.07	0.54
1:F:62:ILE:HG22	1:F:93:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ILE:HG13	1:F:203:ASP:OD1	2.07	0.54
1:F:240:LYS:HB3	1:F:277:GLN:HB3	1.88	0.54
1:G:281:ASN:HB3	1:G:287:ARG:HG2	1.89	0.54
1:G:639:VAL:HA	1:G:642:MET:HG3	1.89	0.54
1:H:506:LYS:H	1:H:506:LYS:HD3	1.70	0.54
1:I:219:ARG:NE	1:I:223:HIS:HA	2.19	0.54
1:I:597:GLN:O	1:I:601:LEU:HB2	2.08	0.54
1:K:406:CYS:SG	1:K:407:VAL:HG23	2.47	0.54
1:L:79:VAL:HG11	1:L:83:LEU:CD1	2.37	0.54
1:A:107:LEU:HD23	1:A:116:LEU:HD11	1.88	0.54
1:A:470:ILE:O	1:A:474:GLN:HG2	2.07	0.54
1:A:574:ARG:HD2	1:A:577:ASP:OD2	2.08	0.54
1:B:84:ASN:ND2	1:B:86:LEU:H	2.04	0.54
1:B:552:ARG:HE	1:B:552:ARG:N	2.04	0.54
1:B:639:VAL:HA	1:B:642:MET:HG3	1.88	0.54
1:C:20:ARG:C	1:C:21:LEU:HD22	2.33	0.54
1:D:188:LEU:HD21	1:D:192:LEU:HD22	1.89	0.54
1:G:13:GLY:N	1:G:14:PRO:HD3	2.22	0.54
1:G:20:ARG:HG3	1:G:30:CYS:SG	2.47	0.54
1:G:362:LEU:HG	1:G:363:ASP:H	1.72	0.54
1:G:574:ARG:NH1	1:K:575:PRO:HB3	2.23	0.54
1:H:590:ILE:O	1:H:594:VAL:HG23	2.07	0.54
1:B:275:TRP:CZ2	1:B:304:MET:HE2	2.43	0.54
1:C:50:LEU:HD13	1:C:90:VAL:HG21	1.90	0.54
1:C:639:VAL:HA	1:C:642:MET:HG3	1.90	0.54
1:E:141:ILE:HG13	1:E:203:ASP:OD1	2.07	0.54
1:G:17:MET:HB3	1:G:32:TYR:CE1	2.42	0.54
1:G:212:PHE:CD2	1:G:220:PRO:HA	2.43	0.54
1:I:55:ARG:HH21	1:I:88:HIS:CE1	2.25	0.54
1:K:392:THR:HG22	1:K:616:GLN:HE22	1.73	0.54
1:A:489:LEU:HD11	1:B:648:LYS:HE3	1.90	0.54
1:C:387:PHE:CZ	1:C:451:ALA:HB2	2.41	0.54
1:D:639:VAL:HA	1:D:642:MET:HG3	1.89	0.54
1:E:115:GLY:HA3	1:E:215:ILE:O	2.07	0.54
1:F:220:PRO:O	1:F:243:PHE:HA	2.06	0.54
1:H:406:CYS:SG	1:H:407:VAL:HG23	2.48	0.54
1:H:412:GLN:HE22	1:J:20:ARG:HG2	1.73	0.54
1:I:303:LEU:O	1:I:307:ILE:HG13	2.08	0.54
1:J:249:SER:HB3	1:L:185:LEU:H	1.73	0.54
1:J:623:PRO:O	1:J:627:VAL:HG23	2.07	0.54
1:L:141:ILE:HG13	1:L:203:ASP:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LYS:O	1:A:513:GLU:HG2	2.06	0.54
1:B:188:LEU:HD21	1:B:192:LEU:HD22	1.90	0.54
1:C:17:MET:HB3	1:C:32:TYR:CE1	2.43	0.54
1:D:17:MET:HB3	1:D:32:TYR:CE1	2.43	0.54
1:E:207:PHE:O	1:E:211:VAL:HG23	2.08	0.54
1:E:514:MET:HA	1:E:642:MET:HE1	1.88	0.54
1:H:222:LEU:HB2	1:H:230:TRP:CD1	2.42	0.54
1:H:233:LYS:HE2	1:H:252:VAL:HG11	1.90	0.54
1:J:589:ILE:HD12	1:J:589:ILE:N	2.21	0.54
1:K:73:VAL:HG22	1:K:74:VAL:H	1.72	0.54
1:K:420:ILE:HG21	1:K:578:HIS:H	1.72	0.54
1:L:420:ILE:HG21	1:L:578:HIS:H	1.72	0.54
1:L:589:ILE:H	1:L:589:ILE:CD1	2.20	0.54
1:C:597:GLN:O	1:C:601:LEU:HB2	2.08	0.54
1:E:291:VAL:HG22	1:E:298:PRO:HB3	1.90	0.54
1:F:320:SER:C	1:F:398:PHE:HB3	2.33	0.54
1:F:470:ILE:O	1:F:474:GLN:HG2	2.08	0.54
1:G:550:GLY:HA3	1:G:604:LEU:HD13	1.90	0.54
1:H:188:LEU:HD21	1:H:192:LEU:HD22	1.90	0.54
1:J:275:TRP:CZ2	1:J:304:MET:HE2	2.41	0.54
1:K:224:HIS:NE2	1:K:424:ARG:HD2	2.22	0.54
1:K:470:ILE:O	1:K:474:GLN:HG2	2.08	0.54
1:L:278:LEU:O	1:L:287:ARG:HG3	2.08	0.54
1:L:427:TRP:CZ3	1:L:567:LEU:HB3	2.41	0.54
1:C:589:ILE:HD12	1:C:589:ILE:N	2.21	0.54
1:E:187:TYR:OH	1:E:219:ARG:HD3	2.08	0.54
1:F:589:ILE:HD12	1:F:589:ILE:N	2.21	0.54
1:G:401:ARG:HH22	1:G:436:GLY:C	2.16	0.54
1:J:7:PRO:C	1:J:9:PHE:H	2.16	0.54
1:J:359:GLY:HA3	1:J:453:LEU:HB2	1.90	0.54
1:K:17:MET:HB3	1:K:32:TYR:CE1	2.43	0.54
1:K:423:LEU:HA	1:K:426:VAL:CG2	2.38	0.54
1:K:465:MET:CB	1:K:625:VAL:HG11	2.38	0.54
1:L:46:CYS:HA	1:L:58:TRP:CH2	2.43	0.54
1:L:207:PHE:O	1:L:211:VAL:HG23	2.07	0.54
1:A:74:VAL:HB	1:A:164:ILE:HG13	1.89	0.54
1:C:237:LYS:NZ	1:C:281:ASN:HA	2.22	0.54
1:D:470:ILE:O	1:D:474:GLN:HG2	2.08	0.54
1:E:427:TRP:HZ3	1:E:567:LEU:HB3	1.72	0.54
1:F:86:LEU:HD23	1:F:87:ILE:CD1	2.38	0.54
1:F:427:TRP:HZ2	1:F:583:SER:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:473:SER:HB2	1:F:524:VAL:HA	1.90	0.54
1:F:552:ARG:HE	1:F:552:ARG:N	2.04	0.54
1:F:589:ILE:H	1:F:589:ILE:CD1	2.20	0.54
1:H:396:GLY:C	1:H:398:PHE:H	2.15	0.54
1:I:50:LEU:HD12	1:I:50:LEU:H	1.73	0.54
1:I:395:GLU:HG2	1:I:396:GLY:H	1.73	0.54
1:I:420:ILE:HG21	1:I:578:HIS:H	1.72	0.54
1:J:639:VAL:HA	1:J:642:MET:HG3	1.90	0.54
1:K:46:CYS:HA	1:K:58:TRP:CH2	2.42	0.54
1:K:204:TYR:HB2	1:K:287:ARG:HH12	1.72	0.54
1:A:204:TYR:HB2	1:A:287:ARG:NH1	2.23	0.54
1:A:362:LEU:HG	1:A:363:ASP:H	1.73	0.54
1:A:654:LEU:HD11	1:B:502:ILE:HD11	1.89	0.54
1:B:46:CYS:HA	1:B:58:TRP:CH2	2.42	0.54
1:D:141:ILE:HG13	1:D:203:ASP:OD1	2.08	0.54
1:G:143:ARG:HG3	1:G:192:LEU:HD21	1.89	0.54
1:I:17:MET:HB3	1:I:32:TYR:CE1	2.43	0.54
1:J:141:ILE:HG13	1:J:203:ASP:OD1	2.08	0.54
1:K:6:ASP:N	1:K:7:PRO:HD2	2.23	0.54
1:K:597:GLN:O	1:K:601:LEU:HB2	2.08	0.54
1:K:639:VAL:HA	1:K:642:MET:HG3	1.89	0.54
1:L:488:GLN:HB3	1:L:515:GLU:OE2	2.07	0.54
2:j:1:5LS:C6	2:j:2:GLC:H5	2.37	0.54
1:B:68:LEU:HD21	1:B:140:ILE:HD12	1.90	0.53
1:B:587:VAL:O	1:B:591:VAL:HG23	2.08	0.53
1:C:82:GLU:CD	1:C:82:GLU:H	2.15	0.53
1:C:406:CYS:SG	1:C:407:VAL:HG23	2.47	0.53
1:E:420:ILE:HG21	1:E:578:HIS:N	2.22	0.53
1:F:303:LEU:O	1:F:307:ILE:HG13	2.08	0.53
1:G:184:THR:OG1	1:I:248:MET:HB3	2.07	0.53
1:G:186:GLN:NE2	1:G:219:ARG:HH11	2.06	0.53
1:H:267:LEU:HD13	1:H:327:LEU:HB2	1.90	0.53
1:I:70:HIS:CG	1:I:71:ALA:H	2.25	0.53
1:J:17:MET:HB3	1:J:32:TYR:CE1	2.43	0.53
1:J:18:ARG:HH21	1:J:33:GLN:NE2	2.04	0.53
1:L:373:LEU:HD23	1:L:373:LEU:N	2.23	0.53
1:B:141:ILE:O	1:B:169:ALA:HB1	2.09	0.53
1:D:18:ARG:HH21	1:D:33:GLN:NE2	2.05	0.53
1:D:50:LEU:H	1:D:50:LEU:HD12	1.74	0.53
1:D:362:LEU:HG	1:D:363:ASP:H	1.72	0.53
1:F:46:CYS:HA	1:F:58:TRP:CH2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:362:LEU:HG	1:H:363:ASP:H	1.73	0.53
1:I:406:CYS:SG	1:I:407:VAL:HG23	2.48	0.53
1:I:426:VAL:HG23	1:I:427:TRP:HD1	1.72	0.53
1:I:427:TRP:O	1:I:431:VAL:HG23	2.08	0.53
1:I:589:ILE:H	1:I:589:ILE:CD1	2.21	0.53
1:K:20:ARG:C	1:K:21:LEU:HD22	2.33	0.53
1:K:98:CYS:HA	1:K:153:GLN:NE2	2.23	0.53
1:K:589:ILE:H	1:K:589:ILE:CD1	2.21	0.53
1:L:470:ILE:O	1:L:474:GLN:HG2	2.09	0.53
1:B:18:ARG:HH21	1:B:33:GLN:NE2	2.06	0.53
1:B:26:PHE:HA	1:F:408:ASN:ND2	2.24	0.53
1:D:275:TRP:CZ2	1:D:304:MET:HE2	2.43	0.53
1:D:502:ILE:HG21	1:D:656:ILE:CD1	2.38	0.53
1:F:17:MET:HB3	1:F:32:TYR:CE1	2.43	0.53
1:F:334:LEU:HD11	1:F:364:PRO:HA	1.90	0.53
1:G:589:ILE:HD12	1:G:589:ILE:N	2.20	0.53
1:J:240:LYS:O	1:J:277:GLN:HG2	2.08	0.53
1:J:551:ARG:HB3	1:J:552:ARG:HH21	1.74	0.53
1:K:46:CYS:N	1:K:86:LEU:HD23	2.22	0.53
1:K:623:PRO:O	1:K:627:VAL:HG23	2.08	0.53
1:L:158:LYS:HD2	1:L:376:VAL:HG13	1.89	0.53
1:A:655:LYS:HA	1:A:658:CYS:SG	2.49	0.53
1:B:176:GLU:HB2	1:B:177:LEU:HD12	1.90	0.53
1:B:406:CYS:SG	1:B:407:VAL:HG23	2.48	0.53
1:C:29:VAL:HG21	4:C:701:5TL:CAE	2.38	0.53
1:D:275:TRP:HZ2	1:D:304:MET:HE2	1.73	0.53
1:E:262:ASN:ND2	1:E:264:LEU:H	2.07	0.53
1:H:552:ARG:HE	1:H:552:ARG:N	2.06	0.53
1:I:589:ILE:HD12	1:I:589:ILE:N	2.22	0.53
1:K:222:LEU:HB2	1:K:230:TRP:CD1	2.44	0.53
1:K:426:VAL:HG23	1:K:427:TRP:HD1	1.72	0.53
1:L:17:MET:HB3	1:L:32:TYR:CE1	2.43	0.53
1:A:589:ILE:HD12	1:A:589:ILE:N	2.21	0.53
1:C:589:ILE:H	1:C:589:ILE:CD1	2.21	0.53
1:D:98:CYS:HA	1:D:153:GLN:NE2	2.23	0.53
1:D:185:LEU:HD13	1:D:186:GLN:H	1.72	0.53
1:E:234:ILE:HG22	1:E:254:PHE:CE1	2.44	0.53
1:E:426:VAL:HG23	1:E:427:TRP:HD1	1.72	0.53
1:F:102:ASP:OD1	4:F:701:5TL:CAN	2.57	0.53
1:F:142:HIS:ND1	1:F:169:ALA:HB2	2.23	0.53
1:H:413:ASP:OD1	1:H:416:ILE:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:600:VAL:HA	1:H:603:GLU:HB3	1.91	0.53
1:J:600:VAL:HA	1:J:603:GLU:HB3	1.90	0.53
1:K:79:VAL:HG21	1:K:83:LEU:HD13	1.90	0.53
1:K:480:LEU:HD22	1:K:518:ALA:HB1	1.91	0.53
1:K:552:ARG:HE	1:K:552:ARG:N	2.06	0.53
1:A:20:ARG:HG3	1:A:30:CYS:SG	2.48	0.53
1:D:180:GLU:HG2	1:D:195:ASN:ND2	2.24	0.53
1:F:207:PHE:O	1:F:211:VAL:HG23	2.08	0.53
1:H:426:VAL:HG23	1:H:427:TRP:HD1	1.73	0.53
1:I:48:LEU:HA	1:I:87:ILE:HG21	1.89	0.53
1:I:551:ARG:HB3	1:I:552:ARG:HH21	1.73	0.53
1:J:98:CYS:HB3	1:J:152:LEU:O	2.08	0.53
1:K:401:ARG:HH22	1:K:440:ASP:CB	2.22	0.53
1:L:406:CYS:SG	1:L:407:VAL:HG23	2.48	0.53
1:A:222:LEU:HD13	1:A:244:ALA:O	2.09	0.53
1:C:50:LEU:H	1:C:50:LEU:HD12	1.74	0.53
1:D:590:ILE:O	1:D:594:VAL:HG23	2.08	0.53
1:D:655:LYS:HA	1:D:658:CYS:SG	2.49	0.53
1:E:6:ASP:N	1:E:7:PRO:HD2	2.24	0.53
1:E:334:LEU:HD11	1:E:364:PRO:HA	1.89	0.53
1:E:423:LEU:HA	1:E:426:VAL:CG2	2.39	0.53
1:G:139:LYS:HD2	1:G:172:VAL:HG21	1.91	0.53
1:G:413:ASP:OD1	1:G:416:ILE:HB	2.09	0.53
1:G:470:ILE:O	1:G:474:GLN:HG2	2.08	0.53
1:H:18:ARG:HH21	1:H:33:GLN:NE2	2.06	0.53
1:H:50:LEU:HD13	1:H:90:VAL:HG21	1.90	0.53
1:I:170:LYS:HG2	1:I:177:LEU:HG	1.91	0.53
1:I:401:ARG:NH2	1:I:440:ASP:HB2	2.24	0.53
1:J:303:LEU:O	1:J:307:ILE:HG13	2.09	0.53
1:J:415:LYS:HA	1:J:584:THR:HB	1.90	0.53
1:K:415:LYS:HA	1:K:584:THR:HB	1.89	0.53
1:A:150:ILE:HD11	1:A:210:MET:HE1	1.91	0.53
1:A:227:PRO:CA	1:A:230:TRP:HB3	2.27	0.53
1:B:219:ARG:CZ	1:B:224:HIS:H	2.22	0.53
1:C:410:ILE:HG23	1:C:583:SER:OG	2.09	0.53
1:C:473:SER:HB2	1:C:524:VAL:HA	1.89	0.53
1:D:600:VAL:HA	1:D:603:GLU:HB3	1.90	0.53
1:E:549:TYR:H	1:E:552:ARG:HD2	1.74	0.53
1:F:267:LEU:HD12	1:F:312:ILE:HG23	1.91	0.53
1:I:219:ARG:HH21	1:I:224:HIS:N	2.07	0.53
1:J:655:LYS:HA	1:J:658:CYS:SG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG21	4:A:701:5TL:CAE	2.39	0.53
1:B:50:LEU:H	1:B:50:LEU:HD12	1.74	0.53
1:G:600:VAL:HA	1:G:603:GLU:HB3	1.91	0.53
1:H:589:ILE:HD12	1:H:589:ILE:N	2.20	0.53
1:I:362:LEU:HG	1:I:363:ASP:H	1.73	0.53
1:J:50:LEU:H	1:J:50:LEU:HD12	1.74	0.53
1:J:334:LEU:HD22	1:J:366:LYS:O	2.08	0.53
1:J:487:ILE:HG12	1:J:515:GLU:HB2	1.90	0.53
1:K:376:VAL:HG13	1:K:377:ARG:H	1.74	0.53
1:B:20:ARG:C	1:B:21:LEU:HD22	2.34	0.53
1:B:413:ASP:OD1	1:B:416:ILE:HB	2.08	0.53
1:B:600:VAL:HA	1:B:603:GLU:HB3	1.91	0.53
1:D:513:GLU:O	1:D:517:LYS:HG3	2.09	0.53
1:E:50:LEU:H	1:E:50:LEU:HD12	1.73	0.53
1:E:362:LEU:HG	1:E:363:ASP:H	1.73	0.53
1:F:150:ILE:HD11	1:F:210:MET:HE1	1.90	0.53
1:G:50:LEU:H	1:G:50:LEU:HD12	1.74	0.53
1:G:547:SER:OG	1:G:548:PRO:HD2	2.09	0.53
1:I:470:ILE:O	1:I:474:GLN:HG2	2.09	0.53
1:K:50:LEU:H	1:K:50:LEU:HD12	1.73	0.53
1:L:221:PHE:HB2	1:L:230:TRP:HE1	1.74	0.53
1:A:275:TRP:HZ2	1:A:304:MET:HE2	1.72	0.52
1:A:413:ASP:OD1	1:A:416:ILE:HB	2.10	0.52
1:D:46:CYS:HA	1:D:58:TRP:CH2	2.44	0.52
1:D:623:PRO:O	1:D:627:VAL:HG23	2.09	0.52
1:E:219:ARG:NH2	1:E:224:HIS:HB2	2.24	0.52
1:G:185:LEU:H	1:I:249:SER:HB3	1.75	0.52
1:J:362:LEU:HG	1:J:363:ASP:H	1.73	0.52
1:J:420:ILE:HG21	1:J:578:HIS:N	2.23	0.52
1:K:600:VAL:HA	1:K:603:GLU:HB3	1.91	0.52
1:L:141:ILE:CG2	1:L:170:LYS:HB2	2.37	0.52
1:A:488:GLN:HB3	1:A:515:GLU:OE2	2.10	0.52
1:C:222:LEU:H	1:C:230:TRP:HE1	1.55	0.52
1:C:362:LEU:HG	1:C:363:ASP:H	1.73	0.52
1:D:303:LEU:O	1:D:307:ILE:HG13	2.09	0.52
1:E:188:LEU:HD21	1:E:192:LEU:HD22	1.91	0.52
1:H:46:CYS:HA	1:H:58:TRP:CH2	2.43	0.52
1:J:470:ILE:O	1:J:474:GLN:HG2	2.10	0.52
1:K:362:LEU:HG	1:K:363:ASP:H	1.73	0.52
1:L:188:LEU:HD21	1:L:192:LEU:HD22	1.91	0.52
1:A:426:VAL:HG23	1:A:427:TRP:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:HD21	1:B:648:LYS:HG3	1.90	0.52
1:A:639:VAL:HA	1:A:642:MET:HG3	1.92	0.52
1:B:465:MET:HB3	1:B:625:VAL:HG11	1.91	0.52
1:B:589:ILE:HD12	1:B:589:ILE:N	2.20	0.52
1:E:224:HIS:C	1:E:225:LEU:HD22	2.34	0.52
1:H:212:PHE:CD2	1:H:220:PRO:HA	2.45	0.52
1:H:410:ILE:O	1:H:587:VAL:HG22	2.09	0.52
1:H:587:VAL:O	1:H:591:VAL:HG23	2.10	0.52
1:I:222:LEU:HB2	1:I:230:TRP:CD1	2.44	0.52
1:J:408:ASN:ND2	1:L:26:PHE:HA	2.25	0.52
1:J:513:GLU:O	1:J:517:LYS:HG3	2.09	0.52
1:K:489:LEU:HD11	1:L:648:LYS:HE3	1.91	0.52
1:A:70:HIS:C	1:A:72:ASN:H	2.18	0.52
1:A:513:GLU:O	1:A:517:LYS:HG3	2.08	0.52
1:A:623:PRO:O	1:A:627:VAL:HG23	2.10	0.52
1:B:234:ILE:HD12	1:B:234:ILE:N	2.24	0.52
1:C:227:PRO:HA	1:C:230:TRP:CB	2.33	0.52
1:E:590:ILE:O	1:E:594:VAL:HG23	2.09	0.52
1:H:50:LEU:H	1:H:50:LEU:HD12	1.74	0.52
1:J:275:TRP:HZ2	1:J:304:MET:HE2	1.75	0.52
1:J:587:VAL:O	1:J:591:VAL:HG23	2.09	0.52
1:L:117:LYS:O	1:L:121:ILE:HG13	2.10	0.52
1:A:50:LEU:HD12	1:A:50:LEU:H	1.74	0.52
1:A:377:ARG:HA	1:A:377:ARG:HE	1.75	0.52
1:D:46:CYS:HB2	1:D:87:ILE:HB	1.92	0.52
1:E:17:MET:HB3	1:E:32:TYR:CE1	2.45	0.52
1:E:513:GLU:O	1:E:517:LYS:HG3	2.10	0.52
1:E:600:VAL:HA	1:E:603:GLU:HB3	1.92	0.52
1:G:73:VAL:HG22	1:G:74:VAL:N	2.22	0.52
1:G:201:THR:C	1:G:287:ARG:HH21	2.17	0.52
1:H:513:GLU:O	1:H:517:LYS:HG3	2.09	0.52
1:I:21:LEU:HD12	4:I:701:5TL:CAJ	2.39	0.52
1:K:185:LEU:HD13	1:K:186:GLN:N	2.20	0.52
1:K:590:ILE:O	1:K:594:VAL:HG23	2.08	0.52
1:L:150:ILE:HD11	1:L:210:MET:HE1	1.91	0.52
1:L:420:ILE:HD11	1:L:571:LEU:HG	1.92	0.52
1:A:17:MET:HB3	1:A:32:TYR:CD1	2.45	0.52
1:B:141:ILE:HG13	1:B:203:ASP:OD1	2.09	0.52
1:B:185:LEU:HD13	1:B:186:GLN:H	1.75	0.52
1:D:416:ILE:HD13	4:F:701:5TL:O4	2.10	0.52
1:F:513:GLU:O	1:F:517:LYS:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:655:LYS:HA	1:F:658:CYS:SG	2.50	0.52
1:G:431:VAL:HG21	1:G:568:TYR:HB2	1.91	0.52
1:H:17:MET:HB3	1:H:32:TYR:CE1	2.44	0.52
1:H:373:LEU:HD22	1:H:373:LEU:N	2.25	0.52
1:H:574:ARG:NH1	1:H:575:PRO:HD2	2.24	0.52
1:I:207:PHE:O	1:I:211:VAL:HG23	2.09	0.52
1:I:234:ILE:HG22	1:I:254:PHE:HE1	1.75	0.52
1:I:550:GLY:HA3	1:I:604:LEU:HD13	1.92	0.52
1:L:328:LEU:HD11	1:L:337:LEU:HD22	1.91	0.52
1:L:517:LYS:HD2	1:L:642:MET:HE1	1.90	0.52
1:B:427:TRP:CZ3	1:B:567:LEU:HB3	2.42	0.52
1:D:118:GLU:HB2	1:D:263:SER:O	2.09	0.52
1:D:222:LEU:HB2	1:D:230:TRP:NE1	2.24	0.52
1:D:240:LYS:O	1:D:277:GLN:HG2	2.10	0.52
1:D:426:VAL:HG23	1:D:427:TRP:HD1	1.74	0.52
1:H:376:VAL:HG23	1:H:377:ARG:H	1.75	0.52
1:I:46:CYS:HA	1:I:58:TRP:CH2	2.44	0.52
1:I:141:ILE:HG13	1:I:203:ASP:OD1	2.10	0.52
1:L:240:LYS:HB3	1:L:277:GLN:HB3	1.92	0.52
1:A:480:LEU:CD2	1:A:518:ALA:HB1	2.40	0.52
1:A:514:MET:HA	1:A:642:MET:HE1	1.92	0.52
1:A:654:LEU:CD2	1:B:497:GLN:HE22	2.23	0.52
1:B:431:VAL:HG21	1:B:568:TYR:HB2	1.92	0.52
1:C:284:PRO:HA	1:C:287:ARG:NH2	2.24	0.52
1:C:470:ILE:O	1:C:474:GLN:HG2	2.10	0.52
1:D:8:GLU:HB2	1:D:87:ILE:HG12	1.91	0.52
1:G:98:CYS:HB3	1:G:152:LEU:O	2.09	0.52
1:G:383:MET:HG2	1:G:384:VAL:N	2.25	0.52
1:I:469:LEU:HD12	1:I:625:VAL:HG13	1.92	0.52
1:J:20:ARG:C	1:J:21:LEU:HD22	2.35	0.52
1:B:17:MET:HB3	1:B:32:TYR:CE1	2.44	0.52
1:B:362:LEU:HG	1:B:363:ASP:H	1.75	0.52
1:D:114:CYS:HB2	1:D:432:HIS:CD2	2.45	0.52
1:D:328:LEU:HD11	1:D:337:LEU:HD22	1.92	0.52
1:E:589:ILE:H	1:E:589:ILE:CD1	2.23	0.52
1:G:185:LEU:HD21	1:G:188:LEU:HB2	1.91	0.52
1:I:284:PRO:HA	1:I:287:ARG:NH2	2.24	0.52
1:J:236:LYS:HD3	1:J:237:LYS:N	2.25	0.52
1:K:513:GLU:O	1:K:517:LYS:HG3	2.10	0.52
1:L:177:LEU:HD11	1:L:198:TYR:CE2	2.45	0.52
1:C:262:ASN:ND2	1:C:264:LEU:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ALA:O	1:C:464:LYS:HG3	2.10	0.52
1:D:248:MET:O	1:F:184:THR:HG23	2.10	0.52
1:F:186:GLN:NE2	1:F:227:PRO:HD3	2.17	0.52
1:G:426:VAL:HG23	1:G:427:TRP:HD1	1.74	0.52
1:G:513:GLU:O	1:G:517:LYS:HG3	2.09	0.52
1:G:523:GLU:HB2	1:G:632:ILE:HG12	1.92	0.52
1:I:62:ILE:HG22	1:I:93:LEU:HD13	1.91	0.52
1:I:298:PRO:O	1:I:302:VAL:HG23	2.10	0.52
1:I:489:LEU:HD11	1:J:648:LYS:HE3	1.92	0.52
1:L:513:GLU:O	1:L:517:LYS:HG3	2.11	0.52
1:A:222:LEU:HB2	1:A:230:TRP:CD1	2.37	0.51
1:C:188:LEU:HD21	1:C:192:LEU:HD22	1.92	0.51
1:C:291:VAL:HG12	1:C:298:PRO:HA	1.92	0.51
1:C:417:GLN:HB3	1:C:581:SER:HB2	1.92	0.51
1:D:283:ASP:HB3	1:D:286:GLN:HB2	1.91	0.51
1:E:212:PHE:CE2	1:E:220:PRO:HA	2.45	0.51
1:F:328:LEU:HD11	1:F:337:LEU:HD22	1.92	0.51
1:G:18:ARG:HH21	1:G:33:GLN:NE2	2.04	0.51
1:H:366:LYS:HB2	1:H:370:GLN:HG2	1.92	0.51
1:H:412:GLN:HB3	1:J:21:LEU:O	2.10	0.51
1:K:18:ARG:HH21	1:K:33:GLN:NE2	2.05	0.51
1:K:88:HIS:O	1:K:90:VAL:HG12	2.10	0.51
1:A:188:LEU:HD21	1:A:192:LEU:HD22	1.91	0.51
1:A:600:VAL:HA	1:A:603:GLU:HB3	1.92	0.51
1:B:29:VAL:HG21	4:B:701:5TL:CAF	2.40	0.51
1:D:20:ARG:C	1:D:21:LEU:HD22	2.36	0.51
1:E:655:LYS:HA	1:E:658:CYS:SG	2.51	0.51
1:J:358:THR:O	1:J:453:LEU:HD13	2.11	0.51
1:J:420:ILE:HG21	1:J:578:HIS:H	1.75	0.51
1:J:426:VAL:HG23	1:J:427:TRP:HD1	1.75	0.51
1:K:473:SER:HB2	1:K:524:VAL:HA	1.92	0.51
1:L:74:VAL:HG11	1:L:95:MET:HE3	1.92	0.51
1:L:320:SER:O	1:L:398:PHE:HB3	2.10	0.51
1:A:408:ASN:HD21	1:E:26:PHE:HD1	1.57	0.51
1:C:222:LEU:HB3	1:C:225:LEU:HB2	1.93	0.51
1:D:316:LEU:HB2	1:D:383:MET:SD	2.50	0.51
1:F:240:LYS:O	1:F:277:GLN:HG2	2.11	0.51
1:F:413:ASP:OD1	1:F:416:ILE:HB	2.11	0.51
1:H:222:LEU:HB2	1:H:230:TRP:HD1	1.76	0.51
1:K:150:ILE:HD11	1:K:210:MET:HE1	1.93	0.51
1:K:188:LEU:HD21	1:K:192:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:413:ASP:OD1	1:K:416:ILE:HB	2.10	0.51
1:K:465:MET:HE3	1:K:625:VAL:HG21	1.92	0.51
1:K:497:GLN:OE1	1:L:655:LYS:HE3	2.09	0.51
1:K:589:ILE:HD12	1:K:589:ILE:N	2.22	0.51
1:L:413:ASP:OD1	1:L:416:ILE:HB	2.11	0.51
1:G:17:MET:HB3	1:G:32:TYR:CD1	2.46	0.51
1:G:33:GLN:HA	1:G:40:LYS:HA	1.92	0.51
1:I:150:ILE:HD11	1:I:210:MET:HE1	1.91	0.51
1:I:262:ASN:ND2	1:I:264:LEU:H	2.09	0.51
1:J:413:ASP:OD1	1:J:416:ILE:HB	2.10	0.51
1:J:473:SER:CB	1:J:527:ILE:HD11	2.41	0.51
1:K:278:LEU:HD23	1:K:288:GLY:HA2	1.92	0.51
1:K:477:LYS:HE3	1:K:524:VAL:HG11	1.93	0.51
1:L:20:ARG:C	1:L:21:LEU:HD22	2.35	0.51
1:A:396:GLY:H	1:A:397:PRO:CD	2.12	0.51
1:C:48:LEU:HA	1:C:87:ILE:CG2	2.39	0.51
1:D:220:PRO:O	1:D:243:PHE:HA	2.09	0.51
1:D:281:ASN:O	1:D:282:TRP:HB2	2.09	0.51
1:D:587:VAL:O	1:D:591:VAL:HG23	2.10	0.51
1:E:18:ARG:HH21	1:E:33:GLN:NE2	2.06	0.51
1:E:84:ASN:HD22	1:E:86:LEU:H	1.56	0.51
1:G:650:ILE:HG21	1:H:650:ILE:HG21	1.92	0.51
1:I:221:PHE:HB2	1:I:230:TRP:NE1	2.22	0.51
1:J:97:TYR:HA	4:J:701:5TL:OAO	2.10	0.51
1:K:230:TRP:O	1:K:234:ILE:HG13	2.10	0.51
1:K:291:VAL:HA	1:K:298:PRO:HA	1.93	0.51
1:L:219:ARG:HE	1:L:223:HIS:HA	1.76	0.51
1:A:219:ARG:HH21	1:A:223:HIS:HB2	1.75	0.51
1:B:410:ILE:HG23	1:B:583:SER:OG	2.11	0.51
1:C:98:CYS:HB3	1:C:152:LEU:O	2.11	0.51
1:C:426:VAL:HG23	1:C:427:TRP:HD1	1.75	0.51
1:C:600:VAL:HA	1:C:603:GLU:HB3	1.92	0.51
1:D:63:GLN:HE22	1:D:174:GLN:NE2	2.05	0.51
1:D:74:VAL:CG1	1:D:164:ILE:HA	2.40	0.51
1:D:294:THR:C	1:D:295:LEU:HD22	2.35	0.51
1:E:413:ASP:OD1	1:E:416:ILE:HB	2.11	0.51
1:F:288:GLY:HA3	1:F:300:CYS:SG	2.50	0.51
1:F:587:VAL:O	1:F:591:VAL:HG23	2.10	0.51
1:I:18:ARG:HH21	1:I:33:GLN:NE2	2.06	0.51
1:I:513:GLU:O	1:I:517:LYS:HG3	2.10	0.51
1:I:600:VAL:HA	1:I:603:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:328:LEU:HD11	1:J:337:LEU:HD22	1.93	0.51
1:K:62:ILE:HG22	1:K:93:LEU:HD13	1.92	0.51
1:B:513:GLU:O	1:B:517:LYS:HG3	2.10	0.51
1:C:18:ARG:HH21	1:C:33:GLN:NE2	2.06	0.51
1:C:328:LEU:HD13	1:C:368:ALA:HB1	1.92	0.51
1:E:227:PRO:HA	1:E:230:TRP:HB3	1.93	0.51
1:G:239:PRO:O	1:G:240:LYS:HB2	2.09	0.51
1:G:392:THR:O	1:G:612:LEU:HD23	2.11	0.51
1:H:133:ARG:CZ	1:H:297:GLN:HE22	2.24	0.51
1:H:543:GLU:HA	1:H:546:LYS:HZ3	1.76	0.51
1:H:589:ILE:H	1:H:589:ILE:CD1	2.19	0.51
1:I:586:MET:O	1:I:590:ILE:HG13	2.11	0.51
1:I:655:LYS:HA	1:I:658:CYS:SG	2.51	0.51
1:K:294:THR:HB	1:K:295:LEU:HD12	1.93	0.51
1:K:487:ILE:CA	1:K:646:ARG:HD2	2.41	0.51
1:L:600:VAL:HA	1:L:603:GLU:HB3	1.91	0.51
1:A:410:ILE:HG23	1:A:583:SER:OG	2.11	0.51
1:A:574:ARG:HH12	1:E:575:PRO:HB3	1.76	0.51
1:C:46:CYS:HA	1:C:58:TRP:CH2	2.44	0.51
1:C:70:HIS:CD2	1:C:72:ASN:H	2.28	0.51
1:D:112:ASN:HB3	1:D:116:LEU:HD23	1.93	0.51
1:E:284:PRO:HG2	1:E:285:GLN:HE21	1.76	0.51
1:E:460:ALA:O	1:E:464:LYS:HG3	2.11	0.51
1:I:423:LEU:HA	1:I:426:VAL:CG2	2.39	0.51
1:I:507:MET:HE1	1:I:653:LEU:HD13	1.92	0.51
1:L:215:ILE:HD13	1:L:264:LEU:HD11	1.91	0.51
1:L:463:THR:HG21	1:L:538:HIS:HD2	1.76	0.51
1:A:33:GLN:HA	1:A:40:LYS:HA	1.93	0.51
1:A:654:LEU:HD21	1:B:497:GLN:HE22	1.75	0.51
1:B:9:PHE:CZ	1:B:82:GLU:HB3	2.46	0.51
1:B:62:ILE:HG22	1:B:93:LEU:HD13	1.93	0.51
1:B:401:ARG:HG2	1:B:433:TYR:CE1	2.46	0.51
1:D:262:ASN:ND2	1:D:264:LEU:H	2.09	0.51
1:D:544:LEU:HD21	1:D:610:LYS:HD2	1.93	0.51
1:E:182:VAL:HG12	1:E:183:GLY:H	1.75	0.51
1:F:98:CYS:HB3	1:F:152:LEU:O	2.10	0.51
1:G:410:ILE:O	1:G:587:VAL:HG22	2.11	0.51
1:G:589:ILE:H	1:G:589:ILE:CD1	2.19	0.51
1:H:328:LEU:HD11	1:H:337:LEU:HD22	1.92	0.51
1:J:204:TYR:O	1:J:279:MET:HE3	2.11	0.51
1:J:581:SER:O	1:J:582:ASP:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:587:VAL:O	1:L:591:VAL:HG23	2.11	0.51
1:D:463:THR:HG21	1:D:538:HIS:CD2	2.45	0.51
1:E:21:LEU:HD12	4:E:701:5TL:CAJ	2.41	0.51
1:G:45:SER:OG	1:G:86:LEU:HD11	2.11	0.51
1:G:219:ARG:HH22	1:G:224:HIS:N	2.09	0.51
1:G:295:LEU:C	1:G:297:GLN:H	2.19	0.51
1:H:62:ILE:HG22	1:H:93:LEU:HD13	1.93	0.51
1:H:411:VAL:HG12	1:H:590:ILE:HG21	1.93	0.51
1:I:33:GLN:HA	1:I:40:LYS:HA	1.92	0.51
1:I:188:LEU:HD21	1:I:192:LEU:HD22	1.93	0.51
1:K:226:GLN:O	1:K:230:TRP:HB2	2.11	0.51
1:L:143:ARG:HB3	1:L:170:LYS:HE3	1.93	0.51
1:B:231:HIS:C	1:B:233:LYS:H	2.19	0.50
1:C:648:LYS:HG3	1:D:489:LEU:HD21	1.92	0.50
1:D:81:GLU:H	1:D:81:GLU:CD	2.19	0.50
1:F:76:ALA:HB1	1:F:93:LEU:HD11	1.94	0.50
1:F:406:CYS:SG	1:F:407:VAL:HG23	2.50	0.50
1:G:275:TRP:HZ2	1:G:304:MET:HE2	1.73	0.50
1:G:574:ARG:NH1	1:G:574:ARG:HB2	2.26	0.50
1:I:186:GLN:CG	1:I:219:ARG:HD3	2.41	0.50
1:J:150:ILE:HD11	1:J:210:MET:HE1	1.91	0.50
1:K:158:LYS:HB3	1:K:376:VAL:HG23	1.93	0.50
1:K:514:MET:HA	1:K:642:MET:HE1	1.93	0.50
1:L:29:VAL:HG21	4:L:701:5TL:CAF	2.41	0.50
1:L:62:ILE:HG22	1:L:93:LEU:HD13	1.93	0.50
1:L:177:LEU:HD11	1:L:198:TYR:HE2	1.76	0.50
1:A:574:ARG:NH1	1:A:574:ARG:HB2	2.26	0.50
1:A:650:ILE:HG21	1:B:650:ILE:HG21	1.93	0.50
1:C:17:MET:HB3	1:C:32:TYR:CD1	2.46	0.50
1:E:11:ALA:O	1:E:14:PRO:HD3	2.10	0.50
1:E:487:ILE:CA	1:E:646:ARG:HD2	2.40	0.50
1:F:192:LEU:H	1:F:192:LEU:HD12	1.76	0.50
1:F:289:GLY:O	1:F:291:VAL:N	2.45	0.50
1:G:219:ARG:HH22	1:G:224:HIS:H	1.60	0.50
1:K:328:LEU:HD11	1:K:337:LEU:HD22	1.93	0.50
1:L:50:LEU:H	1:L:50:LEU:HD12	1.75	0.50
1:L:191:GLU:OE2	1:L:287:ARG:NH2	2.44	0.50
1:B:470:ILE:O	1:B:474:GLN:HG2	2.10	0.50
1:D:423:LEU:HA	1:D:426:VAL:CG2	2.40	0.50
1:E:109:LYS:HZ3	2:X:2:GLC:H4	1.77	0.50
1:F:20:ARG:C	1:F:21:LEU:HD22	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:PRO:HG3	1:G:32:TYR:OH	2.11	0.50
1:G:294:THR:HB	1:G:295:LEU:HD12	1.92	0.50
1:H:655:LYS:HA	1:H:658:CYS:SG	2.51	0.50
1:K:376:VAL:HG13	1:K:377:ARG:N	2.26	0.50
1:K:502:ILE:HD13	1:K:656:ILE:HD12	1.93	0.50
1:A:18:ARG:HH21	1:A:33:GLN:NE2	2.06	0.50
1:A:149:ASN:O	1:A:164:ILE:HG22	2.12	0.50
1:B:73:VAL:HG22	1:B:74:VAL:H	1.76	0.50
1:C:328:LEU:HD11	1:C:337:LEU:HD22	1.93	0.50
1:C:427:TRP:CZ3	1:C:567:LEU:HB3	2.46	0.50
1:F:50:LEU:HD12	1:F:50:LEU:H	1.75	0.50
1:F:188:LEU:HD21	1:F:192:LEU:HD22	1.93	0.50
1:F:284:PRO:HG2	1:F:285:GLN:H	1.77	0.50
1:G:222:LEU:CD2	1:G:230:TRP:HA	2.41	0.50
1:H:20:ARG:C	1:H:21:LEU:HD22	2.36	0.50
1:I:141:ILE:HG23	1:I:170:LYS:HB2	1.94	0.50
1:K:574:ARG:NH1	1:K:575:PRO:HD2	2.26	0.50
1:A:420:ILE:HA	1:A:423:LEU:HB2	1.94	0.50
1:B:215:ILE:HD13	1:B:264:LEU:HD11	1.93	0.50
1:B:328:LEU:HD11	1:B:337:LEU:HD22	1.93	0.50
1:B:460:ALA:O	1:B:464:LYS:HG3	2.12	0.50
1:D:150:ILE:HD11	1:D:210:MET:HE1	1.91	0.50
1:D:413:ASP:OD1	1:D:416:ILE:HB	2.11	0.50
1:E:497:GLN:HE22	1:F:654:LEU:CD2	2.24	0.50
1:G:469:LEU:HD12	1:G:625:VAL:HG13	1.93	0.50
1:G:655:LYS:HA	1:G:658:CYS:SG	2.52	0.50
1:I:77:CYS:H	1:I:95:MET:HA	1.75	0.50
1:K:76:ALA:HA	1:K:95:MET:HA	1.92	0.50
1:A:185:LEU:HD12	1:A:193:PHE:HZ	1.76	0.50
1:A:410:ILE:O	1:A:587:VAL:HG22	2.12	0.50
1:B:212:PHE:CE2	1:B:220:PRO:HA	2.47	0.50
1:B:589:ILE:H	1:B:589:ILE:CD1	2.20	0.50
1:C:507:MET:CE	1:C:653:LEU:HD22	2.40	0.50
1:C:640:MET:HE1	1:D:485:LYS:HG2	1.93	0.50
1:E:547:SER:OG	1:E:548:PRO:HD2	2.12	0.50
1:F:523:GLU:HB2	1:F:632:ILE:HG12	1.93	0.50
1:F:547:SER:HB3	1:F:548:PRO:HD2	1.92	0.50
1:G:46:CYS:SG	1:G:90:VAL:HB	2.52	0.50
1:H:17:MET:HB3	1:H:32:TYR:CD1	2.47	0.50
1:K:17:MET:HB3	1:K:32:TYR:CD1	2.46	0.50
1:K:232:GLU:HA	1:K:235:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:17:MET:HB3	1:L:32:TYR:CD1	2.46	0.50
1:A:561:GLU:O	1:A:565:ILE:HG13	2.12	0.50
1:B:238:ASP:HB3	1:B:239:PRO:HD2	1.92	0.50
1:C:513:GLU:O	1:C:517:LYS:HG3	2.11	0.50
1:D:460:ALA:O	1:D:464:LYS:HG3	2.11	0.50
1:E:587:VAL:O	1:E:591:VAL:HG23	2.11	0.50
1:G:62:ILE:HG22	1:G:93:LEU:HD13	1.94	0.50
1:G:199:THR:HG21	1:G:285:GLN:NE2	2.22	0.50
1:G:234:ILE:O	1:G:237:LYS:HB2	2.12	0.50
1:H:74:VAL:HG21	1:H:95:MET:HE3	1.94	0.50
1:I:29:VAL:HG21	4:I:701:5TL:CAF	2.42	0.50
1:I:212:PHE:CE2	1:I:220:PRO:HA	2.47	0.50
1:I:328:LEU:HD11	1:I:337:LEU:HD22	1.94	0.50
1:A:113:CYS:SG	1:A:428:ALA:HB1	2.52	0.50
1:A:655:LYS:HE3	1:B:497:GLN:OE1	2.12	0.50
1:B:150:ILE:HD11	1:B:210:MET:HE1	1.94	0.50
1:C:33:GLN:HA	1:C:40:LYS:HA	1.93	0.50
1:C:420:ILE:HD11	1:C:571:LEU:HG	1.93	0.50
1:C:658:CYS:HB3	1:D:501:GLY:HA2	1.94	0.50
1:E:62:ILE:HG22	1:E:93:LEU:HD13	1.93	0.50
1:F:33:GLN:HA	1:F:40:LYS:HA	1.93	0.50
1:H:542:MET:HA	1:H:545:GLN:HE21	1.76	0.50
1:I:184:THR:OG1	1:K:248:MET:HB3	2.11	0.50
1:I:318:MET:HE2	1:I:447:GLY:HA3	1.94	0.50
1:J:86:LEU:HD11	1:J:92:LEU:HG	1.94	0.50
1:J:289:GLY:O	1:J:291:VAL:HG23	2.10	0.50
1:J:418:LEU:HB2	1:J:423:LEU:HD21	1.94	0.50
1:L:33:GLN:HA	1:L:40:LYS:HA	1.93	0.50
1:A:395:GLU:HG3	1:A:396:GLY:N	2.27	0.50
1:A:589:ILE:H	1:A:589:ILE:CD1	2.20	0.50
1:B:655:LYS:HA	1:B:658:CYS:SG	2.51	0.50
1:C:62:ILE:HG22	1:C:93:LEU:HD13	1.94	0.50
1:C:65:MET:SD	1:C:166:LEU:HD23	2.51	0.50
1:D:548:PRO:HG2	1:D:607:HIS:NE2	2.27	0.50
1:E:225:LEU:O	1:E:226:GLN:C	2.55	0.50
1:E:589:ILE:HD12	1:E:589:ILE:N	2.24	0.50
1:F:423:LEU:HA	1:F:426:VAL:CG2	2.41	0.50
1:F:600:VAL:HA	1:F:603:GLU:HB3	1.93	0.50
1:G:188:LEU:HD21	1:G:192:LEU:HD22	1.93	0.50
1:H:574:ARG:O	1:H:576:SER:N	2.45	0.50
1:I:576:SER:OG	1:K:580:TYR:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:623:PRO:O	1:I:627:VAL:HG23	2.11	0.50
1:L:18:ARG:HH21	1:L:33:GLN:NE2	2.05	0.50
1:L:73:VAL:O	1:L:162:LYS:HB3	2.12	0.50
1:L:303:LEU:O	1:L:307:ILE:HG13	2.12	0.50
2:j:2:GLC:C6	2:j:3:PDX:H5	2.42	0.50
1:A:62:ILE:HG22	1:A:93:LEU:HD13	1.94	0.49
1:A:170:LYS:HG3	1:A:177:LEU:HA	1.94	0.49
1:A:328:LEU:HD11	1:A:337:LEU:HD22	1.94	0.49
1:A:487:ILE:CG1	1:A:515:GLU:HB2	2.41	0.49
1:C:473:SER:CB	1:C:527:ILE:HD11	2.42	0.49
1:E:415:LYS:HA	1:E:584:THR:HB	1.93	0.49
1:G:222:LEU:CD2	1:G:230:TRP:HD1	2.23	0.49
1:H:31:LEU:HG	1:H:97:TYR:CE2	2.47	0.49
1:H:420:ILE:HD11	1:H:571:LEU:HG	1.94	0.49
1:I:17:MET:HB3	1:I:32:TYR:CD1	2.47	0.49
1:I:192:LEU:H	1:I:192:LEU:HD12	1.77	0.49
1:I:460:ALA:O	1:I:464:LYS:HG3	2.12	0.49
1:J:215:ILE:HG21	1:J:258:LEU:HD21	1.94	0.49
1:J:460:ALA:O	1:J:464:LYS:HG3	2.12	0.49
1:K:460:ALA:O	1:K:464:LYS:HG3	2.12	0.49
1:L:655:LYS:HA	1:L:658:CYS:SG	2.52	0.49
1:A:166:LEU:C	1:A:168:TYR:H	2.19	0.49
1:B:73:VAL:HG22	1:B:74:VAL:N	2.27	0.49
1:D:396:GLY:HA2	1:D:398:PHE:CE2	2.47	0.49
1:E:485:LYS:O	1:E:489:LEU:HB2	2.12	0.49
1:G:150:ILE:HD11	1:G:210:MET:HE1	1.94	0.49
1:G:220:PRO:HG2	1:G:221:PHE:HD2	1.76	0.49
1:H:470:ILE:O	1:H:474:GLN:HG2	2.10	0.49
1:J:251:GLU:HA	1:L:228:PHE:CD1	2.47	0.49
1:J:485:LYS:O	1:J:489:LEU:HB2	2.12	0.49
1:B:262:ASN:ND2	1:B:264:LEU:H	2.10	0.49
1:B:364:PRO:C	1:B:366:LYS:H	2.20	0.49
1:B:392:THR:HG22	1:B:616:GLN:NE2	2.26	0.49
1:B:401:ARG:HH11	1:B:437:LEU:HD23	1.77	0.49
1:D:62:ILE:HG22	1:D:93:LEU:HD13	1.93	0.49
1:E:150:ILE:HD11	1:E:210:MET:HE1	1.94	0.49
1:F:262:ASN:ND2	1:F:264:LEU:H	2.10	0.49
1:F:574:ARG:HB2	1:F:574:ARG:NH1	2.26	0.49
1:G:146:LYS:NZ	1:G:182:VAL:HG11	2.28	0.49
1:J:283:ASP:O	1:J:287:ARG:HG3	2.13	0.49
1:K:587:VAL:O	1:K:591:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:395:GLU:HG3	1:L:397:PRO:HD3	1.94	0.49
1:B:191:GLU:CD	1:B:284:PRO:HB3	2.36	0.49
1:B:401:ARG:HD2	1:B:401:ARG:N	2.27	0.49
1:B:574:ARG:NH1	1:B:574:ARG:HB2	2.26	0.49
1:C:85:ILE:HB	1:C:90:VAL:H	1.78	0.49
1:G:146:LYS:HZ1	1:G:182:VAL:HG11	1.77	0.49
1:H:222:LEU:HD22	1:H:244:ALA:O	2.12	0.49
1:I:29:VAL:HG22	1:I:44:LYS:CB	2.42	0.49
1:J:387:PHE:CZ	1:J:451:ALA:HB2	2.47	0.49
1:L:395:GLU:CG	1:L:396:GLY:H	2.26	0.49
1:C:150:ILE:HD11	1:C:210:MET:HE1	1.92	0.49
1:C:647:GLN:OE1	1:D:489:LEU:HD22	2.13	0.49
1:C:655:LYS:HA	1:C:658:CYS:SG	2.52	0.49
1:D:221:PHE:HB2	1:D:230:TRP:HZ2	1.76	0.49
1:D:406:CYS:SG	1:D:407:VAL:HG23	2.51	0.49
1:D:580:TYR:HB2	1:F:576:SER:OG	2.13	0.49
1:E:141:ILE:HG23	1:E:170:LYS:HB2	1.94	0.49
1:F:112:ASN:HB3	1:F:116:LEU:CD2	2.41	0.49
1:F:225:LEU:O	1:F:226:GLN:C	2.54	0.49
1:F:237:LYS:CE	1:F:281:ASN:HA	2.41	0.49
1:F:473:SER:OG	1:F:524:VAL:HG13	2.13	0.49
1:H:574:ARG:NH1	1:H:574:ARG:HB2	2.27	0.49
1:I:222:LEU:HB2	1:I:230:TRP:HD1	1.77	0.49
1:I:563:ARG:HH12	2:h:2:GLC:H2	1.78	0.49
1:J:33:GLN:HA	1:J:40:LYS:HA	1.93	0.49
1:J:133:ARG:NE	1:J:297:GLN:HE22	2.10	0.49
1:J:574:ARG:NH1	1:J:575:PRO:HD2	2.26	0.49
1:K:185:LEU:O	1:K:186:GLN:HB2	2.12	0.49
1:K:485:LYS:O	1:K:489:LEU:HB2	2.12	0.49
2:P:3:PDX:O3X	2:P:3:PDX:H2	2.12	0.49
1:A:395:GLU:OE2	1:A:397:PRO:HG3	2.12	0.49
1:D:354:LEU:HB3	1:D:384:VAL:CG1	2.43	0.49
1:E:33:GLN:HA	1:E:40:LYS:HA	1.94	0.49
1:F:356:SER:HB2	1:F:382:TYR:CE1	2.47	0.49
1:G:60:HIS:O	1:G:63:GLN:HB3	2.12	0.49
1:H:150:ILE:HD11	1:H:210:MET:HE1	1.94	0.49
1:H:460:ALA:O	1:H:464:LYS:HG3	2.12	0.49
1:J:74:VAL:O	1:J:74:VAL:HG13	2.13	0.49
1:J:315:ILE:HD12	1:J:384:VAL:HB	1.95	0.49
1:K:289:GLY:N	1:K:290:PRO:CD	2.76	0.49
1:L:79:VAL:HG11	1:L:83:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:574:ARG:NH1	1:L:574:ARG:HB2	2.27	0.49
1:A:418:LEU:HB2	1:A:423:LEU:HD21	1.93	0.49
1:C:29:VAL:HG22	1:C:44:LYS:CB	2.42	0.49
1:D:222:LEU:HB3	1:D:225:LEU:HB2	1.95	0.49
1:F:222:LEU:HD23	1:F:225:LEU:HG	1.95	0.49
1:G:489:LEU:HD13	1:H:643:GLN:HG3	1.95	0.49
1:H:33:GLN:HA	1:H:40:LYS:HA	1.94	0.49
1:I:547:SER:HB3	1:I:548:PRO:HD2	1.95	0.49
1:K:574:ARG:HD2	1:K:577:ASP:OD1	2.12	0.49
1:L:423:LEU:HA	1:L:426:VAL:CG2	2.41	0.49
1:A:316:LEU:HB2	1:A:383:MET:HE1	1.93	0.49
1:C:74:VAL:CG2	1:C:95:MET:HB2	2.43	0.49
1:C:395:GLU:HG2	1:C:397:PRO:CD	2.35	0.49
1:C:423:LEU:HA	1:C:426:VAL:CG2	2.40	0.49
1:D:17:MET:HB3	1:D:32:TYR:CD1	2.47	0.49
1:E:98:CYS:HA	1:E:153:GLN:NE2	2.27	0.49
1:F:17:MET:HB3	1:F:32:TYR:CD1	2.47	0.49
1:F:43:ILE:HD12	1:F:43:ILE:N	2.28	0.49
1:F:279:MET:C	1:F:280:LEU:HD12	2.38	0.49
1:G:234:ILE:HG22	1:G:254:PHE:HE1	1.78	0.49
1:H:192:LEU:H	1:H:192:LEU:HD12	1.76	0.49
1:H:549:TYR:N	1:H:552:ARG:HD2	2.28	0.49
1:I:275:TRP:CZ2	1:I:304:MET:HE2	2.47	0.49
1:K:424:ARG:HH11	1:K:572:LYS:HG2	1.78	0.49
1:A:48:LEU:O	1:A:50:LEU:HD12	2.13	0.49
1:A:658:CYS:SG	1:B:501:GLY:HA2	2.53	0.49
1:B:219:ARG:NH1	1:B:224:HIS:H	2.11	0.49
1:C:334:LEU:HD11	1:C:364:PRO:HA	1.95	0.49
1:C:413:ASP:OD1	1:C:416:ILE:HB	2.12	0.49
1:C:653:LEU:HG	1:C:656:ILE:HD11	1.95	0.49
1:D:33:GLN:HA	1:D:40:LYS:HA	1.93	0.49
1:E:29:VAL:HG22	1:E:44:LYS:CB	2.42	0.49
1:E:47:ARG:O	1:E:87:ILE:HB	2.13	0.49
1:G:48:LEU:O	1:G:50:LEU:HD12	2.13	0.49
1:G:147:PRO:C	1:G:149:ASN:H	2.21	0.49
1:G:237:LYS:HD2	1:G:237:LYS:C	2.37	0.49
1:I:191:GLU:CD	1:I:284:PRO:HB3	2.38	0.49
1:I:413:ASP:OD1	1:I:416:ILE:HB	2.12	0.49
1:J:392:THR:O	1:J:612:LEU:HD23	2.13	0.49
1:K:319:THR:HG22	1:K:394:TYR:CE1	2.48	0.49
1:L:316:LEU:HB2	1:L:383:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD22	1:A:166:LEU:N	2.27	0.49
1:A:485:LYS:O	1:A:489:LEU:HB2	2.12	0.49
1:A:513:GLU:HB3	1:A:517:LYS:HE3	1.95	0.49
1:A:523:GLU:OE1	1:A:526:VAL:HG21	2.12	0.49
1:B:17:MET:HB3	1:B:32:TYR:CD1	2.48	0.49
1:B:29:VAL:HG22	1:B:44:LYS:CB	2.42	0.49
1:B:33:GLN:HA	1:B:40:LYS:HA	1.94	0.49
1:C:574:ARG:HB2	1:C:574:ARG:NH1	2.27	0.49
1:D:199:THR:HG21	1:D:284:PRO:HB2	1.95	0.49
1:D:227:PRO:HA	1:D:230:TRP:CB	2.41	0.49
1:D:469:LEU:HD12	1:D:625:VAL:HG13	1.95	0.49
1:D:506:LYS:HE2	1:D:507:MET:HE3	1.95	0.49
1:G:44:LYS:HB3	1:G:93:LEU:HB3	1.95	0.49
1:G:328:LEU:HD11	1:G:337:LEU:HD22	1.95	0.49
1:G:418:LEU:HB2	1:G:423:LEU:HD21	1.93	0.49
1:H:477:LYS:HE3	1:H:524:VAL:HG11	1.94	0.49
1:I:372:VAL:HG13	1:I:372:VAL:O	2.13	0.49
1:J:62:ILE:HG22	1:J:93:LEU:HD13	1.94	0.49
1:K:33:GLN:HA	1:K:40:LYS:HA	1.94	0.49
1:K:654:LEU:HD11	1:L:502:ILE:HD12	1.94	0.49
1:A:373:LEU:HB2	1:A:378:GLY:HA2	1.95	0.48
1:A:427:TRP:HZ2	1:A:583:SER:HA	1.78	0.48
1:B:142:HIS:HA	1:B:169:ALA:HB2	1.94	0.48
1:B:219:ARG:NH2	1:B:224:HIS:H	2.10	0.48
1:D:574:ARG:NH1	1:D:575:PRO:HD2	2.27	0.48
1:E:201:THR:HA	1:E:204:TYR:CD1	2.48	0.48
1:E:523:GLU:OE1	1:E:526:VAL:HG21	2.13	0.48
1:F:186:GLN:CG	1:F:219:ARG:HD3	2.42	0.48
1:F:426:VAL:HG23	1:F:427:TRP:HD1	1.77	0.48
1:G:236:LYS:CG	1:G:237:LYS:N	2.76	0.48
1:G:653:LEU:HG	1:G:656:ILE:HD11	1.95	0.48
1:H:84:ASN:CG	1:H:85:ILE:H	2.21	0.48
1:H:240:LYS:HB3	1:H:277:GLN:HB3	1.94	0.48
1:H:262:ASN:ND2	1:H:264:LEU:H	2.11	0.48
1:H:268:ILE:O	1:H:272:MET:HB2	2.13	0.48
1:H:424:ARG:HD3	1:H:572:LYS:HE2	1.94	0.48
1:I:205:TRP:HB2	1:I:287:ARG:NH1	2.28	0.48
1:I:279:MET:C	1:I:280:LEU:HD12	2.38	0.48
1:I:463:THR:HG21	1:I:538:HIS:HD2	1.79	0.48
1:I:587:VAL:HA	1:I:590:ILE:HD12	1.95	0.48
1:J:29:VAL:HG22	1:J:44:LYS:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:LEU:HG	1:J:97:TYR:CE2	2.48	0.48
1:J:262:ASN:ND2	1:J:264:LEU:H	2.11	0.48
1:J:574:ARG:NH1	1:J:574:ARG:HB2	2.27	0.48
1:K:31:LEU:HG	1:K:97:TYR:CE2	2.48	0.48
1:K:452:MET:SD	1:K:611:LEU:HD22	2.53	0.48
1:L:13:GLY:N	1:L:14:PRO:CD	2.70	0.48
1:B:31:LEU:HG	1:B:97:TYR:CE2	2.48	0.48
1:B:70:HIS:HB3	1:B:73:VAL:HG12	1.96	0.48
1:E:21:LEU:HD23	1:E:29:VAL:C	2.38	0.48
1:E:117:LYS:O	1:E:121:ILE:HG13	2.13	0.48
1:E:224:HIS:O	1:E:225:LEU:HD22	2.12	0.48
1:E:328:LEU:HD11	1:E:337:LEU:HD22	1.95	0.48
1:E:489:LEU:HD22	1:F:647:GLN:OE1	2.12	0.48
1:F:427:TRP:HZ3	1:F:567:LEU:HB3	1.77	0.48
1:F:513:GLU:HB3	1:F:517:LYS:HE3	1.95	0.48
1:G:298:PRO:O	1:G:302:VAL:HG23	2.13	0.48
1:G:460:ALA:O	1:G:464:LYS:HG3	2.14	0.48
1:H:192:LEU:HD12	1:H:192:LEU:N	2.28	0.48
1:H:237:LYS:HE2	1:H:281:ASN:HA	1.95	0.48
1:I:209:THR:HG22	1:I:220:PRO:HG3	1.95	0.48
1:K:79:VAL:HG11	1:K:83:LEU:CD1	2.39	0.48
1:L:410:ILE:HG23	1:L:583:SER:OG	2.13	0.48
1:A:186:GLN:HE21	1:A:227:PRO:HD3	1.78	0.48
1:A:221:PHE:HB2	1:A:230:TRP:NE1	2.25	0.48
1:A:223:HIS:NE2	1:A:425:LYS:HE3	2.28	0.48
1:A:278:LEU:HD23	1:A:288:GLY:HA2	1.95	0.48
1:A:473:SER:O	1:A:524:VAL:HG22	2.12	0.48
1:B:103:LEU:HD22	1:B:150:ILE:HD12	1.96	0.48
1:B:449:ARG:HH12	3:O:1:5LS:C3	2.26	0.48
1:D:29:VAL:HG22	1:D:44:LYS:CB	2.43	0.48
1:D:31:LEU:HG	1:D:97:TYR:CE2	2.49	0.48
1:D:485:LYS:O	1:D:489:LEU:HB2	2.13	0.48
1:E:17:MET:HB3	1:E:32:TYR:CD1	2.48	0.48
1:F:86:LEU:C	1:F:87:ILE:HD12	2.38	0.48
1:F:192:LEU:HD12	1:F:192:LEU:N	2.28	0.48
1:J:367:PRO:O	1:J:370:GLN:HG2	2.11	0.48
1:K:45:SER:HA	1:K:86:LEU:CD2	2.43	0.48
1:L:262:ASN:ND2	1:L:264:LEU:H	2.11	0.48
1:A:60:HIS:O	1:A:63:GLN:HB3	2.13	0.48
1:B:507:MET:HE1	1:B:653:LEU:HD13	1.95	0.48
1:C:192:LEU:H	1:C:192:LEU:HD12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:563:ARG:NH1	2:Y:2:GLC:H2	2.24	0.48
1:G:283:ASP:O	1:G:287:ARG:HG3	2.13	0.48
1:I:574:ARG:NH1	1:I:574:ARG:HB2	2.27	0.48
1:J:13:GLY:N	1:J:14:PRO:CD	2.68	0.48
1:J:201:THR:HA	1:J:204:TYR:CD1	2.49	0.48
1:J:292:ASP:OD2	1:J:294:THR:HB	2.14	0.48
1:J:523:GLU:OE1	1:J:526:VAL:HG21	2.14	0.48
1:K:182:VAL:HG12	1:K:183:GLY:H	1.78	0.48
1:K:185:LEU:HD12	1:K:193:PHE:HZ	1.78	0.48
1:K:574:ARG:NH1	1:K:574:ARG:HB2	2.27	0.48
1:L:31:LEU:HG	1:L:97:TYR:CE2	2.48	0.48
1:L:219:ARG:HG2	1:L:220:PRO:HD2	1.96	0.48
1:L:426:VAL:HG23	1:L:427:TRP:HD1	1.77	0.48
1:L:485:LYS:O	1:L:489:LEU:HB2	2.12	0.48
1:A:31:LEU:HG	1:A:97:TYR:CE2	2.49	0.48
1:A:460:ALA:O	1:A:464:LYS:HG3	2.14	0.48
1:B:430:ALA:O	1:B:434:VAL:HG23	2.14	0.48
1:C:285:GLN:OE1	1:C:285:GLN:HA	2.14	0.48
1:D:201:THR:HA	1:D:204:TYR:CD1	2.49	0.48
1:E:81:GLU:HG2	1:E:82:GLU:OE1	2.14	0.48
1:E:485:LYS:HG2	1:F:640:MET:HE1	1.96	0.48
1:E:513:GLU:HB3	1:E:517:LYS:HE3	1.96	0.48
1:F:485:LYS:O	1:F:489:LEU:HB2	2.12	0.48
1:G:410:ILE:HG23	1:G:583:SER:OG	2.14	0.48
1:G:485:LYS:O	1:G:489:LEU:HB2	2.13	0.48
1:H:47:ARG:O	1:H:87:ILE:HD12	2.13	0.48
1:H:363:ASP:OD1	1:H:365:ARG:HB2	2.12	0.48
1:J:406:CYS:SG	1:J:407:VAL:HG23	2.52	0.48
1:J:473:SER:HB3	1:J:632:ILE:HD13	1.95	0.48
1:J:483:PHE:HZ	1:J:514:MET:HB3	1.78	0.48
1:K:420:ILE:HG21	1:K:578:HIS:N	2.28	0.48
1:K:586:MET:O	1:K:590:ILE:HG13	2.14	0.48
1:L:452:MET:HE1	1:L:455:LEU:HD23	1.95	0.48
1:A:97:TYR:HA	4:A:701:5TL:OAO	2.14	0.48
1:A:334:LEU:HD11	1:A:364:PRO:HA	1.94	0.48
1:C:177:LEU:HD12	1:C:177:LEU:N	2.29	0.48
1:C:418:LEU:HB2	1:C:423:LEU:HD21	1.96	0.48
1:D:513:GLU:HB3	1:D:517:LYS:HE3	1.94	0.48
1:G:31:LEU:HG	1:G:97:TYR:CE2	2.49	0.48
1:H:615:LYS:O	1:H:619:ILE:HG13	2.14	0.48
1:I:74:VAL:HG21	1:I:95:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:410:ILE:HG23	1:I:583:SER:OG	2.13	0.48
1:J:17:MET:HB3	1:J:32:TYR:CD1	2.48	0.48
1:J:473:SER:HB3	1:J:527:ILE:HD11	1.96	0.48
1:L:142:HIS:ND1	1:L:169:ALA:HB2	2.29	0.48
1:L:513:GLU:HB3	1:L:517:LYS:HE3	1.96	0.48
1:L:549:TYR:HD2	1:L:552:ARG:NH1	2.11	0.48
2:e:1:5LS:C6	2:e:2:GLC:H5	2.43	0.48
2:j:2:GLC:H62	2:j:3:PDX:H5	1.95	0.48
1:A:143:ARG:HG2	1:A:143:ARG:HH21	1.78	0.48
1:A:648:LYS:HE3	1:B:489:LEU:HD11	1.96	0.48
1:B:222:LEU:HB2	1:B:230:TRP:NE1	2.28	0.48
1:B:242:ILE:HG22	1:B:280:LEU:HD12	1.95	0.48
1:C:31:LEU:HG	1:C:97:TYR:CE2	2.49	0.48
1:C:178:CYS:HB2	1:C:179:THR:H	1.57	0.48
1:C:410:ILE:HD12	1:C:583:SER:OG	2.13	0.48
1:C:420:ILE:HG21	1:C:578:HIS:N	2.28	0.48
1:D:615:LYS:O	1:D:619:ILE:HG13	2.14	0.48
1:E:143:ARG:HH21	1:E:143:ARG:HG2	1.78	0.48
1:E:158:LYS:HB3	1:E:376:VAL:CG1	2.44	0.48
1:E:648:LYS:HE3	1:F:489:LEU:HD11	1.94	0.48
1:F:71:ALA:C	1:F:73:VAL:N	2.72	0.48
1:F:86:LEU:HD11	1:F:92:LEU:CD1	2.44	0.48
1:G:318:MET:HE2	1:G:447:GLY:HA3	1.95	0.48
1:H:420:ILE:HA	1:H:423:LEU:HB2	1.96	0.48
1:I:192:LEU:HD12	1:I:192:LEU:N	2.29	0.48
1:I:424:ARG:HD3	1:I:572:LYS:HE2	1.95	0.48
1:I:653:LEU:HG	1:I:656:ILE:HD11	1.95	0.48
1:J:506:LYS:HE2	1:J:507:MET:HE3	1.96	0.48
1:K:48:LEU:O	1:K:50:LEU:HD12	2.14	0.48
1:K:655:LYS:HA	1:K:658:CYS:SG	2.54	0.48
1:L:29:VAL:HG22	1:L:44:LYS:CB	2.44	0.48
1:L:170:LYS:HA	1:L:177:LEU:HA	1.95	0.48
1:L:192:LEU:HD12	1:L:192:LEU:H	1.78	0.48
1:L:653:LEU:HG	1:L:656:ILE:HD11	1.95	0.48
1:B:185:LEU:HD13	1:B:186:GLN:N	2.29	0.48
1:B:574:ARG:O	1:B:576:SER:N	2.46	0.48
1:B:615:LYS:O	1:B:619:ILE:HG13	2.14	0.48
1:C:141:ILE:O	1:C:169:ALA:HB1	2.14	0.48
1:C:201:THR:HA	1:C:204:TYR:CD1	2.49	0.48
1:D:60:HIS:O	1:D:63:GLN:HB3	2.14	0.48
1:E:43:ILE:N	1:E:43:ILE:HD12	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:GLU:CD	1:G:180:GLU:H	2.21	0.48
1:G:523:GLU:OE1	1:G:526:VAL:HG21	2.13	0.48
1:G:651:TRP:CZ2	1:H:490:ASP:HB3	2.48	0.48
1:H:29:VAL:HG22	1:H:44:LYS:CB	2.43	0.48
1:H:278:LEU:CD2	1:H:299:ARG:HB3	2.44	0.48
1:H:401:ARG:HH12	1:H:440:ASP:HB2	1.77	0.48
1:H:418:LEU:HB2	1:H:423:LEU:HD21	1.96	0.48
1:I:117:LYS:O	1:I:121:ILE:HG13	2.14	0.48
1:I:227:PRO:HG3	1:K:249:SER:HB2	1.95	0.48
1:J:221:PHE:HB2	1:J:230:TRP:CZ2	2.48	0.48
1:K:227:PRO:HA	1:K:230:TRP:HB2	1.95	0.48
1:B:465:MET:CB	1:B:625:VAL:HG11	2.43	0.48
1:C:44:LYS:HB3	1:C:93:LEU:HB3	1.96	0.48
1:C:485:LYS:O	1:C:489:LEU:HB2	2.14	0.48
1:F:31:LEU:HG	1:F:97:TYR:CE2	2.49	0.48
1:F:452:MET:HE1	1:F:455:LEU:HD23	1.96	0.48
1:G:166:LEU:HD22	1:G:166:LEU:N	2.28	0.48
1:G:494:TYR:HE1	1:G:503:SER:HA	1.79	0.48
1:G:623:PRO:O	1:G:627:VAL:HG23	2.14	0.48
1:H:523:GLU:OE1	1:H:526:VAL:HG21	2.14	0.48
1:I:60:HIS:O	1:I:63:GLN:HB3	2.14	0.48
1:I:513:GLU:HB3	1:I:517:LYS:HE3	1.96	0.48
1:K:29:VAL:HG22	1:K:44:LYS:CB	2.42	0.48
1:K:60:HIS:O	1:K:63:GLN:HB3	2.13	0.48
1:K:587:VAL:HA	1:K:590:ILE:HD12	1.96	0.48
1:B:147:PRO:C	1:B:149:ASN:H	2.22	0.48
1:C:223:HIS:C	1:C:225:LEU:H	2.22	0.48
1:C:267:LEU:HD13	1:C:327:LEU:HB2	1.94	0.48
1:D:653:LEU:HG	1:D:656:ILE:HD11	1.96	0.48
1:E:72:ASN:OD1	1:E:127:ASP:HA	2.14	0.48
1:F:14:PRO:O	1:F:35:ARG:HG2	2.14	0.48
1:F:448:GLN:OE1	1:F:549:TYR:HB3	2.14	0.48
1:H:513:GLU:HB3	1:H:517:LYS:HE3	1.95	0.48
1:I:44:LYS:HB3	1:I:93:LEU:HB3	1.96	0.48
1:I:485:LYS:O	1:I:489:LEU:HB2	2.14	0.48
1:J:70:HIS:HB3	1:J:73:VAL:HG23	1.95	0.48
1:J:480:LEU:HD22	1:J:518:ALA:HB1	1.95	0.48
1:J:653:LEU:HG	1:J:656:ILE:HD11	1.96	0.48
1:K:648:LYS:HE3	1:L:489:LEU:HD11	1.95	0.48
1:L:219:ARG:HH11	1:L:219:ARG:HG3	1.79	0.48
1:L:240:LYS:O	1:L:277:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:VAL:HG12	1:B:385:TYR:N	2.29	0.47
1:B:418:LEU:HB2	1:B:423:LEU:HD21	1.96	0.47
1:B:420:ILE:HA	1:B:423:LEU:HB2	1.96	0.47
1:B:523:GLU:OE1	1:B:526:VAL:HG21	2.14	0.47
1:F:122:LEU:HD12	1:F:379:CYS:SG	2.53	0.47
1:F:586:MET:O	1:F:590:ILE:HG13	2.14	0.47
1:G:334:LEU:HD11	1:G:364:PRO:HA	1.95	0.47
1:G:420:ILE:HA	1:G:423:LEU:HB2	1.96	0.47
1:I:418:LEU:HB2	1:I:423:LEU:HD21	1.96	0.47
1:K:224:HIS:C	1:K:225:LEU:HD22	2.39	0.47
1:A:401:ARG:NH2	1:A:437:LEU:HD23	2.28	0.47
1:B:143:ARG:HH21	1:B:143:ARG:HG2	1.79	0.47
1:B:192:LEU:H	1:B:192:LEU:HD12	1.78	0.47
1:B:290:PRO:HB2	1:B:299:ARG:CB	2.36	0.47
1:B:411:VAL:HG12	1:B:590:ILE:HG21	1.96	0.47
1:D:166:LEU:HD22	1:D:166:LEU:N	2.29	0.47
1:D:192:LEU:HD12	1:D:192:LEU:H	1.77	0.47
1:E:574:ARG:NH1	1:E:574:ARG:HB2	2.28	0.47
1:F:363:ASP:HB3	1:F:370:GLN:HE22	1.79	0.47
1:G:513:GLU:HB3	1:G:517:LYS:HE3	1.96	0.47
1:G:587:VAL:O	1:G:591:VAL:HG23	2.12	0.47
1:H:147:PRO:C	1:H:149:ASN:H	2.22	0.47
1:H:242:ILE:HG22	1:H:280:LEU:HD12	1.96	0.47
1:I:387:PHE:CZ	1:I:451:ALA:HB2	2.49	0.47
1:I:587:VAL:O	1:I:591:VAL:HG23	2.13	0.47
1:J:10:GLY:C	1:J:12:GLY:H	2.22	0.47
1:J:166:LEU:HD22	1:J:166:LEU:N	2.29	0.47
1:J:392:THR:HG22	1:J:616:GLN:HE22	1.79	0.47
1:J:598:ASP:O	1:J:602:LYS:HG2	2.14	0.47
1:K:143:ARG:HG2	1:K:143:ARG:HH21	1.78	0.47
1:L:315:ILE:CD1	1:L:384:VAL:HB	2.45	0.47
1:C:60:HIS:O	1:C:63:GLN:HB3	2.14	0.47
1:D:418:LEU:HB2	1:D:423:LEU:HD21	1.97	0.47
1:D:523:GLU:OE1	1:D:526:VAL:HG21	2.14	0.47
1:D:574:ARG:NH1	1:D:574:ARG:HB2	2.28	0.47
1:D:598:ASP:O	1:D:602:LYS:HG2	2.14	0.47
1:D:633:LYS:HA	1:D:636:ASP:HB3	1.96	0.47
1:E:430:ALA:O	1:E:434:VAL:HG23	2.13	0.47
1:E:466:LYS:HD3	1:E:534:ILE:HG21	1.96	0.47
1:E:487:ILE:CD1	1:E:514:MET:HE3	2.44	0.47
1:F:460:ALA:O	1:F:464:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:561:GLU:O	1:G:565:ILE:HG13	2.15	0.47
1:H:60:HIS:O	1:H:63:GLN:HB3	2.14	0.47
1:H:83:LEU:O	1:H:84:ASN:HB3	2.14	0.47
1:H:275:TRP:HZ2	1:H:304:MET:HE2	1.79	0.47
1:H:635:ALA:HA	1:H:638:THR:OG1	2.14	0.47
1:I:31:LEU:HG	1:I:97:TYR:CE2	2.49	0.47
1:I:537:LEU:O	1:I:541:ILE:HG13	2.14	0.47
1:J:427:TRP:CZ3	1:J:567:LEU:HB3	2.47	0.47
1:K:43:ILE:HD12	1:K:43:ILE:N	2.29	0.47
1:L:396:GLY:HA2	1:L:398:PHE:CE2	2.49	0.47
1:L:417:GLN:HB3	1:L:581:SER:HB2	1.95	0.47
1:L:635:ALA:HA	1:L:638:THR:OG1	2.15	0.47
1:A:643:GLN:HG3	1:B:489:LEU:HD13	1.97	0.47
1:B:268:ILE:O	1:B:272:MET:HB2	2.15	0.47
1:B:623:PRO:O	1:B:627:VAL:HG23	2.14	0.47
1:C:420:ILE:HA	1:C:423:LEU:HB2	1.96	0.47
1:C:466:LYS:HD3	1:C:534:ILE:HD13	1.96	0.47
1:C:473:SER:HB3	1:C:632:ILE:HD13	1.96	0.47
1:D:541:ILE:CD1	1:D:618:ILE:HD11	2.44	0.47
1:E:48:LEU:O	1:E:50:LEU:HD12	2.15	0.47
1:E:418:LEU:HB2	1:E:423:LEU:HD21	1.96	0.47
1:F:356:SER:HB2	1:F:382:TYR:HE1	1.79	0.47
1:F:623:PRO:O	1:F:627:VAL:HG23	2.15	0.47
1:G:199:THR:CG2	1:G:285:GLN:HE22	2.22	0.47
1:H:201:THR:HA	1:H:204:TYR:CD1	2.49	0.47
1:J:77:CYS:H	1:J:95:MET:HA	1.80	0.47
1:J:116:LEU:O	1:J:121:ILE:HD11	2.14	0.47
1:J:192:LEU:H	1:J:192:LEU:HD12	1.78	0.47
1:K:85:ILE:HD12	1:K:89:ASP:HA	1.97	0.47
1:K:523:GLU:OE1	1:K:526:VAL:HG21	2.14	0.47
1:A:44:LYS:HB3	1:A:93:LEU:HB3	1.97	0.47
1:A:51:SER:HB2	1:A:54:ASN:OD1	2.14	0.47
1:A:84:ASN:ND2	1:A:85:ILE:H	2.13	0.47
1:A:147:PRO:C	1:A:149:ASN:H	2.22	0.47
1:B:14:PRO:O	1:B:35:ARG:HG2	2.14	0.47
1:B:317:ASN:ND2	1:B:319:THR:HG23	2.30	0.47
1:B:477:LYS:HE3	1:B:524:VAL:HG11	1.95	0.47
1:C:452:MET:HE1	1:C:455:LEU:HD23	1.97	0.47
1:D:68:LEU:HD21	1:D:140:ILE:HD12	1.96	0.47
1:D:199:THR:CG2	1:D:284:PRO:HB2	2.44	0.47
1:D:635:ALA:HA	1:D:638:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:PRO:O	1:E:240:LYS:HB2	2.15	0.47
1:F:75:LYS:HD2	1:F:76:ALA:N	2.30	0.47
1:F:201:THR:HA	1:F:204:TYR:CD1	2.49	0.47
1:G:396:GLY:N	1:G:397:PRO:CD	2.77	0.47
1:G:506:LYS:HE2	1:G:507:MET:HE3	1.97	0.47
1:I:72:ASN:ND2	1:I:130:SER:HB3	2.29	0.47
1:J:88:HIS:CG	1:J:89:ASP:N	2.80	0.47
1:J:121:ILE:HG21	1:J:264:LEU:HD21	1.96	0.47
1:J:657:ALA:HA	1:J:660:GLN:HG3	1.97	0.47
1:K:48:LEU:HA	1:K:87:ILE:HG21	1.97	0.47
1:K:408:ASN:HA	1:K:411:VAL:HG22	1.97	0.47
1:K:502:ILE:CD1	1:K:656:ILE:HD12	2.45	0.47
1:L:48:LEU:HA	1:L:87:ILE:CD1	2.44	0.47
1:L:387:PHE:CZ	1:L:451:ALA:HB2	2.50	0.47
2:S:2:GLC:H61	2:S:2:GLC:O3	2.14	0.47
1:A:236:LYS:NZ	1:A:237:LYS:H	2.12	0.47
1:A:320:SER:CA	1:A:398:PHE:HB3	2.41	0.47
1:A:653:LEU:HG	1:A:656:ILE:HD11	1.96	0.47
1:B:106:LEU:HD11	1:B:152:LEU:HG	1.96	0.47
1:C:507:MET:HE1	1:C:653:LEU:HD22	1.96	0.47
1:D:420:ILE:HG21	1:D:578:HIS:N	2.24	0.47
1:F:551:ARG:HB3	1:F:552:ARG:HH21	1.80	0.47
1:F:635:ALA:HA	1:F:638:THR:OG1	2.15	0.47
1:H:487:ILE:HG23	1:H:488:GLN:N	2.30	0.47
1:I:201:THR:HA	1:I:204:TYR:CD1	2.50	0.47
1:J:116:LEU:HD12	1:J:116:LEU:N	2.30	0.47
1:K:166:LEU:N	1:K:166:LEU:HD22	2.30	0.47
1:L:86:LEU:CD1	1:L:87:ILE:HG13	2.45	0.47
1:L:267:LEU:HD12	1:L:312:ILE:HG23	1.95	0.47
1:L:418:LEU:HB2	1:L:423:LEU:HD21	1.96	0.47
1:B:21:LEU:HD23	1:B:29:VAL:C	2.39	0.47
1:B:170:LYS:NZ	1:B:192:LEU:HD11	2.29	0.47
1:B:222:LEU:HD22	1:B:244:ALA:O	2.15	0.47
1:B:240:LYS:HB3	1:B:277:GLN:CB	2.43	0.47
1:B:396:GLY:C	1:B:398:PHE:H	2.22	0.47
1:C:316:LEU:HB2	1:C:383:MET:CE	2.45	0.47
1:C:365:ARG:N	1:C:365:ARG:HD2	2.30	0.47
1:C:497:GLN:C	1:C:499:THR:H	2.22	0.47
1:C:537:LEU:O	1:C:541:ILE:HG13	2.15	0.47
1:D:74:VAL:HG21	1:D:164:ILE:HG13	1.97	0.47
1:D:74:VAL:CG2	1:D:95:MET:HE3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:CYS:H	1:D:95:MET:HA	1.80	0.47
1:D:268:ILE:O	1:D:272:MET:HB2	2.15	0.47
1:D:563:ARG:HH22	2:V:1:5LS:C6	2.27	0.47
1:E:31:LEU:HG	1:E:97:TYR:CE2	2.50	0.47
1:E:60:HIS:O	1:E:63:GLN:HB3	2.14	0.47
1:E:323:ILE:HD12	1:E:323:ILE:N	2.30	0.47
1:E:373:LEU:HD22	1:E:373:LEU:N	2.29	0.47
1:E:574:ARG:NH1	1:E:575:PRO:HD2	2.30	0.47
1:F:182:VAL:HB	1:F:185:LEU:HD23	1.96	0.47
1:F:281:ASN:OD1	1:F:286:GLN:HB3	2.15	0.47
1:G:143:ARG:HG2	1:G:143:ARG:HH21	1.80	0.47
1:G:408:ASN:HA	1:G:411:VAL:HG22	1.95	0.47
1:G:420:ILE:HG21	1:G:578:HIS:N	2.29	0.47
1:H:43:ILE:HD12	1:H:43:ILE:N	2.29	0.47
1:H:44:LYS:HB3	1:H:93:LEU:HB3	1.96	0.47
1:H:117:LYS:O	1:H:121:ILE:HG13	2.15	0.47
1:H:485:LYS:O	1:H:489:LEU:HB2	2.14	0.47
1:H:633:LYS:HA	1:H:636:ASP:HB3	1.97	0.47
1:J:319:THR:HG22	1:J:394:TYR:CE1	2.49	0.47
1:K:7:PRO:HG3	1:K:17:MET:SD	2.54	0.47
1:K:51:SER:HB2	1:K:54:ASN:OD1	2.15	0.47
1:K:201:THR:HA	1:K:204:TYR:CD1	2.50	0.47
1:K:387:PHE:CZ	1:K:451:ALA:HB2	2.49	0.47
1:K:420:ILE:HA	1:K:423:LEU:HB2	1.97	0.47
1:L:60:HIS:O	1:L:63:GLN:HB3	2.13	0.47
1:L:201:THR:HA	1:L:204:TYR:CD1	2.49	0.47
1:L:507:MET:HE1	1:L:653:LEU:HD13	1.96	0.47
1:L:523:GLU:HB2	1:L:632:ILE:HG12	1.97	0.47
1:L:623:PRO:O	1:L:627:VAL:HG23	2.15	0.47
1:B:103:LEU:HB3	1:B:147:PRO:O	2.15	0.47
1:C:506:LYS:HE2	1:C:507:MET:HE3	1.97	0.47
1:C:513:GLU:HB3	1:C:517:LYS:HE3	1.97	0.47
1:D:74:VAL:HG11	1:D:164:ILE:HA	1.96	0.47
1:D:473:SER:HB3	1:D:632:ILE:HD13	1.95	0.47
1:E:268:ILE:C	1:E:271:PRO:HD2	2.39	0.47
1:E:548:PRO:HG2	1:E:607:HIS:NE2	2.30	0.47
1:F:219:ARG:NE	1:F:224:HIS:H	2.02	0.47
1:F:653:LEU:HG	1:F:656:ILE:HD11	1.96	0.47
1:G:576:SER:HB2	1:I:577:ASP:HA	1.97	0.47
1:H:45:SER:OG	1:H:86:LEU:HD11	2.14	0.47
1:H:51:SER:HB2	1:H:54:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:PRO:HG3	1:L:249:SER:HB2	1.97	0.47
1:H:229:THR:C	1:H:231:HIS:H	2.22	0.47
1:H:395:GLU:H	1:H:395:GLU:CD	2.22	0.47
1:I:501:GLY:HA2	1:J:658:CYS:HB3	1.97	0.47
1:I:633:LYS:HA	1:I:636:ASP:HB3	1.97	0.47
1:J:44:LYS:HB3	1:J:93:LEU:HB3	1.97	0.47
1:J:452:MET:HE1	1:J:455:LEU:HD23	1.97	0.47
1:J:615:LYS:O	1:J:619:ILE:HG13	2.15	0.47
1:K:192:LEU:H	1:K:192:LEU:HD12	1.80	0.47
1:K:401:ARG:HG2	1:K:433:TYR:HE1	1.78	0.47
1:K:513:GLU:HB3	1:K:517:LYS:HE3	1.97	0.47
1:L:192:LEU:HD12	1:L:192:LEU:N	2.30	0.47
1:B:192:LEU:HD12	1:B:192:LEU:N	2.30	0.47
1:B:635:ALA:HA	1:B:638:THR:OG1	2.15	0.47
1:C:317:ASN:ND2	1:C:319:THR:HG23	2.30	0.47
1:C:424:ARG:HD3	1:C:572:LYS:HE2	1.97	0.47
1:C:587:VAL:O	1:C:591:VAL:HG23	2.14	0.47
1:C:633:LYS:HA	1:C:636:ASP:HB3	1.97	0.47
1:D:51:SER:HB2	1:D:54:ASN:OD1	2.15	0.47
1:E:88:HIS:O	1:E:90:VAL:N	2.47	0.47
1:E:408:ASN:HA	1:E:411:VAL:HG22	1.97	0.47
1:E:420:ILE:HA	1:E:423:LEU:HB2	1.97	0.47
1:F:418:LEU:HB2	1:F:423:LEU:HD21	1.96	0.47
1:F:523:GLU:OE1	1:F:526:VAL:HG21	2.15	0.47
1:H:401:ARG:H	1:H:401:ARG:NE	2.12	0.47
1:I:43:ILE:HD12	1:I:43:ILE:N	2.29	0.47
1:I:223:HIS:C	1:I:225:LEU:H	2.22	0.47
1:I:404:SER:HB2	1:I:406:CYS:SG	2.54	0.47
1:J:420:ILE:HA	1:J:423:LEU:HB2	1.96	0.47
1:K:73:VAL:HG22	1:K:74:VAL:N	2.30	0.47
1:K:541:ILE:HD11	1:K:618:ILE:HD11	1.97	0.47
1:L:586:MET:O	1:L:590:ILE:HG13	2.15	0.47
1:A:29:VAL:HG22	1:A:44:LYS:CB	2.44	0.47
1:A:452:MET:HE1	1:A:455:LEU:HD23	1.96	0.47
1:A:586:MET:O	1:A:590:ILE:HG13	2.15	0.47
1:B:44:LYS:HB3	1:B:93:LEU:HB3	1.97	0.47
1:B:219:ARG:HH11	1:B:219:ARG:HB2	1.80	0.47
1:C:404:SER:HB2	1:C:406:CYS:SG	2.54	0.47
1:D:387:PHE:CZ	1:D:451:ALA:HB2	2.49	0.47
1:G:219:ARG:HH12	1:G:224:HIS:H	1.62	0.47
1:I:430:ALA:O	1:I:434:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:HIS:O	1:J:63:GLN:HB3	2.15	0.47
1:J:88:HIS:HD2	1:J:90:VAL:HG22	1.80	0.47
1:J:513:GLU:HB3	1:J:517:LYS:HE3	1.95	0.47
1:J:633:LYS:HA	1:J:636:ASP:HB3	1.97	0.47
1:K:396:GLY:HA2	1:K:398:PHE:CE2	2.50	0.47
1:K:452:MET:O	1:K:456:LEU:HG	2.15	0.47
1:L:44:LYS:HB3	1:L:93:LEU:HB3	1.97	0.47
1:A:587:VAL:O	1:A:591:VAL:HG23	2.14	0.46
1:B:408:ASN:ND2	1:D:26:PHE:HA	2.29	0.46
1:C:192:LEU:HD12	1:C:192:LEU:N	2.30	0.46
1:D:14:PRO:O	1:D:35:ARG:HG2	2.15	0.46
1:D:192:LEU:HD12	1:D:192:LEU:N	2.30	0.46
1:E:465:MET:HE3	1:E:625:VAL:HG21	1.97	0.46
1:F:29:VAL:HG22	1:F:44:LYS:CB	2.45	0.46
1:F:240:LYS:HA	1:F:240:LYS:NZ	2.30	0.46
1:G:201:THR:HA	1:G:204:TYR:CD1	2.51	0.46
1:G:404:SER:HB2	1:G:406:CYS:SG	2.55	0.46
1:H:166:LEU:HD22	1:H:166:LEU:N	2.29	0.46
1:H:215:ILE:HD13	1:H:264:LEU:HD11	1.97	0.46
1:I:98:CYS:HA	1:I:153:GLN:NE2	2.29	0.46
1:I:236:LYS:HG2	1:I:237:LYS:N	2.30	0.46
1:I:452:MET:HE1	1:I:455:LEU:HD23	1.97	0.46
1:I:487:ILE:HA	1:I:646:ARG:HD2	1.97	0.46
1:I:615:LYS:O	1:I:619:ILE:HG13	2.15	0.46
1:J:219:ARG:NH2	1:J:224:HIS:H	2.13	0.46
1:J:408:ASN:HA	1:J:411:VAL:HG22	1.97	0.46
1:K:502:ILE:HG12	1:K:656:ILE:HD12	1.96	0.46
1:L:268:ILE:O	1:L:272:MET:HB2	2.14	0.46
1:L:506:LYS:HE2	1:L:507:MET:HE3	1.96	0.46
2:j:2:GLC:H61	2:j:3:PDX:C3	2.39	0.46
1:B:60:HIS:O	1:B:63:GLN:HB3	2.15	0.46
1:B:103:LEU:HB2	1:B:150:ILE:HB	1.96	0.46
1:B:401:ARG:NH1	1:B:437:LEU:HD23	2.29	0.46
1:B:595:GLN:CB	2:Q:2:GLC:H62	2.45	0.46
1:C:523:GLU:OE1	1:C:526:VAL:HG21	2.14	0.46
1:C:635:ALA:HA	1:C:638:THR:OG1	2.15	0.46
1:E:633:LYS:HA	1:E:636:ASP:HB3	1.97	0.46
1:F:70:HIS:O	1:F:71:ALA:HB3	2.15	0.46
1:G:560:LEU:O	1:G:563:ARG:HB2	2.15	0.46
1:H:430:ALA:O	1:H:434:VAL:HG23	2.15	0.46
1:I:560:LEU:O	1:I:563:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:635:ALA:HA	1:I:638:THR:OG1	2.15	0.46
1:I:657:ALA:HA	1:I:660:GLN:HG3	1.97	0.46
1:L:275:TRP:CZ2	1:L:304:MET:HE2	2.50	0.46
1:A:74:VAL:CG2	1:A:95:MET:HE3	2.46	0.46
1:A:151:VAL:C	1:A:152:LEU:HD22	2.40	0.46
1:B:117:LYS:HE2	1:B:117:LYS:N	2.31	0.46
1:B:275:TRP:HZ2	1:B:304:MET:HE2	1.79	0.46
1:B:485:LYS:O	1:B:489:LEU:HB2	2.14	0.46
1:D:452:MET:HE1	1:D:455:LEU:HD23	1.98	0.46
1:D:657:ALA:HA	1:D:660:GLN:HG3	1.97	0.46
1:E:166:LEU:HD22	1:E:166:LEU:N	2.31	0.46
1:G:70:HIS:O	1:G:73:VAL:HG12	2.14	0.46
1:I:523:GLU:OE1	1:I:526:VAL:HG21	2.14	0.46
1:J:51:SER:HB2	1:J:54:ASN:OD1	2.16	0.46
1:J:268:ILE:O	1:J:272:MET:HB2	2.15	0.46
1:K:418:LEU:HB2	1:K:423:LEU:HD21	1.97	0.46
1:L:323:ILE:N	1:L:323:ILE:HD12	2.31	0.46
1:A:284:PRO:HG2	1:A:285:GLN:H	1.80	0.46
1:B:513:GLU:HB3	1:B:517:LYS:HE3	1.98	0.46
1:B:653:LEU:HG	1:B:656:ILE:HD11	1.96	0.46
1:C:445:PHE:HE1	1:C:549:TYR:HB3	1.81	0.46
1:C:586:MET:O	1:C:590:ILE:HG13	2.16	0.46
1:D:249:SER:HB3	1:F:184:THR:CA	2.45	0.46
1:E:51:SER:HB2	1:E:54:ASN:OD1	2.15	0.46
1:E:497:GLN:HE22	1:F:654:LEU:HD21	1.81	0.46
1:E:635:ALA:HA	1:E:638:THR:OG1	2.15	0.46
1:F:268:ILE:O	1:F:272:MET:HB2	2.14	0.46
1:G:51:SER:HB2	1:G:54:ASN:OD1	2.14	0.46
1:G:621:LEU:O	1:G:625:VAL:HG23	2.16	0.46
1:J:238:ASP:CB	1:J:239:PRO:HD2	2.45	0.46
1:L:424:ARG:HD3	1:L:572:LYS:HE2	1.97	0.46
1:L:523:GLU:OE1	1:L:526:VAL:HG21	2.16	0.46
1:A:473:SER:HB2	1:A:524:VAL:HG22	1.97	0.46
1:B:281:ASN:HD22	1:B:282:TRP:H	1.63	0.46
1:B:657:ALA:HA	1:B:660:GLN:HG3	1.98	0.46
1:C:142:HIS:HA	1:C:169:ALA:HB2	1.98	0.46
1:E:463:THR:HA	1:E:534:ILE:HD11	1.97	0.46
1:E:477:LYS:HE3	1:E:524:VAL:HG11	1.98	0.46
1:F:44:LYS:HB3	1:F:93:LEU:HB3	1.98	0.46
1:F:60:HIS:O	1:F:63:GLN:HB3	2.14	0.46
1:G:423:LEU:HA	1:G:426:VAL:CG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:452:MET:HE1	1:G:455:LEU:HD23	1.96	0.46
1:H:48:LEU:HA	1:H:87:ILE:CD1	2.45	0.46
1:H:143:ARG:HH21	1:H:143:ARG:HG2	1.81	0.46
1:H:537:LEU:O	1:H:541:ILE:HG13	2.15	0.46
1:I:445:PHE:CE2	1:I:551:ARG:HD2	2.51	0.46
1:J:537:LEU:O	1:J:541:ILE:HG13	2.16	0.46
1:J:586:MET:O	1:J:590:ILE:HG13	2.15	0.46
1:L:43:ILE:N	1:L:43:ILE:HD12	2.31	0.46
1:C:49:GLU:HA	1:C:88:HIS:HB2	1.98	0.46
1:C:267:LEU:HD12	1:C:312:ILE:HG23	1.97	0.46
1:E:192:LEU:H	1:E:192:LEU:HD12	1.81	0.46
1:F:141:ILE:CG2	1:F:170:LYS:HB2	2.46	0.46
1:F:396:GLY:HA2	1:F:398:PHE:CE2	2.50	0.46
1:G:29:VAL:HG22	1:G:44:LYS:CB	2.44	0.46
1:G:43:ILE:N	1:G:43:ILE:HD12	2.30	0.46
1:G:403:LEU:HD12	1:G:407:VAL:HG12	1.98	0.46
1:G:487:ILE:HG23	1:G:488:GLN:N	2.31	0.46
1:G:579:SER:HB3	1:K:577:ASP:N	2.28	0.46
1:H:74:VAL:O	1:H:74:VAL:HG13	2.15	0.46
1:I:396:GLY:HA2	1:I:398:PHE:CE2	2.50	0.46
1:I:420:ILE:HA	1:I:423:LEU:HB2	1.97	0.46
1:J:219:ARG:H	1:J:219:ARG:NE	2.14	0.46
1:K:363:ASP:OD1	1:K:365:ARG:HB2	2.15	0.46
1:A:249:SER:HB2	1:E:227:PRO:HG3	1.98	0.46
1:A:576:SER:OG	1:C:577:ASP:HA	2.15	0.46
1:B:117:LYS:O	1:B:121:ILE:HG13	2.16	0.46
1:B:201:THR:HA	1:B:204:TYR:CD1	2.51	0.46
1:C:48:LEU:O	1:C:50:LEU:HD12	2.16	0.46
1:C:205:TRP:HE3	1:C:287:ARG:HH12	1.62	0.46
1:D:274:ASN:HA	1:D:277:GLN:NE2	2.31	0.46
1:E:147:PRO:C	1:E:149:ASN:H	2.24	0.46
1:E:586:MET:O	1:E:590:ILE:HG13	2.16	0.46
1:F:487:ILE:HG12	1:F:515:GLU:HB2	1.98	0.46
1:F:592:HIS:CD2	2:Z:2:GLC:H2	2.51	0.46
1:G:13:GLY:H	1:G:14:PRO:HD3	1.81	0.46
1:G:143:ARG:C	1:G:145:LEU:H	2.24	0.46
1:G:320:SER:HA	1:G:398:PHE:HB3	1.97	0.46
1:H:27:GLY:O	1:H:45:SER:HB3	2.16	0.46
1:H:657:ALA:HA	1:H:660:GLN:HG3	1.98	0.46
1:I:21:LEU:HD23	1:I:29:VAL:C	2.41	0.46
1:I:143:ARG:CD	1:I:143:ARG:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:GLY:O	1:I:185:LEU:N	2.49	0.46
1:I:408:ASN:HA	1:I:411:VAL:HG22	1.97	0.46
1:J:192:LEU:HD12	1:J:192:LEU:N	2.31	0.46
1:K:151:VAL:C	1:K:152:LEU:HD22	2.41	0.46
1:K:268:ILE:C	1:K:271:PRO:HD2	2.40	0.46
1:A:182:VAL:HG12	1:A:183:GLY:N	2.28	0.46
1:A:201:THR:HA	1:A:204:TYR:CD1	2.51	0.46
1:A:323:ILE:N	1:A:323:ILE:HD12	2.31	0.46
1:A:633:LYS:HA	1:A:636:ASP:HB3	1.97	0.46
1:B:170:LYS:HG2	1:B:177:LEU:HG	1.98	0.46
1:B:222:LEU:HB2	1:B:230:TRP:CD1	2.51	0.46
1:B:408:ASN:HA	1:B:411:VAL:HG22	1.97	0.46
1:D:72:ASN:O	1:D:162:LYS:HA	2.16	0.46
1:F:51:SER:HB2	1:F:54:ASN:OD1	2.15	0.46
1:F:166:LEU:HD22	1:F:166:LEU:N	2.30	0.46
1:G:77:CYS:SG	1:G:78:ASP:N	2.88	0.46
1:G:192:LEU:N	1:G:192:LEU:HD12	2.31	0.46
1:G:192:LEU:HD12	1:G:192:LEU:H	1.80	0.46
1:G:323:ILE:HD12	1:G:323:ILE:N	2.31	0.46
1:G:537:LEU:O	1:G:541:ILE:HG13	2.16	0.46
1:H:201:THR:C	1:H:287:ARG:HH21	2.23	0.46
1:I:274:ASN:HA	1:I:277:GLN:NE2	2.31	0.46
1:I:401:ARG:HH21	1:I:440:ASP:HB2	1.80	0.46
1:J:477:LYS:HE3	1:J:524:VAL:HG11	1.97	0.46
1:J:635:ALA:HA	1:J:638:THR:OG1	2.16	0.46
1:K:268:ILE:O	1:K:272:MET:HB2	2.16	0.46
1:A:281:ASN:HB3	1:A:287:ARG:HG3	1.98	0.46
1:A:598:ASP:O	1:A:602:LYS:HG2	2.15	0.46
1:A:651:TRP:HZ2	1:B:490:ASP:HB3	1.81	0.46
1:B:51:SER:HB2	1:B:54:ASN:OD1	2.16	0.46
1:B:537:LEU:O	1:B:541:ILE:HG13	2.16	0.46
1:B:598:ASP:O	1:B:602:LYS:HG2	2.15	0.46
1:B:633:LYS:HA	1:B:636:ASP:HB3	1.98	0.46
1:C:274:ASN:HA	1:C:277:GLN:NE2	2.31	0.46
1:C:615:LYS:O	1:C:619:ILE:HG13	2.15	0.46
1:D:323:ILE:HD12	1:D:323:ILE:N	2.31	0.46
1:E:279:MET:O	1:E:287:ARG:HD2	2.15	0.46
1:F:80:PRO:HB3	1:F:92:LEU:H	1.80	0.46
1:F:147:PRO:C	1:F:149:ASN:H	2.23	0.46
1:G:219:ARG:HH12	1:G:224:HIS:N	2.14	0.46
1:G:420:ILE:HG21	1:G:578:HIS:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:408:ASN:HA	1:H:411:VAL:HG22	1.98	0.46
1:H:465:MET:HE3	1:H:625:VAL:HG21	1.97	0.46
1:H:480:LEU:HD22	1:H:518:ALA:HB1	1.97	0.46
1:H:549:TYR:H	1:H:552:ARG:HD2	1.80	0.46
1:I:420:ILE:HD11	1:I:571:LEU:HG	1.98	0.46
1:L:51:SER:HB2	1:L:54:ASN:OD1	2.16	0.46
1:L:615:LYS:O	1:L:619:ILE:HG13	2.16	0.46
1:A:268:ILE:C	1:A:271:PRO:HD2	2.41	0.46
1:B:27:GLY:O	1:B:45:SER:HB3	2.16	0.46
1:B:487:ILE:HG23	1:B:488:GLN:N	2.31	0.46
1:C:143:ARG:HG2	1:C:143:ARG:HH21	1.80	0.46
1:C:393:VAL:HG13	1:C:609:SER:OG	2.16	0.46
1:C:598:ASP:O	1:C:602:LYS:HG2	2.16	0.46
1:C:616:GLN:O	1:C:620:ASP:HB2	2.15	0.46
1:C:623:PRO:O	1:C:627:VAL:HG23	2.15	0.46
1:C:657:ALA:HA	1:C:660:GLN:HG3	1.98	0.46
1:D:44:LYS:HB3	1:D:93:LEU:HB3	1.98	0.46
1:D:359:GLY:HA3	1:D:453:LEU:HB2	1.98	0.46
1:E:44:LYS:HB3	1:E:93:LEU:HB3	1.98	0.46
1:E:465:MET:HB3	1:E:625:VAL:HG11	1.97	0.46
1:E:623:PRO:O	1:E:627:VAL:HG23	2.15	0.46
1:F:395:GLU:HG2	1:F:396:GLY:N	2.24	0.46
1:F:430:ALA:O	1:F:434:VAL:HG23	2.16	0.46
1:F:615:LYS:O	1:F:619:ILE:HG13	2.16	0.46
1:G:489:LEU:HD13	1:H:643:GLN:CG	2.45	0.46
1:G:598:ASP:O	1:G:602:LYS:HG2	2.16	0.46
1:H:141:ILE:HG13	1:H:203:ASP:CG	2.40	0.46
1:H:274:ASN:HA	1:H:277:GLN:NE2	2.31	0.46
1:I:143:ARG:HG2	1:I:143:ARG:HH21	1.80	0.46
1:I:403:LEU:HD12	1:I:407:VAL:HG12	1.98	0.46
1:I:427:TRP:CZ3	1:I:567:LEU:HB3	2.49	0.46
1:I:473:SER:HB2	1:I:524:VAL:HA	1.97	0.46
1:I:501:GLY:HA3	1:J:655:LYS:HE2	1.98	0.46
1:I:506:LYS:HE2	1:I:507:MET:HE3	1.98	0.46
1:K:466:LYS:HD3	1:K:534:ILE:HG21	1.98	0.46
1:K:537:LEU:O	1:K:541:ILE:HG13	2.15	0.46
1:L:212:PHE:CD2	1:L:220:PRO:HA	2.51	0.46
1:A:84:ASN:CG	1:A:85:ILE:N	2.74	0.45
1:A:295:LEU:C	1:A:297:GLN:H	2.24	0.45
1:A:616:GLN:O	1:A:620:ASP:HB2	2.16	0.45
1:B:142:HIS:HA	1:B:169:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:H	1:B:293:LEU:HD22	1.80	0.45
1:B:542:MET:HE2	1:B:545:GLN:HE22	1.81	0.45
1:C:51:SER:HB2	1:C:54:ASN:OD1	2.15	0.45
1:C:408:ASN:HA	1:C:411:VAL:HG22	1.97	0.45
1:D:408:ASN:HA	1:D:411:VAL:HG22	1.98	0.45
1:E:140:ILE:HG12	1:E:171:ASP:OD2	2.15	0.45
1:E:615:LYS:O	1:E:619:ILE:HG13	2.15	0.45
1:E:653:LEU:HG	1:E:656:ILE:HD11	1.97	0.45
1:F:420:ILE:HA	1:F:423:LEU:HB2	1.97	0.45
1:G:616:GLN:O	1:G:620:ASP:HB2	2.16	0.45
1:H:21:LEU:HD23	1:H:29:VAL:C	2.40	0.45
1:H:26:PHE:HA	1:L:408:ASN:ND2	2.31	0.45
1:H:139:LYS:HB3	1:H:172:VAL:HG11	1.97	0.45
1:H:220:PRO:O	1:H:243:PHE:HA	2.17	0.45
1:H:408:ASN:HD21	1:J:26:PHE:HA	1.78	0.45
1:I:21:LEU:HD12	4:I:701:5TL:CAL	2.46	0.45
1:I:227:PRO:HA	1:I:230:TRP:CB	2.46	0.45
1:I:598:ASP:O	1:I:602:LYS:HG2	2.16	0.45
1:J:71:ALA:C	1:J:73:VAL:H	2.24	0.45
1:J:170:LYS:HZ1	1:J:192:LEU:HD11	1.81	0.45
1:J:267:LEU:HD13	1:J:327:LEU:HB2	1.98	0.45
1:K:147:PRO:C	1:K:149:ASN:H	2.24	0.45
1:K:149:ASN:O	1:K:164:ILE:HG22	2.16	0.45
1:K:190:PRO:HA	1:K:193:PHE:CD1	2.52	0.45
1:L:65:MET:HB3	1:L:76:ALA:CB	2.41	0.45
1:L:147:PRO:C	1:L:149:ASN:H	2.23	0.45
1:L:420:ILE:HA	1:L:423:LEU:HB2	1.97	0.45
1:A:651:TRP:CZ2	1:B:490:ASP:HB3	2.51	0.45
1:D:8:GLU:O	1:D:9:PHE:HB2	2.16	0.45
1:D:209:THR:N	1:D:280:LEU:HD21	2.32	0.45
1:D:430:ALA:O	1:D:434:VAL:HG23	2.16	0.45
1:D:586:MET:O	1:D:590:ILE:HG13	2.16	0.45
1:E:452:MET:O	1:E:456:LEU:HG	2.16	0.45
1:E:587:VAL:HA	1:E:590:ILE:HD12	1.98	0.45
1:E:621:LEU:O	1:E:625:VAL:HG23	2.16	0.45
1:F:427:TRP:CZ2	1:F:583:SER:HA	2.51	0.45
1:G:219:ARG:HH12	1:G:224:HIS:HA	1.81	0.45
1:G:237:LYS:CE	1:G:282:TRP:H	2.29	0.45
1:G:268:ILE:C	1:G:271:PRO:HD2	2.41	0.45
1:G:586:MET:O	1:G:590:ILE:HG13	2.15	0.45
1:G:635:ALA:HA	1:G:638:THR:OG1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:GLU:O	1:H:277:GLN:HG3	2.16	0.45
1:H:317:ASN:ND2	1:H:319:THR:HG23	2.32	0.45
1:I:466:LYS:HD3	1:I:534:ILE:HD13	1.98	0.45
1:J:48:LEU:O	1:J:50:LEU:HD12	2.16	0.45
1:L:185:LEU:HD11	1:L:188:LEU:CB	2.30	0.45
1:L:238:ASP:CB	1:L:239:PRO:HD2	2.46	0.45
1:L:537:LEU:O	1:L:541:ILE:HG13	2.15	0.45
1:A:487:ILE:HG23	1:A:488:GLN:N	2.31	0.45
1:A:579:SER:HB2	1:E:578:HIS:ND1	2.31	0.45
1:B:37:LEU:HB3	1:B:38:ASP:H	1.67	0.45
1:B:423:LEU:HA	1:B:426:VAL:CG2	2.42	0.45
1:C:43:ILE:HD12	1:C:43:ILE:N	2.31	0.45
1:C:292:ASP:O	1:C:296:LYS:HA	2.17	0.45
1:D:147:PRO:C	1:D:149:ASN:H	2.23	0.45
1:D:283:ASP:OD2	1:D:284:PRO:HD2	2.17	0.45
1:D:537:LEU:O	1:D:541:ILE:HG13	2.17	0.45
1:E:144:ASP:OD1	1:E:182:VAL:HG11	2.16	0.45
1:F:101:GLY:HA2	4:F:701:5TL:CAR	2.46	0.45
1:F:143:ARG:HG2	1:F:143:ARG:HH21	1.81	0.45
1:G:149:ASN:O	1:G:164:ILE:HG22	2.16	0.45
1:H:29:VAL:HG21	4:H:701:5TL:CAF	2.47	0.45
1:H:586:MET:O	1:H:590:ILE:HG13	2.16	0.45
1:H:587:VAL:HA	1:H:590:ILE:HD12	1.98	0.45
1:I:83:LEU:HB3	1:I:84:ASN:H	1.59	0.45
1:I:268:ILE:O	1:I:272:MET:HB2	2.16	0.45
1:I:550:GLY:C	1:I:552:ARG:H	2.25	0.45
1:J:273:GLU:O	1:J:277:GLN:HG3	2.17	0.45
1:J:423:LEU:HA	1:J:426:VAL:CG2	2.42	0.45
1:K:502:ILE:HD12	1:L:654:LEU:CD1	2.41	0.45
1:K:506:LYS:HE2	1:K:507:MET:HE3	1.98	0.45
1:L:411:VAL:HG12	1:L:590:ILE:HG21	1.97	0.45
1:L:430:ALA:O	1:L:434:VAL:HG23	2.16	0.45
1:L:657:ALA:HA	1:L:660:GLN:HG3	1.98	0.45
1:A:21:LEU:HD23	1:A:29:VAL:C	2.41	0.45
1:A:27:GLY:HA2	1:C:412:GLN:NE2	2.31	0.45
1:A:587:VAL:HA	1:A:590:ILE:HD12	1.97	0.45
1:B:143:ARG:H	1:B:143:ARG:CD	2.30	0.45
1:B:324:ILE:HD12	1:B:324:ILE:N	2.30	0.45
1:C:166:LEU:N	1:C:166:LEU:HD22	2.32	0.45
1:C:410:ILE:O	1:C:587:VAL:HG22	2.16	0.45
1:D:237:LYS:CG	1:D:241:CYS:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ILE:HD13	1:E:264:LEU:HD11	1.97	0.45
1:E:616:GLN:O	1:E:620:ASP:HB2	2.16	0.45
1:F:141:ILE:HG13	1:F:203:ASP:CG	2.41	0.45
1:F:238:ASP:CB	1:F:239:PRO:HD2	2.45	0.45
1:F:633:LYS:HA	1:F:636:ASP:HB3	1.97	0.45
1:G:222:LEU:HD12	1:G:244:ALA:O	2.16	0.45
1:G:417:GLN:HB3	1:G:581:SER:HB3	1.98	0.45
1:H:212:PHE:CE2	1:H:220:PRO:HA	2.52	0.45
1:H:563:ARG:HH12	2:d:2:GLC:H2	1.80	0.45
1:H:616:GLN:O	1:H:620:ASP:HB2	2.17	0.45
1:I:230:TRP:O	1:I:234:ILE:HG12	2.16	0.45
1:I:392:THR:O	1:I:612:LEU:HD23	2.17	0.45
1:J:37:LEU:HB3	1:J:38:ASP:H	1.67	0.45
1:J:240:LYS:HD3	1:J:281:ASN:OD1	2.17	0.45
1:K:445:PHE:HA	1:K:604:LEU:HD21	1.98	0.45
1:K:633:LYS:HA	1:K:636:ASP:HB3	1.98	0.45
1:K:657:ALA:HA	1:K:660:GLN:HG3	1.99	0.45
1:L:141:ILE:HG13	1:L:203:ASP:CG	2.41	0.45
1:L:459:ASN:HD21	1:L:538:HIS:CD2	2.34	0.45
1:A:540:GLU:O	1:A:544:LEU:HG	2.16	0.45
1:A:621:LEU:O	1:A:625:VAL:HG23	2.17	0.45
1:B:34:HIS:CE1	1:B:37:LEU:HD23	2.52	0.45
1:B:373:LEU:N	1:B:373:LEU:HD22	2.31	0.45
1:B:420:ILE:HD11	1:B:571:LEU:HG	1.98	0.45
1:D:143:ARG:HG2	1:D:143:ARG:HH21	1.81	0.45
1:D:548:PRO:CB	1:D:552:ARG:HG3	2.46	0.45
1:G:231:HIS:O	1:G:235:LYS:N	2.49	0.45
1:G:587:VAL:HA	1:G:590:ILE:HD12	1.97	0.45
1:I:68:LEU:HD21	1:I:140:ILE:HD12	1.98	0.45
1:I:85:ILE:C	1:I:86:LEU:HD22	2.41	0.45
1:J:279:MET:O	1:J:287:ARG:HD2	2.16	0.45
1:K:273:GLU:O	1:K:277:GLN:HG3	2.17	0.45
1:K:551:ARG:HG2	1:K:551:ARG:O	2.17	0.45
1:L:27:GLY:O	1:L:45:SER:HB3	2.17	0.45
1:L:212:PHE:CE2	1:L:220:PRO:HA	2.52	0.45
1:L:427:TRP:HZ2	1:L:583:SER:HA	1.81	0.45
1:L:616:GLN:O	1:L:620:ASP:HB2	2.16	0.45
1:A:74:VAL:HG11	1:A:164:ILE:HA	1.98	0.45
1:A:354:LEU:HB3	1:A:384:VAL:HG11	1.99	0.45
1:A:373:LEU:HD22	1:A:373:LEU:N	2.32	0.45
1:A:408:ASN:HA	1:A:411:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ALA:HA	1:A:660:GLN:HG3	1.99	0.45
1:C:107:LEU:HD23	1:C:116:LEU:HD11	1.99	0.45
1:E:87:ILE:O	1:E:88:HIS:HB3	2.16	0.45
1:G:657:ALA:HA	1:G:660:GLN:HG3	1.99	0.45
1:H:34:HIS:CE1	1:H:37:LEU:HD23	2.52	0.45
1:H:79:VAL:CG1	1:H:83:LEU:HD11	2.46	0.45
1:H:185:LEU:HB3	1:L:249:SER:HB3	1.99	0.45
1:H:549:TYR:HB2	1:H:552:ARG:CZ	2.47	0.45
1:H:560:LEU:O	1:H:563:ARG:HB2	2.16	0.45
1:I:395:GLU:HG2	1:I:396:GLY:N	2.31	0.45
1:J:314:HIS:ND1	1:J:380:ASP:HA	2.32	0.45
1:J:412:GLN:NE2	1:L:27:GLY:HA2	2.32	0.45
1:K:21:LEU:HD23	1:K:29:VAL:C	2.41	0.45
1:K:115:GLY:HA3	1:K:215:ILE:O	2.15	0.45
1:K:403:LEU:HD12	1:K:407:VAL:HG12	1.99	0.45
1:K:615:LYS:O	1:K:619:ILE:HG13	2.16	0.45
1:L:21:LEU:HD23	1:L:29:VAL:C	2.42	0.45
1:L:275:TRP:HZ2	1:L:304:MET:HE2	1.81	0.45
1:A:190:PRO:HA	1:A:193:PHE:CD1	2.52	0.45
1:A:615:LYS:O	1:A:619:ILE:HG13	2.16	0.45
1:B:415:LYS:HD3	1:B:584:THR:HG21	1.98	0.45
1:C:268:ILE:O	1:C:272:MET:HB2	2.16	0.45
1:C:430:ALA:O	1:C:434:VAL:HG23	2.16	0.45
1:D:70:HIS:C	1:D:72:ASN:H	2.24	0.45
1:D:404:SER:HB2	1:D:406:CYS:SG	2.56	0.45
1:D:477:LYS:HE3	1:D:524:VAL:HG11	1.98	0.45
1:D:544:LEU:HD21	1:D:610:LYS:CD	2.46	0.45
1:E:151:VAL:C	1:E:152:LEU:HD22	2.42	0.45
1:E:506:LYS:HE2	1:E:507:MET:HE3	1.99	0.45
1:E:537:LEU:O	1:E:541:ILE:HG13	2.15	0.45
1:F:8:GLU:HB2	1:F:45:SER:OG	2.16	0.45
1:F:657:ALA:HA	1:F:660:GLN:HG3	1.99	0.45
1:G:142:HIS:HA	1:G:169:ALA:CB	2.46	0.45
1:G:220:PRO:HG2	1:G:221:PHE:CD2	2.52	0.45
1:G:236:LYS:HG2	1:G:237:LYS:H	1.82	0.45
1:G:408:ASN:HD21	1:K:26:PHE:HD1	1.63	0.45
1:H:323:ILE:HD12	1:H:323:ILE:N	2.32	0.45
1:I:48:LEU:O	1:I:50:LEU:HD12	2.16	0.45
1:I:65:MET:SD	1:I:166:LEU:HD23	2.56	0.45
1:I:275:TRP:CH2	1:I:279:MET:HG3	2.52	0.45
1:L:89:ASP:O	1:L:90:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:460:ALA:O	1:L:464:LYS:HG3	2.16	0.45
1:L:560:LEU:HB3	1:L:593:THR:HG22	1.97	0.45
1:L:587:VAL:HA	1:L:590:ILE:HD12	1.98	0.45
1:L:589:ILE:O	1:L:593:THR:HG23	2.16	0.45
1:A:430:ALA:O	1:A:434:VAL:HG23	2.16	0.45
1:A:459:ASN:HD21	1:A:538:HIS:CD2	2.34	0.45
1:A:537:LEU:O	1:A:541:ILE:HG13	2.16	0.45
1:B:27:GLY:HA2	1:F:412:GLN:CD	2.42	0.45
1:B:367:PRO:C	1:B:369:SER:H	2.24	0.45
1:B:506:LYS:HE2	1:B:507:MET:HE3	1.98	0.45
1:C:50:LEU:HD22	1:C:90:VAL:HG11	1.99	0.45
1:C:57:ARG:O	1:C:60:HIS:HB3	2.17	0.45
1:C:89:ASP:O	1:C:90:VAL:HG13	2.17	0.45
1:C:147:PRO:C	1:C:149:ASN:H	2.23	0.45
1:C:323:ILE:N	1:C:323:ILE:HD12	2.31	0.45
1:D:37:LEU:HB3	1:D:38:ASP:H	1.67	0.45
1:E:657:ALA:HA	1:E:660:GLN:HG3	1.99	0.45
1:F:72:ASN:O	1:F:162:LYS:HA	2.17	0.45
1:G:143:ARG:H	1:G:143:ARG:CD	2.30	0.45
1:G:236:LYS:HG2	1:G:237:LYS:N	2.32	0.45
1:H:420:ILE:HG12	1:H:577:ASP:HB3	1.98	0.45
1:I:147:PRO:C	1:I:149:ASN:H	2.23	0.45
1:I:487:ILE:HG23	1:I:488:GLN:N	2.32	0.45
1:J:77:CYS:SG	1:J:78:ASP:N	2.90	0.45
1:J:141:ILE:HG13	1:J:203:ASP:CG	2.42	0.45
1:J:147:PRO:C	1:J:149:ASN:H	2.24	0.45
1:L:143:ARG:HG2	1:L:143:ARG:HH21	1.81	0.45
1:L:273:GLU:O	1:L:277:GLN:HG3	2.17	0.45
3:T:3:5TM:C1	3:T:3:5TM:O6	2.65	0.45
1:A:141:ILE:HG13	1:A:203:ASP:CG	2.42	0.45
1:A:143:ARG:C	1:A:145:LEU:H	2.25	0.45
1:A:404:SER:HB2	1:A:406:CYS:SG	2.56	0.45
1:A:647:GLN:OE1	1:B:489:LEU:HD22	2.17	0.45
1:B:43:ILE:N	1:B:43:ILE:HD12	2.31	0.45
1:C:26:PHE:HD2	1:C:47:ARG:HA	1.81	0.45
1:C:68:LEU:HD21	1:C:140:ILE:HD12	1.99	0.45
1:C:143:ARG:CD	1:C:143:ARG:H	2.30	0.45
1:C:223:HIS:O	1:C:224:HIS:HB3	2.16	0.45
1:C:549:TYR:H	1:C:552:ARG:HD2	1.82	0.45
1:D:143:ARG:H	1:D:143:ARG:CD	2.30	0.45
1:D:514:MET:SD	1:D:645:LYS:HD3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:GLU:O	1:D:565:ILE:HG13	2.16	0.45
1:E:85:ILE:HD12	1:E:89:ASP:HA	1.98	0.45
1:E:143:ARG:H	1:E:143:ARG:CD	2.30	0.45
1:E:236:LYS:O	1:E:237:LYS:C	2.59	0.45
1:F:27:GLY:O	1:F:45:SER:HB3	2.17	0.45
1:F:229:THR:C	1:F:231:HIS:H	2.25	0.45
1:F:273:GLU:O	1:F:277:GLN:HG3	2.17	0.45
1:F:408:ASN:HA	1:F:411:VAL:HG22	1.97	0.45
1:G:370:GLN:HE21	1:G:370:GLN:HB2	1.52	0.45
1:G:427:TRP:HZ2	1:G:583:SER:HA	1.81	0.45
1:H:72:ASN:ND2	1:H:127:ASP:O	2.50	0.45
1:H:370:GLN:HE21	1:H:370:GLN:HB2	1.61	0.45
1:H:473:SER:CB	1:H:527:ILE:HD11	2.47	0.45
1:I:268:ILE:C	1:I:271:PRO:HD2	2.42	0.45
1:J:430:ALA:O	1:J:434:VAL:HG23	2.17	0.45
1:J:497:GLN:HA	1:J:500:TYR:HD2	1.82	0.45
1:J:560:LEU:HB3	1:J:593:THR:HG22	1.98	0.45
1:J:561:GLU:O	1:J:565:ILE:HG13	2.17	0.45
1:K:65:MET:SD	1:K:166:LEU:HD23	2.57	0.45
1:K:192:LEU:HD12	1:K:192:LEU:N	2.31	0.45
1:K:238:ASP:OD2	1:K:239:PRO:HD2	2.16	0.45
1:K:274:ASN:HA	1:K:277:GLN:NE2	2.31	0.45
1:A:143:ARG:CD	1:A:143:ARG:H	2.30	0.45
1:A:506:LYS:HE2	1:A:507:MET:HE3	1.99	0.45
1:B:273:GLU:O	1:B:277:GLN:HG3	2.17	0.45
1:C:141:ILE:HG13	1:C:203:ASP:CG	2.42	0.45
1:C:452:MET:O	1:C:456:LEU:HG	2.16	0.45
1:D:126:SER:HB2	1:D:308:LEU:CD1	2.47	0.45
1:D:420:ILE:HA	1:D:423:LEU:HB2	1.98	0.45
1:E:237:LYS:CE	1:E:282:TRP:H	2.24	0.45
1:F:560:LEU:HB3	1:F:593:THR:HG22	1.98	0.45
1:F:616:GLN:O	1:F:620:ASP:HB2	2.17	0.45
1:G:9:PHE:HZ	1:G:17:MET:HG2	1.82	0.45
1:G:141:ILE:HG13	1:G:203:ASP:CG	2.42	0.45
1:H:452:MET:HE1	1:H:455:LEU:HD23	1.99	0.45
1:I:29:VAL:HG21	4:I:701:5TL:CAE	2.47	0.45
1:J:323:ILE:HD12	1:J:323:ILE:N	2.32	0.45
1:L:232:GLU:C	1:L:234:ILE:H	2.25	0.45
1:A:274:ASN:HA	1:A:277:GLN:NE2	2.32	0.44
1:A:373:LEU:HD21	1:A:382:TYR:HB3	1.98	0.44
1:A:420:ILE:HG21	1:A:578:HIS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LEU:HB2	1:B:230:TRP:HE1	1.81	0.44
1:D:222:LEU:HD23	1:D:230:TRP:HE1	1.81	0.44
1:F:140:ILE:HG12	1:F:171:ASP:OD2	2.16	0.44
1:F:275:TRP:CH2	1:F:279:MET:HG3	2.52	0.44
1:F:506:LYS:HE2	1:F:507:MET:HE3	1.98	0.44
1:G:21:LEU:HD23	1:G:29:VAL:C	2.42	0.44
1:H:149:ASN:O	1:H:164:ILE:HG22	2.18	0.44
1:H:506:LYS:HE2	1:H:507:MET:HE3	1.98	0.44
1:H:653:LEU:HG	1:H:656:ILE:HD11	1.98	0.44
1:I:324:ILE:HD12	1:I:324:ILE:N	2.31	0.44
1:J:541:ILE:CD1	1:J:618:ILE:HD11	2.47	0.44
1:K:34:HIS:CE1	1:K:37:LEU:HD23	2.52	0.44
1:K:222:LEU:HD13	1:K:244:ALA:O	2.17	0.44
1:K:635:ALA:HA	1:K:638:THR:OG1	2.16	0.44
1:L:143:ARG:HD2	1:L:170:LYS:HE3	1.99	0.44
1:L:274:ASN:HA	1:L:277:GLN:NE2	2.32	0.44
1:L:423:LEU:O	1:L:427:TRP:HB2	2.17	0.44
1:A:8:GLU:O	1:A:9:PHE:HB2	2.17	0.44
1:A:13:GLY:N	1:A:14:PRO:CD	2.76	0.44
1:A:249:SER:HB2	1:E:227:PRO:CG	2.47	0.44
1:A:317:ASN:ND2	1:A:319:THR:HG23	2.33	0.44
1:C:231:HIS:C	1:C:233:LYS:H	2.26	0.44
1:C:541:ILE:HD11	1:C:618:ILE:HD11	2.00	0.44
1:C:587:VAL:HA	1:C:590:ILE:HD12	1.98	0.44
1:D:185:LEU:HD13	1:D:186:GLN:N	2.32	0.44
1:D:502:ILE:HD13	1:D:656:ILE:HD12	1.99	0.44
1:E:268:ILE:O	1:E:272:MET:HB2	2.17	0.44
1:E:316:LEU:HB2	1:E:383:MET:CE	2.36	0.44
1:E:417:GLN:HB3	1:E:581:SER:CB	2.46	0.44
1:G:87:ILE:HG22	1:G:88:HIS:N	2.33	0.44
1:G:151:VAL:C	1:G:152:LEU:HD22	2.42	0.44
1:G:314:HIS:HB2	1:G:383:MET:HB2	1.98	0.44
1:G:334:LEU:HD22	1:G:366:LYS:O	2.17	0.44
1:I:151:VAL:C	1:I:152:LEU:HD22	2.43	0.44
1:I:452:MET:O	1:I:456:LEU:HG	2.16	0.44
1:J:311:LYS:O	1:J:372:VAL:HG11	2.17	0.44
1:J:366:LYS:CE	1:J:367:PRO:HD2	2.46	0.44
1:K:143:ARG:CD	1:K:143:ARG:H	2.30	0.44
1:K:430:ALA:O	1:K:434:VAL:HG23	2.16	0.44
1:L:218:TYR:HB2	1:L:223:HIS:ND1	2.32	0.44
1:A:268:ILE:O	1:A:272:MET:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:HIS:HB2	1:A:383:MET:HB3	1.99	0.44
1:A:410:ILE:HD12	1:A:583:SER:OG	2.17	0.44
1:B:166:LEU:HD22	1:B:166:LEU:N	2.31	0.44
1:B:616:GLN:O	1:B:620:ASP:HB2	2.18	0.44
1:C:487:ILE:HG23	1:C:488:GLN:N	2.32	0.44
1:D:141:ILE:HG13	1:D:203:ASP:CG	2.42	0.44
1:D:395:GLU:OE2	1:D:397:PRO:HG3	2.17	0.44
1:E:34:HIS:CE1	1:E:37:LEU:HD23	2.52	0.44
1:E:141:ILE:HG13	1:E:203:ASP:CG	2.42	0.44
1:E:190:PRO:HA	1:E:193:PHE:CD1	2.53	0.44
1:F:537:LEU:O	1:F:541:ILE:HG13	2.16	0.44
1:G:190:PRO:HA	1:G:193:PHE:CD1	2.52	0.44
1:H:462:LEU:HD22	1:H:618:ILE:HG23	1.99	0.44
1:H:598:ASP:O	1:H:602:LYS:HG2	2.17	0.44
1:I:34:HIS:CE1	1:I:37:LEU:HD23	2.52	0.44
1:I:452:MET:SD	1:I:611:LEU:HD22	2.57	0.44
1:I:592:HIS:CD2	2:h:2:GLC:H2	2.52	0.44
1:J:143:ARG:HH21	1:J:143:ARG:HG2	1.82	0.44
1:J:274:ASN:HA	1:J:277:GLN:NE2	2.33	0.44
1:J:411:VAL:HG12	1:J:590:ILE:HG21	1.99	0.44
1:J:514:MET:HA	1:J:642:MET:HE1	1.98	0.44
1:K:35:ARG:HG3	1:K:36:GLU:HG3	2.00	0.44
1:K:427:TRP:CZ3	1:K:567:LEU:HB3	2.49	0.44
1:K:616:GLN:O	1:K:620:ASP:HB2	2.17	0.44
1:K:621:LEU:O	1:K:625:VAL:HG23	2.17	0.44
1:L:483:PHE:HZ	1:L:514:MET:HB3	1.81	0.44
1:A:333:SER:C	1:A:368:ALA:HB2	2.42	0.44
1:A:635:ALA:HA	1:A:638:THR:OG1	2.16	0.44
1:B:404:SER:HB2	1:B:406:CYS:SG	2.57	0.44
1:C:151:VAL:C	1:C:152:LEU:HD22	2.43	0.44
1:C:427:TRP:HZ2	1:C:583:SER:HA	1.82	0.44
1:D:396:GLY:N	1:D:397:PRO:CD	2.79	0.44
1:E:199:THR:HG21	1:E:285:GLN:NE2	2.32	0.44
1:E:387:PHE:CZ	1:E:451:ALA:HB2	2.52	0.44
1:F:487:ILE:HG23	1:F:488:GLN:N	2.32	0.44
1:F:498:MET:HA	1:F:503:SER:HB2	1.99	0.44
1:F:587:VAL:HA	1:F:590:ILE:HD12	1.99	0.44
1:G:180:GLU:CB	1:G:192:LEU:HD23	2.46	0.44
1:H:143:ARG:H	1:H:143:ARG:CD	2.30	0.44
1:H:334:LEU:HD11	1:H:364:PRO:HA	1.99	0.44
1:H:354:LEU:HB3	1:H:384:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:473:SER:HB3	1:H:527:ILE:HD11	2.00	0.44
1:I:621:LEU:O	1:I:625:VAL:HG23	2.18	0.44
1:J:383:MET:HG2	1:J:385:TYR:CE1	2.53	0.44
1:K:323:ILE:N	1:K:323:ILE:HD12	2.32	0.44
1:K:487:ILE:CD1	1:K:514:MET:HE3	2.47	0.44
1:L:14:PRO:HG2	1:L:81:GLU:HG2	1.99	0.44
1:L:166:LEU:HD22	1:L:166:LEU:N	2.32	0.44
1:L:494:TYR:HE2	1:L:508:LEU:HD13	1.83	0.44
1:A:290:PRO:HB2	1:A:299:ARG:HB2	1.99	0.44
1:B:268:ILE:C	1:B:271:PRO:HD2	2.42	0.44
1:C:29:VAL:HG21	4:C:701:5TL:CAF	2.47	0.44
1:C:401:ARG:HH21	1:C:436:GLY:C	2.25	0.44
1:D:48:LEU:O	1:D:50:LEU:HD12	2.18	0.44
1:D:65:MET:SD	1:D:166:LEU:HD23	2.57	0.44
1:D:381:SER:O	1:D:383:MET:N	2.51	0.44
1:D:587:VAL:HA	1:D:590:ILE:HD12	1.99	0.44
1:D:616:GLN:O	1:D:620:ASP:HB2	2.17	0.44
1:E:149:ASN:O	1:E:164:ILE:HG22	2.17	0.44
1:E:152:LEU:HD13	1:E:161:HIS:HA	1.99	0.44
1:E:541:ILE:HD11	1:E:618:ILE:HD11	2.00	0.44
1:E:561:GLU:O	1:E:565:ILE:HG13	2.17	0.44
1:F:231:HIS:O	1:F:235:LYS:N	2.51	0.44
1:F:323:ILE:N	1:F:323:ILE:HD12	2.32	0.44
1:F:404:SER:HB2	1:F:406:CYS:SG	2.58	0.44
1:F:445:PHE:CD1	1:F:551:ARG:HB2	2.53	0.44
1:G:74:VAL:CG2	1:G:95:MET:HE3	2.48	0.44
1:G:116:LEU:HD12	1:G:116:LEU:N	2.30	0.44
1:G:191:GLU:CD	1:G:284:PRO:HB3	2.43	0.44
1:G:403:LEU:HD23	1:G:403:LEU:N	2.33	0.44
1:H:275:TRP:CH2	1:H:279:MET:HG3	2.53	0.44
1:H:319:THR:HG22	1:H:394:TYR:CE1	2.52	0.44
1:H:423:LEU:HA	1:H:426:VAL:CG2	2.43	0.44
1:I:51:SER:HB2	1:I:54:ASN:OD1	2.16	0.44
1:I:142:HIS:ND1	1:I:169:ALA:HB2	2.33	0.44
1:I:212:PHE:CD2	1:I:220:PRO:HA	2.52	0.44
1:J:288:GLY:HA3	1:J:300:CYS:SG	2.57	0.44
1:J:318:MET:HE2	1:J:447:GLY:HA3	2.00	0.44
1:K:44:LYS:HB3	1:K:93:LEU:HB3	1.99	0.44
1:K:143:ARG:C	1:K:145:LEU:H	2.26	0.44
1:K:497:GLN:HE22	1:L:654:LEU:HD21	1.81	0.44
1:K:561:GLU:O	1:K:565:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:26:PHE:HD2	1:L:47:ARG:HA	1.83	0.44
1:L:235:LYS:HA	1:L:282:TRP:CH2	2.53	0.44
1:L:393:VAL:HG13	1:L:609:SER:OG	2.18	0.44
1:A:417:GLN:HB3	1:A:581:SER:HB3	1.99	0.44
1:A:423:LEU:HA	1:A:426:VAL:CG2	2.43	0.44
1:B:48:LEU:O	1:B:50:LEU:HD12	2.17	0.44
1:B:149:ASN:O	1:B:164:ILE:HG22	2.18	0.44
1:B:423:LEU:O	1:B:427:TRP:HB2	2.16	0.44
1:C:117:LYS:HD3	1:C:117:LYS:HA	1.85	0.44
1:C:318:MET:HE1	1:C:444:LEU:O	2.17	0.44
1:D:26:PHE:HD2	1:D:47:ARG:HA	1.83	0.44
1:D:43:ILE:N	1:D:43:ILE:HD12	2.32	0.44
1:D:112:ASN:CB	1:D:116:LEU:HD23	2.48	0.44
1:D:209:THR:CG2	1:D:220:PRO:HG3	2.42	0.44
1:D:423:LEU:O	1:D:427:TRP:HB2	2.18	0.44
1:D:560:LEU:HB3	1:D:593:THR:HG22	1.99	0.44
1:E:487:ILE:HG23	1:E:488:GLN:N	2.32	0.44
1:F:77:CYS:SG	1:F:94:ALA:HB3	2.58	0.44
1:G:563:ARG:HH12	2:b:2:GLC:H2	1.82	0.44
1:I:616:GLN:O	1:I:620:ASP:HB2	2.17	0.44
1:J:34:HIS:CE1	1:J:37:LEU:HD23	2.53	0.44
1:J:404:SER:HB2	1:J:406:CYS:SG	2.57	0.44
1:J:424:ARG:HD3	1:J:572:LYS:HE2	1.99	0.44
1:J:616:GLN:O	1:J:620:ASP:HB2	2.18	0.44
1:K:396:GLY:HA2	1:K:398:PHE:CZ	2.52	0.44
1:L:541:ILE:CD1	1:L:618:ILE:HD11	2.48	0.44
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.48	0.44
1:B:141:ILE:HG13	1:B:203:ASP:CG	2.42	0.44
1:C:149:ASN:O	1:C:164:ILE:HG22	2.18	0.44
1:C:298:PRO:O	1:C:302:VAL:HG23	2.17	0.44
1:D:273:GLU:O	1:D:277:GLN:HG3	2.18	0.44
1:D:487:ILE:HG23	1:D:488:GLN:N	2.31	0.44
1:F:236:LYS:HB2	1:F:236:LYS:NZ	2.32	0.44
1:F:274:ASN:HA	1:F:277:GLN:NE2	2.33	0.44
1:H:561:GLU:O	1:H:565:ILE:HG13	2.17	0.44
1:I:238:ASP:HB3	1:I:239:PRO:HD2	1.99	0.44
1:I:283:ASP:OD1	1:I:285:GLN:HB2	2.18	0.44
1:I:613:GLY:O	1:I:617:LYS:HG3	2.17	0.44
1:J:43:ILE:N	1:J:43:ILE:HD12	2.32	0.44
1:J:473:SER:OG	1:J:524:VAL:HG13	2.18	0.44
1:J:621:LEU:O	1:J:625:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:653:LEU:HG	1:K:656:ILE:HD11	1.98	0.44
1:L:116:LEU:O	1:L:121:ILE:HD11	2.17	0.44
1:L:219:ARG:HB2	1:L:223:HIS:HB3	1.99	0.44
1:L:473:SER:HB3	1:L:632:ILE:HD13	1.98	0.44
1:L:633:LYS:HA	1:L:636:ASP:HB3	1.98	0.44
1:A:237:LYS:CD	1:A:241:CYS:HB3	2.48	0.44
1:A:283:ASP:HB3	1:A:286:GLN:HB3	2.00	0.44
1:A:507:MET:HB3	1:A:511:TRP:CD1	2.53	0.44
1:A:507:MET:CE	1:A:653:LEU:HD22	2.47	0.44
1:C:395:GLU:HG2	1:C:396:GLY:H	1.83	0.44
1:D:149:ASN:O	1:D:164:ILE:HG22	2.18	0.44
1:E:423:LEU:O	1:E:427:TRP:HB2	2.18	0.44
1:E:459:ASN:HD21	1:E:538:HIS:CD2	2.36	0.44
1:E:598:ASP:O	1:E:602:LYS:HG2	2.18	0.44
1:F:26:PHE:HD2	1:F:47:ARG:HA	1.83	0.44
1:F:320:SER:CA	1:F:398:PHE:HB3	2.47	0.44
1:F:328:LEU:HD21	1:F:337:LEU:HD22	2.00	0.44
1:F:393:VAL:HG13	1:F:609:SER:OG	2.18	0.44
1:G:117:LYS:HE2	1:G:117:LYS:N	2.33	0.44
1:G:185:LEU:HD21	1:G:188:LEU:CB	2.48	0.44
1:G:317:ASN:ND2	1:G:319:THR:HG23	2.33	0.44
1:G:469:LEU:HD11	1:G:628:ALA:HB3	1.99	0.44
1:G:615:LYS:O	1:G:619:ILE:HG13	2.17	0.44
1:G:633:LYS:HA	1:G:636:ASP:HB3	1.98	0.44
1:H:177:LEU:HD11	1:H:198:TYR:OH	2.18	0.44
1:H:186:GLN:HG2	1:H:219:ARG:NH1	2.33	0.44
1:H:238:ASP:HB3	1:H:239:PRO:CD	2.43	0.44
1:H:404:SER:HB2	1:H:406:CYS:SG	2.58	0.44
1:J:21:LEU:HD23	1:J:29:VAL:C	2.43	0.44
1:J:393:VAL:HG13	1:J:609:SER:OG	2.18	0.44
1:J:408:ASN:CG	1:L:26:PHE:HA	2.42	0.44
1:K:74:VAL:HB	1:K:164:ILE:HG13	2.00	0.44
1:K:118:GLU:HA	1:K:121:ILE:HD12	2.00	0.44
1:K:404:SER:HB2	1:K:406:CYS:SG	2.57	0.44
1:K:502:ILE:CG1	1:K:656:ILE:HD12	2.47	0.44
1:L:53:LYS:HG3	1:L:54:ASN:OD1	2.18	0.44
1:L:275:TRP:CH2	1:L:279:MET:HG3	2.52	0.44
1:L:485:LYS:O	1:L:485:LYS:HD3	2.18	0.44
1:L:598:ASP:O	1:L:602:LYS:HG2	2.16	0.44
1:L:613:GLY:O	1:L:617:LYS:HG3	2.18	0.44
1:A:27:GLY:O	1:A:45:SER:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HG3	1:A:36:GLU:HG3	1.99	0.44
1:A:231:HIS:O	1:A:235:LYS:N	2.51	0.44
1:A:577:ASP:HB3	1:A:578:HIS:H	1.58	0.44
1:B:587:VAL:HA	1:B:590:ILE:HD12	2.00	0.44
1:C:116:LEU:O	1:C:121:ILE:HD11	2.18	0.44
1:C:174:GLN:HG2	1:H:350:GLY:HA2	2.00	0.44
1:C:220:PRO:O	1:C:243:PHE:HA	2.18	0.44
1:D:219:ARG:HB2	1:D:223:HIS:HA	1.99	0.44
1:D:452:MET:O	1:D:456:LEU:HG	2.18	0.44
1:D:560:LEU:O	1:D:563:ARG:HB2	2.17	0.44
1:E:404:SER:HB2	1:E:406:CYS:SG	2.58	0.44
1:F:190:PRO:HA	1:F:193:PHE:CD1	2.53	0.44
1:F:423:LEU:O	1:F:427:TRP:HB2	2.18	0.44
1:F:614:CYS:HA	1:F:617:LYS:HD3	2.00	0.44
1:G:234:ILE:HD11	1:G:282:TRP:CZ3	2.53	0.44
1:G:237:LYS:O	1:G:238:ASP:C	2.59	0.44
1:I:317:ASN:ND2	1:I:319:THR:HG23	2.32	0.44
1:J:88:HIS:CD2	1:J:90:VAL:HG22	2.53	0.44
1:J:236:LYS:H	1:J:236:LYS:HG3	1.63	0.44
1:K:26:PHE:HD2	1:K:47:ARG:HA	1.83	0.44
1:K:27:GLY:O	1:K:45:SER:HB3	2.17	0.44
1:L:577:ASP:O	1:L:578:HIS:HB2	2.18	0.44
1:A:43:ILE:HD12	1:A:43:ILE:N	2.32	0.43
1:A:152:LEU:HD13	1:A:161:HIS:HA	1.99	0.43
1:B:251:GLU:HA	1:D:228:PHE:CD1	2.53	0.43
1:B:420:ILE:HG21	1:B:578:HIS:N	2.32	0.43
1:B:452:MET:O	1:B:456:LEU:HG	2.17	0.43
1:B:485:LYS:O	1:B:485:LYS:HD3	2.17	0.43
1:C:170:LYS:HD3	1:C:198:TYR:CZ	2.53	0.43
1:D:395:GLU:HG3	1:D:397:PRO:CD	2.38	0.43
1:D:424:ARG:HD3	1:D:572:LYS:HE2	1.99	0.43
1:D:487:ILE:HA	1:D:646:ARG:HD2	1.99	0.43
1:E:65:MET:SD	1:E:166:LEU:HD23	2.57	0.43
1:E:273:GLU:O	1:E:277:GLN:HG3	2.18	0.43
1:E:274:ASN:HA	1:E:277:GLN:NE2	2.32	0.43
1:F:21:LEU:HD23	1:F:29:VAL:C	2.43	0.43
1:F:84:ASN:HB3	1:F:85:ILE:H	1.68	0.43
1:G:274:ASN:HA	1:G:277:GLN:NE2	2.33	0.43
1:G:507:MET:HB3	1:G:511:TRP:CD1	2.53	0.43
1:H:318:MET:HE2	1:H:447:GLY:HA3	2.00	0.43
1:H:581:SER:O	1:H:582:ASP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:LEU:HD22	1:I:166:LEU:N	2.33	0.43
1:I:265:CYS:SG	1:I:267:LEU:HB2	2.58	0.43
1:J:275:TRP:NE1	1:J:300:CYS:O	2.51	0.43
1:J:452:MET:O	1:J:456:LEU:HG	2.18	0.43
1:K:452:MET:HE1	1:K:455:LEU:HD23	1.99	0.43
1:L:81:GLU:HG3	1:L:82:GLU:N	2.34	0.43
1:L:185:LEU:HD12	1:L:193:PHE:CZ	2.49	0.43
1:A:328:LEU:HD21	1:A:337:LEU:HD22	2.01	0.43
1:B:152:LEU:HD13	1:B:161:HIS:HA	1.99	0.43
1:C:265:CYS:SG	1:C:267:LEU:HB2	2.58	0.43
1:C:485:LYS:O	1:C:485:LYS:HD3	2.17	0.43
1:C:613:GLY:O	1:C:617:LYS:HG3	2.18	0.43
1:C:621:LEU:O	1:C:625:VAL:HG23	2.18	0.43
1:D:6:ASP:N	1:D:7:PRO:CD	2.82	0.43
1:D:215:ILE:HG21	1:D:258:LEU:HD21	2.00	0.43
1:D:420:ILE:HD11	1:D:571:LEU:HG	1.98	0.43
1:E:84:ASN:CG	1:E:85:ILE:H	2.26	0.43
1:E:333:SER:HA	1:E:367:PRO:HB2	2.00	0.43
1:E:548:PRO:CB	1:E:552:ARG:HG3	2.49	0.43
1:E:560:LEU:O	1:E:563:ARG:HB2	2.17	0.43
1:F:143:ARG:CD	1:F:143:ARG:H	2.31	0.43
1:F:392:THR:HG22	1:F:616:GLN:HE22	1.84	0.43
1:G:26:PHE:HD2	1:G:47:ARG:HA	1.83	0.43
1:G:73:VAL:CG2	1:G:163:ILE:HB	2.45	0.43
1:G:219:ARG:H	1:G:219:ARG:NE	2.16	0.43
1:G:548:PRO:CB	1:G:552:ARG:HG3	2.48	0.43
1:H:517:LYS:HD2	1:H:642:MET:HE1	1.99	0.43
1:I:592:HIS:CG	2:h:2:GLC:H4	2.53	0.43
1:J:149:ASN:O	1:J:164:ILE:HG22	2.18	0.43
1:K:187:TYR:CZ	1:K:219:ARG:HD2	2.53	0.43
1:K:334:LEU:HD22	1:K:366:LYS:O	2.18	0.43
1:L:48:LEU:O	1:L:50:LEU:HD12	2.19	0.43
1:L:143:ARG:H	1:L:143:ARG:CD	2.31	0.43
1:L:550:GLY:H	1:L:552:ARG:HG2	1.82	0.43
1:A:192:LEU:HD12	1:A:192:LEU:H	1.82	0.43
1:A:227:PRO:CG	1:C:249:SER:HB2	2.48	0.43
1:A:560:LEU:O	1:A:563:ARG:HB2	2.18	0.43
1:B:118:GLU:HB2	1:B:263:SER:O	2.18	0.43
1:B:323:ILE:HD12	1:B:323:ILE:N	2.33	0.43
1:B:328:LEU:HD21	1:B:337:LEU:HD22	2.00	0.43
1:B:560:LEU:O	1:B:563:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LEU:HD22	1:C:293:LEU:N	2.33	0.43
1:D:621:LEU:O	1:D:625:VAL:HG23	2.18	0.43
1:E:80:PRO:HB2	1:E:81:GLU:OE2	2.18	0.43
1:E:192:LEU:HD12	1:E:192:LEU:N	2.33	0.43
1:E:324:ILE:HD12	1:E:324:ILE:N	2.33	0.43
1:F:317:ASN:ND2	1:F:319:THR:HG23	2.34	0.43
1:F:598:ASP:O	1:F:602:LYS:HG2	2.17	0.43
1:G:141:ILE:O	1:G:169:ALA:HB1	2.17	0.43
1:G:485:LYS:O	1:G:485:LYS:HD3	2.18	0.43
1:H:78:ASP:HB3	1:H:79:VAL:H	1.59	0.43
1:H:328:LEU:HD21	1:H:337:LEU:HD22	2.00	0.43
1:H:507:MET:HB3	1:H:511:TRP:CD1	2.53	0.43
1:I:8:GLU:HB2	1:I:86:LEU:HD12	2.00	0.43
1:I:26:PHE:HD2	1:I:47:ARG:HA	1.83	0.43
1:I:190:PRO:HA	1:I:193:PHE:CD1	2.53	0.43
1:J:423:LEU:O	1:J:427:TRP:HB2	2.18	0.43
1:J:487:ILE:HG23	1:J:488:GLN:N	2.32	0.43
1:L:452:MET:O	1:L:456:LEU:HG	2.18	0.43
1:A:192:LEU:HD12	1:A:192:LEU:N	2.33	0.43
1:A:258:LEU:HB2	1:A:273:GLU:HG2	2.00	0.43
1:A:424:ARG:NH1	1:A:572:LYS:HG2	2.33	0.43
1:A:455:LEU:HD13	1:A:615:LYS:CG	2.49	0.43
1:B:248:MET:HB3	1:D:184:THR:HG22	2.00	0.43
1:B:452:MET:HE1	1:B:455:LEU:HD23	2.00	0.43
1:B:507:MET:HB3	1:B:511:TRP:CD1	2.53	0.43
1:C:7:PRO:HG3	1:C:32:TYR:OH	2.17	0.43
1:C:560:LEU:O	1:C:563:ARG:HB2	2.19	0.43
1:D:151:VAL:C	1:D:152:LEU:HD22	2.43	0.43
1:E:396:GLY:H	1:E:397:PRO:CD	2.22	0.43
1:F:268:ILE:C	1:F:271:PRO:HD2	2.44	0.43
1:F:387:PHE:CZ	1:F:451:ALA:HB2	2.54	0.43
1:F:424:ARG:NH1	1:F:572:LYS:HG2	2.33	0.43
1:F:613:GLY:O	1:F:617:LYS:HG3	2.18	0.43
1:G:473:SER:HB2	1:G:524:VAL:HG22	1.99	0.43
1:G:648:LYS:HE3	1:H:489:LEU:CD1	2.46	0.43
1:H:423:LEU:O	1:H:427:TRP:HB2	2.17	0.43
1:H:441:TYR:HE2	1:H:551:ARG:HA	1.83	0.43
1:I:273:GLU:O	1:I:277:GLN:HG3	2.18	0.43
1:K:165:ASP:C	1:K:166:LEU:HD22	2.43	0.43
1:K:324:ILE:HD12	1:K:324:ILE:N	2.33	0.43
1:L:149:ASN:O	1:L:164:ILE:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:HG22	1:C:95:MET:HB2	2.01	0.43
1:C:239:PRO:O	1:C:240:LYS:HB2	2.17	0.43
1:C:268:ILE:C	1:C:271:PRO:HD2	2.43	0.43
1:C:324:ILE:HD12	1:C:324:ILE:N	2.32	0.43
1:D:275:TRP:CH2	1:D:279:MET:HG3	2.53	0.43
1:D:317:ASN:ND2	1:D:319:THR:HG23	2.34	0.43
1:D:410:ILE:HD12	1:D:583:SER:OG	2.19	0.43
1:E:35:ARG:HG3	1:E:36:GLU:HG3	2.01	0.43
1:E:338:GLN:HA	1:E:341:ILE:HD12	2.01	0.43
1:E:489:LEU:HD11	1:F:648:LYS:HE3	2.01	0.43
1:E:502:ILE:HD12	1:F:654:LEU:CD1	2.49	0.43
1:E:502:ILE:HB	1:F:654:LEU:HD21	2.00	0.43
1:E:639:VAL:O	1:E:642:MET:HB2	2.19	0.43
1:F:74:VAL:HG11	1:F:164:ILE:HD12	1.99	0.43
1:F:283:ASP:OD2	1:F:286:GLN:HB2	2.19	0.43
1:F:401:ARG:NH2	1:F:440:ASP:HB2	2.33	0.43
1:G:27:GLY:O	1:G:45:SER:HB3	2.19	0.43
1:G:35:ARG:HG3	1:G:36:GLU:HG3	2.00	0.43
1:G:37:LEU:HB3	1:G:38:ASP:H	1.65	0.43
1:G:95:MET:CE	1:G:164:ILE:HD11	2.48	0.43
1:G:430:ALA:O	1:G:434:VAL:HG23	2.17	0.43
1:H:7:PRO:HD2	1:H:17:MET:SD	2.58	0.43
1:I:515:GLU:O	1:I:519:ILE:HG13	2.19	0.43
1:J:275:TRP:CH2	1:J:279:MET:HG3	2.53	0.43
1:J:541:ILE:HD11	1:J:618:ILE:HD11	2.00	0.43
1:J:613:GLY:O	1:J:617:LYS:HG3	2.19	0.43
1:K:141:ILE:HG13	1:K:203:ASP:CG	2.43	0.43
1:K:141:ILE:HG23	1:K:170:LYS:HB2	2.00	0.43
1:L:487:ILE:HG23	1:L:488:GLN:N	2.33	0.43
1:L:515:GLU:O	1:L:519:ILE:HG13	2.18	0.43
1:A:324:ILE:HD12	1:A:324:ILE:N	2.30	0.43
1:A:411:VAL:HG23	1:A:412:GLN:N	2.33	0.43
1:A:423:LEU:O	1:A:427:TRP:HB2	2.19	0.43
1:B:462:LEU:HD22	1:B:618:ILE:HG23	2.00	0.43
1:C:21:LEU:HD23	1:C:29:VAL:C	2.44	0.43
1:D:152:LEU:HD13	1:D:161:HIS:HA	2.00	0.43
1:D:281:ASN:H	1:D:287:ARG:HH12	1.65	0.43
1:D:485:LYS:O	1:D:485:LYS:HD3	2.18	0.43
1:F:222:LEU:HD12	1:F:244:ALA:O	2.18	0.43
1:H:48:LEU:O	1:H:50:LEU:HD12	2.17	0.43
1:H:49:GLU:HA	1:H:88:HIS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:268:ILE:C	1:H:271:PRO:HD2	2.43	0.43
1:H:324:ILE:HD12	1:H:324:ILE:N	2.32	0.43
1:H:621:LEU:O	1:H:625:VAL:HG23	2.19	0.43
1:I:75:LYS:HD2	1:I:76:ALA:H	1.83	0.43
1:I:281:ASN:ND2	1:I:286:GLN:HB2	2.33	0.43
1:J:83:LEU:HD12	1:J:92:LEU:HD13	2.00	0.43
1:J:587:VAL:HA	1:J:590:ILE:HD12	2.00	0.43
1:K:560:LEU:O	1:K:563:ARG:HB2	2.18	0.43
1:K:598:ASP:O	1:K:602:LYS:HG2	2.19	0.43
1:L:190:PRO:HB3	1:L:231:HIS:CD2	2.53	0.43
1:L:227:PRO:HA	1:L:230:TRP:CB	2.41	0.43
1:L:316:LEU:HB2	1:L:383:MET:CE	2.46	0.43
1:B:26:PHE:HD2	1:B:47:ARG:HA	1.83	0.43
1:B:333:SER:HA	1:B:368:ALA:H	1.84	0.43
1:C:328:LEU:HD21	1:C:337:LEU:HD22	2.01	0.43
1:C:359:GLY:HA3	1:C:453:LEU:HB2	2.01	0.43
1:C:543:GLU:O	1:C:546:LYS:HD3	2.19	0.43
1:C:648:LYS:HE3	1:D:489:LEU:HD11	2.01	0.43
1:D:21:LEU:HD23	1:D:29:VAL:C	2.43	0.43
1:D:117:LYS:O	1:D:121:ILE:HG13	2.19	0.43
1:D:142:HIS:HA	1:D:169:ALA:HB1	1.99	0.43
1:D:190:PRO:HA	1:D:193:PHE:CD1	2.54	0.43
1:D:268:ILE:C	1:D:271:PRO:HD2	2.43	0.43
1:E:473:SER:OG	1:E:524:VAL:HG13	2.19	0.43
1:F:515:GLU:O	1:F:519:ILE:HG13	2.19	0.43
1:G:324:ILE:HD12	1:G:324:ILE:N	2.30	0.43
1:H:227:PRO:CG	1:L:249:SER:HB2	2.48	0.43
1:I:118:GLU:HA	1:I:121:ILE:HD12	2.01	0.43
1:I:223:HIS:O	1:I:224:HIS:HB3	2.18	0.43
1:I:227:PRO:CG	1:K:249:SER:HB2	2.48	0.43
1:I:323:ILE:N	1:I:323:ILE:HD12	2.33	0.43
1:I:395:GLU:CG	1:I:396:GLY:H	2.30	0.43
1:J:27:GLY:O	1:J:45:SER:HB3	2.19	0.43
1:J:116:LEU:H	1:J:116:LEU:CD1	2.31	0.43
1:K:487:ILE:HG23	1:K:488:GLN:N	2.33	0.43
1:L:190:PRO:HA	1:L:193:PHE:CD1	2.54	0.43
1:L:408:ASN:HA	1:L:411:VAL:HG22	1.99	0.43
1:L:614:CYS:HA	1:L:617:LYS:HD3	2.01	0.43
1:A:57:ARG:O	1:A:60:HIS:HB3	2.18	0.43
1:A:166:LEU:C	1:A:168:TYR:N	2.77	0.43
1:A:234:ILE:HA	1:A:236:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LYS:HD2	1:A:241:CYS:HB3	2.00	0.43
1:A:403:LEU:HD12	1:A:407:VAL:HG12	2.01	0.43
1:A:427:TRP:CZ3	1:A:567:LEU:HB3	2.53	0.43
1:A:560:LEU:HB3	1:A:593:THR:HG22	2.01	0.43
1:B:586:MET:O	1:B:590:ILE:HG13	2.18	0.43
1:C:236:LYS:O	1:C:237:LYS:O	2.35	0.43
1:D:34:HIS:CE1	1:D:37:LEU:HD23	2.54	0.43
1:D:244:ALA:HA	1:D:253:ARG:O	2.19	0.43
1:E:26:PHE:HD2	1:E:47:ARG:HA	1.84	0.43
1:E:219:ARG:HE	1:E:219:ARG:HB2	1.66	0.43
1:E:445:PHE:HA	1:E:604:LEU:HD21	2.01	0.43
1:G:43:ILE:HG23	1:G:93:LEU:C	2.44	0.43
1:G:114:CYS:HB2	1:G:432:HIS:CD2	2.54	0.43
1:I:231:HIS:N	1:I:231:HIS:ND1	2.66	0.43
1:I:427:TRP:HZ2	1:I:583:SER:HA	1.84	0.43
1:I:489:LEU:HD22	1:J:647:GLN:OE1	2.19	0.43
1:J:143:ARG:C	1:J:145:LEU:H	2.27	0.43
1:J:152:LEU:HD13	1:J:161:HIS:HA	2.00	0.43
1:K:410:ILE:O	1:K:587:VAL:HG22	2.18	0.43
1:A:655:LYS:HE2	1:B:501:GLY:HA3	2.01	0.43
1:B:274:ASN:HA	1:B:277:GLN:NE2	2.34	0.43
1:B:334:LEU:HD11	1:B:364:PRO:HA	2.01	0.43
1:B:473:SER:CB	1:B:527:ILE:HD11	2.49	0.43
1:C:152:LEU:HD13	1:C:161:HIS:HA	2.00	0.43
1:C:507:MET:HB3	1:C:511:TRP:CD1	2.53	0.43
1:D:8:GLU:OE2	1:D:87:ILE:HG23	2.19	0.43
1:D:35:ARG:HG3	1:D:36:GLU:HG3	2.01	0.43
1:D:186:GLN:NE2	1:D:219:ARG:HG2	2.34	0.43
1:D:392:THR:HG22	1:D:616:GLN:HE22	1.82	0.43
1:E:401:ARG:NH2	1:E:436:GLY:C	2.70	0.43
1:F:621:LEU:O	1:F:625:VAL:HG23	2.18	0.43
1:G:171:ASP:CG	1:G:172:VAL:H	2.27	0.43
1:G:613:GLY:O	1:G:617:LYS:HG3	2.19	0.43
1:H:392:THR:HG22	1:H:616:GLN:HE22	1.84	0.43
1:I:228:PHE:HA	1:K:251:GLU:OE2	2.19	0.43
1:I:415:LYS:HA	1:I:584:THR:HB	2.01	0.43
1:K:57:ARG:O	1:K:60:HIS:HB3	2.19	0.43
1:L:34:HIS:CE1	1:L:37:LEU:HD23	2.54	0.43
1:L:507:MET:HB3	1:L:511:TRP:CD1	2.53	0.43
1:A:270:GLU:N	1:A:271:PRO:HD2	2.34	0.43
1:A:284:PRO:C	1:A:286:GLN:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:GLY:O	1:A:617:LYS:HG3	2.19	0.43
1:B:515:GLU:O	1:B:519:ILE:HG13	2.19	0.43
1:C:35:ARG:HG3	1:C:36:GLU:HG3	2.00	0.43
1:C:273:GLU:O	1:C:277:GLN:HG3	2.18	0.43
1:C:515:GLU:O	1:C:519:ILE:HG13	2.19	0.43
1:C:614:CYS:HA	1:C:617:LYS:HD3	2.00	0.43
1:D:27:GLY:O	1:D:45:SER:HB3	2.19	0.43
1:D:473:SER:CB	1:D:527:ILE:HD11	2.49	0.43
1:E:27:GLY:O	1:E:45:SER:HB3	2.18	0.43
1:E:90:VAL:HG13	1:E:91:PRO:HD2	2.00	0.43
1:E:143:ARG:C	1:E:145:LEU:H	2.27	0.43
1:E:201:THR:O	1:E:287:ARG:NH1	2.52	0.43
1:E:289:GLY:O	1:E:291:VAL:N	2.52	0.43
1:E:497:GLN:OE1	1:F:655:LYS:HE3	2.18	0.43
1:F:315:ILE:CD1	1:F:384:VAL:HB	2.49	0.43
1:F:589:ILE:O	1:F:593:THR:HG23	2.18	0.43
1:G:480:LEU:CD2	1:G:518:ALA:HB1	2.49	0.43
1:H:204:TYR:O	1:H:279:MET:HE3	2.19	0.43
1:H:240:LYS:O	1:H:277:GLN:HG2	2.19	0.43
1:H:412:GLN:OE1	1:J:20:ARG:HB3	2.19	0.43
1:H:613:GLY:O	1:H:617:LYS:HG3	2.19	0.43
1:I:86:LEU:HD22	1:I:86:LEU:N	2.34	0.43
1:I:143:ARG:H	1:I:143:ARG:HD3	1.84	0.43
1:I:328:LEU:HD21	1:I:337:LEU:HD22	2.01	0.43
1:J:86:LEU:C	1:J:88:HIS:H	2.26	0.43
1:J:244:ALA:HA	1:J:253:ARG:O	2.18	0.43
1:J:268:ILE:C	1:J:271:PRO:HD2	2.43	0.43
1:J:589:ILE:O	1:J:593:THR:HG23	2.18	0.43
1:K:95:MET:CE	1:K:164:ILE:HD11	2.49	0.43
1:K:318:MET:CE	1:K:447:GLY:HA3	2.47	0.43
1:L:244:ALA:HA	1:L:253:ARG:O	2.19	0.43
1:L:317:ASN:ND2	1:L:319:THR:HG23	2.34	0.43
1:L:420:ILE:HG21	1:L:578:HIS:N	2.34	0.43
1:A:95:MET:CE	1:A:164:ILE:HD11	2.49	0.42
1:A:165:ASP:C	1:A:166:LEU:HD22	2.43	0.42
1:A:292:ASP:C	1:A:294:THR:H	2.26	0.42
1:A:396:GLY:C	1:A:398:PHE:H	2.26	0.42
1:A:574:ARG:O	1:A:576:SER:N	2.52	0.42
1:B:118:GLU:HA	1:B:121:ILE:HD12	2.00	0.42
1:B:180:GLU:HB3	1:B:181:PHE:H	1.68	0.42
1:C:91:PRO:C	1:C:92:LEU:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:HIS:C	1:C:233:LYS:N	2.74	0.42
1:E:236:LYS:HB2	1:E:236:LYS:NZ	2.33	0.42
1:E:396:GLY:C	1:E:398:PHE:H	2.26	0.42
1:G:57:ARG:O	1:G:60:HIS:HB3	2.19	0.42
1:G:79:VAL:HG11	1:G:83:LEU:HD23	2.00	0.42
1:G:515:GLU:O	1:G:519:ILE:HG13	2.19	0.42
1:H:106:LEU:HD11	1:H:152:LEU:HG	2.01	0.42
1:H:515:GLU:O	1:H:519:ILE:HG13	2.19	0.42
1:H:548:PRO:HB2	1:H:552:ARG:HG3	2.01	0.42
1:I:143:ARG:C	1:I:145:LEU:H	2.27	0.42
1:J:143:ARG:H	1:J:143:ARG:CD	2.32	0.42
1:K:507:MET:HB3	1:K:511:TRP:CD1	2.54	0.42
1:K:515:GLU:O	1:K:519:ILE:HG13	2.19	0.42
1:L:328:LEU:HD21	1:L:337:LEU:HD22	2.01	0.42
1:A:46:CYS:SG	1:A:90:VAL:HB	2.59	0.42
1:B:190:PRO:HA	1:B:193:PHE:CD1	2.54	0.42
1:C:143:ARG:C	1:C:145:LEU:H	2.27	0.42
1:C:533:GLN:HE21	1:C:621:LEU:HD21	1.84	0.42
1:D:212:PHE:CE2	1:D:220:PRO:HA	2.54	0.42
1:E:48:LEU:HB2	1:E:49:GLU:H	1.64	0.42
1:E:452:MET:HE1	1:E:455:LEU:HD23	2.00	0.42
1:E:507:MET:HB3	1:E:511:TRP:CD1	2.53	0.42
1:F:83:LEU:HB3	1:F:84:ASN:H	1.70	0.42
1:F:502:ILE:HD13	1:F:656:ILE:HD12	2.01	0.42
1:G:184:THR:H	1:I:248:MET:HB2	1.83	0.42
1:G:240:LYS:O	1:G:277:GLN:HG2	2.19	0.42
1:G:258:LEU:HB2	1:G:273:GLU:HG2	2.01	0.42
1:G:473:SER:HA	1:G:632:ILE:CG2	2.49	0.42
1:G:507:MET:HA	1:G:510:ALA:HB3	2.01	0.42
1:G:658:CYS:SG	1:H:502:ILE:HG13	2.59	0.42
1:H:199:THR:OG1	1:H:284:PRO:HB2	2.18	0.42
1:H:215:ILE:HG21	1:H:258:LEU:HD21	2.00	0.42
1:H:622:LEU:N	1:H:623:PRO:CD	2.82	0.42
1:I:27:GLY:O	1:I:45:SER:HB3	2.18	0.42
1:I:220:PRO:HG2	1:I:221:PHE:CD2	2.54	0.42
1:J:118:GLU:HA	1:J:121:ILE:HD12	2.01	0.42
1:J:236:LYS:HD3	1:J:237:LYS:H	1.84	0.42
1:J:410:ILE:HG23	1:J:583:SER:HG	1.83	0.42
1:K:463:THR:HA	1:K:534:ILE:HD11	1.99	0.42
1:K:560:LEU:HB3	1:K:593:THR:HG22	2.01	0.42
1:L:487:ILE:CD1	1:L:514:MET:HE3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HG3	1:A:54:ASN:OD1	2.19	0.42
1:A:338:GLN:HA	1:A:341:ILE:HD12	2.02	0.42
1:A:485:LYS:O	1:A:485:LYS:HD3	2.19	0.42
1:B:265:CYS:SG	1:B:267:LEU:HB2	2.60	0.42
1:B:473:SER:OG	1:B:524:VAL:HG13	2.18	0.42
1:B:561:GLU:O	1:B:565:ILE:HG13	2.19	0.42
1:B:621:LEU:O	1:B:625:VAL:HG23	2.19	0.42
1:C:190:PRO:HA	1:C:193:PHE:CD1	2.53	0.42
1:C:401:ARG:H	1:C:401:ARG:HG2	1.72	0.42
1:C:449:ARG:HH22	3:T:5:Z4K:C6	2.32	0.42
1:C:561:GLU:O	1:C:565:ILE:HG13	2.19	0.42
1:C:576:SER:OG	1:E:580:TYR:HB2	2.19	0.42
1:C:596:SER:O	1:C:600:VAL:HG22	2.19	0.42
1:D:79:VAL:HG21	1:D:83:LEU:CD1	2.49	0.42
1:D:287:ARG:HH11	1:D:287:ARG:HG3	1.84	0.42
1:D:473:SER:OG	1:D:524:VAL:HG13	2.18	0.42
1:D:550:GLY:C	1:D:552:ARG:H	2.26	0.42
1:E:165:ASP:C	1:E:166:LEU:HD22	2.44	0.42
1:E:170:LYS:HZ1	1:E:192:LEU:HG	1.84	0.42
1:E:275:TRP:CH2	1:E:279:MET:HG3	2.54	0.42
1:F:170:LYS:HA	1:F:177:LEU:HA	2.00	0.42
1:G:147:PRO:HB2	1:G:148:GLU:OE2	2.20	0.42
1:G:270:GLU:N	1:G:271:PRO:HD2	2.35	0.42
1:G:396:GLY:HA2	1:G:398:PHE:CE2	2.54	0.42
1:G:511:TRP:CZ3	1:G:646:ARG:HA	2.54	0.42
1:H:152:LEU:HD13	1:H:161:HIS:HA	2.00	0.42
1:H:244:ALA:HA	1:H:253:ARG:O	2.20	0.42
1:H:485:LYS:O	1:H:485:LYS:HD3	2.18	0.42
1:I:507:MET:HB3	1:I:511:TRP:CD1	2.53	0.42
1:I:549:TYR:H	1:I:552:ARG:HD2	1.85	0.42
1:J:26:PHE:HD2	1:J:47:ARG:HA	1.85	0.42
1:J:403:LEU:HD23	1:L:26:PHE:HE1	1.84	0.42
1:J:410:ILE:O	1:J:587:VAL:HG22	2.19	0.42
1:K:29:VAL:HG21	4:K:701:5TL:CAE	2.50	0.42
1:K:53:LYS:HG3	1:K:54:ASN:OD1	2.19	0.42
1:L:77:CYS:HB3	1:L:94:ALA:CB	2.49	0.42
1:L:118:GLU:HB2	1:L:263:SER:O	2.19	0.42
1:L:550:GLY:HA3	1:L:604:LEU:HD13	2.01	0.42
1:L:561:GLU:O	1:L:565:ILE:HG13	2.19	0.42
1:A:37:LEU:HB3	1:A:38:ASP:H	1.65	0.42
1:A:420:ILE:HG21	1:A:578:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HG3	1:B:36:GLU:HG3	2.00	0.42
1:B:237:LYS:HE3	1:B:281:ASN:HA	2.02	0.42
1:B:387:PHE:HD1	1:B:394:TYR:OH	2.01	0.42
1:B:396:GLY:N	1:B:397:PRO:CD	2.80	0.42
1:C:174:GLN:CG	1:H:350:GLY:HA2	2.49	0.42
1:C:581:SER:O	1:C:582:ASP:HB2	2.19	0.42
1:D:143:ARG:C	1:D:145:LEU:H	2.28	0.42
1:E:204:TYR:O	1:E:279:MET:HE3	2.20	0.42
1:E:489:LEU:HD13	1:F:643:GLN:CG	2.50	0.42
1:E:614:CYS:O	1:E:618:ILE:HG13	2.19	0.42
1:F:35:ARG:HG3	1:F:36:GLU:HG3	2.00	0.42
1:F:53:LYS:HG3	1:F:54:ASN:OD1	2.20	0.42
1:G:165:ASP:C	1:G:166:LEU:HD22	2.44	0.42
1:G:411:VAL:HG23	1:G:412:GLN:N	2.34	0.42
1:G:504:SER:OG	1:G:653:LEU:HD21	2.18	0.42
1:J:6:ASP:HB3	1:J:7:PRO:HD2	2.00	0.42
1:J:28:ASN:HB2	1:J:29:VAL:H	1.67	0.42
1:J:235:LYS:HA	1:J:282:TRP:CH2	2.54	0.42
1:J:313:VAL:HG11	1:J:371:CYS:SG	2.59	0.42
1:K:274:ASN:O	1:K:277:GLN:HB2	2.19	0.42
1:B:53:LYS:HG3	1:B:54:ASN:OD1	2.20	0.42
1:B:70:HIS:HB2	1:B:134:TYR:CD2	2.54	0.42
1:B:244:ALA:HA	1:B:253:ARG:O	2.20	0.42
1:B:411:VAL:HG23	1:B:412:GLN:N	2.34	0.42
1:B:412:GLN:HB3	1:D:21:LEU:O	2.20	0.42
1:B:473:SER:HB3	1:B:527:ILE:HD11	2.01	0.42
1:D:393:VAL:HG22	1:D:609:SER:HB3	2.02	0.42
1:D:613:GLY:O	1:D:617:LYS:HG3	2.20	0.42
1:E:118:GLU:HB2	1:E:263:SER:O	2.20	0.42
1:E:411:VAL:HG23	1:E:412:GLN:N	2.35	0.42
1:F:485:LYS:O	1:F:485:LYS:HD3	2.19	0.42
1:G:118:GLU:HB2	1:G:263:SER:O	2.20	0.42
1:G:219:ARG:HH12	1:G:224:HIS:CA	2.33	0.42
1:G:222:LEU:HD22	1:G:230:TRP:HA	2.01	0.42
1:H:265:CYS:SG	1:H:267:LEU:HB2	2.60	0.42
1:I:98:CYS:HB3	1:I:152:LEU:O	2.20	0.42
1:I:141:ILE:HG13	1:I:203:ASP:CG	2.45	0.42
1:I:149:ASN:O	1:I:164:ILE:HG22	2.20	0.42
1:I:376:VAL:O	1:I:377:ARG:HG2	2.19	0.42
1:I:589:ILE:O	1:I:593:THR:HG23	2.20	0.42
1:J:151:VAL:C	1:J:152:LEU:HD22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:507:MET:HB3	1:J:511:TRP:CD1	2.54	0.42
1:K:68:LEU:HD21	1:K:140:ILE:HD12	2.01	0.42
1:K:270:GLU:N	1:K:271:PRO:HD2	2.35	0.42
1:K:613:GLY:O	1:K:617:LYS:HG3	2.20	0.42
1:A:26:PHE:HD2	1:A:47:ARG:HA	1.83	0.42
1:A:74:VAL:HG23	1:A:95:MET:HE3	2.01	0.42
1:A:95:MET:HE2	1:A:164:ILE:HD11	2.02	0.42
1:A:228:PHE:HA	1:C:251:GLU:OE2	2.19	0.42
1:B:410:ILE:HD12	1:B:583:SER:OG	2.19	0.42
1:B:415:LYS:HD3	1:B:584:THR:CG2	2.50	0.42
1:D:57:ARG:O	1:D:60:HIS:HB3	2.20	0.42
1:D:319:THR:HG22	1:D:394:TYR:CE1	2.55	0.42
1:D:363:ASP:N	1:D:364:PRO:HD3	2.34	0.42
1:D:411:VAL:CG1	1:D:590:ILE:HG21	2.49	0.42
1:E:270:GLU:N	1:E:271:PRO:HD2	2.35	0.42
1:F:34:HIS:CE1	1:F:37:LEU:HD23	2.55	0.42
1:F:48:LEU:O	1:F:50:LEU:HD12	2.20	0.42
1:F:294:THR:C	1:F:295:LEU:HD12	2.45	0.42
1:F:355:LEU:HD12	1:F:355:LEU:N	2.35	0.42
1:F:507:MET:HB3	1:F:511:TRP:CD1	2.54	0.42
1:F:560:LEU:O	1:F:563:ARG:HB2	2.18	0.42
1:G:152:LEU:HD13	1:G:161:HIS:HA	2.00	0.42
1:G:275:TRP:CH2	1:G:279:MET:HG3	2.55	0.42
1:I:50:LEU:HD22	1:I:90:VAL:HG11	2.01	0.42
1:I:281:ASN:HD22	1:I:286:GLN:HB2	1.84	0.42
1:I:578:HIS:HB2	1:K:579:SER:HB2	2.01	0.42
1:I:639:VAL:O	1:I:642:MET:HB2	2.19	0.42
1:J:14:PRO:HG2	1:J:82:GLU:OE1	2.19	0.42
1:L:68:LEU:HD21	1:L:140:ILE:HD12	2.01	0.42
1:L:560:LEU:O	1:L:563:ARG:HB2	2.18	0.42
1:L:621:LEU:O	1:L:625:VAL:HG23	2.19	0.42
1:A:655:LYS:N	1:A:655:LYS:HD2	2.35	0.42
1:B:549:TYR:H	1:B:552:ARG:HD2	1.85	0.42
1:B:614:CYS:O	1:B:618:ILE:HG13	2.19	0.42
1:E:237:LYS:O	1:E:238:ASP:C	2.63	0.42
1:E:328:LEU:HD21	1:E:337:LEU:HD22	2.01	0.42
1:E:395:GLU:HG3	1:E:396:GLY:H	1.85	0.42
1:E:515:GLU:O	1:E:519:ILE:HG13	2.20	0.42
1:F:143:ARG:C	1:F:145:LEU:H	2.27	0.42
1:F:424:ARG:HH11	1:F:572:LYS:HG2	1.85	0.42
1:G:265:CYS:SG	1:G:267:LEU:HB2	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:588:LYS:HB3	1:G:589:ILE:HD12	2.01	0.42
1:H:28:ASN:HB2	1:H:29:VAL:H	1.68	0.42
1:H:165:ASP:C	1:H:166:LEU:HD22	2.44	0.42
1:H:238:ASP:CB	1:H:239:PRO:HD2	2.40	0.42
1:I:35:ARG:HG3	1:I:36:GLU:HG3	2.00	0.42
1:I:43:ILE:HG23	1:I:93:LEU:C	2.45	0.42
1:I:485:LYS:O	1:I:485:LYS:HD3	2.19	0.42
1:I:614:CYS:HA	1:I:617:LYS:HD3	2.01	0.42
1:J:57:ARG:O	1:J:60:HIS:HB3	2.20	0.42
1:J:485:LYS:O	1:J:485:LYS:HD3	2.19	0.42
1:K:152:LEU:HD13	1:K:161:HIS:HA	2.01	0.42
1:L:83:LEU:O	1:L:92:LEU:HD13	2.20	0.42
1:L:392:THR:HG22	1:L:616:GLN:HE22	1.84	0.42
1:L:547:SER:HB2	1:L:548:PRO:HD2	2.01	0.42
1:A:412:GLN:NE2	1:E:27:GLY:HA2	2.35	0.42
1:A:549:TYR:HB2	1:A:552:ARG:NE	2.35	0.42
1:A:630:SER:O	1:A:634:GLU:HB2	2.20	0.42
1:B:230:TRP:O	1:B:234:ILE:HD13	2.19	0.42
1:B:535:MET:HA	1:B:538:HIS:HB3	2.02	0.42
1:C:27:GLY:O	1:C:45:SER:HB3	2.19	0.42
1:C:191:GLU:OE2	1:C:284:PRO:HB3	2.20	0.42
1:C:403:LEU:HD12	1:C:407:VAL:HG12	2.02	0.42
1:C:449:ARG:HH22	3:T:5:Z4K:C5	2.32	0.42
1:D:318:MET:HE2	1:D:447:GLY:HA3	2.02	0.42
1:F:324:ILE:HD12	1:F:324:ILE:N	2.32	0.42
1:F:561:GLU:O	1:F:565:ILE:HG13	2.19	0.42
1:G:107:LEU:HD23	1:G:116:LEU:HD11	2.02	0.42
1:G:338:GLN:HA	1:G:341:ILE:HD12	2.02	0.42
1:G:507:MET:HE1	1:G:653:LEU:HD13	2.01	0.42
1:G:614:CYS:HA	1:G:617:LYS:HD3	2.01	0.42
1:H:396:GLY:N	1:H:397:PRO:CD	2.82	0.42
1:I:411:VAL:HG23	1:I:412:GLN:N	2.35	0.42
1:J:35:ARG:HG3	1:J:36:GLU:HG3	2.01	0.42
1:J:53:LYS:HG3	1:J:54:ASN:OD1	2.19	0.42
1:J:237:LYS:HE3	1:J:282:TRP:HB2	2.02	0.42
1:J:317:ASN:ND2	1:J:319:THR:HG23	2.35	0.42
1:K:236:LYS:O	1:K:237:LYS:C	2.62	0.42
1:K:279:MET:O	1:K:287:ARG:HD2	2.20	0.42
1:L:268:ILE:C	1:L:271:PRO:HD2	2.45	0.42
1:L:596:SER:O	1:L:600:VAL:HG22	2.20	0.42
1:A:86:LEU:HB3	1:A:87:ILE:H	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD23	1:A:207:PHE:CZ	2.54	0.42
1:B:28:ASN:HB2	1:B:29:VAL:H	1.68	0.42
1:B:240:LYS:NZ	1:B:240:LYS:H	2.18	0.42
1:B:420:ILE:HG21	1:B:578:HIS:H	1.85	0.42
1:B:639:VAL:O	1:B:642:MET:HB2	2.20	0.42
1:C:653:LEU:CD1	1:C:656:ILE:HD11	2.50	0.42
1:D:55:ARG:HG3	1:D:90:VAL:HG13	2.02	0.42
1:D:142:HIS:HA	1:D:169:ALA:CB	2.50	0.42
1:D:319:THR:HG22	1:D:394:TYR:CZ	2.55	0.42
1:E:403:LEU:HD12	1:E:407:VAL:HG12	2.02	0.42
1:F:342:GLU:HB2	1:F:352:GLN:HE22	1.85	0.42
1:F:363:ASP:HB3	1:F:370:GLN:NE2	2.34	0.42
1:F:567:LEU:CD2	1:F:589:ILE:HD13	2.50	0.42
1:G:219:ARG:NH1	1:G:224:HIS:N	2.66	0.42
1:H:186:GLN:HG2	1:H:219:ARG:HH11	1.85	0.42
1:H:452:MET:O	1:H:456:LEU:HG	2.19	0.42
1:I:514:MET:HA	1:I:642:MET:HE1	2.02	0.42
1:K:167:GLY:O	1:K:178:CYS:HB3	2.20	0.42
1:K:221:PHE:O	1:K:223:HIS:N	2.53	0.42
1:K:244:ALA:HA	1:K:253:ARG:O	2.20	0.42
1:K:275:TRP:CH2	1:K:279:MET:HG3	2.55	0.42
1:L:232:GLU:C	1:L:234:ILE:N	2.77	0.42
1:L:313:VAL:HG11	1:L:371:CYS:SG	2.60	0.42
1:L:639:VAL:O	1:L:642:MET:HB2	2.19	0.42
1:B:84:ASN:CG	1:B:85:ILE:N	2.77	0.42
1:B:223:HIS:O	1:B:225:LEU:HD23	2.19	0.42
1:B:415:LYS:CA	1:B:584:THR:HB	2.44	0.42
1:C:95:MET:HE2	1:C:164:ILE:HD11	2.02	0.42
1:C:477:LYS:HE3	1:C:524:VAL:CG1	2.46	0.42
1:C:507:MET:HA	1:C:510:ALA:HB3	2.02	0.42
1:C:643:GLN:HG3	1:D:489:LEU:HD13	2.01	0.42
1:D:507:MET:HB3	1:D:511:TRP:CD1	2.54	0.42
1:D:541:ILE:HD11	1:D:618:ILE:HD11	2.00	0.42
1:E:13:GLY:H	1:E:14:PRO:CD	2.24	0.42
1:E:13:GLY:N	1:E:14:PRO:HD3	2.21	0.42
1:E:34:HIS:ND1	1:E:37:LEU:HB2	2.35	0.42
1:E:401:ARG:HH22	1:E:440:ASP:CB	2.32	0.42
1:E:485:LYS:O	1:E:485:LYS:HD3	2.20	0.42
1:E:536:SER:O	1:E:540:GLU:HB2	2.20	0.42
1:F:401:ARG:HB2	1:F:433:TYR:HE1	1.83	0.42
1:G:268:ILE:O	1:G:272:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:651:TRP:HZ2	1:H:490:ASP:HB3	1.83	0.42
1:H:151:VAL:C	1:H:152:LEU:HD22	2.45	0.42
1:H:411:VAL:HG23	1:H:412:GLN:N	2.35	0.42
1:H:589:ILE:O	1:H:593:THR:HG23	2.20	0.42
1:I:186:GLN:OE1	1:I:227:PRO:HD3	2.19	0.42
1:I:473:SER:HB3	1:I:632:ILE:HD13	2.01	0.42
1:K:13:GLY:N	1:K:14:PRO:CD	2.80	0.42
1:K:48:LEU:HB2	1:K:49:GLU:H	1.64	0.42
1:K:630:SER:O	1:K:634:GLU:HB2	2.20	0.42
1:L:404:SER:HB2	1:L:406:CYS:SG	2.60	0.42
1:B:403:LEU:HD12	1:B:407:VAL:HG12	2.02	0.41
1:B:458:TYR:HB3	1:B:618:ILE:HG21	2.02	0.41
1:C:63:GLN:NE2	1:H:349:THR:OG1	2.52	0.41
1:C:560:LEU:HB3	1:C:593:THR:HG22	2.01	0.41
1:D:95:MET:CE	1:D:164:ILE:HD11	2.50	0.41
1:D:165:ASP:C	1:D:166:LEU:HD22	2.45	0.41
1:D:417:GLN:HB3	1:D:581:SER:CB	2.48	0.41
1:E:73:VAL:HG22	1:E:74:VAL:N	2.35	0.41
1:E:139:LYS:HD2	1:E:172:VAL:CG1	2.50	0.41
1:F:37:LEU:HB3	1:F:38:ASP:H	1.67	0.41
1:G:204:TYR:O	1:G:279:MET:HE3	2.19	0.41
1:G:215:ILE:HD13	1:G:264:LEU:HD11	2.01	0.41
1:G:219:ARG:H	1:G:219:ARG:HE	1.68	0.41
1:G:234:ILE:O	1:G:235:LYS:C	2.63	0.41
1:G:379:CYS:C	1:G:381:SER:H	2.28	0.41
1:G:401:ARG:HH22	1:G:437:LEU:N	2.18	0.41
1:H:118:GLU:HA	1:H:121:ILE:HD12	2.01	0.41
1:H:560:LEU:HB3	1:H:593:THR:HG22	2.02	0.41
1:I:57:ARG:O	1:I:60:HIS:HB3	2.20	0.41
1:I:482:PHE:HD2	1:J:482:PHE:HD2	1.67	0.41
1:I:561:GLU:O	1:I:565:ILE:HG13	2.19	0.41
1:J:630:SER:O	1:J:634:GLU:HB2	2.20	0.41
1:K:411:VAL:HG23	1:K:412:GLN:N	2.35	0.41
1:L:9:PHE:CZ	1:L:82:GLU:HB2	2.55	0.41
1:A:25:GLY:HA3	1:A:47:ARG:NH1	2.35	0.41
1:A:34:HIS:CE1	1:A:37:LEU:HD23	2.55	0.41
1:A:185:LEU:HD21	1:A:188:LEU:CD2	2.51	0.41
1:A:411:VAL:HG12	1:A:590:ILE:HG21	2.03	0.41
1:B:171:ASP:HB3	1:B:173:ASP:OD1	2.20	0.41
1:B:270:GLU:N	1:B:271:PRO:HD2	2.36	0.41
1:B:480:LEU:HD22	1:B:518:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:PRO:HB2	1:C:86:LEU:CD1	2.50	0.41
1:D:118:GLU:HA	1:D:121:ILE:HD12	2.02	0.41
1:D:403:LEU:HD23	1:D:403:LEU:N	2.34	0.41
1:D:403:LEU:HD12	1:D:407:VAL:HG12	2.02	0.41
1:D:473:SER:HB3	1:D:527:ILE:HD11	2.01	0.41
1:E:53:LYS:HG3	1:E:54:ASN:OD1	2.20	0.41
1:E:410:ILE:O	1:E:587:VAL:HG22	2.20	0.41
1:E:452:MET:SD	1:E:611:LEU:HD22	2.61	0.41
1:E:478:ALA:HB2	1:F:475:GLN:HA	2.01	0.41
1:F:149:ASN:O	1:F:164:ILE:HG22	2.20	0.41
1:F:295:LEU:HD12	1:F:295:LEU:N	2.34	0.41
1:G:53:LYS:HG3	1:G:54:ASN:OD1	2.20	0.41
1:G:403:LEU:HD11	1:G:408:ASN:HA	2.03	0.41
1:G:622:LEU:N	1:G:623:PRO:CD	2.83	0.41
1:H:170:LYS:HD3	1:H:198:TYR:CZ	2.55	0.41
1:H:614:CYS:HA	1:H:617:LYS:HD3	2.02	0.41
1:I:507:MET:HA	1:I:510:ALA:HB3	2.03	0.41
1:I:563:ARG:HH12	2:h:2:GLC:C2	2.33	0.41
1:I:630:SER:O	1:I:634:GLU:HB2	2.20	0.41
1:J:272:MET:HA	1:J:272:MET:HE3	2.02	0.41
1:J:283:ASP:HB2	1:J:286:GLN:HB2	2.02	0.41
1:J:485:LYS:HE2	1:J:485:LYS:HB2	1.91	0.41
1:K:237:LYS:NZ	1:K:240:LYS:H	2.18	0.41
1:K:328:LEU:HD21	1:K:337:LEU:HD22	2.01	0.41
1:K:455:LEU:HD22	1:K:611:LEU:O	2.20	0.41
1:K:614:CYS:O	1:K:618:ILE:HG13	2.20	0.41
1:L:151:VAL:C	1:L:152:LEU:HD22	2.45	0.41
2:j:1:5LS:C6	2:j:2:GLC:C5	2.98	0.41
1:A:227:PRO:HG2	1:C:249:SER:HB2	2.02	0.41
1:A:229:THR:C	1:A:231:HIS:H	2.27	0.41
1:A:295:LEU:C	1:A:296:LYS:HG2	2.45	0.41
1:A:515:GLU:O	1:A:519:ILE:HG13	2.20	0.41
1:A:550:GLY:C	1:A:552:ARG:H	2.27	0.41
1:B:577:ASP:C	1:B:579:SER:H	2.28	0.41
1:C:34:HIS:CE1	1:C:37:LEU:HD23	2.55	0.41
1:C:117:LYS:O	1:C:121:ILE:HG13	2.20	0.41
1:C:244:ALA:HA	1:C:253:ARG:O	2.20	0.41
1:E:70:HIS:HB3	1:E:73:VAL:HG12	2.02	0.41
1:E:274:ASN:O	1:E:277:GLN:HB2	2.21	0.41
1:E:489:LEU:HD13	1:F:643:GLN:HG3	2.01	0.41
1:F:211:VAL:HG21	1:F:275:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:LYS:CD	1:F:277:GLN:HB3	2.50	0.41
1:F:517:LYS:HD2	1:F:642:MET:HE1	2.03	0.41
1:F:639:VAL:O	1:F:642:MET:HB2	2.19	0.41
1:G:142:HIS:ND1	1:G:169:ALA:HB2	2.35	0.41
1:H:26:PHE:HD2	1:H:47:ARG:HA	1.85	0.41
1:H:536:SER:O	1:H:540:GLU:HB2	2.21	0.41
1:I:152:LEU:HD13	1:I:161:HIS:HA	2.01	0.41
1:I:215:ILE:HD13	1:I:264:LEU:HD11	2.02	0.41
1:I:489:LEU:HD21	1:J:648:LYS:HG3	2.01	0.41
1:K:45:SER:HA	1:K:86:LEU:HD21	2.02	0.41
1:K:213:GLU:C	1:K:215:ILE:H	2.27	0.41
1:K:423:LEU:O	1:K:427:TRP:HB2	2.21	0.41
1:K:596:SER:O	1:K:600:VAL:HG22	2.20	0.41
1:K:653:LEU:CD1	1:K:656:ILE:HD11	2.50	0.41
1:L:311:LYS:CD	1:L:372:VAL:HG21	2.44	0.41
1:L:394:TYR:CE2	1:L:612:LEU:HD22	2.56	0.41
1:L:396:GLY:H	1:L:397:PRO:HD3	1.84	0.41
1:A:183:GLY:O	1:A:184:THR:C	2.63	0.41
1:A:233:LYS:O	1:A:236:LYS:HE3	2.20	0.41
1:C:143:ARG:H	1:C:143:ARG:HD3	1.86	0.41
1:C:237:LYS:O	1:C:237:LYS:HG3	2.20	0.41
1:D:53:LYS:HG3	1:D:54:ASN:OD1	2.19	0.41
1:D:342:GLU:HB2	1:D:352:GLN:HE22	1.85	0.41
1:D:366:LYS:HB3	1:D:367:PRO:HD2	2.01	0.41
1:D:393:VAL:HG13	1:D:609:SER:OG	2.19	0.41
1:D:596:SER:O	1:D:600:VAL:HG22	2.21	0.41
1:E:523:GLU:HA	1:E:526:VAL:HG23	2.03	0.41
1:E:567:LEU:CD2	1:E:589:ILE:HD13	2.51	0.41
1:E:596:SER:O	1:E:600:VAL:HG22	2.20	0.41
1:F:118:GLU:HA	1:F:121:ILE:HD12	2.01	0.41
1:G:69:ASN:ND2	1:G:75:LYS:HE2	2.35	0.41
1:G:143:ARG:H	1:G:143:ARG:HD3	1.86	0.41
1:G:234:ILE:O	1:G:237:LYS:N	2.54	0.41
1:G:249:SER:O	1:K:227:PRO:HG2	2.20	0.41
1:H:8:GLU:HB3	1:H:86:LEU:HG	2.02	0.41
1:H:69:ASN:CG	1:H:75:LYS:HE2	2.45	0.41
1:H:372:VAL:C	1:H:373:LEU:HD13	2.45	0.41
1:H:445:PHE:CG	1:H:551:ARG:HB2	2.55	0.41
1:I:53:LYS:HG3	1:I:54:ASN:OD1	2.20	0.41
1:I:219:ARG:CZ	1:I:224:HIS:H	2.33	0.41
1:J:614:CYS:HA	1:J:617:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:292:ASP:C	1:K:294:THR:H	2.28	0.41
1:K:510:ALA:O	1:K:645:LYS:HE2	2.21	0.41
1:K:639:VAL:O	1:K:642:MET:HB2	2.21	0.41
1:L:240:LYS:HD2	1:L:277:GLN:HB3	2.01	0.41
1:L:411:VAL:HG23	1:L:412:GLN:N	2.34	0.41
1:A:392:THR:O	1:A:612:LEU:HD23	2.20	0.41
1:A:658:CYS:HB3	1:B:501:GLY:HA2	2.03	0.41
1:B:141:ILE:CG2	1:B:170:LYS:HB2	2.49	0.41
1:B:313:VAL:HG21	1:B:371:CYS:HB2	2.03	0.41
1:B:507:MET:HA	1:B:510:ALA:HB3	2.02	0.41
1:B:577:ASP:HB2	1:B:578:HIS:H	1.58	0.41
1:C:158:LYS:HE3	1:C:377:ARG:HH21	1.85	0.41
1:C:189:ALA:C	1:C:191:GLU:H	2.29	0.41
1:C:501:GLY:HA2	1:D:658:CYS:HB3	2.02	0.41
1:C:536:SER:O	1:C:540:GLU:HB2	2.21	0.41
1:C:639:VAL:O	1:C:642:MET:HB2	2.20	0.41
1:D:328:LEU:HD21	1:D:337:LEU:HD22	2.01	0.41
1:D:515:GLU:O	1:D:519:ILE:HG13	2.19	0.41
1:E:589:ILE:O	1:E:593:THR:HG23	2.21	0.41
1:F:152:LEU:HD13	1:F:161:HIS:HA	2.02	0.41
1:F:168:TYR:CD1	1:F:182:VAL:HG22	2.56	0.41
1:F:168:TYR:CE1	1:F:182:VAL:HG22	2.56	0.41
1:F:452:MET:O	1:F:456:LEU:HG	2.19	0.41
1:G:328:LEU:HD21	1:G:337:LEU:HD22	2.03	0.41
1:G:452:MET:O	1:G:456:LEU:HG	2.20	0.41
1:G:560:LEU:HB3	1:G:593:THR:HG22	2.03	0.41
1:H:283:ASP:HB3	1:H:286:GLN:HB2	2.01	0.41
1:I:180:GLU:HB3	1:I:181:PHE:H	1.62	0.41
1:I:258:LEU:HB2	1:I:273:GLU:HG2	2.00	0.41
1:I:423:LEU:O	1:I:427:TRP:HB2	2.20	0.41
1:I:536:SER:O	1:I:540:GLU:HB2	2.21	0.41
1:I:596:SER:O	1:I:600:VAL:HG22	2.21	0.41
1:J:560:LEU:O	1:J:563:ARG:HB2	2.20	0.41
1:K:478:ALA:HB1	1:L:475:GLN:HA	2.03	0.41
1:K:485:LYS:O	1:K:485:LYS:HD3	2.21	0.41
1:K:487:ILE:HD11	1:K:514:MET:HE3	2.01	0.41
1:L:35:ARG:HG3	1:L:36:GLU:HG3	2.01	0.41
3:T:6:5TK:C6	3:T:7:5TH:O2	2.68	0.41
1:A:463:THR:HG21	1:A:538:HIS:HD2	1.86	0.41
1:B:414:SER:HA	1:B:587:VAL:HG21	2.02	0.41
1:C:21:LEU:HD12	4:C:701:5TL:CAJ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:HIS:HA	1:C:169:ALA:HB1	2.02	0.41
1:D:87:ILE:O	1:D:89:ASP:N	2.54	0.41
1:D:589:ILE:O	1:D:593:THR:HG23	2.20	0.41
1:E:95:MET:CE	1:E:164:ILE:HD11	2.51	0.41
1:E:118:GLU:HA	1:E:121:ILE:HD12	2.03	0.41
1:E:231:HIS:O	1:E:235:LYS:N	2.54	0.41
1:E:613:GLY:O	1:E:617:LYS:HG3	2.21	0.41
1:F:244:ALA:HA	1:F:253:ARG:O	2.20	0.41
1:F:411:VAL:HG23	1:F:412:GLN:N	2.35	0.41
1:F:596:SER:O	1:F:600:VAL:HG22	2.21	0.41
1:G:126:SER:HB2	1:G:308:LEU:CD1	2.51	0.41
1:H:53:LYS:HG3	1:H:54:ASN:OD1	2.21	0.41
1:H:630:SER:O	1:H:634:GLU:HB2	2.20	0.41
1:I:77:CYS:O	1:I:94:ALA:HB3	2.20	0.41
1:I:97:TYR:HA	4:I:701:5TL:OAO	2.21	0.41
1:I:142:HIS:HA	1:I:169:ALA:CB	2.50	0.41
1:J:190:PRO:HA	1:J:193:PHE:CD1	2.55	0.41
1:J:639:VAL:O	1:J:642:MET:HB2	2.20	0.41
1:K:97:TYR:HA	4:K:701:5TL:OAO	2.20	0.41
1:K:482:PHE:HB2	1:L:479:LYS:HZ3	1.85	0.41
1:K:589:ILE:O	1:K:593:THR:HG23	2.21	0.41
1:L:237:LYS:HD2	1:L:238:ASP:N	2.25	0.41
1:A:372:VAL:O	1:A:373:LEU:HD13	2.20	0.41
1:A:473:SER:CB	1:A:524:VAL:HA	2.44	0.41
1:A:475:GLN:HA	1:B:478:ALA:HB2	2.02	0.41
1:A:507:MET:HA	1:A:510:ALA:HB3	2.02	0.41
1:A:614:CYS:HA	1:A:617:LYS:HD3	2.01	0.41
1:B:34:HIS:ND1	1:B:37:LEU:HB2	2.35	0.41
1:B:258:LEU:HB2	1:B:273:GLU:HG2	2.03	0.41
1:B:481:GLU:C	1:B:483:PHE:H	2.29	0.41
1:B:595:GLN:CG	2:Q:2:GLC:H62	2.49	0.41
1:C:275:TRP:CH2	1:C:279:MET:HG3	2.56	0.41
1:C:342:GLU:HB2	1:C:352:GLN:HE22	1.86	0.41
1:C:574:ARG:NH1	1:C:575:PRO:HD2	2.36	0.41
1:C:589:ILE:O	1:C:593:THR:HG23	2.21	0.41
1:D:41:ILE:HG13	1:D:41:ILE:O	2.21	0.41
1:D:221:PHE:HB2	1:D:230:TRP:CZ2	2.54	0.41
1:D:485:LYS:HE2	1:D:485:LYS:HB2	1.92	0.41
1:F:151:VAL:C	1:F:152:LEU:HD22	2.46	0.41
1:F:215:ILE:HD13	1:F:264:LEU:HD11	2.02	0.41
1:G:83:LEU:O	1:G:84:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:PRO:C	1:G:300:CYS:N	2.76	0.41
1:H:165:ASP:O	1:H:166:LEU:HD13	2.20	0.41
1:H:481:GLU:C	1:H:483:PHE:H	2.29	0.41
1:I:189:ALA:C	1:I:191:GLU:H	2.29	0.41
1:I:249:SER:C	1:I:251:GLU:H	2.29	0.41
1:J:109:LYS:HB3	1:J:111:GLU:HG2	2.03	0.41
1:J:143:ARG:HD2	1:J:170:LYS:HG3	2.03	0.41
1:J:165:ASP:C	1:J:166:LEU:HD22	2.45	0.41
1:J:371:CYS:HB2	1:J:372:VAL:H	1.62	0.41
1:J:655:LYS:N	1:J:655:LYS:HD2	2.36	0.41
1:K:6:ASP:C	1:K:8:GLU:H	2.29	0.41
1:K:567:LEU:CD2	1:K:589:ILE:HD13	2.51	0.41
1:L:86:LEU:HD13	1:L:87:ILE:HG13	2.03	0.41
1:L:122:LEU:HD12	1:L:379:CYS:SG	2.60	0.41
1:L:324:ILE:HD12	1:L:324:ILE:N	2.33	0.41
1:A:43:ILE:HG23	1:A:93:LEU:C	2.46	0.41
1:A:143:ARG:H	1:A:143:ARG:HD3	1.86	0.41
1:A:536:SER:O	1:A:540:GLU:HB2	2.21	0.41
1:A:658:CYS:HB3	1:B:500:TYR:O	2.20	0.41
1:B:125:LEU:HD23	1:B:207:PHE:CZ	2.56	0.41
1:B:234:ILE:HD12	1:B:234:ILE:H	1.85	0.41
1:B:560:LEU:HB3	1:B:593:THR:HG22	2.02	0.41
1:B:579:SER:HB2	1:D:578:HIS:CE1	2.55	0.41
1:C:158:LYS:HE3	1:C:377:ARG:NH2	2.36	0.41
1:C:395:GLU:HG2	1:C:396:GLY:N	2.36	0.41
1:C:411:VAL:HG23	1:C:412:GLN:N	2.35	0.41
1:C:465:MET:O	1:C:469:LEU:HB2	2.21	0.41
1:C:541:ILE:CD1	1:C:618:ILE:HD11	2.51	0.41
1:C:630:SER:O	1:C:634:GLU:HB2	2.20	0.41
1:D:69:ASN:HD22	1:D:69:ASN:HA	1.61	0.41
1:D:536:SER:O	1:D:540:GLU:HB2	2.20	0.41
1:D:614:CYS:HA	1:D:617:LYS:HD3	2.02	0.41
1:E:83:LEU:O	1:E:92:LEU:HD13	2.20	0.41
1:E:143:ARG:H	1:E:143:ARG:HD3	1.85	0.41
1:E:507:MET:HA	1:E:510:ALA:HB3	2.03	0.41
1:E:535:MET:HA	1:E:538:HIS:HB3	2.03	0.41
1:F:199:THR:OG1	1:F:284:PRO:HB2	2.20	0.41
1:G:34:HIS:CE1	1:G:37:LEU:HD23	2.56	0.41
1:G:74:VAL:HG21	1:G:95:MET:HE3	2.02	0.41
1:G:237:LYS:HD2	1:G:241:CYS:HB3	2.03	0.41
1:G:237:LYS:NZ	1:G:240:LYS:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ARG:HG3	1:H:36:GLU:HG3	2.01	0.41
1:H:57:ARG:O	1:H:60:HIS:HB3	2.21	0.41
1:I:278:LEU:O	1:I:287:ARG:HG3	2.21	0.41
1:I:348:ASN:O	1:I:352:GLN:HG3	2.21	0.41
1:J:395:GLU:HG3	1:J:397:PRO:CD	2.45	0.41
1:J:549:TYR:H	1:J:552:ARG:HD2	1.85	0.41
1:K:70:HIS:HB2	1:K:134:TYR:CD2	2.55	0.41
1:K:79:VAL:CG1	1:K:83:LEU:HD13	2.46	0.41
1:K:143:ARG:H	1:K:143:ARG:HD3	1.85	0.41
1:K:193:PHE:CE2	1:K:231:HIS:NE2	2.86	0.41
1:K:535:MET:HA	1:K:538:HIS:HB3	2.03	0.41
1:K:536:SER:O	1:K:540:GLU:HB2	2.21	0.41
1:A:521:TYR:CD1	1:A:635:ALA:HB1	2.56	0.41
1:A:589:ILE:O	1:A:593:THR:HG23	2.21	0.41
1:B:204:TYR:O	1:B:279:MET:HE3	2.21	0.41
1:B:275:TRP:CH2	1:B:279:MET:HG3	2.56	0.41
1:B:296:LYS:NZ	1:B:296:LYS:HB3	2.35	0.41
1:B:613:GLY:O	1:B:617:LYS:HG3	2.20	0.41
1:B:653:LEU:CD1	1:B:656:ILE:HD11	2.50	0.41
1:C:274:ASN:O	1:C:277:GLN:HB2	2.21	0.41
1:C:318:MET:CE	1:C:447:GLY:HA3	2.50	0.41
1:C:319:THR:HG22	1:C:394:TYR:CE1	2.56	0.41
1:C:396:GLY:N	1:C:397:PRO:CD	2.80	0.41
1:C:423:LEU:O	1:C:427:TRP:HB2	2.20	0.41
1:C:455:LEU:HD22	1:C:611:LEU:O	2.21	0.41
1:C:540:GLU:O	1:C:544:LEU:HG	2.21	0.41
1:C:548:PRO:CB	1:C:552:ARG:HG3	2.49	0.41
1:D:125:LEU:HD23	1:D:207:PHE:CZ	2.56	0.41
1:D:204:TYR:O	1:D:279:MET:HE3	2.21	0.41
1:D:342:GLU:HB2	1:D:352:GLN:NE2	2.36	0.41
1:D:372:VAL:HG13	1:D:372:VAL:O	2.20	0.41
1:D:630:SER:O	1:D:634:GLU:HB2	2.21	0.41
1:E:37:LEU:HB3	1:E:38:ASP:H	1.67	0.41
1:E:42:ALA:C	1:E:43:ILE:HD12	2.46	0.41
1:E:221:PHE:HB2	1:E:230:TRP:CE2	2.56	0.41
1:E:258:LEU:HB2	1:E:273:GLU:HG2	2.02	0.41
1:E:289:GLY:N	1:E:290:PRO:CD	2.84	0.41
1:E:318:MET:HE1	1:E:444:LEU:O	2.20	0.41
1:E:342:GLU:HB2	1:E:352:GLN:HE22	1.85	0.41
1:E:424:ARG:HH11	1:E:572:LYS:HG2	1.86	0.41
1:E:560:LEU:HB3	1:E:593:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:630:SER:O	1:E:634:GLU:HB2	2.21	0.41
1:F:186:GLN:HG2	1:F:219:ARG:HD3	2.02	0.41
1:F:225:LEU:HD13	1:F:225:LEU:HA	1.91	0.41
1:G:189:ALA:C	1:G:191:GLU:H	2.29	0.41
1:G:273:GLU:O	1:G:277:GLN:HG3	2.20	0.41
1:G:403:LEU:HD12	1:G:407:VAL:HB	2.02	0.41
1:G:550:GLY:C	1:G:552:ARG:H	2.29	0.41
1:H:34:HIS:ND1	1:H:37:LEU:HB2	2.35	0.41
1:H:190:PRO:HA	1:H:193:PHE:CD1	2.56	0.41
1:H:342:GLU:HB2	1:H:352:GLN:HE22	1.86	0.41
1:I:37:LEU:HB3	1:I:38:ASP:H	1.68	0.41
1:I:64:ILE:O	1:I:67:LYS:HB3	2.20	0.41
1:I:117:LYS:HA	1:I:117:LYS:HD3	1.94	0.41
1:I:275:TRP:HZ2	1:I:304:MET:HE2	1.86	0.41
1:I:342:GLU:HB2	1:I:352:GLN:HE22	1.86	0.41
1:I:393:VAL:HG13	1:I:609:SER:OG	2.20	0.41
1:I:653:LEU:CD1	1:I:656:ILE:HD11	2.51	0.41
1:J:279:MET:SD	1:J:300:CYS:HB3	2.60	0.41
1:J:328:LEU:HD21	1:J:337:LEU:HD22	2.01	0.41
1:J:342:GLU:HB2	1:J:352:GLN:HE22	1.85	0.41
1:J:403:LEU:HD12	1:J:407:VAL:HG12	2.02	0.41
1:J:515:GLU:O	1:J:519:ILE:HG13	2.19	0.41
1:K:43:ILE:HG23	1:K:93:LEU:C	2.45	0.41
1:K:86:LEU:HB3	1:K:87:ILE:H	1.59	0.41
1:K:189:ALA:C	1:K:191:GLU:H	2.29	0.41
1:K:342:GLU:HB2	1:K:352:GLN:HE22	1.85	0.41
1:K:469:LEU:HD12	1:K:625:VAL:HG13	2.03	0.41
1:K:622:LEU:N	1:K:623:PRO:CD	2.84	0.41
1:L:106:LEU:HD11	1:L:152:LEU:HG	2.03	0.41
1:L:112:ASN:OD1	1:L:116:LEU:HA	2.21	0.41
1:L:118:GLU:HA	1:L:121:ILE:HD12	2.01	0.41
1:L:125:LEU:HD23	1:L:207:PHE:CZ	2.56	0.41
1:L:567:LEU:CD2	1:L:589:ILE:HD13	2.51	0.41
1:L:574:ARG:NH1	1:L:575:PRO:HD2	2.36	0.41
1:A:186:GLN:OE1	1:A:219:ARG:HD2	2.21	0.41
1:B:143:ARG:H	1:B:143:ARG:HD3	1.85	0.41
1:C:173:ASP:O	1:C:175:GLY:N	2.53	0.41
1:C:209:THR:HG22	1:C:280:LEU:HD11	2.03	0.41
1:C:279:MET:C	1:C:280:LEU:HD22	2.46	0.41
1:C:317:ASN:C	1:C:319:THR:H	2.29	0.41
1:C:338:GLN:HA	1:C:341:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:HIS:ND1	1:D:37:LEU:HB2	2.35	0.41
1:D:408:ASN:ND2	1:F:26:PHE:HA	2.36	0.41
1:E:213:GLU:C	1:E:215:ILE:H	2.28	0.41
1:F:95:MET:CE	1:F:164:ILE:HD11	2.50	0.41
1:F:420:ILE:HG21	1:F:578:HIS:H	1.86	0.41
1:G:7:PRO:C	1:G:9:PHE:H	2.29	0.41
1:G:272:MET:HA	1:G:272:MET:HE3	2.03	0.41
1:G:423:LEU:O	1:G:427:TRP:HB2	2.21	0.41
1:G:627:VAL:HG12	1:G:631:ASN:ND2	2.35	0.41
1:H:103:LEU:HB2	1:H:150:ILE:HB	2.03	0.41
1:H:219:ARG:HD2	1:H:223:HIS:HA	2.03	0.41
1:H:473:SER:OG	1:H:524:VAL:HG13	2.20	0.41
1:H:507:MET:CE	1:H:653:LEU:HD13	2.51	0.41
1:H:627:VAL:HG12	1:H:631:ASN:ND2	2.36	0.41
1:H:653:LEU:CD1	1:H:656:ILE:HD11	2.50	0.41
1:J:41:ILE:HG13	1:J:41:ILE:O	2.21	0.41
1:K:47:ARG:O	1:K:87:ILE:HB	2.20	0.41
1:K:85:ILE:HB	1:K:90:VAL:H	1.86	0.41
1:K:338:GLN:HA	1:K:341:ILE:HD12	2.03	0.41
1:L:225:LEU:O	1:L:226:GLN:C	2.63	0.41
1:L:418:LEU:O	1:L:581:SER:HA	2.21	0.41
1:L:653:LEU:CD1	1:L:656:ILE:HD11	2.51	0.41
1:A:452:MET:HE3	1:A:452:MET:HA	2.03	0.40
1:B:413:ASP:CG	1:B:416:ILE:HB	2.46	0.40
1:B:455:LEU:HD12	1:B:618:ILE:HD12	2.03	0.40
1:B:465:MET:SD	1:B:625:VAL:HG11	2.61	0.40
1:C:53:LYS:HG3	1:C:54:ASN:OD1	2.20	0.40
1:C:125:LEU:HD23	1:C:207:PHE:CZ	2.56	0.40
1:D:320:SER:C	1:D:398:PHE:HB3	2.46	0.40
1:D:507:MET:HA	1:D:510:ALA:HB3	2.03	0.40
1:E:57:ARG:O	1:E:60:HIS:HB3	2.21	0.40
1:E:244:ALA:HA	1:E:253:ARG:O	2.22	0.40
1:E:563:ARG:HB3	1:E:589:ILE:CG1	2.52	0.40
1:F:7:PRO:CG	1:F:17:MET:HE1	2.48	0.40
1:F:32:TYR:HD2	1:F:43:ILE:H	1.69	0.40
1:F:57:ARG:O	1:F:60:HIS:HB3	2.20	0.40
1:F:348:ASN:O	1:F:352:GLN:HG3	2.21	0.40
1:G:29:VAL:HG13	1:G:43:ILE:C	2.47	0.40
1:G:383:MET:SD	1:G:385:TYR:CE1	3.14	0.40
1:G:639:VAL:O	1:G:642:MET:HB2	2.21	0.40
1:H:323:ILE:HG23	1:H:383:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:507:MET:HA	1:H:510:ALA:HB3	2.02	0.40
1:H:535:MET:HA	1:H:538:HIS:HB3	2.03	0.40
1:I:50:LEU:HD13	1:I:90:VAL:HG21	2.02	0.40
1:I:270:GLU:N	1:I:271:PRO:HD2	2.35	0.40
1:J:34:HIS:ND1	1:J:37:LEU:HB2	2.35	0.40
1:J:657:ALA:C	1:J:659:THR:H	2.30	0.40
1:K:478:ALA:HB2	1:L:475:GLN:HA	2.02	0.40
1:L:270:GLU:N	1:L:271:PRO:HD2	2.36	0.40
1:L:355:LEU:HD12	1:L:355:LEU:N	2.36	0.40
1:A:29:VAL:HG13	1:A:43:ILE:C	2.47	0.40
1:A:89:ASP:O	1:A:90:VAL:HG13	2.21	0.40
1:A:588:LYS:HB3	1:A:589:ILE:HD12	2.03	0.40
1:B:43:ILE:HG23	1:B:93:LEU:C	2.47	0.40
1:B:57:ARG:O	1:B:60:HIS:HB3	2.21	0.40
1:B:237:LYS:HD3	1:B:238:ASP:O	2.20	0.40
1:B:317:ASN:HD21	1:B:319:THR:HG23	1.86	0.40
1:B:342:GLU:HB2	1:B:352:GLN:HE22	1.87	0.40
1:B:574:ARG:NH1	1:B:575:PRO:HD2	2.36	0.40
1:C:65:MET:HB3	1:C:76:ALA:HB2	2.03	0.40
1:C:147:PRO:HB2	1:C:148:GLU:OE2	2.21	0.40
1:C:270:GLU:N	1:C:271:PRO:HD2	2.35	0.40
1:C:284:PRO:HG2	1:C:285:GLN:H	1.86	0.40
1:C:473:SER:HA	1:C:632:ILE:HG21	2.04	0.40
1:C:567:LEU:CD2	1:C:589:ILE:HD13	2.52	0.40
1:D:72:ASN:HD21	1:D:127:ASP:HA	1.87	0.40
1:D:639:VAL:O	1:D:642:MET:HB2	2.20	0.40
1:D:657:ALA:C	1:D:659:THR:H	2.30	0.40
1:F:76:ALA:HA	1:F:94:ALA:O	2.20	0.40
1:F:342:GLU:HB2	1:F:352:GLN:NE2	2.36	0.40
1:G:448:GLN:OE1	1:G:549:TYR:HB3	2.22	0.40
1:G:482:PHE:HD2	1:H:482:PHE:HD2	1.69	0.40
1:G:630:SER:O	1:G:634:GLU:HB2	2.22	0.40
1:H:574:ARG:HH11	1:H:575:PRO:HD2	1.85	0.40
1:I:34:HIS:ND1	1:I:37:LEU:HB2	2.35	0.40
1:I:455:LEU:HD22	1:I:611:LEU:O	2.21	0.40
1:I:588:LYS:HB3	1:I:589:ILE:HD12	2.03	0.40
1:J:617:LYS:O	1:J:621:LEU:HG	2.22	0.40
1:K:37:LEU:HB3	1:K:38:ASP:H	1.65	0.40
1:K:42:ALA:C	1:K:43:ILE:HD12	2.47	0.40
1:K:95:MET:HE2	1:K:164:ILE:HD11	2.02	0.40
1:K:223:HIS:O	1:K:225:LEU:HD23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:507:MET:HA	1:K:510:ALA:HB3	2.03	0.40
1:L:37:LEU:HB3	1:L:38:ASP:H	1.67	0.40
1:L:85:ILE:O	1:L:90:VAL:HG23	2.21	0.40
1:L:215:ILE:HG21	1:L:258:LEU:HD21	2.04	0.40
1:L:265:CYS:SG	1:L:267:LEU:HB2	2.61	0.40
1:L:373:LEU:O	1:L:378:GLY:HA3	2.22	0.40
1:L:627:VAL:HG12	1:L:631:ASN:ND2	2.36	0.40
1:A:244:ALA:HA	1:A:253:ARG:O	2.21	0.40
1:A:577:ASP:H	1:C:579:SER:CB	2.31	0.40
1:A:644:GLY:O	1:A:648:LYS:HB2	2.22	0.40
1:B:151:VAL:C	1:B:152:LEU:HD22	2.46	0.40
1:B:213:GLU:C	1:B:215:ILE:H	2.29	0.40
1:B:237:LYS:NZ	1:B:281:ASN:HA	2.35	0.40
1:B:238:ASP:CB	1:B:239:PRO:HD2	2.51	0.40
1:B:445:PHE:HA	1:B:604:LEU:HD21	2.03	0.40
1:B:536:SER:O	1:B:540:GLU:HB2	2.21	0.40
1:B:563:ARG:HB3	1:B:589:ILE:CG1	2.51	0.40
1:B:589:ILE:O	1:B:593:THR:HG23	2.22	0.40
1:B:596:SER:O	1:B:600:VAL:HG22	2.21	0.40
1:B:655:LYS:HD2	1:B:655:LYS:N	2.36	0.40
1:C:176:GLU:O	1:C:177:LEU:HB2	2.21	0.40
1:C:317:ASN:HD21	1:C:319:THR:HG23	1.86	0.40
1:D:109:LYS:HB3	1:D:111:GLU:HG2	2.04	0.40
1:D:324:ILE:HD12	1:D:324:ILE:N	2.32	0.40
1:D:655:LYS:N	1:D:655:LYS:HD2	2.36	0.40
1:E:32:TYR:HD2	1:E:43:ILE:H	1.70	0.40
1:E:171:ASP:OD1	1:E:172:VAL:N	2.52	0.40
1:F:523:GLU:HA	1:F:526:VAL:HG23	2.04	0.40
1:F:550:GLY:HA3	1:F:604:LEU:HD13	2.02	0.40
1:G:42:ALA:C	1:G:43:ILE:HD12	2.46	0.40
1:G:314:HIS:O	1:G:315:ILE:HD13	2.21	0.40
1:H:484:HIS:O	1:H:488:GLN:HG2	2.22	0.40
1:I:42:ALA:C	1:I:43:ILE:HD12	2.46	0.40
1:I:125:LEU:HD23	1:I:207:PHE:CZ	2.56	0.40
1:I:392:THR:HG22	1:I:616:GLN:NE2	2.35	0.40
1:I:560:LEU:HB3	1:I:593:THR:HG22	2.02	0.40
1:J:222:LEU:HD12	1:J:225:LEU:HD23	2.03	0.40
1:J:653:LEU:CD1	1:J:656:ILE:HD11	2.51	0.40
1:K:128:ILE:O	1:K:132:ILE:HG22	2.21	0.40
1:K:165:ASP:O	1:K:166:LEU:HD13	2.21	0.40
1:L:143:ARG:C	1:L:145:LEU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:258:LEU:HB2	1:L:273:GLU:HG2	2.02	0.40
1:L:342:GLU:HB2	1:L:352:GLN:HE22	1.87	0.40
1:L:473:SER:HA	1:L:632:ILE:HG21	2.03	0.40
1:A:73:VAL:HA	1:A:162:LYS:HB3	2.03	0.40
1:A:222:LEU:N	1:A:222:LEU:HD22	2.36	0.40
1:A:354:LEU:HB3	1:A:384:VAL:CG1	2.51	0.40
1:A:396:GLY:HA2	1:A:398:PHE:CE2	2.57	0.40
1:A:481:GLU:C	1:A:483:PHE:H	2.30	0.40
1:A:579:SER:OG	1:E:577:ASP:HB2	2.22	0.40
1:A:639:VAL:O	1:A:642:MET:HB2	2.22	0.40
1:B:41:ILE:O	1:B:41:ILE:HG13	2.21	0.40
1:B:182:VAL:HG12	1:B:183:GLY:H	1.86	0.40
1:B:630:SER:O	1:B:634:GLU:HB2	2.21	0.40
1:C:43:ILE:HG23	1:C:93:LEU:C	2.47	0.40
1:D:95:MET:HE2	1:D:164:ILE:HD11	2.02	0.40
1:D:272:MET:HA	1:D:272:MET:HE3	2.04	0.40
1:E:29:VAL:HG12	1:E:30:CYS:N	2.37	0.40
1:E:97:TYR:HA	4:E:701:5TL:OAO	2.22	0.40
1:E:355:LEU:N	1:E:355:LEU:HD12	2.36	0.40
1:E:653:LEU:CD1	1:E:656:ILE:HD11	2.51	0.40
1:F:258:LEU:HB2	1:F:273:GLU:HG2	2.02	0.40
1:F:653:LEU:CD1	1:F:656:ILE:HD11	2.51	0.40
1:G:536:SER:O	1:G:540:GLU:HB2	2.21	0.40
1:H:213:GLU:C	1:H:215:ILE:H	2.29	0.40
1:H:403:LEU:HD12	1:H:407:VAL:HG12	2.04	0.40
1:I:226:GLN:O	1:I:230:TRP:HB2	2.21	0.40
1:I:271:PRO:HB2	1:I:307:ILE:HD11	2.02	0.40
1:I:627:VAL:HG12	1:I:631:ASN:ND2	2.36	0.40
1:J:98:CYS:HA	1:J:153:GLN:NE2	2.36	0.40
1:J:342:GLU:HB2	1:J:352:GLN:NE2	2.37	0.40
1:J:396:GLY:N	1:J:397:PRO:CD	2.80	0.40
1:J:473:SER:O	1:J:524:VAL:HG22	2.22	0.40
1:K:25:GLY:HA3	1:K:47:ARG:NH1	2.36	0.40
1:K:34:HIS:ND1	1:K:37:LEU:HB2	2.36	0.40
1:K:46:CYS:H	1:K:86:LEU:CD2	2.25	0.40
1:K:317:ASN:ND2	1:K:319:THR:HG23	2.35	0.40
1:L:465:MET:O	1:L:469:LEU:HB2	2.21	0.40
1:L:536:SER:O	1:L:540:GLU:HB2	2.20	0.40
1:L:549:TYR:H	1:L:552:ARG:HD2	1.87	0.40
2:R:1:5LS:C1	2:R:3:PDX:H5	2.52	0.40
1:A:234:ILE:HA	1:A:236:LYS:HZ2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ILE:HD11	1:A:511:TRP:O	2.21	0.40
1:B:165:ASP:C	1:B:166:LEU:HD22	2.46	0.40
1:C:237:LYS:HD3	1:C:282:TRP:H	1.86	0.40
1:C:363:ASP:HB3	1:C:370:GLN:NE2	2.34	0.40
1:D:588:LYS:HB3	1:D:589:ILE:HD12	2.04	0.40
1:E:128:ILE:O	1:E:132:ILE:HG22	2.21	0.40
1:F:427:TRP:CZ3	1:F:567:LEU:HB3	2.55	0.40
1:F:630:SER:O	1:F:634:GLU:HB2	2.21	0.40
1:G:288:GLY:O	1:G:289:GLY:C	2.64	0.40
1:G:481:GLU:C	1:G:483:PHE:H	2.30	0.40
1:H:143:ARG:C	1:H:145:LEU:H	2.29	0.40
1:H:317:ASN:C	1:H:319:THR:H	2.30	0.40
1:H:465:MET:O	1:H:469:LEU:HB2	2.20	0.40
1:H:596:SER:O	1:H:600:VAL:HG22	2.21	0.40
1:I:244:ALA:HA	1:I:253:ARG:O	2.21	0.40
1:J:222:LEU:HD13	1:J:222:LEU:HA	1.89	0.40
1:K:126:SER:HB2	1:K:308:LEU:CD1	2.51	0.40
1:K:239:PRO:O	1:K:240:LYS:HB2	2.20	0.40
1:K:334:LEU:HD21	1:K:364:PRO:HA	2.03	0.40
1:K:420:ILE:HD11	1:K:571:LEU:HG	2.03	0.40
1:K:523:GLU:HA	1:K:526:VAL:HG23	2.04	0.40
1:L:79:VAL:O	1:L:79:VAL:HG23	2.22	0.40
1:L:313:VAL:HG21	1:L:371:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	653/655 (100%)	504 (77%)	113 (17%)	36 (6%)	1	15
1	B	653/655 (100%)	514 (79%)	106 (16%)	33 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	653/655 (100%)	511 (78%)	105 (16%)	37 (6%)	1	14
1	D	653/655 (100%)	515 (79%)	104 (16%)	34 (5%)	1	15
1	E	653/655 (100%)	511 (78%)	104 (16%)	38 (6%)	1	14
1	F	653/655 (100%)	505 (77%)	111 (17%)	37 (6%)	1	14
1	G	653/655 (100%)	508 (78%)	114 (18%)	31 (5%)	2	17
1	H	653/655 (100%)	507 (78%)	99 (15%)	47 (7%)	1	11
1	I	653/655 (100%)	502 (77%)	110 (17%)	41 (6%)	1	13
1	J	653/655 (100%)	515 (79%)	98 (15%)	40 (6%)	1	13
1	K	653/655 (100%)	506 (78%)	105 (16%)	42 (6%)	1	13
1	L	653/655 (100%)	500 (77%)	113 (17%)	40 (6%)	1	13
All	All	7836/7860 (100%)	6098 (78%)	1282 (16%)	456 (6%)	1	14

All (456) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	521	TYR
1	A	549	TYR
1	B	48	LEU
1	B	173	ASP
1	B	180	GLU
1	B	521	TYR
1	C	7	PRO
1	C	48	LEU
1	C	180	GLU
1	C	186	GLN
1	C	237	LYS
1	C	521	TYR
1	C	549	TYR
1	D	8	GLU
1	D	48	LEU
1	D	282	TRP
1	D	521	TYR
1	E	48	LEU
1	E	89	ASP
1	E	173	ASP
1	E	180	GLU
1	E	186	GLN

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Mol	Chain	Res	Type
1	E	521	TYR
1	F	48	LEU
1	F	70	HIS
1	F	521	TYR
1	F	579	SER
1	G	48	LEU
1	G	395	GLU
1	G	521	TYR
1	H	8	GLU
1	H	14	PRO
1	H	48	LEU
1	H	80	PRO
1	H	87	ILE
1	H	172	VAL
1	H	173	ASP
1	H	180	GLU
1	H	365	ARG
1	H	521	TYR
1	I	48	LEU
1	I	184	THR
1	I	370	GLN
1	I	521	TYR
1	I	549	TYR
1	J	48	LEU
1	J	395	GLU
1	J	521	TYR
1	J	549	TYR
1	K	14	PRO
1	K	48	LEU
1	K	186	GLN
1	K	365	ARG
1	K	521	TYR
1	L	14	PRO
1	L	48	LEU
1	L	80	PRO
1	L	521	TYR
1	A	28	ASN
1	A	47	ARG
1	A	86	LEU
1	A	237	LYS
1	A	583	SER
1	B	28	ASN

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Mol	Chain	Res	Type
1	B	47	ARG
1	B	175	GLY
1	B	549	TYR
1	B	575	PRO
1	B	583	SER
1	C	28	ASN
1	C	47	ARG
1	C	174	GLN
1	C	367	PRO
1	C	377	ARG
1	C	395	GLU
1	C	501	GLY
1	C	583	SER
1	D	28	ASN
1	D	47	ARG
1	D	89	ASP
1	D	186	GLN
1	D	237	LYS
1	D	579	SER
1	D	583	SER
1	E	14	PRO
1	E	28	ASN
1	E	222	LEU
1	E	579	SER
1	E	583	SER
1	F	28	ASN
1	F	47	ARG
1	F	365	ARG
1	F	583	SER
1	G	14	PRO
1	G	28	ASN
1	G	73	VAL
1	G	91	PRO
1	G	367	PRO
1	G	579	SER
1	G	583	SER
1	H	28	ASN
1	H	47	ARG
1	H	78	ASP
1	H	186	GLN
1	H	233	LYS
1	H	575	PRO

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Mol	Chain	Res	Type
1	H	579	SER
1	H	583	SER
1	I	11	ALA
1	I	28	ASN
1	I	47	ARG
1	I	83	LEU
1	I	237	LYS
1	I	365	ARG
1	I	395	GLU
1	I	579	SER
1	I	583	SER
1	J	28	ASN
1	J	87	ILE
1	J	173	ASP
1	J	175	GLY
1	J	186	GLN
1	J	579	SER
1	J	583	SER
1	K	28	ASN
1	K	172	VAL
1	K	222	LEU
1	K	237	LYS
1	K	395	GLU
1	K	549	TYR
1	K	579	SER
1	K	583	SER
1	L	28	ASN
1	L	47	ARG
1	L	73	VAL
1	L	77	CYS
1	L	81	GLU
1	L	174	GLN
1	L	365	ARG
1	L	367	PRO
1	L	400	SER
1	L	579	SER
1	L	583	SER
1	A	13	GLY
1	A	14	PRO
1	A	71	ALA
1	A	165	ASP
1	A	174	GLN

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Mol	Chain	Res	Type
1	A	361	SER
1	A	362	LEU
1	A	550	GLY
1	A	575	PRO
1	A	579	SER
1	A	588	LYS
1	B	165	ASP
1	B	169	ALA
1	B	186	GLN
1	B	361	SER
1	B	362	LEU
1	B	365	ARG
1	B	588	LYS
1	C	14	PRO
1	C	80	PRO
1	C	165	ASP
1	C	361	SER
1	C	362	LEU
1	C	505	GLU
1	C	550	GLY
1	C	588	LYS
1	D	86	LEU
1	D	88	HIS
1	D	165	ASP
1	D	177	LEU
1	D	361	SER
1	D	362	LEU
1	D	382	TYR
1	D	395	GLU
1	D	575	PRO
1	D	588	LYS
1	E	13	GLY
1	E	47	ARG
1	E	165	ASP
1	E	169	ALA
1	E	182	VAL
1	E	237	LYS
1	E	290	PRO
1	E	361	SER
1	E	362	LEU
1	E	365	ARG
1	E	396	GLY

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Mol	Chain	Res	Type
1	E	575	PRO
1	E	588	LYS
1	F	9	PHE
1	F	69	ASN
1	F	88	HIS
1	F	165	ASP
1	F	180	GLU
1	F	237	LYS
1	F	290	PRO
1	F	292	ASP
1	F	361	SER
1	F	362	LEU
1	F	367	PRO
1	F	575	PRO
1	F	588	LYS
1	G	9	PHE
1	G	47	ARG
1	G	80	PRO
1	G	165	ASP
1	G	237	LYS
1	G	361	SER
1	G	362	LEU
1	G	575	PRO
1	G	588	LYS
1	H	11	ALA
1	H	165	ASP
1	H	237	LYS
1	H	290	PRO
1	H	361	SER
1	H	362	LEU
1	H	367	PRO
1	H	549	TYR
1	H	588	LYS
1	I	9	PHE
1	I	80	PRO
1	I	165	ASP
1	I	361	SER
1	I	362	LEU
1	I	505	GLU
1	I	588	LYS
1	J	47	ARG
1	J	88	HIS

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Mol	Chain	Res	Type
1	J	165	ASP
1	J	180	GLU
1	J	224	HIS
1	J	237	LYS
1	J	361	SER
1	J	362	LEU
1	J	400	SER
1	J	550	GLY
1	J	575	PRO
1	J	588	LYS
1	K	47	ARG
1	K	165	ASP
1	K	179	THR
1	K	290	PRO
1	K	361	SER
1	K	362	LEU
1	K	575	PRO
1	K	588	LYS
1	L	8	GLU
1	L	165	ASP
1	L	180	GLU
1	L	361	SER
1	L	362	LEU
1	L	395	GLU
1	L	575	PRO
1	L	588	LYS
1	A	8	GLU
1	A	91	PRO
1	A	157	GLY
1	A	186	GLN
1	A	284	PRO
1	A	414	SER
1	B	237	LYS
1	B	414	SER
1	C	85	ILE
1	C	157	GLY
1	C	365	ARG
1	C	414	SER
1	C	575	PRO
1	D	14	PRO
1	D	157	GLY
1	D	290	PRO

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Mol	Chain	Res	Type
1	D	414	SER
1	E	157	GLY
1	E	414	SER
1	F	113	CYS
1	F	173	ASP
1	F	381	SER
1	F	396	GLY
1	F	414	SER
1	G	157	GLY
1	G	414	SER
1	H	9	PHE
1	H	414	SER
1	H	576	SER
1	I	10	GLY
1	I	70	HIS
1	I	157	GLY
1	I	381	SER
1	I	414	SER
1	J	157	GLY
1	J	284	PRO
1	J	414	SER
1	K	77	CYS
1	K	80	PRO
1	K	89	ASP
1	K	157	GLY
1	K	180	GLU
1	K	367	PRO
1	K	383	MET
1	K	414	SER
1	K	576	SER
1	L	222	LEU
1	L	237	LYS
1	L	290	PRO
1	L	414	SER
1	L	576	SER
1	A	290	PRO
1	A	367	PRO
1	A	396	GLY
1	A	522	ALA
1	B	83	LEU
1	B	157	GLY
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	182	VAL
1	B	312	ILE
1	B	379	CYS
1	B	522	ALA
1	C	182	VAL
1	C	312	ILE
1	C	522	ALA
1	D	37	LEU
1	D	312	ILE
1	D	522	ALA
1	E	88	HIS
1	E	367	PRO
1	E	395	GLU
1	E	522	ALA
1	F	117	LYS
1	F	157	GLY
1	F	312	ILE
1	F	522	ALA
1	G	84	ASN
1	G	178	CYS
1	G	522	ALA
1	H	10	GLY
1	H	77	CYS
1	H	157	GLY
1	H	182	VAL
1	H	312	ILE
1	H	522	ALA
1	I	85	ILE
1	I	290	PRO
1	I	312	ILE
1	I	504	SER
1	I	522	ALA
1	I	575	PRO
1	I	576	SER
1	J	14	PRO
1	J	37	LEU
1	J	290	PRO
1	J	312	ILE
1	J	379	CYS
1	J	522	ALA
1	K	312	ILE
1	K	400	SER

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Mol	Chain	Res	Type
1	K	522	ALA
1	K	550	GLY
1	L	84	ASN
1	L	85	ILE
1	L	157	GLY
1	L	522	ALA
1	A	312	ILE
1	B	37	LEU
1	C	37	LEU
1	E	37	LEU
1	E	312	ILE
1	F	14	PRO
1	F	284	PRO
1	G	312	ILE
1	H	37	LEU
1	H	89	ASP
1	I	37	LEU
1	I	175	GLY
1	I	377	ARG
1	I	550	GLY
1	J	13	GLY
1	K	37	LEU
1	K	182	VAL
1	K	399	ALA
1	L	37	LEU
1	L	312	ILE
1	A	182	VAL
1	A	197	PRO
1	B	197	PRO
1	B	550	GLY
1	C	197	PRO
1	D	197	PRO
1	E	197	PRO
1	F	197	PRO
1	G	197	PRO
1	H	13	GLY
1	H	197	PRO
1	I	197	PRO
1	J	80	PRO
1	J	197	PRO
1	J	376	VAL
1	K	197	PRO

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Mol	Chain	Res	Type
1	L	10	GLY
1	L	197	PRO
1	B	290	PRO
1	E	85	ILE
1	E	115	GLY
1	H	550	GLY
1	A	155	VAL
1	B	155	VAL
1	C	91	PRO
1	C	155	VAL
1	C	239	PRO
1	D	80	PRO
1	D	155	VAL
1	E	155	VAL
1	G	155	VAL
1	G	376	VAL
1	H	155	VAL
1	I	155	VAL
1	J	10	GLY
1	J	375	GLY
1	K	73	VAL
1	K	155	VAL
1	L	155	VAL
1	A	121	ILE
1	A	175	GLY
1	B	22	GLY
1	B	121	ILE
1	C	22	GLY
1	E	121	ILE
1	F	22	GLY
1	F	121	ILE
1	F	155	VAL
1	F	550	GLY
1	G	259	PRO
1	G	550	GLY
1	H	22	GLY
1	H	121	ILE
1	H	259	PRO
1	H	376	VAL
1	J	22	GLY
1	J	155	VAL
1	K	121	ILE

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Mol	Chain	Res	Type
1	L	22	GLY
1	L	182	VAL
1	A	259	PRO
1	D	22	GLY
1	D	121	ILE
1	D	259	PRO
1	E	22	GLY
1	G	121	ILE
1	H	397	PRO
1	I	22	GLY
1	I	259	PRO
1	K	22	GLY
1	L	121	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	589/589 (100%)	564 (96%)	25 (4%)	26	48
1	B	589/589 (100%)	562 (95%)	27 (5%)	24	46
1	C	589/589 (100%)	568 (96%)	21 (4%)	31	52
1	D	589/589 (100%)	573 (97%)	16 (3%)	39	59
1	E	589/589 (100%)	566 (96%)	23 (4%)	28	50
1	F	589/589 (100%)	567 (96%)	22 (4%)	30	51
1	G	589/589 (100%)	561 (95%)	28 (5%)	23	45
1	H	589/589 (100%)	565 (96%)	24 (4%)	27	49
1	I	589/589 (100%)	570 (97%)	19 (3%)	34	55
1	J	589/589 (100%)	569 (97%)	20 (3%)	32	54
1	K	589/589 (100%)	570 (97%)	19 (3%)	34	55
1	L	589/589 (100%)	564 (96%)	25 (4%)	26	48
All	All	7068/7068 (100%)	6799 (96%)	269 (4%)	29	51

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	56	GLU
1	A	64	ILE
1	A	65	MET
1	A	81	GLU
1	A	83	LEU
1	A	90	VAL
1	A	113	CYS
1	A	170	LYS
1	A	180	GLU
1	A	185	LEU
1	A	191	GLU
1	A	219	ARG
1	A	223	HIS
1	A	231	HIS
1	A	236	LYS
1	A	295	LEU
1	A	371	CYS
1	A	373	LEU
1	A	377	ARG
1	A	485	LYS
1	A	543	GLU
1	A	574	ARG
1	A	601	LEU
1	A	646	ARG
1	B	9	PHE
1	B	48	LEU
1	B	56	GLU
1	B	65	MET
1	B	81	GLU
1	B	83	LEU
1	B	88	HIS
1	B	90	VAL
1	B	176	GLU
1	B	185	LEU
1	B	191	GLU
1	B	219	ARG
1	B	230	TRP
1	B	234	ILE
1	B	238	ASP
1	B	240	LYS
1	B	296	LYS

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Mol	Chain	Res	Type
1	B	297	GLN
1	B	366	LYS
1	B	395	GLU
1	B	401	ARG
1	B	485	LYS
1	B	543	GLU
1	B	574	ARG
1	B	577	ASP
1	B	601	LEU
1	B	646	ARG
1	C	48	LEU
1	C	56	GLU
1	C	64	ILE
1	C	65	MET
1	C	82	GLU
1	C	83	LEU
1	C	85	ILE
1	C	90	VAL
1	C	178	CYS
1	C	182	VAL
1	C	185	LEU
1	C	191	GLU
1	C	297	GLN
1	C	366	LYS
1	C	377	ARG
1	C	485	LYS
1	C	543	GLU
1	C	574	ARG
1	C	579	SER
1	C	601	LEU
1	C	646	ARG
1	D	48	LEU
1	D	56	GLU
1	D	65	MET
1	D	174	GLN
1	D	185	LEU
1	D	191	GLU
1	D	225	LEU
1	D	237	LYS
1	D	370	GLN
1	D	401	ARG
1	D	485	LYS

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Mol	Chain	Res	Type
1	D	543	GLU
1	D	544	LEU
1	D	574	ARG
1	D	601	LEU
1	D	646	ARG
1	E	48	LEU
1	E	56	GLU
1	E	65	MET
1	E	69	ASN
1	E	82	GLU
1	E	83	LEU
1	E	86	LEU
1	E	177	LEU
1	E	185	LEU
1	E	186	GLN
1	E	191	GLU
1	E	222	LEU
1	E	234	ILE
1	E	236	LYS
1	E	238	ASP
1	E	371	CYS
1	E	373	LEU
1	E	395	GLU
1	E	485	LYS
1	E	543	GLU
1	E	574	ARG
1	E	601	LEU
1	E	646	ARG
1	F	48	LEU
1	F	56	GLU
1	F	81	GLU
1	F	87	ILE
1	F	116	LEU
1	F	176	GLU
1	F	184	THR
1	F	185	LEU
1	F	191	GLU
1	F	222	LEU
1	F	225	LEU
1	F	231	HIS
1	F	232	GLU
1	F	236	LYS

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Mol	Chain	Res	Type
1	F	240	LYS
1	F	286	GLN
1	F	371	CYS
1	F	485	LYS
1	F	543	GLU
1	F	574	ARG
1	F	601	LEU
1	F	646	ARG
1	G	48	LEU
1	G	56	GLU
1	G	64	ILE
1	G	65	MET
1	G	84	ASN
1	G	86	LEU
1	G	90	VAL
1	G	170	LYS
1	G	173	ASP
1	G	174	GLN
1	G	191	GLU
1	G	219	ARG
1	G	222	LEU
1	G	225	LEU
1	G	231	HIS
1	G	233	LYS
1	G	234	ILE
1	G	281	ASN
1	G	370	GLN
1	G	373	LEU
1	G	383	MET
1	G	395	GLU
1	G	485	LYS
1	G	503	SER
1	G	543	GLU
1	G	574	ARG
1	G	601	LEU
1	G	646	ARG
1	H	9	PHE
1	H	48	LEU
1	H	56	GLU
1	H	83	LEU
1	H	85	ILE
1	H	86	LEU

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Mol	Chain	Res	Type
1	H	90	VAL
1	H	114	CYS
1	H	171	ASP
1	H	173	ASP
1	H	191	GLU
1	H	219	ARG
1	H	224	HIS
1	H	235	LYS
1	H	370	GLN
1	H	373	LEU
1	H	376	VAL
1	H	382	TYR
1	H	401	ARG
1	H	485	LYS
1	H	543	GLU
1	H	574	ARG
1	H	601	LEU
1	H	646	ARG
1	I	6	ASP
1	I	48	LEU
1	I	56	GLU
1	I	64	ILE
1	I	65	MET
1	I	83	LEU
1	I	85	ILE
1	I	86	LEU
1	I	90	VAL
1	I	191	GLU
1	I	287	ARG
1	I	366	LYS
1	I	377	ARG
1	I	395	GLU
1	I	485	LYS
1	I	543	GLU
1	I	574	ARG
1	I	601	LEU
1	I	646	ARG
1	J	48	LEU
1	J	56	GLU
1	J	65	MET
1	J	73	VAL
1	J	114	CYS

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Mol	Chain	Res	Type
1	J	191	GLU
1	J	219	ARG
1	J	222	LEU
1	J	223	HIS
1	J	225	LEU
1	J	230	TRP
1	J	236	LYS
1	J	283	ASP
1	J	379	CYS
1	J	485	LYS
1	J	499	THR
1	J	543	GLU
1	J	574	ARG
1	J	601	LEU
1	J	646	ARG
1	K	48	LEU
1	K	56	GLU
1	K	65	MET
1	K	78	ASP
1	K	114	CYS
1	K	182	VAL
1	K	185	LEU
1	K	191	GLU
1	K	219	ARG
1	K	236	LYS
1	K	238	ASP
1	K	373	LEU
1	K	374	ASP
1	K	395	GLU
1	K	485	LYS
1	K	543	GLU
1	K	574	ARG
1	K	601	LEU
1	K	646	ARG
1	L	48	LEU
1	L	56	GLU
1	L	70	HIS
1	L	72	ASN
1	L	74	VAL
1	L	75	LYS
1	L	84	ASN
1	L	86	LEU

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Mol	Chain	Res	Type
1	L	88	HIS
1	L	172	VAL
1	L	184	THR
1	L	191	GLU
1	L	237	LYS
1	L	238	ASP
1	L	286	GLN
1	L	370	GLN
1	L	373	LEU
1	L	377	ARG
1	L	395	GLU
1	L	401	ARG
1	L	485	LYS
1	L	543	GLU
1	L	574	ARG
1	L	601	LEU
1	L	646	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (340) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	33	GLN
1	A	112	ASN
1	A	195	ASN
1	A	260	GLN
1	A	262	ASN
1	A	286	GLN
1	A	309	ASN
1	A	317	ASN
1	A	335	HIS
1	A	352	GLN
1	A	370	GLN
1	A	408	ASN
1	A	422	GLN
1	A	448	GLN
1	A	459	ASN
1	A	475	GLN
1	A	488	GLN
1	A	538	HIS
1	A	573	HIS
1	A	597	GLN

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Mol	Chain	Res	Type
1	A	616	GLN
1	A	631	ASN
1	A	643	GLN
1	B	28	ASN
1	B	33	GLN
1	B	72	ASN
1	B	84	ASN
1	B	112	ASN
1	B	120	GLN
1	B	226	GLN
1	B	260	GLN
1	B	262	ASN
1	B	281	ASN
1	B	286	GLN
1	B	297	GLN
1	B	309	ASN
1	B	317	ASN
1	B	335	HIS
1	B	352	GLN
1	B	408	ASN
1	B	422	GLN
1	B	475	GLN
1	B	488	GLN
1	B	538	HIS
1	B	545	GLN
1	B	573	HIS
1	B	595	GLN
1	B	597	GLN
1	B	607	HIS
1	B	616	GLN
1	B	631	ASN
1	B	643	GLN
1	C	28	ASN
1	C	33	GLN
1	C	63	GLN
1	C	72	ASN
1	C	195	ASN
1	C	257	HIS
1	C	260	GLN
1	C	262	ASN
1	C	297	GLN
1	C	309	ASN

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Mol	Chain	Res	Type
1	C	317	ASN
1	C	335	HIS
1	C	352	GLN
1	C	370	GLN
1	C	422	GLN
1	C	432	HIS
1	C	446	GLN
1	C	448	GLN
1	C	474	GLN
1	C	475	GLN
1	C	488	GLN
1	C	533	GLN
1	C	538	HIS
1	C	573	HIS
1	C	597	GLN
1	C	616	GLN
1	C	631	ASN
1	C	643	GLN
1	D	28	ASN
1	D	33	GLN
1	D	69	ASN
1	D	84	ASN
1	D	88	HIS
1	D	174	GLN
1	D	186	GLN
1	D	195	ASN
1	D	257	HIS
1	D	260	GLN
1	D	262	ASN
1	D	286	GLN
1	D	309	ASN
1	D	317	ASN
1	D	352	GLN
1	D	408	ASN
1	D	412	GLN
1	D	432	HIS
1	D	446	GLN
1	D	459	ASN
1	D	475	GLN
1	D	488	GLN
1	D	538	HIS
1	D	545	GLN

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Mol	Chain	Res	Type
1	D	573	HIS
1	D	597	GLN
1	D	616	GLN
1	D	631	ASN
1	D	643	GLN
1	E	28	ASN
1	E	33	GLN
1	E	72	ASN
1	E	84	ASN
1	E	120	GLN
1	E	195	ASN
1	E	257	HIS
1	E	260	GLN
1	E	262	ASN
1	E	281	ASN
1	E	285	GLN
1	E	297	GLN
1	E	309	ASN
1	E	317	ASN
1	E	335	HIS
1	E	352	GLN
1	E	422	GLN
1	E	475	GLN
1	E	484	HIS
1	E	488	GLN
1	E	533	GLN
1	E	538	HIS
1	E	573	HIS
1	E	597	GLN
1	E	616	GLN
1	E	631	ASN
1	E	643	GLN
1	F	28	ASN
1	F	33	GLN
1	F	84	ASN
1	F	186	GLN
1	F	195	ASN
1	F	226	GLN
1	F	257	HIS
1	F	260	GLN
1	F	262	ASN
1	F	281	ASN

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Mol	Chain	Res	Type
1	F	309	ASN
1	F	317	ASN
1	F	335	HIS
1	F	352	GLN
1	F	370	GLN
1	F	408	ASN
1	F	422	GLN
1	F	446	GLN
1	F	459	ASN
1	F	475	GLN
1	F	488	GLN
1	F	497	GLN
1	F	533	GLN
1	F	538	HIS
1	F	545	GLN
1	F	573	HIS
1	F	597	GLN
1	F	616	GLN
1	F	631	ASN
1	F	643	GLN
1	G	33	GLN
1	G	69	ASN
1	G	84	ASN
1	G	112	ASN
1	G	120	GLN
1	G	186	GLN
1	G	195	ASN
1	G	257	HIS
1	G	260	GLN
1	G	262	ASN
1	G	281	ASN
1	G	285	GLN
1	G	286	GLN
1	G	309	ASN
1	G	317	ASN
1	G	335	HIS
1	G	352	GLN
1	G	370	GLN
1	G	408	ASN
1	G	422	GLN
1	G	459	ASN
1	G	475	GLN

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Mol	Chain	Res	Type
1	G	488	GLN
1	G	538	HIS
1	G	573	HIS
1	G	597	GLN
1	G	616	GLN
1	G	631	ASN
1	G	643	GLN
1	H	28	ASN
1	H	33	GLN
1	H	69	ASN
1	H	72	ASN
1	H	84	ASN
1	H	120	GLN
1	H	186	GLN
1	H	195	ASN
1	H	260	GLN
1	H	262	ASN
1	H	297	GLN
1	H	309	ASN
1	H	317	ASN
1	H	352	GLN
1	H	370	GLN
1	H	422	GLN
1	H	446	GLN
1	H	475	GLN
1	H	488	GLN
1	H	533	GLN
1	H	538	HIS
1	H	545	GLN
1	H	573	HIS
1	H	597	GLN
1	H	616	GLN
1	H	631	ASN
1	H	643	GLN
1	I	28	ASN
1	I	33	GLN
1	I	69	ASN
1	I	72	ASN
1	I	120	GLN
1	I	195	ASN
1	I	257	HIS
1	I	260	GLN

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Mol	Chain	Res	Type
1	I	262	ASN
1	I	281	ASN
1	I	297	GLN
1	I	309	ASN
1	I	314	HIS
1	I	317	ASN
1	I	335	HIS
1	I	352	GLN
1	I	370	GLN
1	I	412	GLN
1	I	422	GLN
1	I	446	GLN
1	I	448	GLN
1	I	459	ASN
1	I	474	GLN
1	I	475	GLN
1	I	488	GLN
1	I	533	GLN
1	I	538	HIS
1	I	545	GLN
1	I	573	HIS
1	I	597	GLN
1	I	616	GLN
1	I	631	ASN
1	I	643	GLN
1	J	28	ASN
1	J	33	GLN
1	J	63	GLN
1	J	88	HIS
1	J	112	ASN
1	J	186	GLN
1	J	195	ASN
1	J	257	HIS
1	J	260	GLN
1	J	262	ASN
1	J	297	GLN
1	J	309	ASN
1	J	317	ASN
1	J	335	HIS
1	J	352	GLN
1	J	370	GLN
1	J	408	ASN

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Mol	Chain	Res	Type
1	J	412	GLN
1	J	422	GLN
1	J	446	GLN
1	J	459	ASN
1	J	475	GLN
1	J	488	GLN
1	J	533	GLN
1	J	538	HIS
1	J	573	HIS
1	J	597	GLN
1	J	616	GLN
1	J	631	ASN
1	J	643	GLN
1	K	28	ASN
1	K	33	GLN
1	K	69	ASN
1	K	72	ASN
1	K	195	ASN
1	K	257	HIS
1	K	260	GLN
1	K	262	ASN
1	K	297	GLN
1	K	309	ASN
1	K	317	ASN
1	K	408	ASN
1	K	422	GLN
1	K	475	GLN
1	K	488	GLN
1	K	533	GLN
1	K	538	HIS
1	K	573	HIS
1	K	595	GLN
1	K	597	GLN
1	K	607	HIS
1	K	616	GLN
1	K	631	ASN
1	K	643	GLN
1	L	28	ASN
1	L	33	GLN
1	L	69	ASN
1	L	120	GLN
1	L	174	GLN

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Mol	Chain	Res	Type
1	L	186	GLN
1	L	195	ASN
1	L	231	HIS
1	L	257	HIS
1	L	260	GLN
1	L	262	ASN
1	L	297	GLN
1	L	309	ASN
1	L	317	ASN
1	L	335	HIS
1	L	352	GLN
1	L	408	ASN
1	L	422	GLN
1	L	446	GLN
1	L	459	ASN
1	L	475	GLN
1	L	488	GLN
1	L	497	GLN
1	L	538	HIS
1	L	545	GLN
1	L	573	HIS
1	L	597	GLN
1	L	616	GLN
1	L	631	ASN
1	L	643	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

100 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5LS	M	1	2	20,20,20	1.34	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	M	2	2	11,11,12	0.58	0	15,15,17	0.37	0
2	PDX	M	3	2	19,19,20	1.36	2 (10%)	22,29,31	1.02	2 (9%)
2	5LS	N	1	2	20,20,20	1.27	1 (5%)	25,31,31	0.96	2 (8%)
2	GLC	N	2	2	11,11,12	0.85	0	15,15,17	0.99	1 (6%)
2	PDX	N	3	2	19,19,20	1.31	2 (10%)	22,29,31	1.02	2 (9%)
3	5LS	O	1	3	20,20,20	1.08	0	25,31,31	1.01	2 (8%)
3	5TJ	O	2	3	14,17,18	0.98	0	19,24,26	0.93	2 (10%)
3	5TM	O	3	3	14,17,18	1.21	1 (7%)	18,24,26	0.88	1 (5%)
3	5TJ	O	4	3	14,17,18	1.00	0	19,24,26	0.75	1 (5%)
3	Z4K	O	5	3	15,15,16	1.20	1 (6%)	17,22,24	0.76	0
3	5TK	O	6	3	10,13,14	0.60	0	15,17,19	0.36	0
3	5TH	O	7	3	14,17,18	1.40	2 (14%)	17,24,26	0.71	1 (5%)
2	5LS	P	1	2	20,20,20	1.22	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	P	2	2	11,11,12	0.67	0	15,15,17	0.40	0
2	PDX	P	3	2	19,19,20	1.25	2 (10%)	22,29,31	0.95	1 (4%)
2	5LS	Q	1	2	20,20,20	1.18	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	Q	2	2	11,11,12	0.58	0	15,15,17	0.34	0
2	PDX	Q	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.06	3 (13%)
2	5LS	R	1	2	20,20,20	1.28	1 (5%)	25,31,31	0.96	2 (8%)
2	GLC	R	2	2	11,11,12	0.54	0	15,15,17	0.34	0
2	PDX	R	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.05	2 (9%)
2	5LS	S	1	2	20,20,20	1.40	1 (5%)	25,31,31	0.85	1 (4%)
2	GLC	S	2	2	11,11,12	0.49	0	15,15,17	0.37	0
2	PDX	S	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.07	2 (9%)
3	5LS	T	1	3	20,20,20	1.30	1 (5%)	25,31,31	0.97	2 (8%)
3	5TJ	T	2	3	14,17,18	0.96	0	19,24,26	0.81	1 (5%)
3	5TM	T	3	3	14,17,18	1.15	1 (7%)	18,24,26	0.93	1 (5%)
3	5TJ	T	4	3	14,17,18	0.95	0	19,24,26	0.80	1 (5%)
3	Z4K	T	5	3	15,15,16	1.13	1 (6%)	17,22,24	0.73	1 (5%)
3	5TK	T	6	3	10,13,14	0.67	0	15,17,19	0.55	0
3	5TH	T	7	3	14,17,18	1.42	2 (14%)	17,24,26	0.84	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5LS	U	1	2	20,20,20	1.29	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	U	2	2	11,11,12	0.56	0	15,15,17	0.36	0
2	PDX	U	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.04	2 (9%)
2	5LS	V	1	2	20,20,20	1.16	1 (5%)	25,31,31	1.02	2 (8%)
2	GLC	V	2	2	11,11,12	0.60	0	15,15,17	0.47	0
2	PDX	V	3	2	19,19,20	1.34	2 (10%)	22,29,31	0.99	2 (9%)
2	5LS	W	1	2	20,20,20	1.25	1 (5%)	25,31,31	1.00	2 (8%)
2	GLC	W	2	2	11,11,12	0.62	0	15,15,17	0.50	0
2	PDX	W	3	2	19,19,20	1.44	2 (10%)	22,29,31	1.13	3 (13%)
2	5LS	X	1	2	20,20,20	1.28	1 (5%)	25,31,31	1.00	3 (12%)
2	GLC	X	2	2	11,11,12	0.66	0	15,15,17	0.62	0
2	PDX	X	3	2	19,19,20	1.37	2 (10%)	22,29,31	1.04	2 (9%)
2	5LS	Y	1	2	20,20,20	1.37	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	Y	2	2	11,11,12	0.60	0	15,15,17	0.55	0
2	PDX	Y	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.02	2 (9%)
2	5LS	Z	1	2	20,20,20	1.22	1 (5%)	25,31,31	1.02	2 (8%)
2	GLC	Z	2	2	11,11,12	0.70	0	15,15,17	0.46	0
2	PDX	Z	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.00	2 (9%)
2	5LS	a	1	2	20,20,20	1.37	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	a	2	2	11,11,12	0.58	0	15,15,17	0.32	0
2	PDX	a	3	2	19,19,20	1.35	2 (10%)	22,29,31	1.05	2 (9%)
2	5LS	b	1	2	20,20,20	1.37	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	b	2	2	11,11,12	0.56	0	15,15,17	0.44	0
2	PDX	b	3	2	19,19,20	1.32	2 (10%)	22,29,31	1.03	2 (9%)
3	5LS	c	1	3	20,20,20	1.08	1 (5%)	25,31,31	0.99	2 (8%)
3	5TJ	c	2	3	14,17,18	0.97	0	19,24,26	0.76	1 (5%)
3	5TM	c	3	3	14,17,18	1.26	2 (14%)	18,24,26	0.98	1 (5%)
3	5TJ	c	4	3	14,17,18	1.00	0	19,24,26	0.79	1 (5%)
3	Z4K	c	5	3	15,15,16	1.17	1 (6%)	17,22,24	0.71	1 (5%)
3	5TK	c	6	3	10,13,14	0.66	0	15,17,19	0.36	0
3	5TH	c	7	3	14,17,18	1.29	2 (14%)	17,24,26	0.79	1 (5%)
2	5LS	d	1	2	20,20,20	1.32	1 (5%)	25,31,31	1.00	2 (8%)
2	GLC	d	2	2	11,11,12	0.79	0	15,15,17	0.42	0
2	PDX	d	3	2	19,19,20	1.39	2 (10%)	22,29,31	1.01	2 (9%)
2	5LS	e	1	2	20,20,20	1.29	1 (5%)	25,31,31	0.97	2 (8%)
2	GLC	e	2	2	11,11,12	0.80	0	15,15,17	1.08	1 (6%)
2	PDX	e	3	2	19,19,20	1.36	2 (10%)	22,29,31	1.03	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5LS	f	1	2	20,20,20	1.35	1 (5%)	25,31,31	0.98	2 (8%)
2	GLC	f	2	2	11,11,12	0.68	0	15,15,17	0.35	0
2	PDX	f	3	2	19,19,20	1.49	2 (10%)	22,29,31	1.23	3 (13%)
2	5LS	g	1	2	20,20,20	1.06	0	25,31,31	1.01	3 (12%)
2	GLC	g	2	2	11,11,12	0.67	0	15,15,17	0.53	0
2	PDX	g	3	2	19,19,20	1.39	2 (10%)	22,29,31	1.03	3 (13%)
2	5LS	h	1	2	20,20,20	1.28	1 (5%)	25,31,31	0.99	2 (8%)
2	GLC	h	2	2	11,11,12	0.61	0	15,15,17	0.47	0
2	PDX	h	3	2	19,19,20	1.34	2 (10%)	22,29,31	1.01	2 (9%)
3	5LS	i	1	3	20,20,20	1.23	1 (5%)	25,31,31	0.97	2 (8%)
3	5TJ	i	2	3	14,17,18	0.97	0	19,24,26	0.83	1 (5%)
3	5TM	i	3	3	14,17,18	1.22	1 (7%)	18,24,26	0.89	1 (5%)
3	5TJ	i	4	3	14,17,18	0.97	0	19,24,26	0.84	1 (5%)
3	Z4K	i	5	3	15,15,16	1.22	1 (6%)	17,22,24	0.67	0
3	5TK	i	6	3	10,13,14	0.56	0	15,17,19	0.34	0
3	5TH	i	7	3	14,17,18	1.36	2 (14%)	17,24,26	0.76	0
2	5LS	j	1	2	20,20,20	1.08	0	25,31,31	1.00	3 (12%)
2	GLC	j	2	2	11,11,12	0.93	0	15,15,17	1.04	2 (13%)
2	PDX	j	3	2	19,19,20	1.41	2 (10%)	22,29,31	1.22	3 (13%)
2	5LS	k	1	2	20,20,20	1.27	1 (5%)	25,31,31	0.97	2 (8%)
2	GLC	k	2	2	11,11,12	0.61	0	15,15,17	0.33	0
2	PDX	k	3	2	19,19,20	1.39	2 (10%)	22,29,31	1.00	2 (9%)
2	5LS	l	1	2	20,20,20	1.14	1 (5%)	25,31,31	0.89	1 (4%)
2	GLC	l	2	2	11,11,12	0.55	0	15,15,17	0.44	0
2	PDX	l	3	2	19,19,20	1.36	2 (10%)	22,29,31	1.03	2 (9%)
2	5LS	m	1	2	20,20,20	1.32	1 (5%)	25,31,31	0.93	2 (8%)
2	GLC	m	2	2	11,11,12	0.64	0	15,15,17	0.43	0
2	PDX	m	3	2	19,19,20	1.43	2 (10%)	22,29,31	1.16	3 (13%)
2	5LS	n	1	2	20,20,20	1.23	1 (5%)	25,31,31	1.52	3 (12%)
2	GLC	n	2	2	11,11,12	0.58	0	15,15,17	0.46	0
2	PDX	n	3	2	19,19,20	1.36	2 (10%)	22,29,31	0.96	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5LS	M	1	2	-	2/12/32/32	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	PDX	M	3	2	-	0/12/29/32	0/1/1/1
2	5LS	N	1	2	-	2/12/32/32	0/1/1/1
2	GLC	N	2	2	-	2/2/19/22	0/1/1/1
2	PDX	N	3	2	-	1/12/29/32	0/1/1/1
3	5LS	O	1	3	-	0/12/32/32	0/1/1/1
3	5TJ	O	2	3	-	1/9/27/30	0/1/1/1
3	5TM	O	3	3	-	2/9/27/30	0/1/1/1
3	5TJ	O	4	3	-	2/9/27/30	0/1/1/1
3	Z4K	O	5	3	-	1/7/24/27	0/1/1/1
3	5TK	O	6	3	-	0/4/22/25	0/1/1/1
3	5TH	O	7	3	-	1/9/27/30	0/1/1/1
2	5LS	P	1	2	-	2/12/32/32	0/1/1/1
2	GLC	P	2	2	-	2/2/19/22	0/1/1/1
2	PDX	P	3	2	-	3/12/29/32	0/1/1/1
2	5LS	Q	1	2	-	2/12/32/32	0/1/1/1
2	GLC	Q	2	2	-	0/2/19/22	0/1/1/1
2	PDX	Q	3	2	-	0/12/29/32	0/1/1/1
2	5LS	R	1	2	-	0/12/32/32	0/1/1/1
2	GLC	R	2	2	-	0/2/19/22	0/1/1/1
2	PDX	R	3	2	-	2/12/29/32	0/1/1/1
2	5LS	S	1	2	-	2/12/32/32	0/1/1/1
2	GLC	S	2	2	-	0/2/19/22	0/1/1/1
2	PDX	S	3	2	-	0/12/29/32	0/1/1/1
3	5LS	T	1	3	-	0/12/32/32	0/1/1/1
3	5TJ	T	2	3	-	1/9/27/30	0/1/1/1
3	5TM	T	3	3	-	0/9/27/30	0/1/1/1
3	5TJ	T	4	3	-	0/9/27/30	0/1/1/1
3	Z4K	T	5	3	-	0/7/24/27	0/1/1/1
3	5TK	T	6	3	-	1/4/22/25	0/1/1/1
3	5TH	T	7	3	-	0/9/27/30	0/1/1/1
2	5LS	U	1	2	-	0/12/32/32	0/1/1/1
2	GLC	U	2	2	-	1/2/19/22	0/1/1/1
2	PDX	U	3	2	-	0/12/29/32	0/1/1/1
2	5LS	V	1	2	-	1/12/32/32	0/1/1/1
2	GLC	V	2	2	-	0/2/19/22	0/1/1/1
2	PDX	V	3	2	-	2/12/29/32	0/1/1/1
2	5LS	W	1	2	-	2/12/32/32	0/1/1/1
2	GLC	W	2	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PDX	W	3	2	-	2/12/29/32	0/1/1/1
2	5LS	X	1	2	-	0/12/32/32	0/1/1/1
2	GLC	X	2	2	-	0/2/19/22	0/1/1/1
2	PDX	X	3	2	-	2/12/29/32	0/1/1/1
2	5LS	Y	1	2	-	0/12/32/32	0/1/1/1
2	GLC	Y	2	2	-	0/2/19/22	0/1/1/1
2	PDX	Y	3	2	-	1/12/29/32	0/1/1/1
2	5LS	Z	1	2	-	0/12/32/32	0/1/1/1
2	GLC	Z	2	2	-	2/2/19/22	0/1/1/1
2	PDX	Z	3	2	-	0/12/29/32	0/1/1/1
2	5LS	a	1	2	-	0/12/32/32	0/1/1/1
2	GLC	a	2	2	-	2/2/19/22	0/1/1/1
2	PDX	a	3	2	-	2/12/29/32	0/1/1/1
2	5LS	b	1	2	-	0/12/32/32	0/1/1/1
2	GLC	b	2	2	-	0/2/19/22	0/1/1/1
2	PDX	b	3	2	-	0/12/29/32	0/1/1/1
3	5LS	c	1	3	-	0/12/32/32	0/1/1/1
3	5TJ	c	2	3	-	3/9/27/30	0/1/1/1
3	5TM	c	3	3	-	2/9/27/30	0/1/1/1
3	5TJ	c	4	3	-	0/9/27/30	0/1/1/1
3	Z4K	c	5	3	-	1/7/24/27	0/1/1/1
3	5TK	c	6	3	-	2/4/22/25	0/1/1/1
3	5TH	c	7	3	-	4/9/27/30	0/1/1/1
2	5LS	d	1	2	-	0/12/32/32	0/1/1/1
2	GLC	d	2	2	-	0/2/19/22	0/1/1/1
2	PDX	d	3	2	-	0/12/29/32	0/1/1/1
2	5LS	e	1	2	-	1/12/32/32	0/1/1/1
2	GLC	e	2	2	-	1/2/19/22	0/1/1/1
2	PDX	e	3	2	-	2/12/29/32	0/1/1/1
2	5LS	f	1	2	-	0/12/32/32	0/1/1/1
2	GLC	f	2	2	-	2/2/19/22	0/1/1/1
2	PDX	f	3	2	-	0/12/29/32	0/1/1/1
2	5LS	g	1	2	-	0/12/32/32	0/1/1/1
2	GLC	g	2	2	-	0/2/19/22	0/1/1/1
2	PDX	g	3	2	-	2/12/29/32	0/1/1/1
2	5LS	h	1	2	-	0/12/32/32	0/1/1/1
2	GLC	h	2	2	-	2/2/19/22	0/1/1/1
2	PDX	h	3	2	-	0/12/29/32	0/1/1/1
3	5LS	i	1	3	-	2/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5TJ	i	2	3	-	1/9/27/30	0/1/1/1
3	5TM	i	3	3	-	2/9/27/30	0/1/1/1
3	5TJ	i	4	3	-	2/9/27/30	0/1/1/1
3	Z4K	i	5	3	-	2/7/24/27	0/1/1/1
3	5TK	i	6	3	-	0/4/22/25	0/1/1/1
3	5TH	i	7	3	-	2/9/27/30	0/1/1/1
2	5LS	j	1	2	-	2/12/32/32	0/1/1/1
2	GLC	j	2	2	-	2/2/19/22	0/1/1/1
2	PDX	j	3	2	-	1/12/29/32	0/1/1/1
2	5LS	k	1	2	-	2/12/32/32	0/1/1/1
2	GLC	k	2	2	-	0/2/19/22	0/1/1/1
2	PDX	k	3	2	-	0/12/29/32	0/1/1/1
2	5LS	l	1	2	-	3/12/32/32	0/1/1/1
2	GLC	l	2	2	-	0/2/19/22	0/1/1/1
2	PDX	l	3	2	-	0/12/29/32	0/1/1/1
2	5LS	m	1	2	-	1/12/32/32	0/1/1/1
2	GLC	m	2	2	-	2/2/19/22	0/1/1/1
2	PDX	m	3	2	-	0/12/29/32	0/1/1/1
2	5LS	n	1	2	-	2/12/32/32	0/1/1/1
2	GLC	n	2	2	-	2/2/19/22	0/1/1/1
2	PDX	n	3	2	-	2/12/29/32	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1	5LS	C1-C2	4.65	1.56	1.52
2	b	1	5LS	C1-C2	4.15	1.56	1.52
2	a	1	5LS	C1-C2	4.11	1.56	1.52
2	Y	1	5LS	C1-C2	4.09	1.56	1.52
2	f	1	5LS	C1-C2	4.08	1.56	1.52
2	f	3	PDX	C1-C2	4.04	1.58	1.51
2	M	1	5LS	C1-C2	3.94	1.56	1.52
2	m	1	5LS	C1-C2	3.90	1.56	1.52
2	d	1	5LS	C1-C2	3.83	1.56	1.52
2	U	1	5LS	C1-C2	3.71	1.55	1.52
2	R	1	5LS	C1-C2	3.68	1.55	1.52
2	W	3	PDX	C1-C2	3.67	1.57	1.51
2	n	1	5LS	C1-C2	3.66	1.55	1.52
3	T	1	5LS	C1-C2	3.65	1.55	1.52
2	h	1	5LS	C1-C2	3.61	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	m	3	PDX	C1-C2	3.60	1.57	1.51
2	e	1	5LS	C1-C2	3.53	1.55	1.52
2	j	3	PDX	C1-C2	3.49	1.57	1.51
2	k	1	5LS	C1-C2	3.44	1.55	1.52
2	g	3	PDX	C1-C2	3.43	1.57	1.51
2	X	1	5LS	C1-C2	3.42	1.55	1.52
2	d	3	PDX	C1-C2	3.38	1.57	1.51
2	b	3	PDX	O2-C2	-3.37	1.42	1.47
2	N	1	5LS	C1-C2	3.36	1.55	1.52
3	T	7	5TH	C1-C2	3.35	1.57	1.51
2	h	3	PDX	O2-C2	-3.31	1.42	1.47
2	N	3	PDX	O2-C2	-3.28	1.42	1.47
2	l	3	PDX	O2-C2	-3.27	1.42	1.47
2	R	3	PDX	O2-C2	-3.27	1.42	1.47
2	a	3	PDX	O2-C2	-3.25	1.42	1.47
3	i	7	5TH	O2-C2	-3.23	1.42	1.47
2	Q	3	PDX	O2-C2	-3.22	1.42	1.47
2	M	3	PDX	O2-C2	-3.21	1.42	1.47
2	Z	3	PDX	O2-C2	-3.21	1.42	1.47
3	O	7	5TH	C1-C2	3.20	1.56	1.51
2	W	1	5LS	C1-C2	3.19	1.55	1.52
2	n	3	PDX	O2-C2	-3.17	1.42	1.47
3	i	3	5TM	O2-C2	-3.16	1.42	1.47
2	k	3	PDX	C1-C2	3.16	1.56	1.51
3	i	5	Z4K	O2-C2	-3.15	1.42	1.47
3	O	5	Z4K	O2-C2	-3.11	1.42	1.47
3	O	7	5TH	O2-C2	-3.11	1.42	1.47
2	e	3	PDX	O2-C2	-3.11	1.42	1.47
2	X	3	PDX	C1-C2	3.10	1.56	1.51
2	f	3	PDX	O2-C2	-3.10	1.42	1.47
2	V	3	PDX	O2-C2	-3.09	1.42	1.47
2	Y	3	PDX	O2-C2	-3.08	1.42	1.47
2	U	3	PDX	O2-C2	-3.08	1.42	1.47
2	S	3	PDX	C1-C2	3.08	1.56	1.51
2	W	3	PDX	O2-C2	-3.08	1.42	1.47
2	S	3	PDX	O2-C2	-3.07	1.42	1.47
2	k	3	PDX	O2-C2	-3.07	1.42	1.47
2	X	3	PDX	O2-C2	-3.07	1.42	1.47
3	i	1	5LS	C1-C2	3.06	1.55	1.52
3	c	3	5TM	O2-C2	-3.06	1.42	1.47
2	Z	1	5LS	C1-C2	3.06	1.55	1.52
2	m	3	PDX	O2-C2	-3.03	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	5	Z4K	O2-C2	-3.02	1.42	1.47
3	T	3	5TM	O2-C2	-3.02	1.42	1.47
2	d	3	PDX	O2-C2	-3.01	1.42	1.47
2	P	3	PDX	O2-C2	-2.98	1.42	1.47
2	P	1	5LS	C1-C2	2.98	1.55	1.52
2	j	3	PDX	O2-C2	-2.96	1.42	1.47
3	c	5	Z4K	O2-C2	-2.95	1.42	1.47
2	n	3	PDX	C1-C2	2.95	1.56	1.51
2	V	3	PDX	C1-C2	2.94	1.56	1.51
2	Q	3	PDX	C1-C2	2.92	1.56	1.51
2	Y	3	PDX	C1-C2	2.91	1.56	1.51
2	g	3	PDX	O2-C2	-2.90	1.43	1.47
2	R	3	PDX	C1-C2	2.90	1.56	1.51
3	O	3	5TM	O2-C2	-2.90	1.43	1.47
2	M	3	PDX	C1-C2	2.90	1.56	1.51
3	T	7	5TH	O2-C2	-2.90	1.43	1.47
2	U	3	PDX	C1-C2	2.87	1.56	1.51
3	i	7	5TH	C1-C2	2.83	1.56	1.51
2	e	3	PDX	C1-C2	2.83	1.56	1.51
2	l	1	5LS	C1-C2	2.78	1.55	1.52
3	c	7	5TH	O2-C2	-2.70	1.43	1.47
2	Z	3	PDX	C1-C2	2.70	1.56	1.51
2	a	3	PDX	C1-C2	2.69	1.56	1.51
2	l	3	PDX	C1-C2	2.63	1.55	1.51
2	h	3	PDX	C1-C2	2.58	1.55	1.51
3	c	7	5TH	C1-C2	2.58	1.55	1.51
2	P	3	PDX	C1-C2	2.52	1.55	1.51
2	V	1	5LS	C1-C2	2.45	1.54	1.52
2	Q	1	5LS	C1-C2	2.44	1.54	1.52
3	c	3	5TM	C1-C2	2.42	1.55	1.51
2	b	3	PDX	C1-C2	2.29	1.55	1.51
2	N	3	PDX	C1-C2	2.14	1.55	1.51
3	c	1	5LS	C1-C2	2.03	1.54	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	n	1	5LS	O2-C2-C1	6.16	115.86	107.58
2	f	3	PDX	C1-C2-C3	3.53	114.69	109.40
3	c	3	5TM	O2-C2-C3	3.37	110.38	106.65
2	S	3	PDX	O2-C2-C3	3.33	110.34	106.65
2	U	3	PDX	O2-C2-C3	3.32	110.33	106.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	3	PDX	O2-C2-C3	3.24	110.23	106.65
2	a	3	PDX	O2-C2-C3	3.19	110.19	106.65
2	P	3	PDX	O2-C2-C3	3.18	110.17	106.65
2	e	3	PDX	O2-C2-C3	3.09	110.07	106.65
2	l	3	PDX	O2-C2-C3	3.08	110.07	106.65
2	X	3	PDX	O2-C2-C3	3.07	110.05	106.65
2	e	2	GLC	C1-C2-C3	3.05	114.09	109.64
2	b	3	PDX	O2-C2-C3	3.05	110.03	106.65
2	W	3	PDX	C1-C2-C3	3.03	113.94	109.40
2	M	3	PDX	O2-C2-C3	2.99	109.96	106.65
2	h	3	PDX	O2-C2-C3	2.97	109.94	106.65
3	O	3	5TM	O2-C2-C3	2.95	109.92	106.65
2	Y	3	PDX	O2-C2-C3	2.94	109.91	106.65
3	T	3	5TM	O2-C2-C3	2.89	109.85	106.65
2	N	3	PDX	O2-C2-C3	2.88	109.84	106.65
2	Q	1	5LS	C2-O2-S1	-2.83	112.26	119.04
2	N	2	GLC	C1-C2-C3	2.82	113.74	109.64
2	V	3	PDX	O2-C2-C3	2.80	109.75	106.65
2	Z	3	PDX	O2-C2-C3	2.80	109.75	106.65
2	g	1	5LS	C2-O2-S1	-2.79	112.35	119.04
2	a	3	PDX	C3-O3-S'	-2.78	112.37	119.04
2	Y	1	5LS	C4-O4-S2	-2.78	112.38	119.04
3	i	1	5LS	C2-O2-S1	-2.77	112.40	119.04
2	l	1	5LS	C2-O2-S1	-2.76	112.42	119.04
2	P	1	5LS	C2-O2-S1	-2.76	112.42	119.04
3	i	3	5TM	O2-C2-C3	2.75	109.70	106.65
2	N	3	PDX	C3-O3-S'	-2.74	112.47	119.04
2	Z	1	5LS	C2-O2-S1	-2.74	112.47	119.04
2	a	1	5LS	C4-O4-S2	-2.73	112.48	119.04
2	l	3	PDX	C3-O3-S'	-2.73	112.49	119.04
2	f	1	5LS	C4-O4-S2	-2.72	112.52	119.04
2	S	3	PDX	C3-O3-S'	-2.72	112.52	119.04
2	b	3	PDX	C3-O3-S'	-2.71	112.53	119.04
3	i	2	5TJ	C3-O3-S3	-2.71	112.54	119.04
2	m	3	PDX	C3-O3-S'	-2.71	112.54	119.04
2	h	1	5LS	C2-O2-S1	-2.71	112.55	119.04
2	W	1	5LS	C4-O4-S2	-2.71	112.55	119.04
3	i	1	5LS	C4-O4-S2	-2.70	112.57	119.04
2	N	1	5LS	C2-O2-S1	-2.69	112.58	119.04
3	i	4	5TJ	C3-O3-S3	-2.69	112.59	119.04
2	k	1	5LS	C2-O2-S1	-2.68	112.61	119.04
2	b	1	5LS	C4-O4-S2	-2.68	112.62	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	5LS	C4-O4-S2	-2.68	112.62	119.04
2	a	1	5LS	C2-O2-S1	-2.68	112.62	119.04
2	j	1	5LS	C2-O2-S1	-2.67	112.63	119.04
2	n	1	5LS	C4-O4-S2	-2.67	112.64	119.04
2	f	1	5LS	C2-O2-S1	-2.66	112.65	119.04
2	V	1	5LS	C4-O4-S2	-2.66	112.66	119.04
2	V	1	5LS	C2-O2-S1	-2.66	112.67	119.04
2	m	1	5LS	C4-O4-S2	-2.65	112.68	119.04
3	O	1	5LS	C2-O2-S1	-2.65	112.68	119.04
2	d	1	5LS	C4-O4-S2	-2.65	112.68	119.04
2	d	3	PDX	O2-C2-C3	2.65	109.59	106.65
3	T	7	5TH	O2-C2-C3	2.65	110.65	106.95
2	d	1	5LS	C2-O2-S1	-2.64	112.70	119.04
2	R	1	5LS	C4-O4-S2	-2.64	112.70	119.04
3	T	1	5LS	C4-O4-S2	-2.64	112.70	119.04
2	j	2	GLC	C1-C2-C3	2.64	113.48	109.64
2	W	1	5LS	C2-O2-S1	-2.63	112.72	119.04
2	U	1	5LS	C4-O4-S2	-2.63	112.74	119.04
2	n	3	PDX	C3-O3-S'	-2.63	112.74	119.04
2	P	1	5LS	C4-O4-S2	-2.62	112.75	119.04
2	j	3	PDX	C3-O3-S'	-2.62	112.76	119.04
3	T	2	5TJ	C3-O3-S3	-2.62	112.77	119.04
3	c	2	5TJ	C3-O3-S3	-2.61	112.77	119.04
2	Y	1	5LS	C2-O2-S1	-2.61	112.78	119.04
2	b	1	5LS	C2-O2-S1	-2.61	112.78	119.04
2	n	3	PDX	O2-C2-C3	2.61	109.54	106.65
2	h	1	5LS	C4-O4-S2	-2.61	112.79	119.04
2	h	3	PDX	C3-O3-S'	-2.61	112.79	119.04
2	Z	1	5LS	C4-O4-S2	-2.60	112.81	119.04
2	j	1	5LS	C4-O4-S2	-2.60	112.81	119.04
2	N	1	5LS	C4-O4-S2	-2.59	112.82	119.04
2	f	3	PDX	O2-C2-C3	2.59	109.52	106.65
2	R	1	5LS	C2-O2-S1	-2.59	112.83	119.04
3	T	1	5LS	C2-O2-S1	-2.59	112.83	119.04
3	T	4	5TJ	C3-O3-S3	-2.57	112.87	119.04
3	c	4	5TJ	C3-O3-S3	-2.57	112.88	119.04
2	Z	3	PDX	C3-O3-S'	-2.56	112.89	119.04
2	U	1	5LS	C2-O2-S1	-2.56	112.90	119.04
2	X	3	PDX	C3-O3-S'	-2.56	112.91	119.04
2	m	1	5LS	C2-O2-S1	-2.55	112.92	119.04
2	e	1	5LS	C4-O4-S2	-2.55	112.93	119.04
2	U	3	PDX	C3-O3-S'	-2.54	112.94	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	e	3	PDX	C3-O3-S'	-2.54	112.95	119.04
2	X	1	5LS	C4-O4-S2	-2.53	112.96	119.04
2	m	3	PDX	O2-C2-C3	2.53	109.46	106.65
2	R	3	PDX	C3-O3-S'	-2.53	112.97	119.04
2	M	1	5LS	C4-O4-S2	-2.53	112.98	119.04
2	Q	3	PDX	C3-O3-S'	-2.53	112.98	119.04
2	j	2	GLC	C1-O5-C5	2.52	115.56	112.19
2	S	1	5LS	C2-O2-S1	-2.51	113.02	119.04
3	O	1	5LS	C4-O4-S2	-2.50	113.04	119.04
2	k	3	PDX	C3-O3-S'	-2.49	113.08	119.04
2	e	1	5LS	C2-O2-S1	-2.49	113.08	119.04
3	O	4	5TJ	C3-O3-S3	-2.49	113.08	119.04
2	g	3	PDX	C3-O3-S'	-2.48	113.09	119.04
2	j	3	PDX	O2-C2-C3	2.48	109.40	106.65
2	k	1	5LS	C4-O4-S2	-2.47	113.11	119.04
2	k	3	PDX	O2-C2-C3	2.47	109.38	106.65
2	d	3	PDX	C3-O3-S'	-2.47	113.12	119.04
2	g	1	5LS	C4-O4-S2	-2.47	113.12	119.04
3	c	1	5LS	C2-O2-S1	-2.47	113.12	119.04
2	M	3	PDX	C3-O3-S'	-2.45	113.16	119.04
2	M	1	5LS	C2-O2-S1	-2.45	113.17	119.04
2	Y	3	PDX	C3-O3-S'	-2.43	113.21	119.04
3	O	2	5TJ	C3-O3-S3	-2.42	113.23	119.04
3	c	7	5TH	O2-C2-C3	2.37	110.26	106.95
2	X	1	5LS	C2-O2-S1	-2.35	113.41	119.04
2	V	3	PDX	C3-O3-S'	-2.32	113.49	119.04
2	W	3	PDX	C3-O3-S'	-2.30	113.53	119.04
2	Q	3	PDX	O2-C2-C3	2.26	109.16	106.65
2	W	3	PDX	O2-C2-C3	2.26	109.16	106.65
3	c	1	5LS	C4-O4-S2	-2.25	113.65	119.04
2	g	3	PDX	C1-C2-C3	2.22	112.73	109.40
2	Q	3	PDX	C1-C2-C3	2.18	112.67	109.40
2	m	3	PDX	C1-C2-C3	2.16	112.63	109.40
2	X	1	5LS	C4-C3-C2	2.15	113.46	109.11
2	j	3	PDX	C1-C2-C3	2.12	112.58	109.40
3	T	5	Z4K	O2-C2-C3	2.11	109.90	106.95
3	c	5	Z4K	O2-C2-C3	2.11	109.89	106.95
3	O	7	5TH	O2-C2-C3	2.11	109.89	106.95
2	g	3	PDX	O2-C2-C3	2.10	108.98	106.65
3	O	2	5TJ	C2-C3-C4	-2.09	109.47	111.03
2	g	1	5LS	O2-C2-C1	2.07	110.37	107.58
2	f	3	PDX	C3-O3-S'	-2.07	114.08	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	1	5LS	O2-C2-C1	2.06	110.35	107.58
2	n	1	5LS	O7-S1-O2	2.01	110.98	106.37

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	3	PDX	C2-C3-O3-S'
2	P	3	PDX	C4-C3-O3-S'
2	S	1	5LS	C3-C4-O4-S2
2	S	1	5LS	C5-C4-O4-S2
2	l	1	5LS	C3-C4-O4-S2
2	l	1	5LS	C5-C4-O4-S2
2	n	1	5LS	C1-C2-O2-S1
2	n	1	5LS	C3-C2-O2-S1
3	c	7	5TH	C3-C4-O4-S2
3	c	7	5TH	C5-C4-O4-S2
2	j	2	GLC	O5-C5-C6-O6
3	i	5	Z4K	O5-C5-C6-O6
2	g	3	PDX	O5-C5-C6-O6
3	O	3	5TM	O5-C5-C6-O6
2	a	3	PDX	O5-C5-C6-O6
3	i	3	5TM	O5-C5-C6-O6
3	i	1	5LS	O5-C5-C6-O6
3	c	7	5TH	O5-C5-C6-O6
3	i	4	5TJ	O5-C5-C6-O6
3	c	7	5TH	C4-C5-C6-O6
3	c	3	5TM	O5-C5-C6-O6
2	a	3	PDX	C4-C5-C6-O6
2	g	3	PDX	C4-C5-C6-O6
3	O	3	5TM	C4-C5-C6-O6
3	i	3	5TM	C4-C5-C6-O6
3	i	5	Z4K	C4-C5-C6-O6
2	P	1	5LS	O5-C5-C6-O6
2	f	2	GLC	O5-C5-C6-O6
2	m	2	GLC	O5-C5-C6-O6
2	k	1	5LS	C4-C5-C6-O6
2	e	3	PDX	C4-C5-C6-O6
2	j	2	GLC	C4-C5-C6-O6
2	n	3	PDX	C4-C5-C6-O6
3	i	7	5TH	O5-C5-C6-O6
2	M	1	5LS	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	c	6	5TK	O5-C5-C6-O6
3	i	7	5TH	C4-C5-C6-O6
2	m	2	GLC	C4-C5-C6-O6
3	i	1	5LS	C4-C5-C6-O6
3	O	4	5TJ	O5-C5-C6-O6
2	W	3	PDX	O5-C5-C6-O6
2	e	3	PDX	O5-C5-C6-O6
2	k	1	5LS	O5-C5-C6-O6
2	n	3	PDX	O5-C5-C6-O6
2	f	2	GLC	C4-C5-C6-O6
2	j	1	5LS	O5-C5-C6-O6
2	M	1	5LS	O5-C5-C6-O6
2	V	3	PDX	O5-C5-C6-O6
2	W	1	5LS	O5-C5-C6-O6
3	c	3	5TM	C4-C5-C6-O6
3	i	4	5TJ	C4-C5-C6-O6
2	X	3	PDX	O5-C5-C6-O6
3	c	2	5TJ	O5-C5-C6-O6
2	j	1	5LS	C4-C5-C6-O6
2	N	2	GLC	O5-C5-C6-O6
2	h	2	GLC	C4-C5-C6-O6
2	N	1	5LS	O5-C5-C6-O6
2	N	1	5LS	C4-C5-C6-O6
2	P	2	GLC	C4-C5-C6-O6
2	P	1	5LS	C4-C5-C6-O6
3	c	5	Z4K	O5-C5-C6-O6
2	P	2	GLC	O5-C5-C6-O6
2	Q	1	5LS	C4-C5-C6-O6
3	c	6	5TK	C4-C5-C6-O6
2	Z	2	GLC	C4-C5-C6-O6
2	W	3	PDX	C4-C5-C6-O6
2	Y	3	PDX	O5-C5-C6-O6
3	O	4	5TJ	C4-C5-C6-O6
2	P	3	PDX	O5-C5-C6-O6
2	N	3	PDX	O5-C5-C6-O6
2	h	2	GLC	O5-C5-C6-O6
2	Q	1	5LS	O5-C5-C6-O6
2	R	3	PDX	C4-C5-C6-O6
2	m	1	5LS	O5-C5-C6-O6
3	O	2	5TJ	O5-C5-C6-O6
2	V	3	PDX	C4-C5-C6-O6
2	a	2	GLC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	e	1	5LS	O5-C5-C6-O6
2	W	1	5LS	C4-C5-C6-O6
2	n	2	GLC	C4-C5-C6-O6
3	i	2	5TJ	O5-C5-C6-O6
2	X	3	PDX	C4-C5-C6-O6
2	a	2	GLC	O5-C5-C6-O6
2	j	3	PDX	O5-C5-C6-O6
3	O	7	5TH	C4-C5-C6-O6
3	T	2	5TJ	O5-C5-C6-O6
3	c	2	5TJ	C4-C5-C6-O6
2	e	2	GLC	O5-C5-C6-O6
2	W	2	GLC	C4-C5-C6-O6
2	Z	2	GLC	O5-C5-C6-O6
2	R	3	PDX	O5-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	n	2	GLC	O5-C5-C6-O6
2	l	1	5LS	C4-O4-S2-O07
3	O	5	Z4K	O5-C5-C6-O6
2	V	1	5LS	C4-C5-C6-O6
3	c	2	5TJ	C3-C4-O4-S4
3	T	6	5TK	O5-C5-C6-O6
2	U	2	GLC	C4-C5-C6-O6

There are no ring outliers.

31 monomers are involved in 41 short contacts:

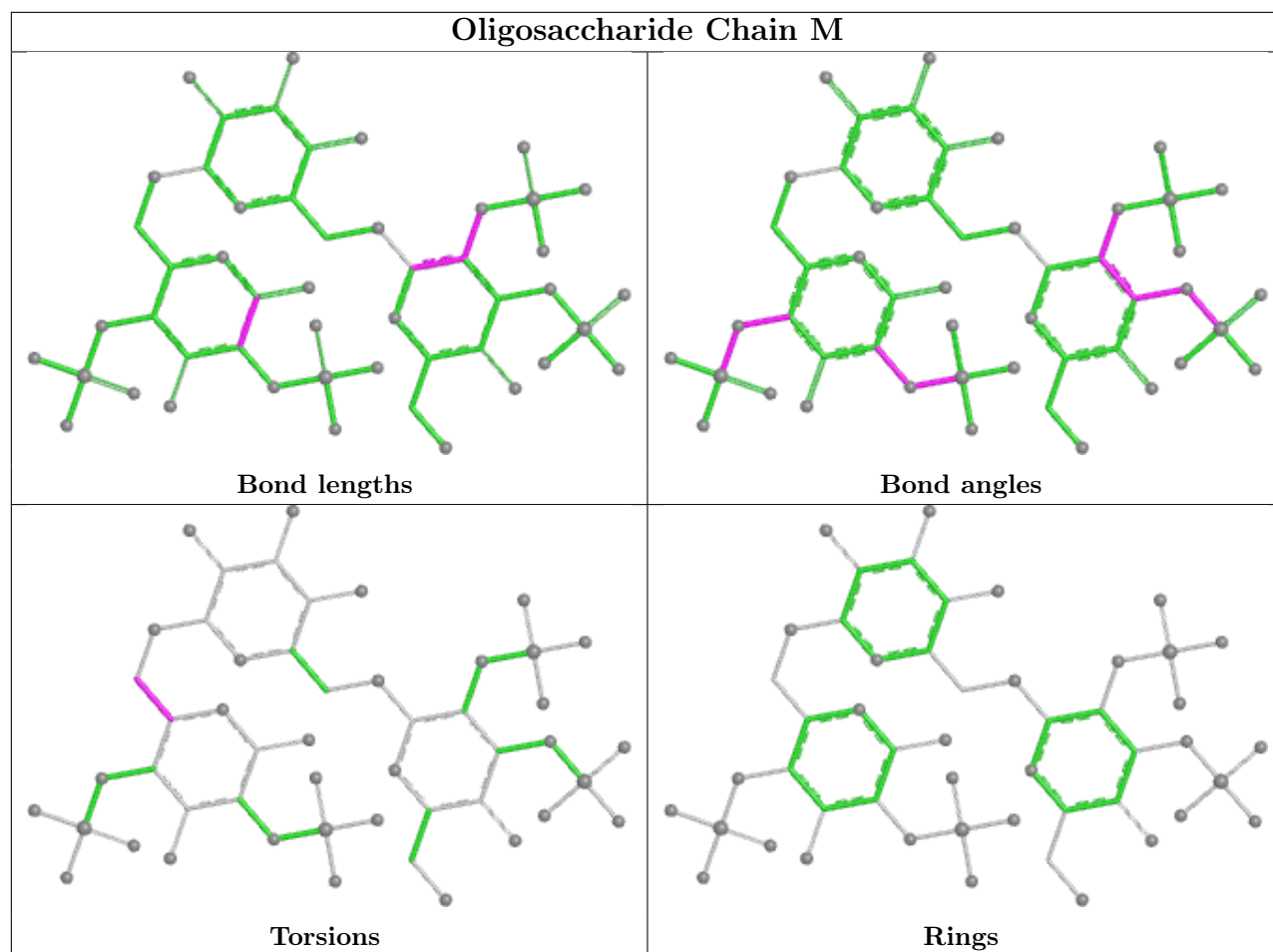
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	3	PDX	1	0
2	l	3	PDX	1	0
2	S	2	GLC	3	0
3	T	5	Z4K	2	0
3	T	6	5TK	1	0
2	Y	2	GLC	2	0
2	N	2	GLC	1	0
2	W	2	GLC	1	0
2	j	2	GLC	6	0
2	e	1	5LS	1	0
2	h	2	GLC	4	0
2	V	1	5LS	1	0
2	m	3	PDX	2	0
3	T	2	5TJ	1	0
2	Q	2	GLC	3	0

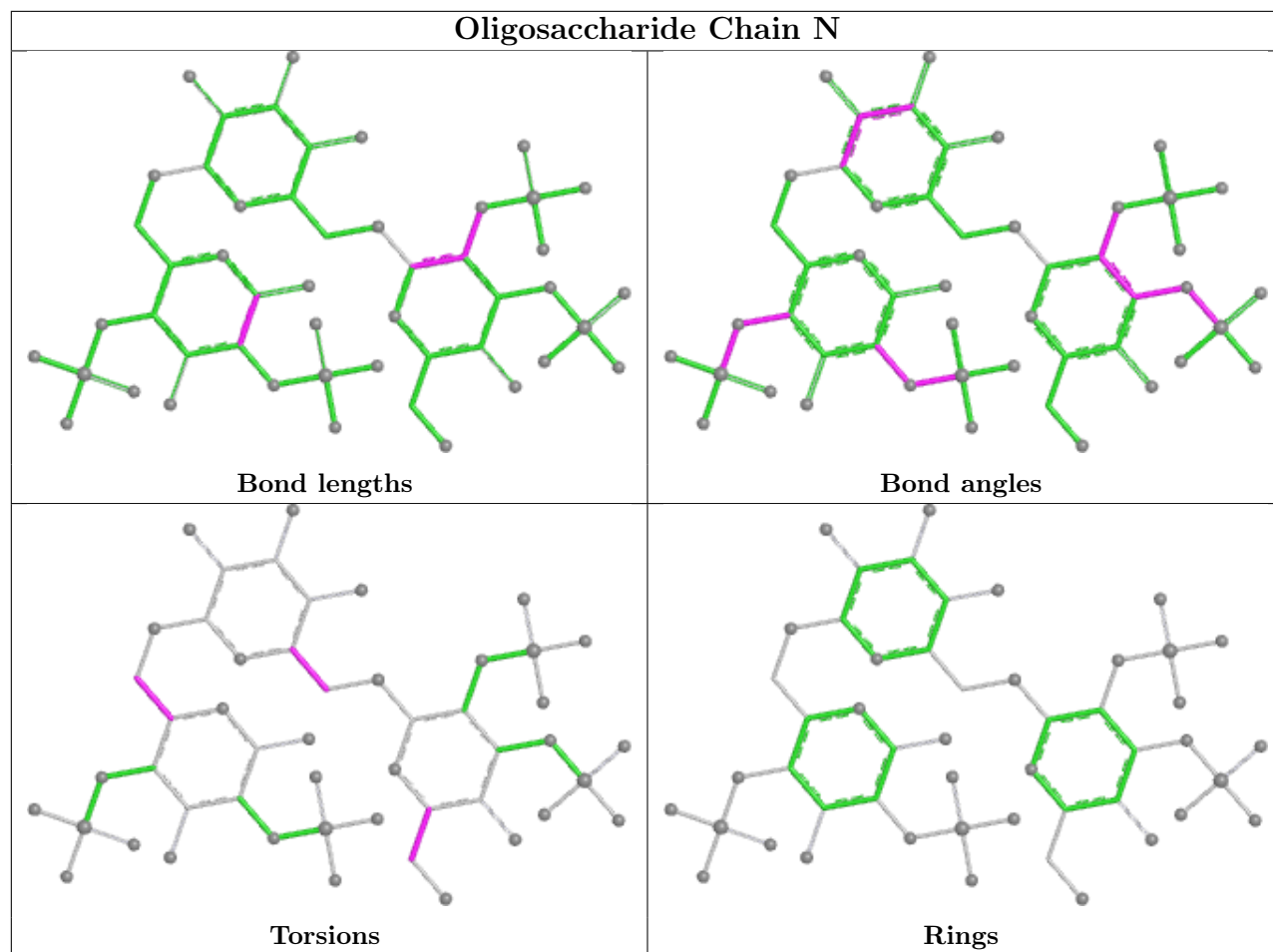
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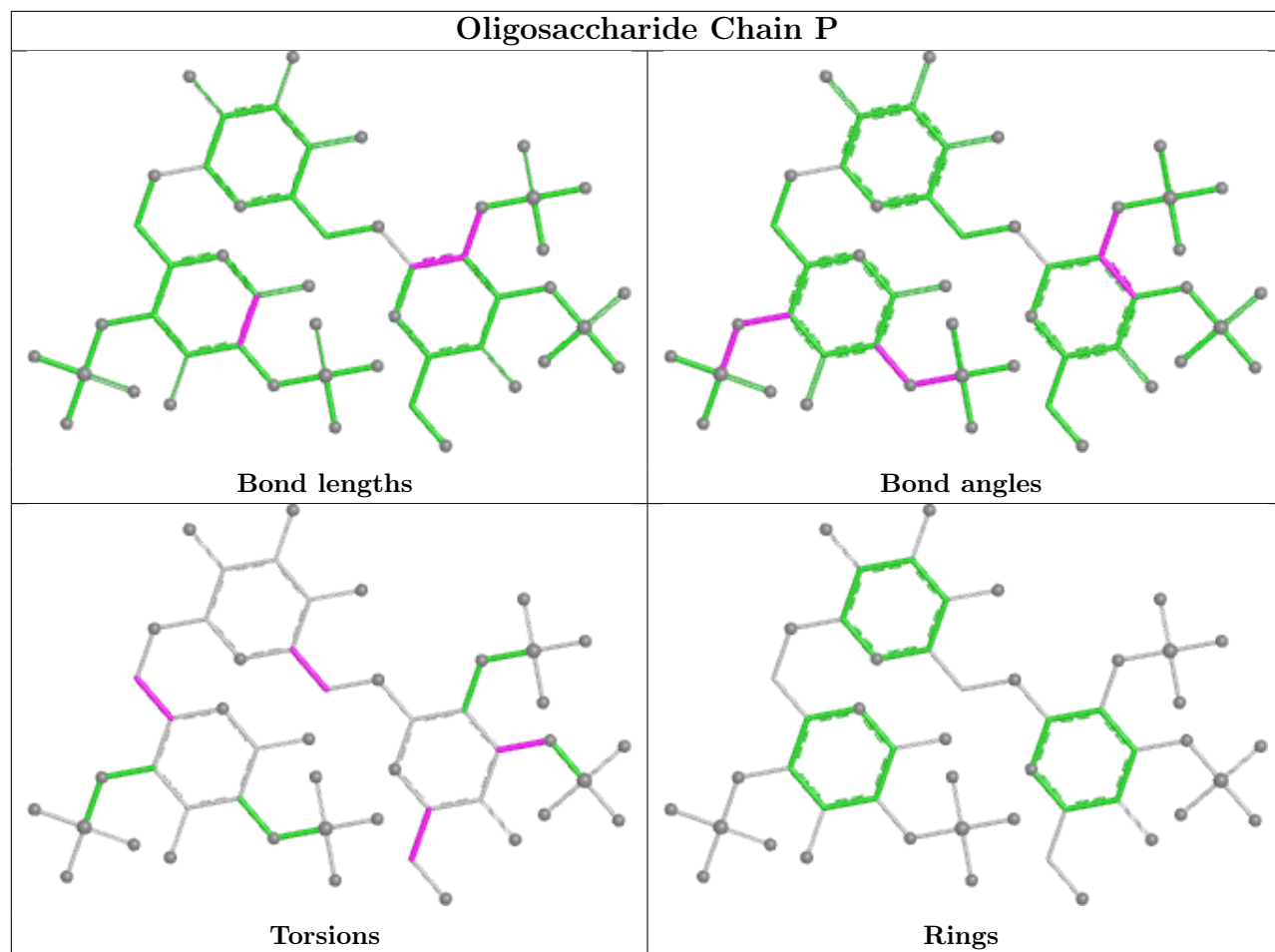
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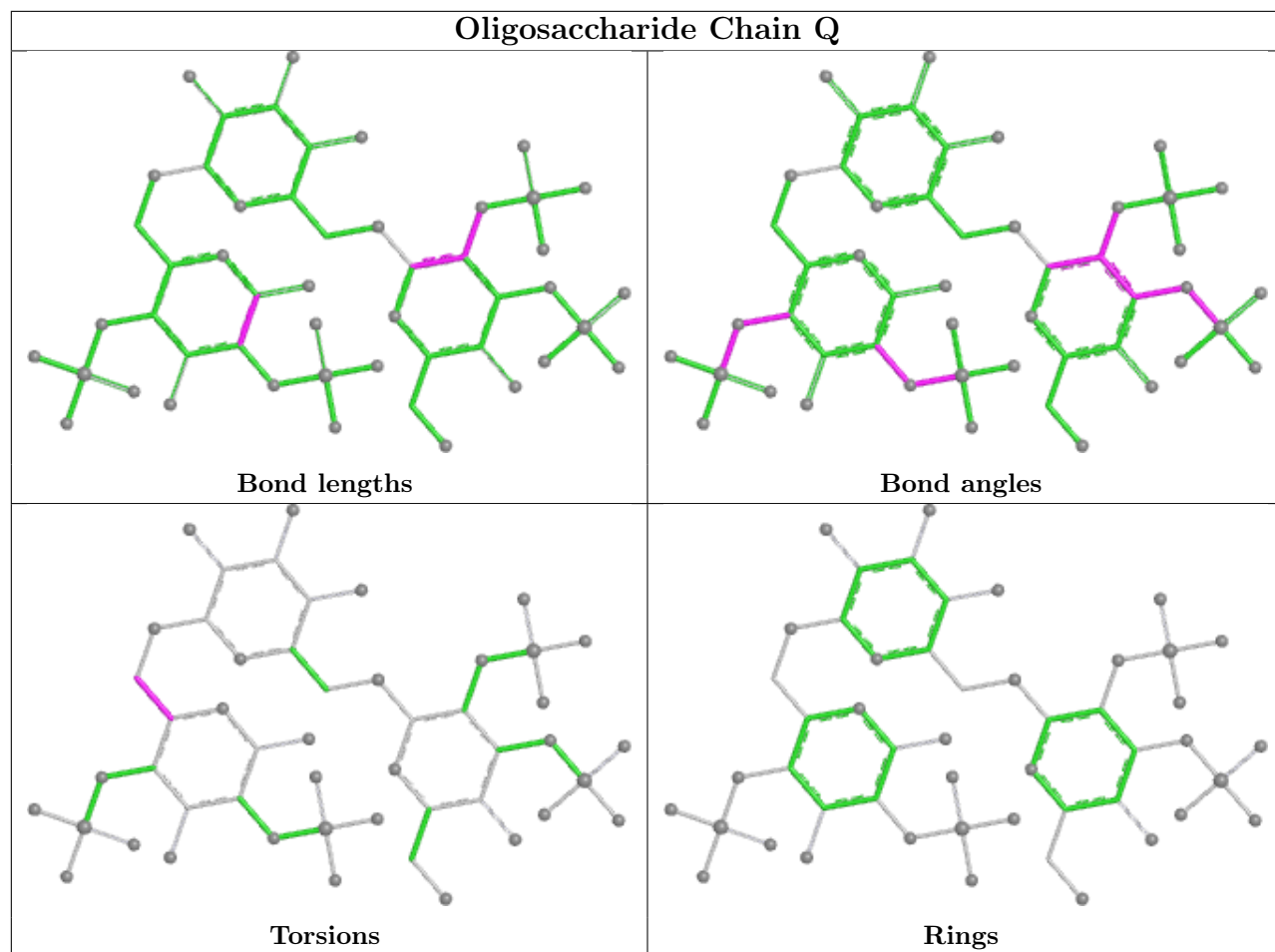
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	b	2	GLC	1	0
3	O	1	5LS	2	0
3	T	3	5TM	1	0
2	e	2	GLC	1	0
3	T	7	5TH	1	0
2	R	1	5LS	1	0
2	j	3	PDX	4	0
2	Z	2	GLC	1	0
2	X	2	GLC	1	0
2	m	2	GLC	2	0
2	P	3	PDX	1	0
2	n	2	GLC	2	0
2	N	1	5LS	1	0
2	j	1	5LS	2	0
2	R	3	PDX	1	0
2	d	2	GLC	1	0

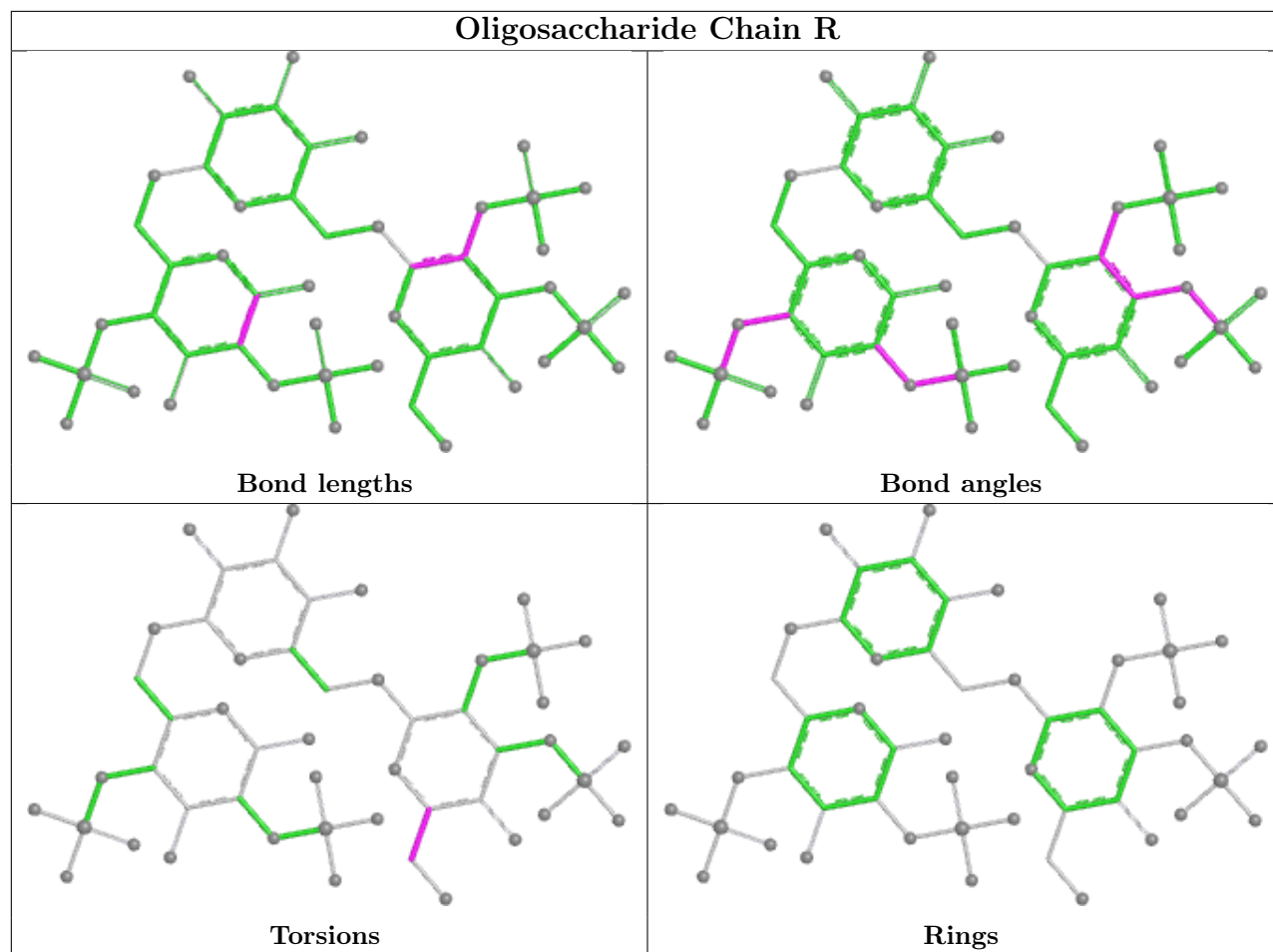
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

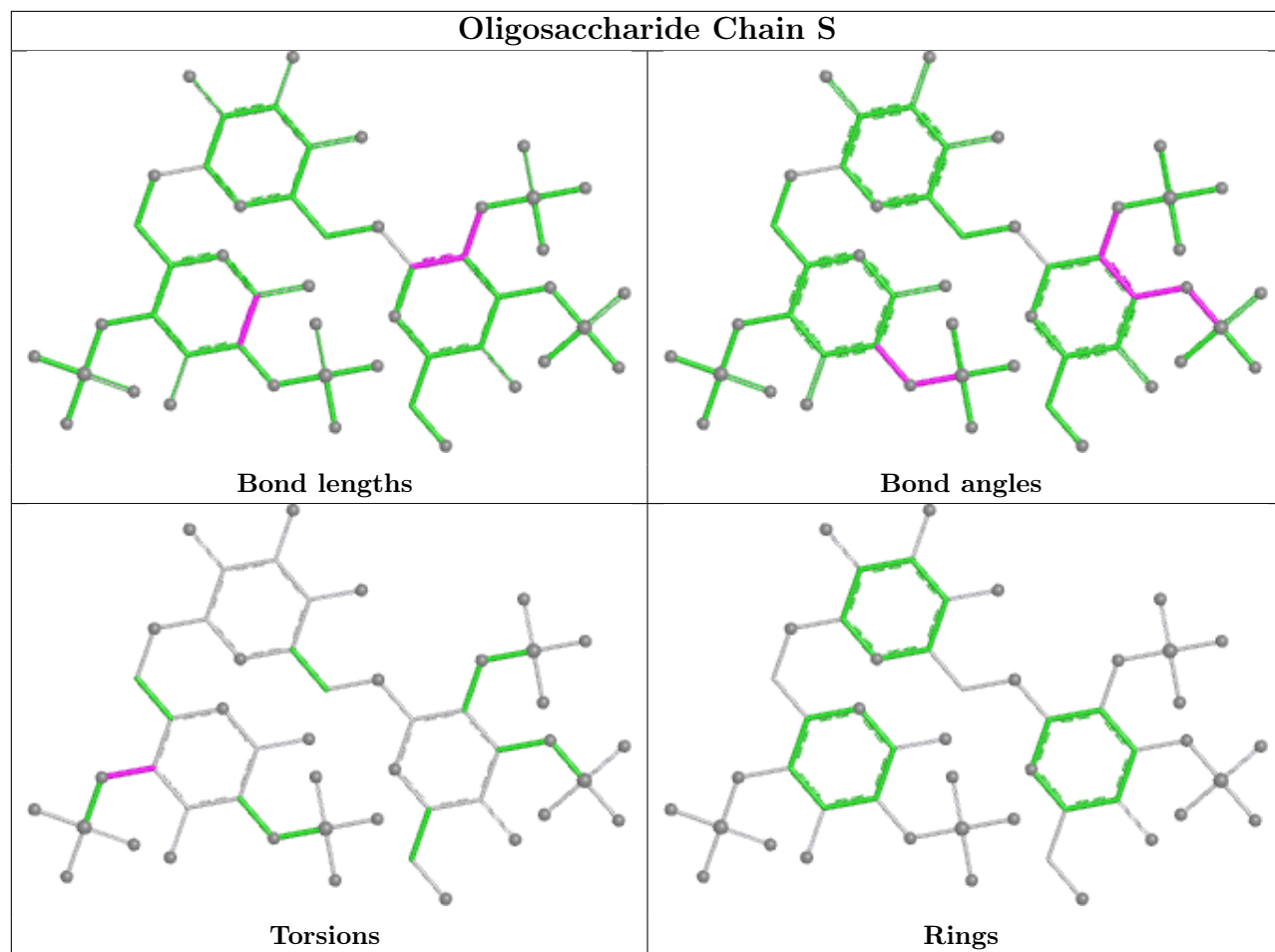


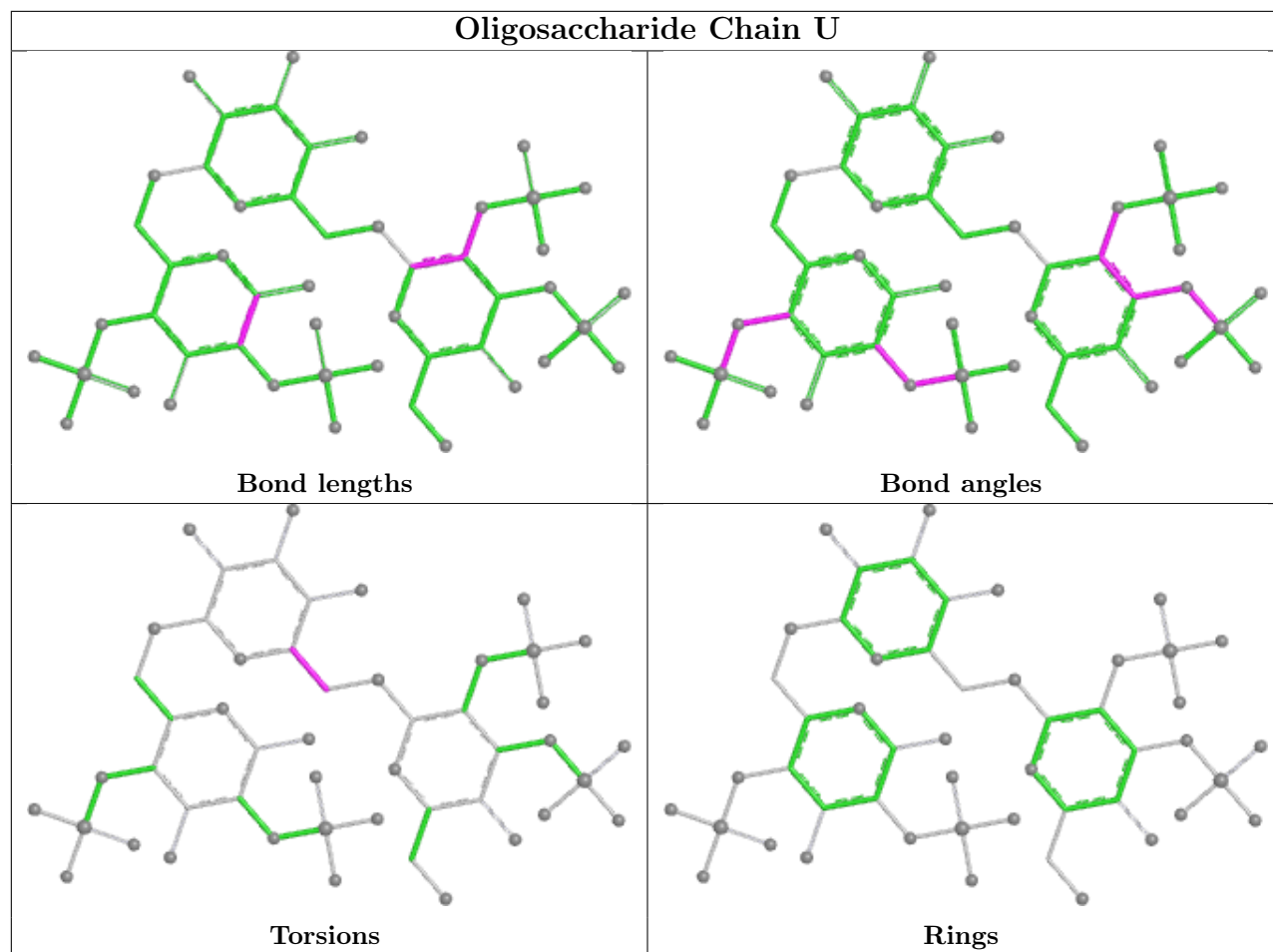


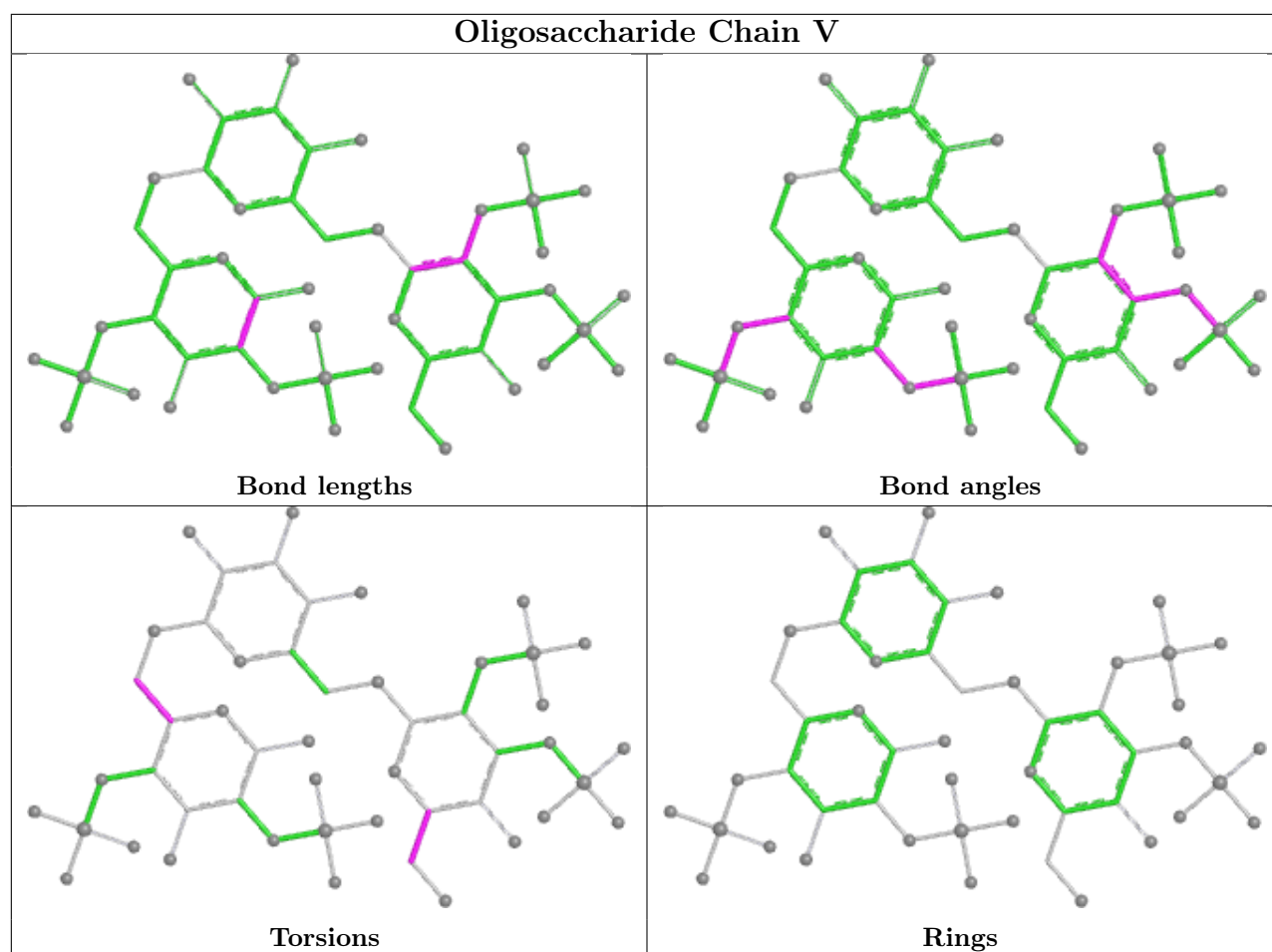




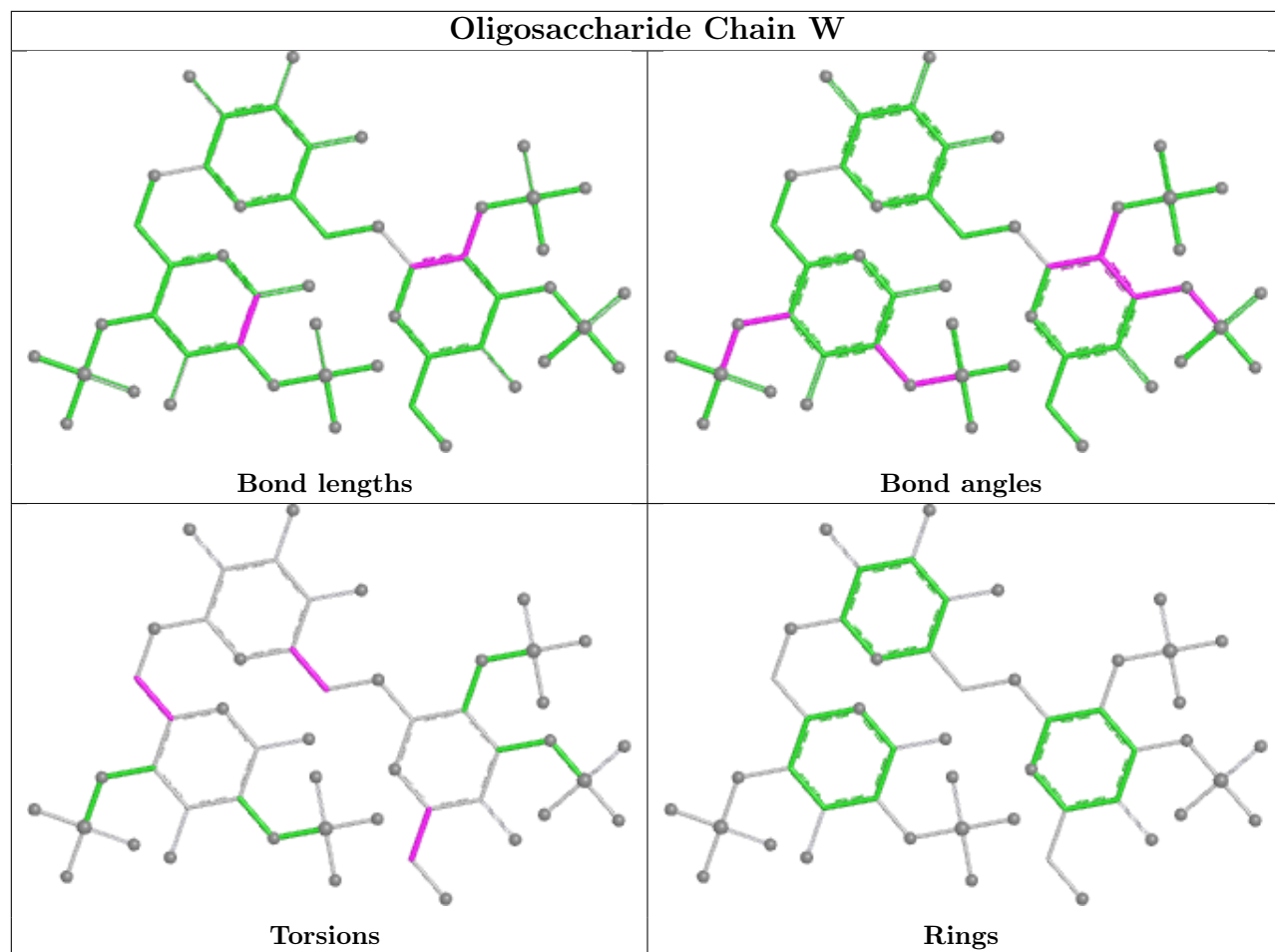


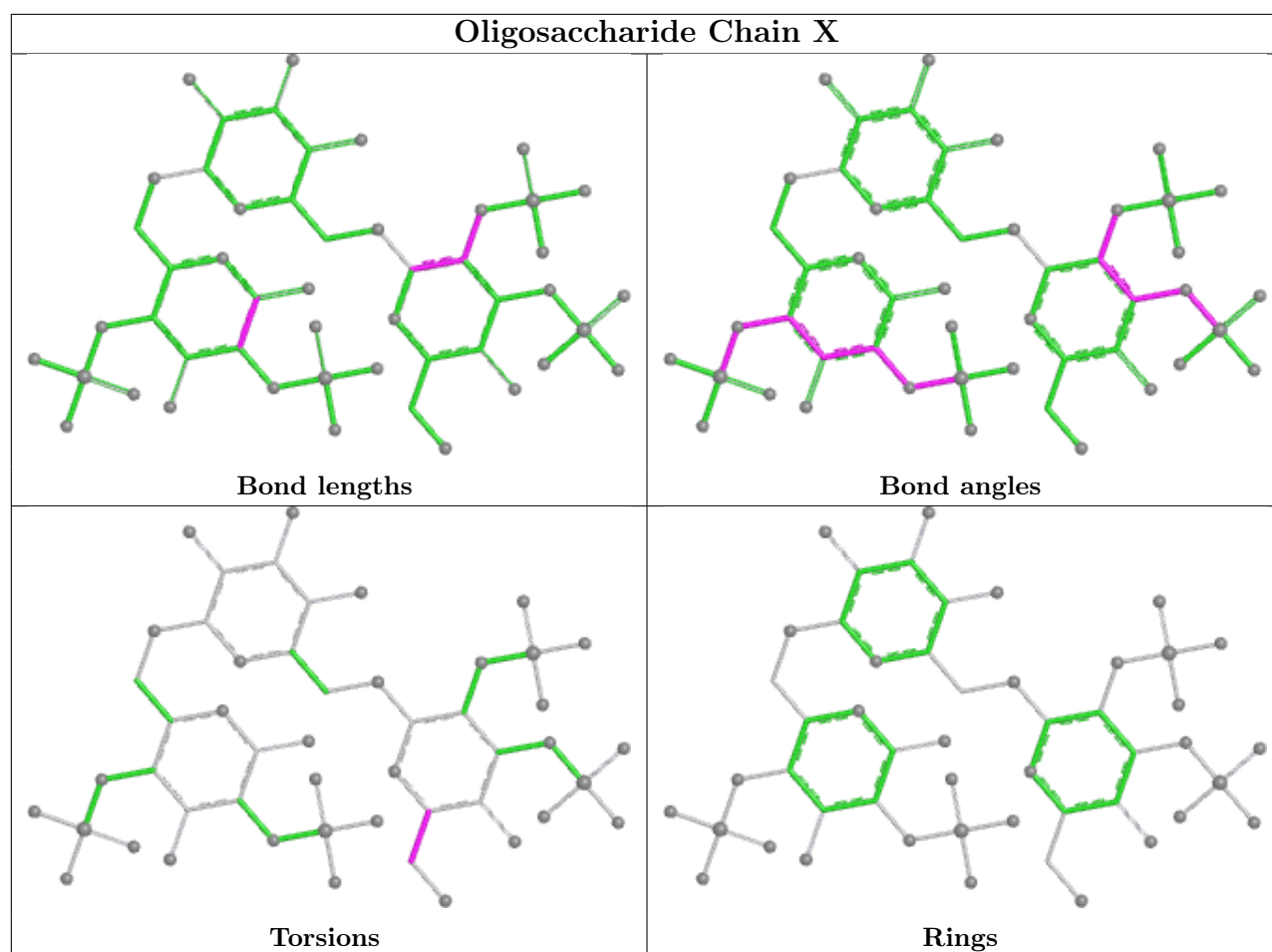


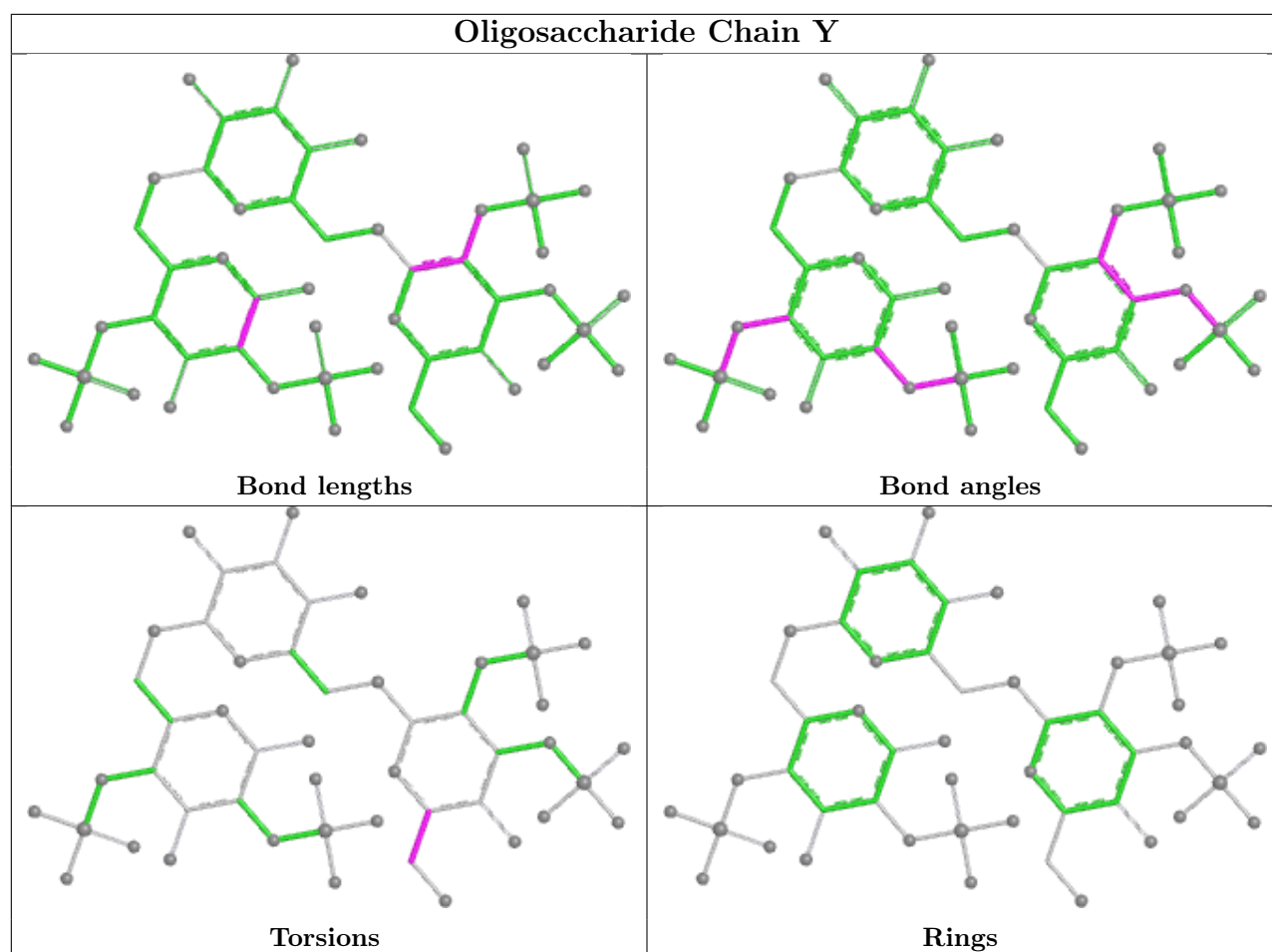


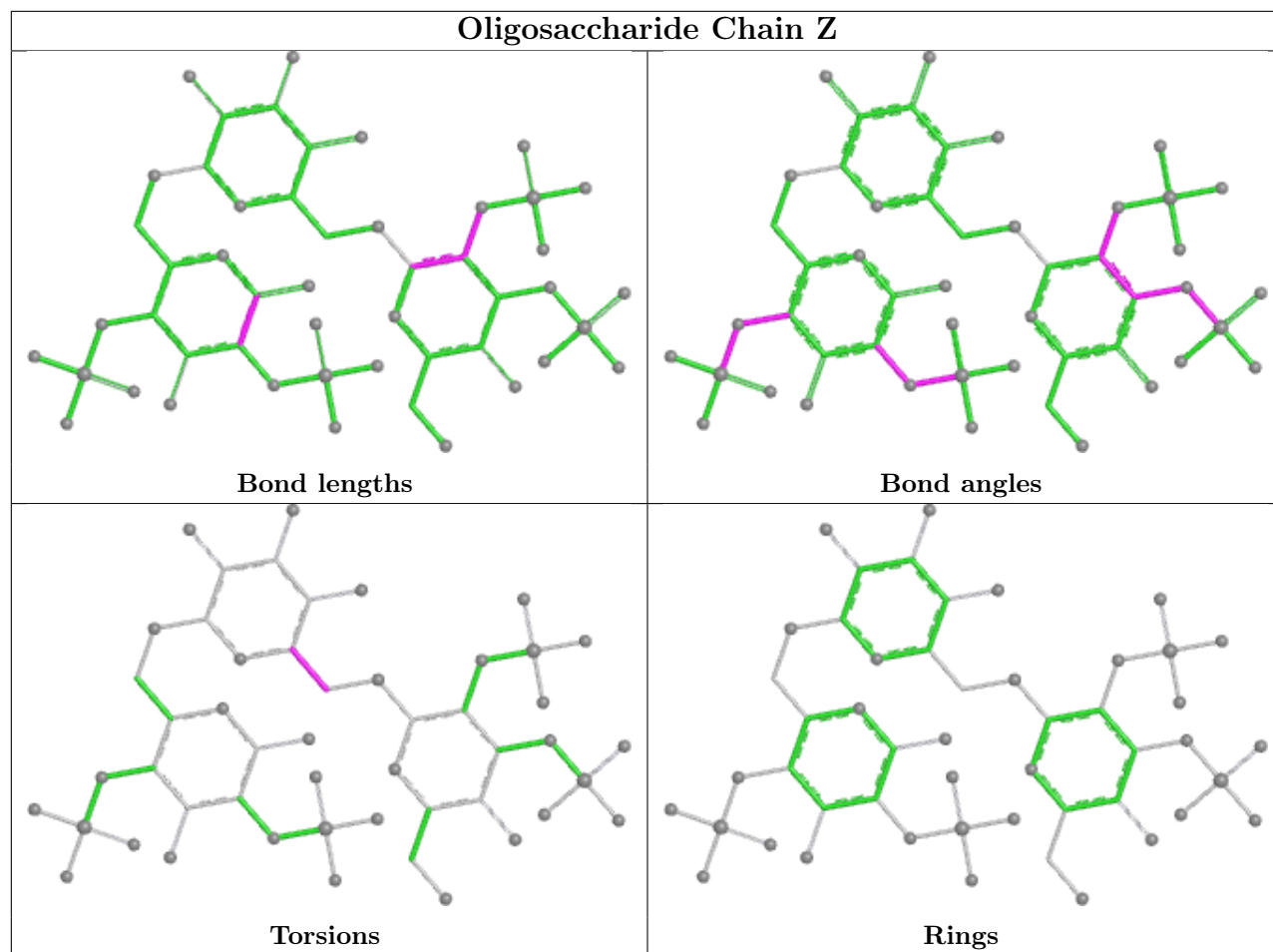


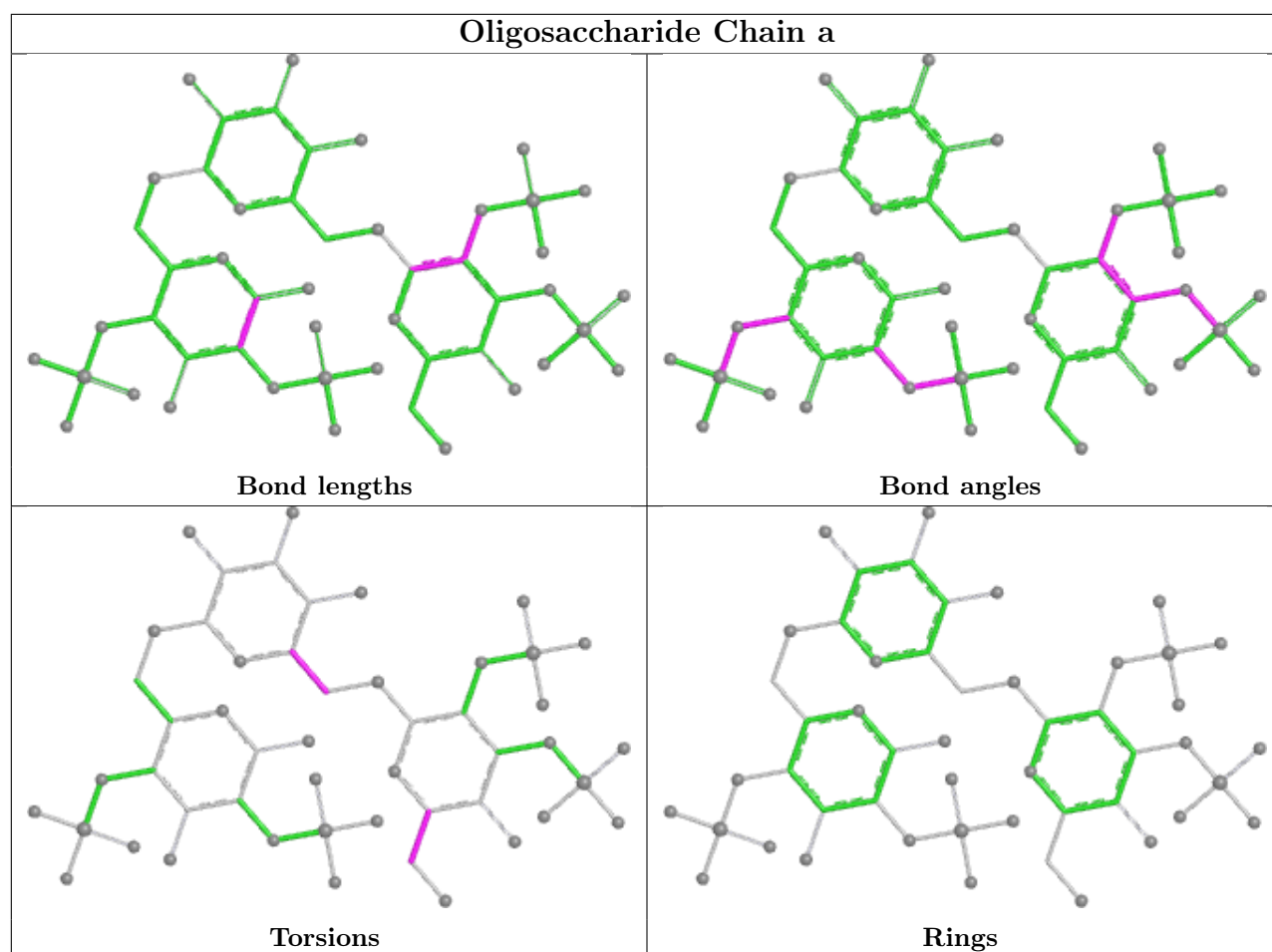
Oligosaccharide Chain W

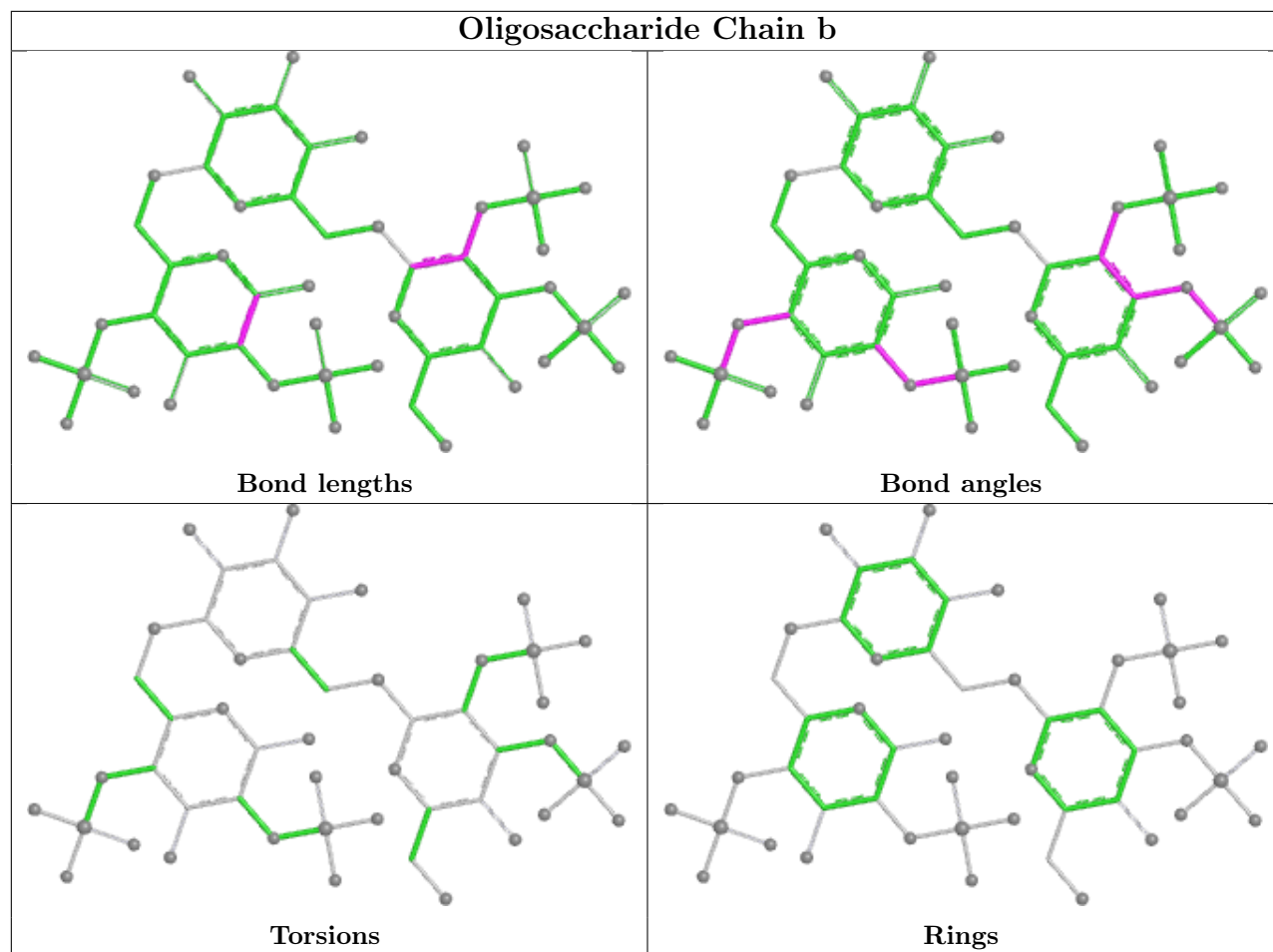


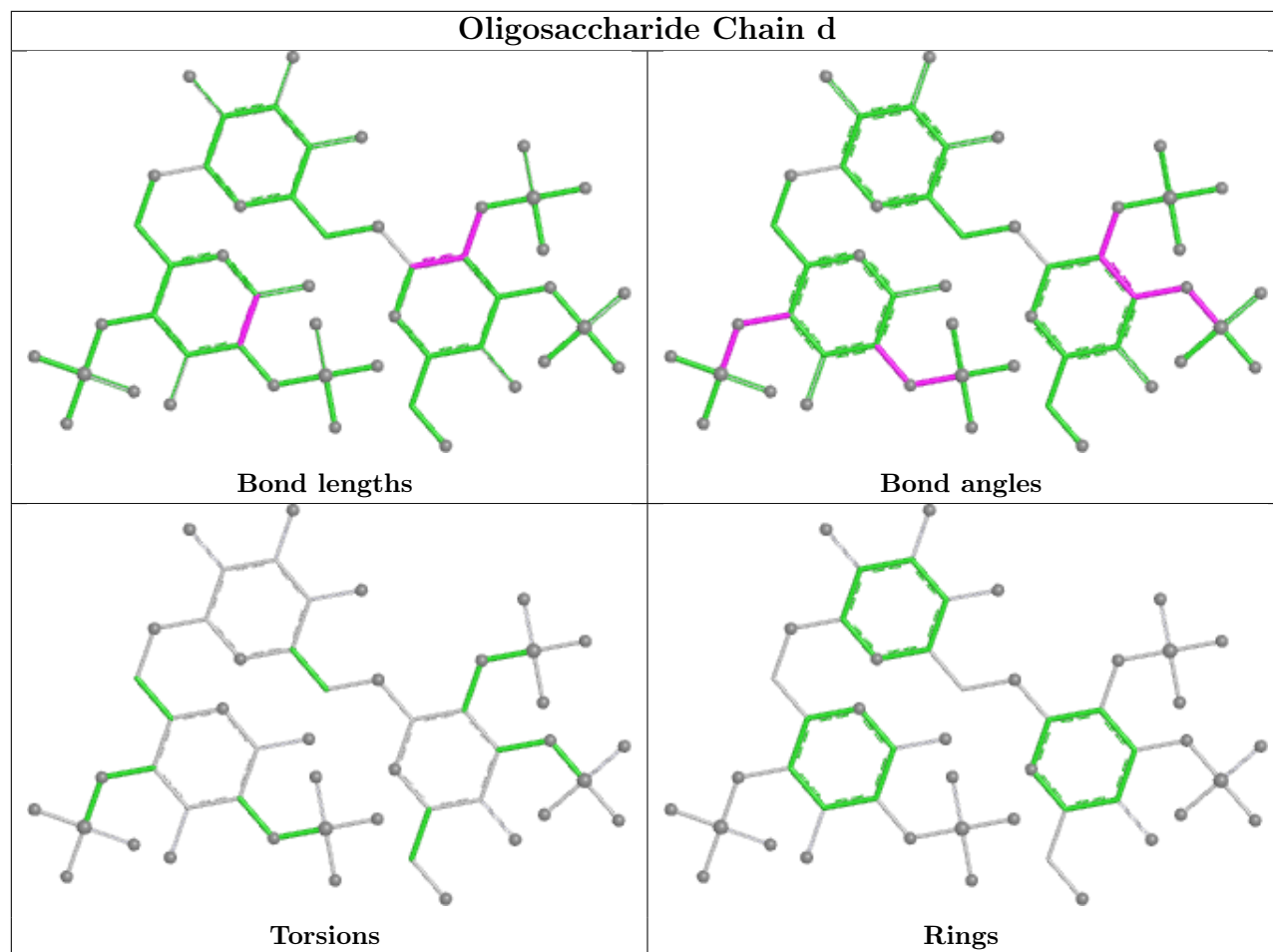


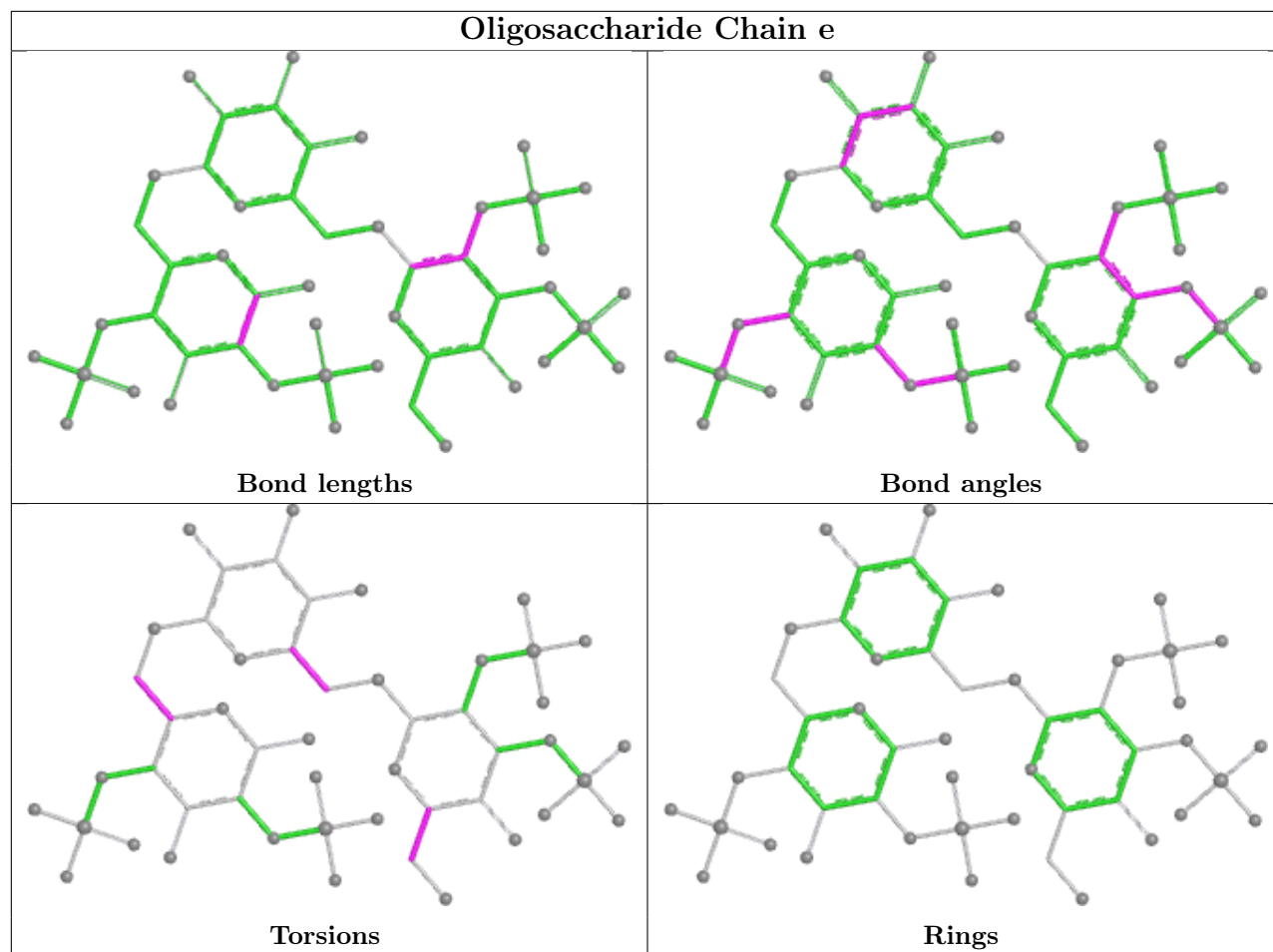


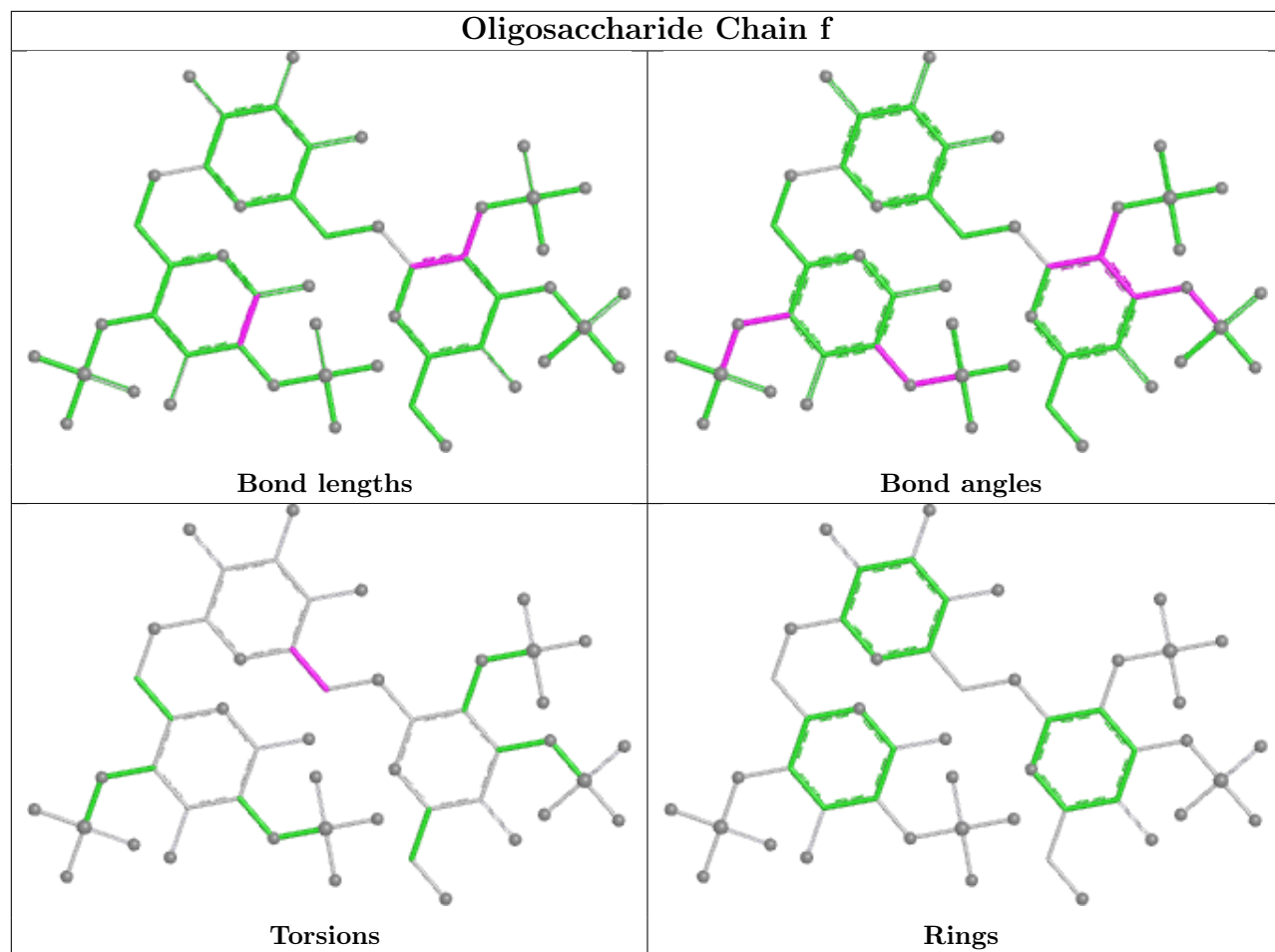


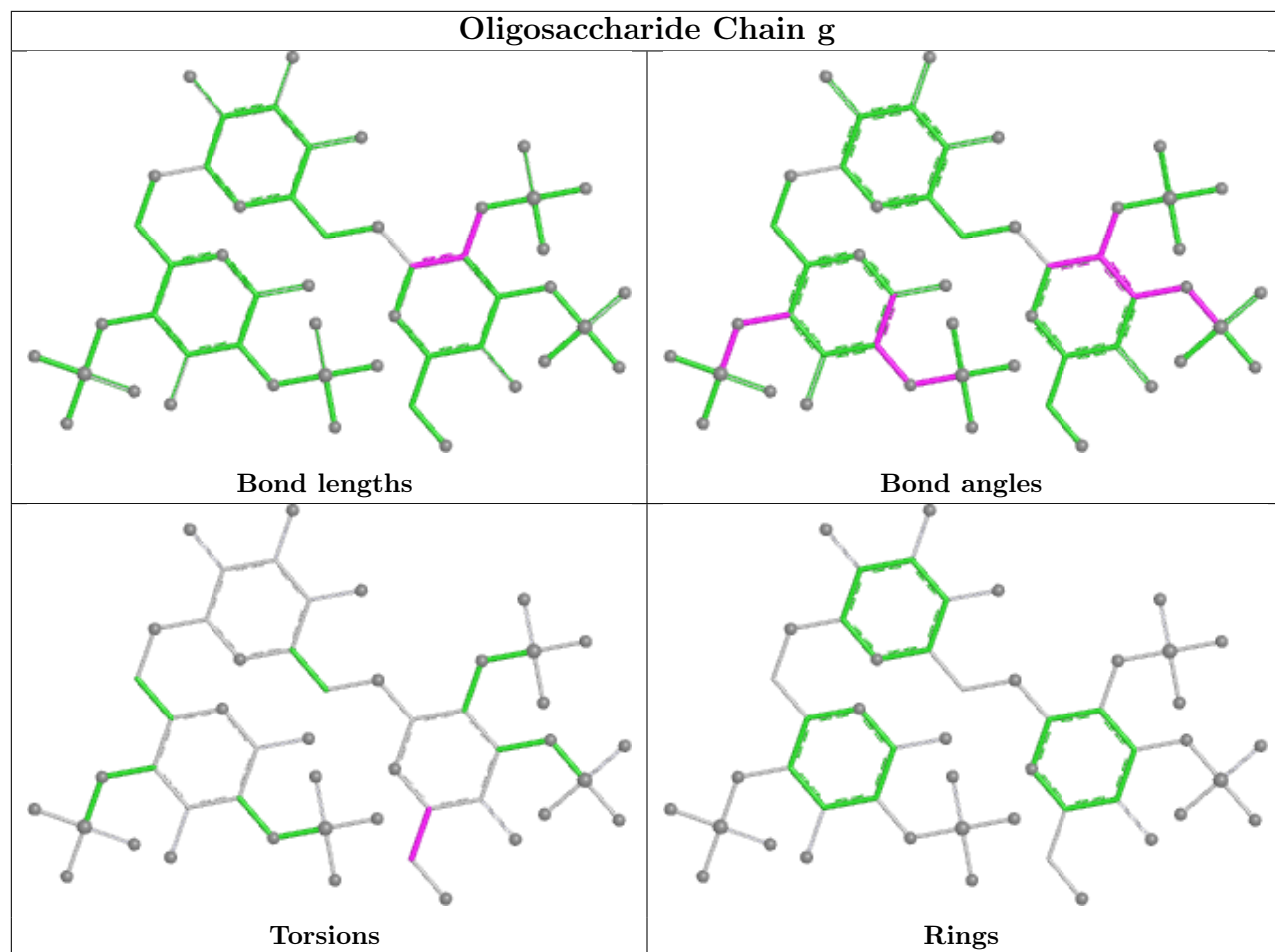


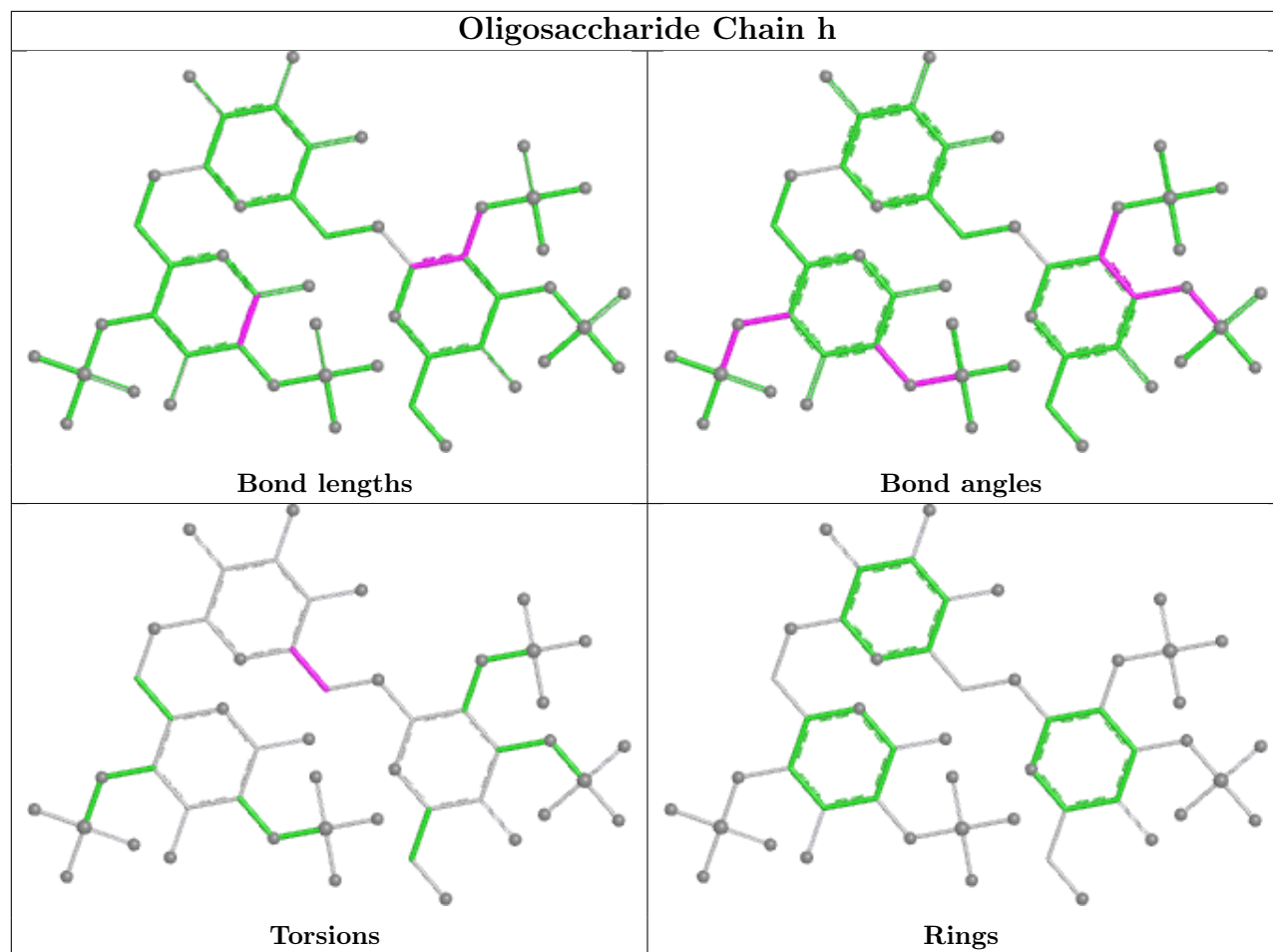


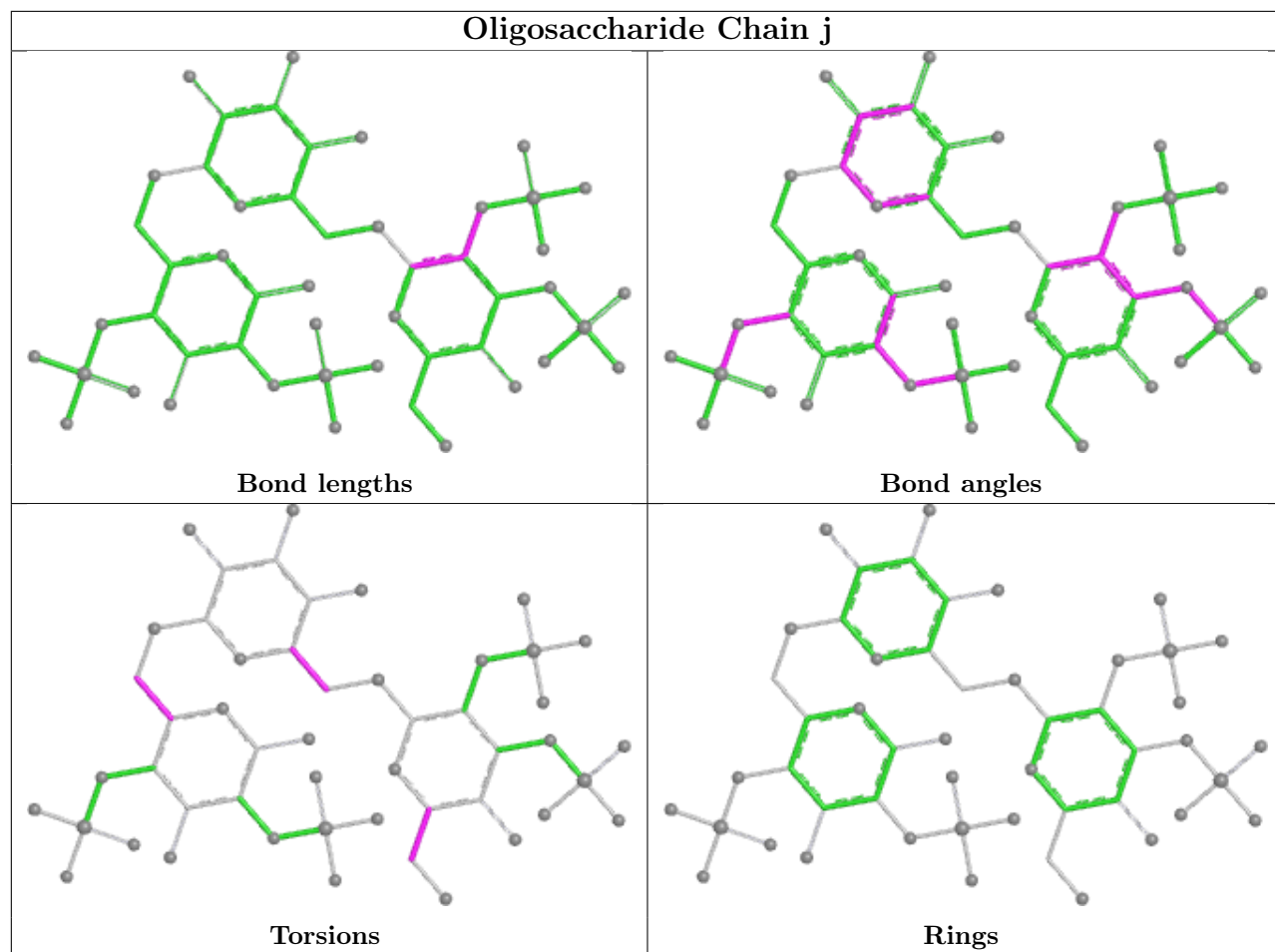


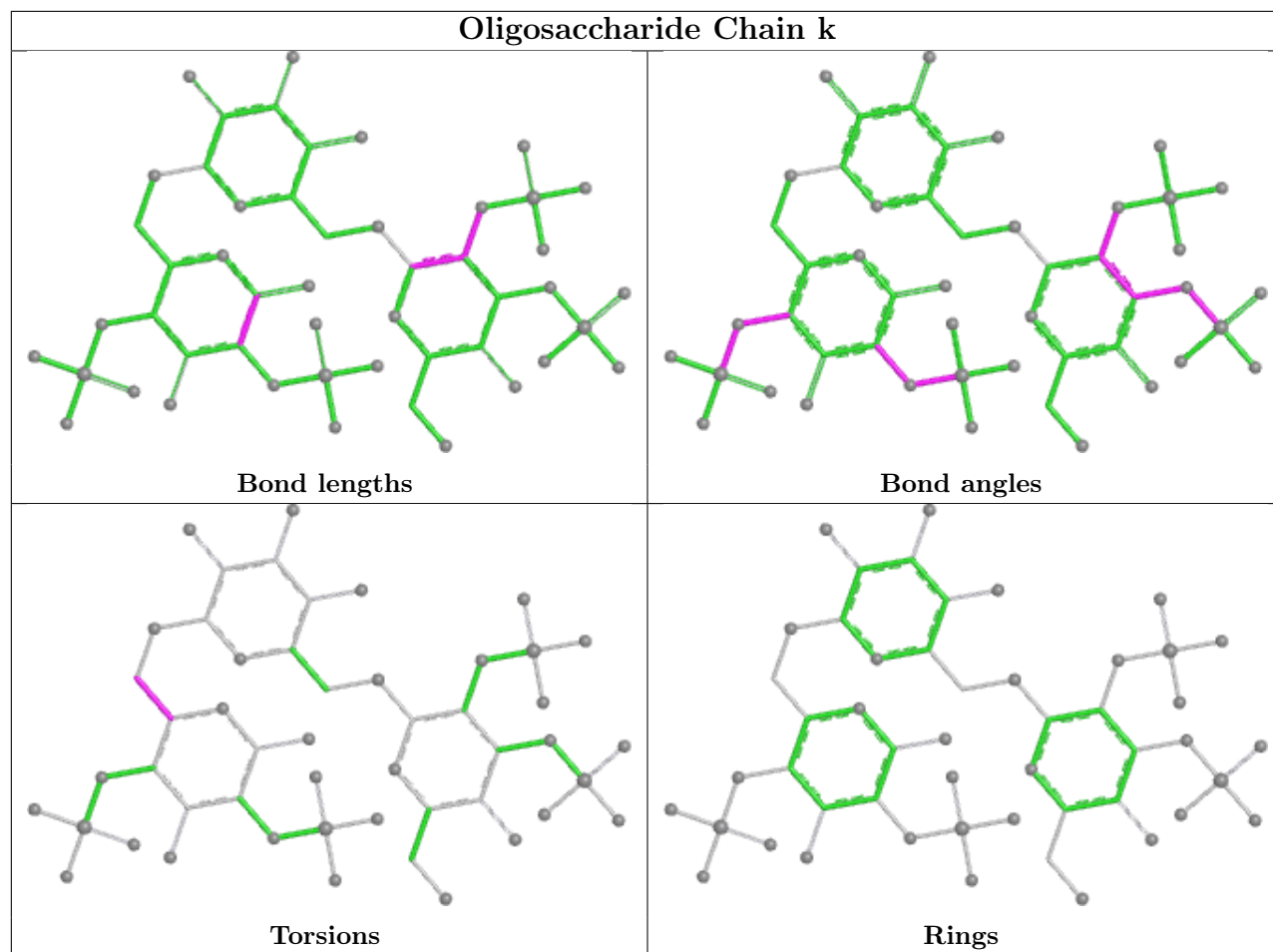


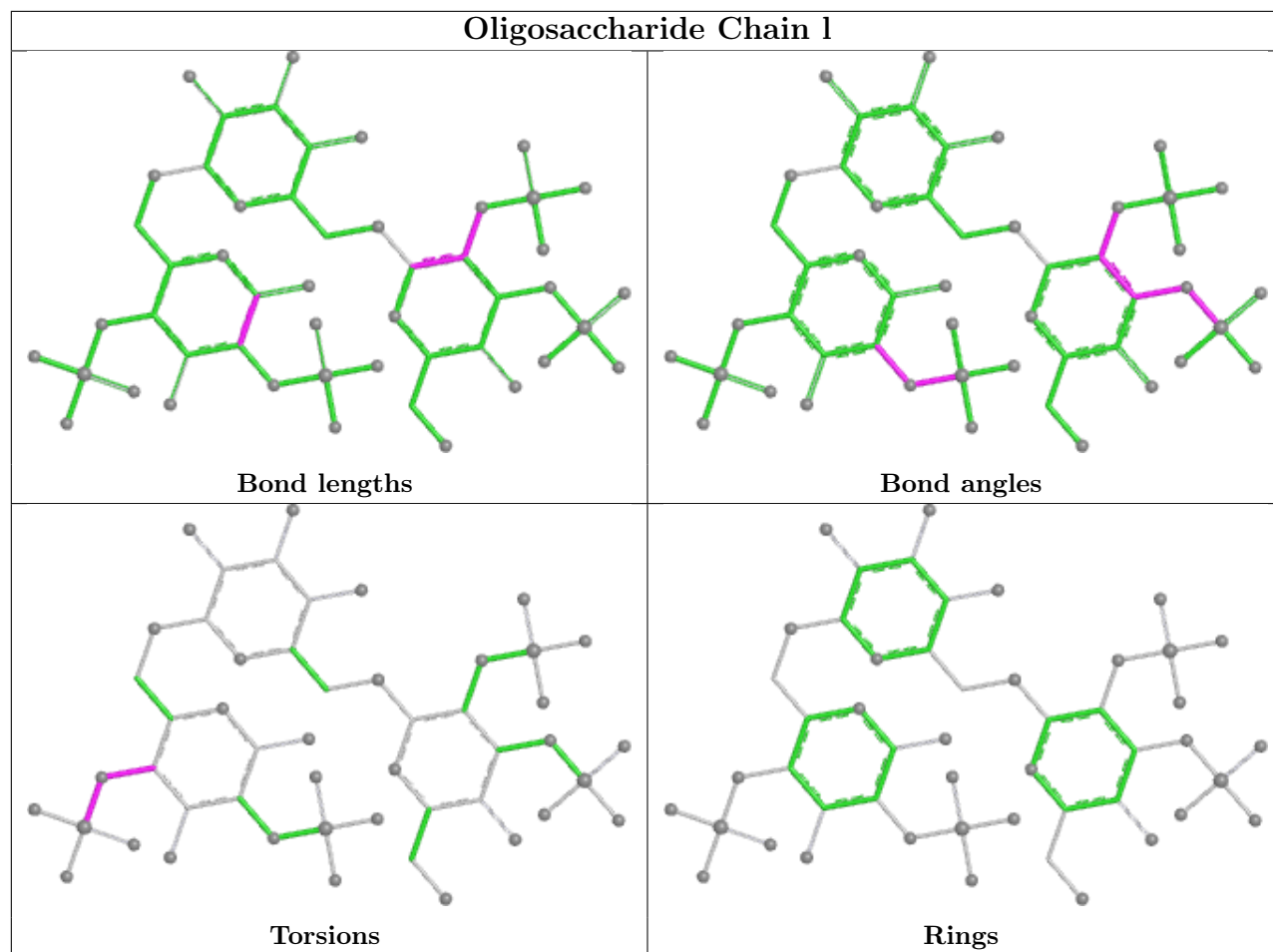


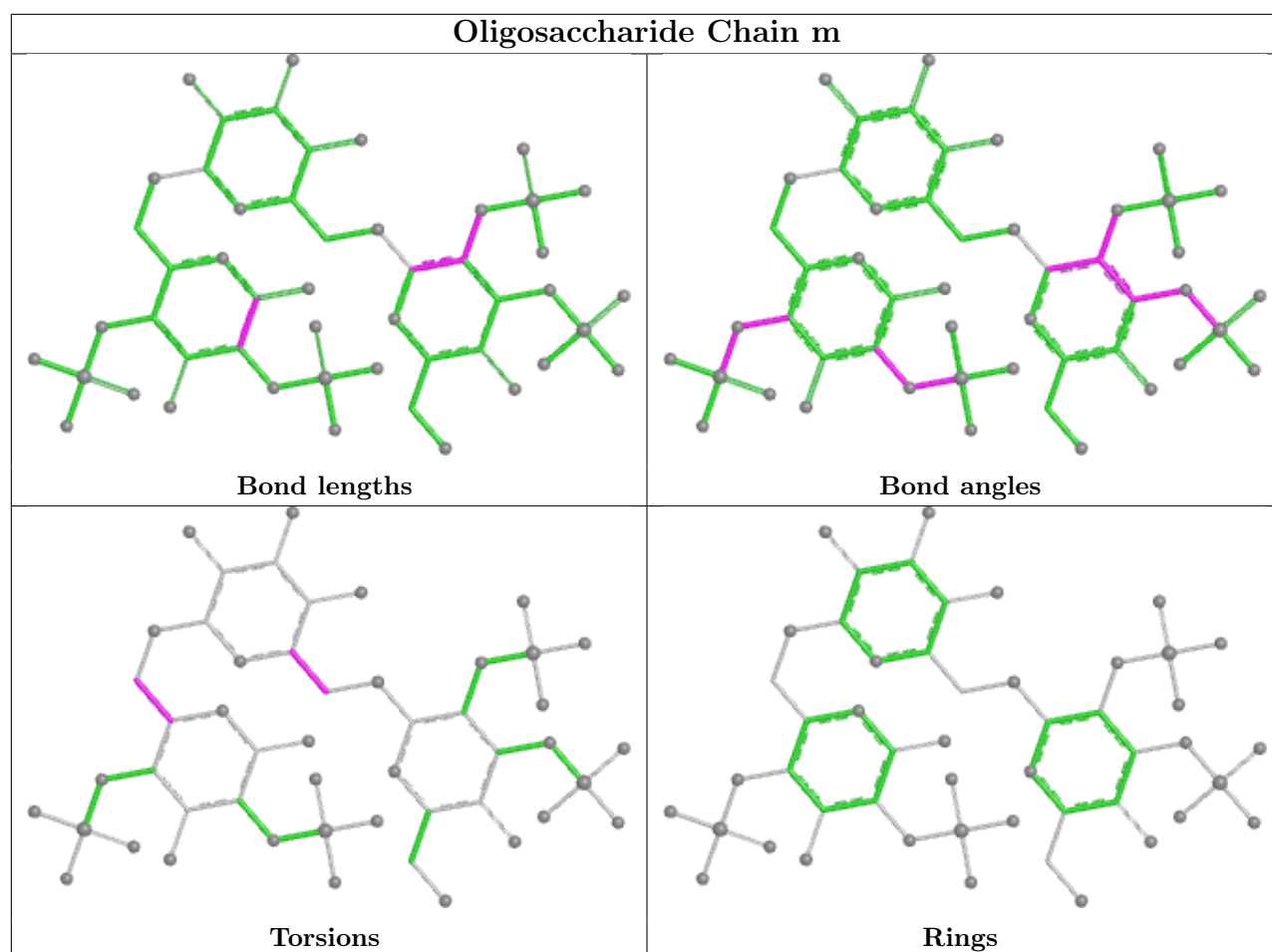


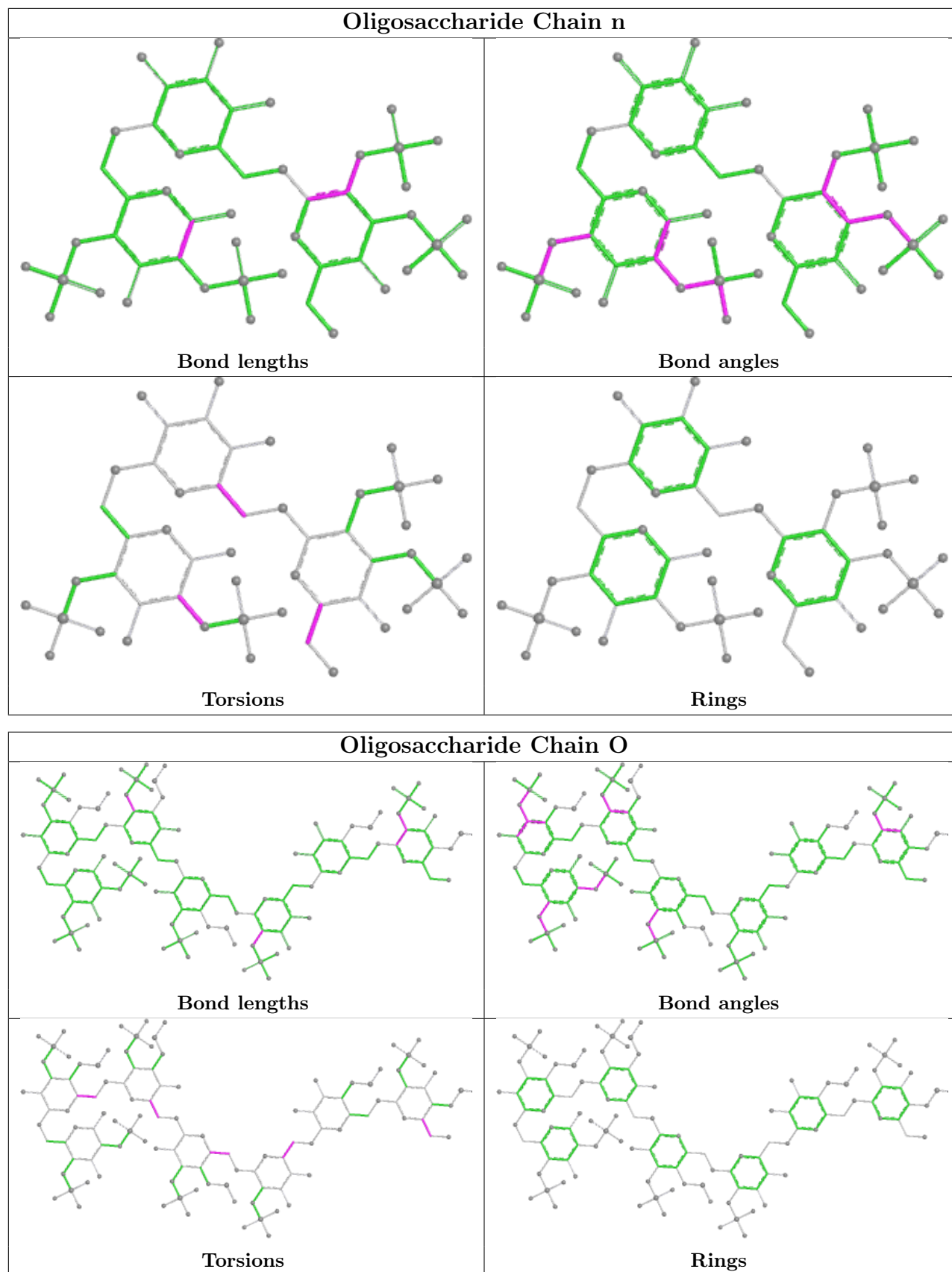




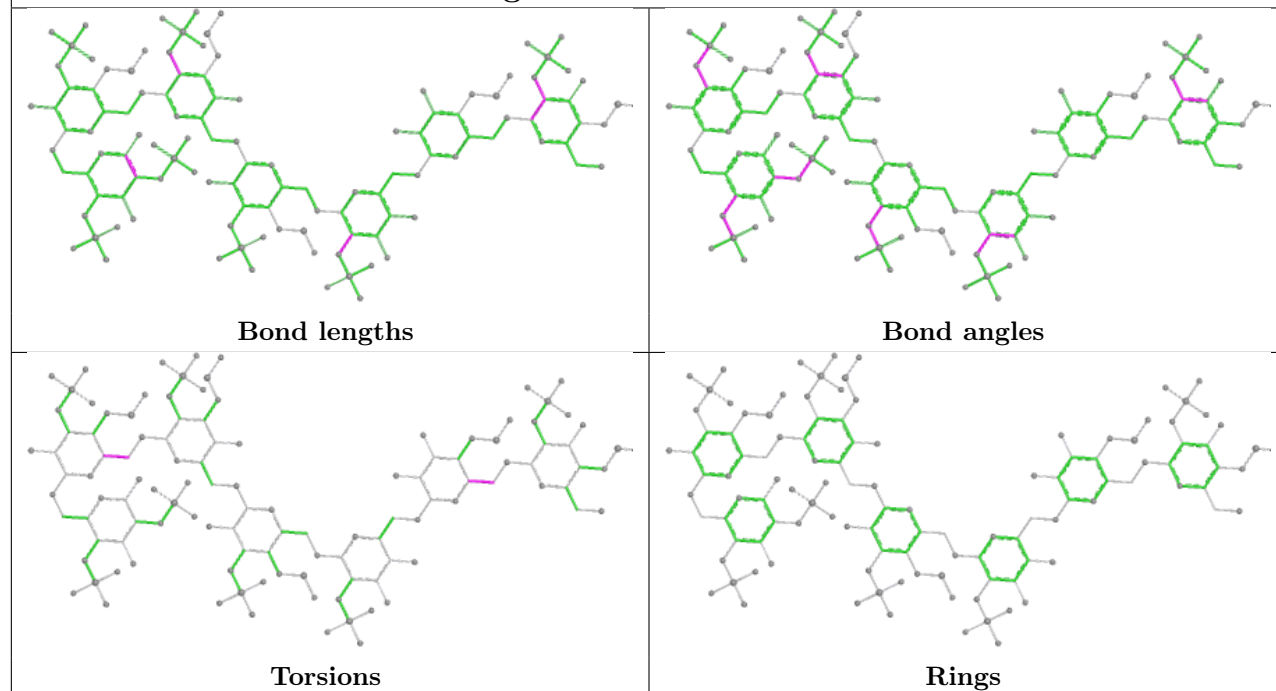




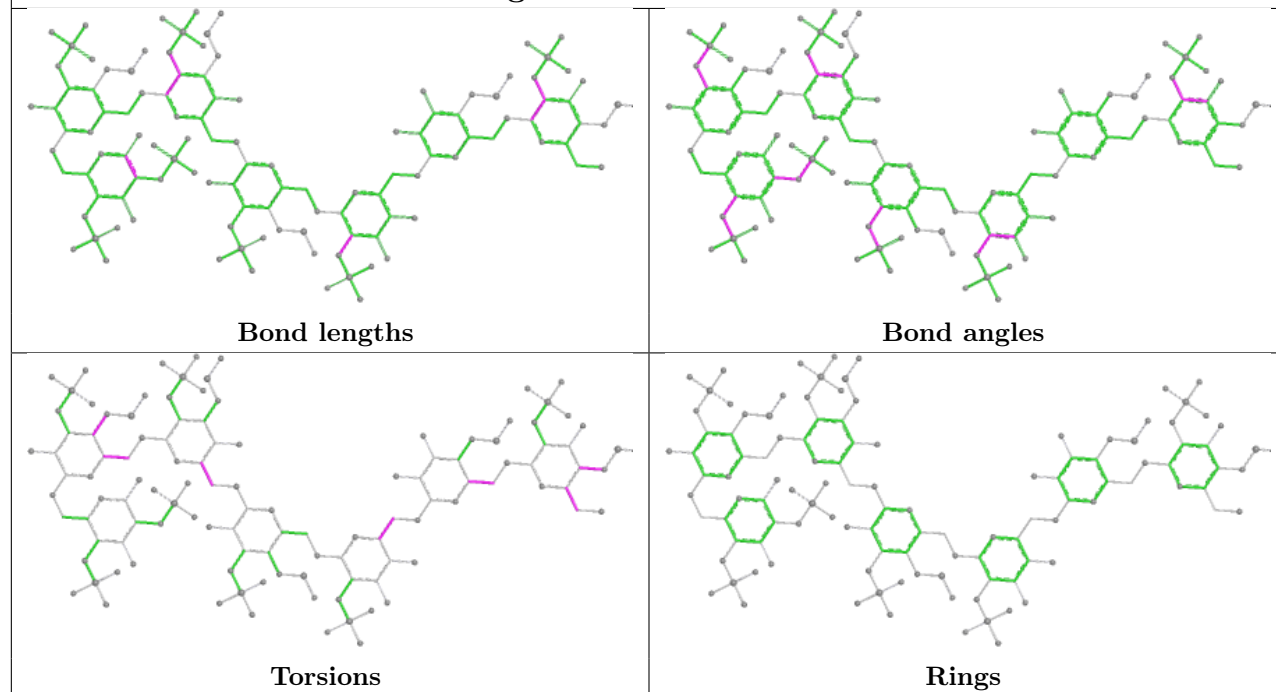


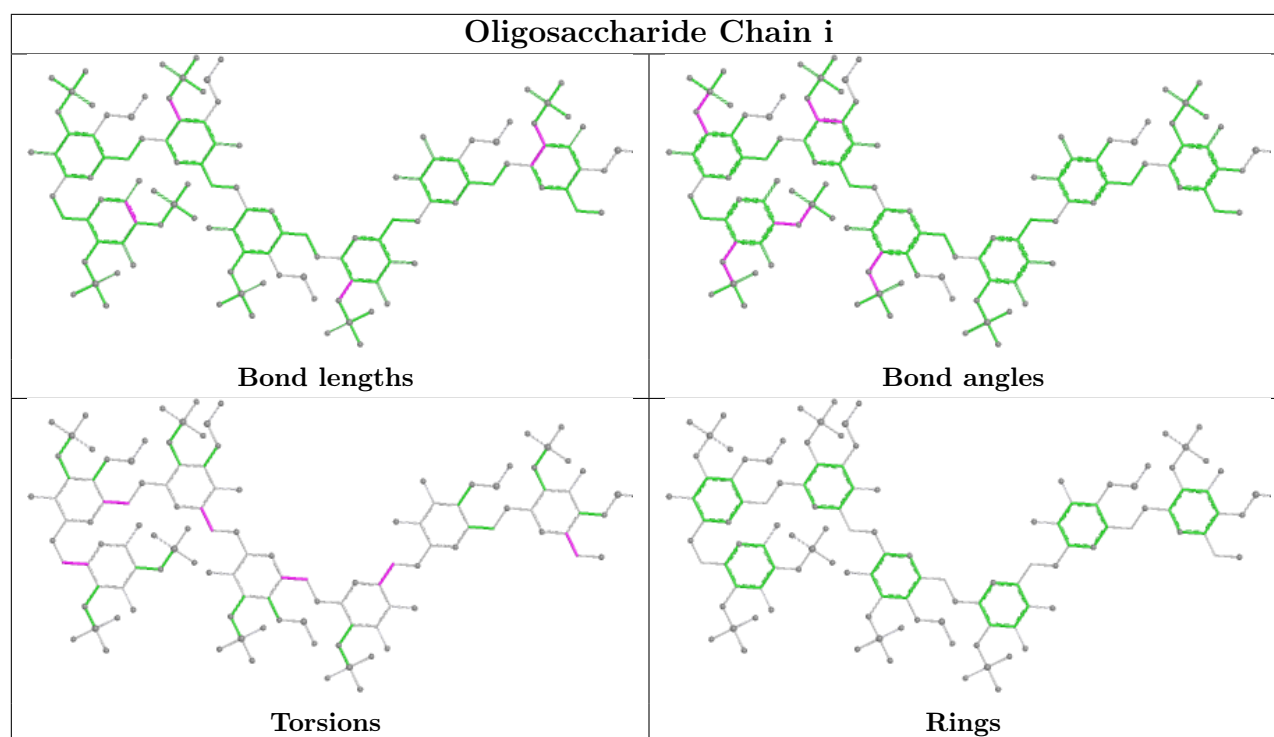


Oligosaccharide Chain T



Oligosaccharide Chain c





5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	5TL	D	701	-	28,28,28	2.74	10 (35%)	41,41,41	5.01	20 (48%)
4	5TL	C	701	-	28,28,28	2.70	11 (39%)	41,41,41	4.97	22 (53%)
4	5TL	G	701	-	28,28,28	2.69	11 (39%)	41,41,41	4.99	25 (60%)
4	5TL	J	701	-	28,28,28	2.74	12 (42%)	41,41,41	5.02	23 (56%)
4	5TL	A	701	-	28,28,28	2.71	13 (46%)	41,41,41	4.95	23 (56%)
4	5TL	I	701	-	28,28,28	2.71	10 (35%)	41,41,41	4.92	22 (53%)
4	5TL	B	701	-	28,28,28	2.75	12 (42%)	41,41,41	4.89	24 (58%)
4	5TL	K	701	-	28,28,28	2.67	11 (39%)	41,41,41	5.05	21 (51%)
4	5TL	F	701	-	28,28,28	2.73	10 (35%)	41,41,41	4.93	19 (46%)
4	5TL	E	701	-	28,28,28	2.70	10 (35%)	41,41,41	4.95	21 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5TL	L	701	-	28,28,28	2.73	12 (42%)	41,41,41	4.95	21 (51%)
4	5TL	H	701	-	28,28,28	2.74	12 (42%)	41,41,41	4.92	22 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5TL	D	701	-	-	7/18/18/18	0/3/3/3
4	5TL	C	701	-	-	8/18/18/18	0/3/3/3
4	5TL	G	701	-	-	5/18/18/18	0/3/3/3
4	5TL	J	701	-	-	8/18/18/18	0/3/3/3
4	5TL	A	701	-	-	8/18/18/18	0/3/3/3
4	5TL	I	701	-	-	8/18/18/18	0/3/3/3
4	5TL	B	701	-	-	6/18/18/18	0/3/3/3
4	5TL	K	701	-	-	8/18/18/18	0/3/3/3
4	5TL	F	701	-	-	8/18/18/18	0/3/3/3
4	5TL	E	701	-	-	8/18/18/18	0/3/3/3
4	5TL	L	701	-	-	6/18/18/18	0/3/3/3
4	5TL	H	701	-	-	6/18/18/18	0/3/3/3

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	701	5TL	S-N1	-6.33	1.48	1.60
4	H	701	5TL	S-N1	-6.29	1.48	1.60
4	F	701	5TL	S-N1	-6.26	1.48	1.60
4	B	701	5TL	S-N1	-6.20	1.48	1.60
4	L	701	5TL	S-N1	-6.11	1.48	1.60
4	I	701	5TL	S-N1	-6.10	1.48	1.60
4	J	701	5TL	S-N1	-6.06	1.48	1.60
4	C	701	5TL	S-N1	-6.03	1.48	1.60
4	A	701	5TL	S-N1	-5.85	1.49	1.60
4	D	701	5TL	S-N1	-5.83	1.49	1.60
4	K	701	5TL	S-N1	-5.79	1.49	1.60
4	E	701	5TL	S-N1	-5.77	1.49	1.60
4	G	701	5TL	CAQ-CAR	-5.25	1.33	1.42
4	I	701	5TL	CAQ-CAR	-5.19	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	5TL	CAQ-CAR	-5.12	1.34	1.42
4	C	701	5TL	CAQ-CAR	-5.11	1.34	1.42
4	J	701	5TL	CAQ-CAR	-5.06	1.34	1.42
4	H	701	5TL	CAQ-CAR	-5.06	1.34	1.42
4	F	701	5TL	CAQ-CAR	-5.04	1.34	1.42
4	B	701	5TL	CAQ-CAR	-4.94	1.34	1.42
4	D	701	5TL	CAQ-CAR	-4.91	1.34	1.42
4	K	701	5TL	CAQ-CAR	-4.88	1.34	1.42
4	E	701	5TL	CAQ-CAR	-4.87	1.34	1.42
4	E	701	5TL	CAV-NAW	4.82	1.41	1.33
4	L	701	5TL	CAQ-CAR	-4.81	1.34	1.42
4	D	701	5TL	CAT-CAU	4.75	1.46	1.38
4	D	701	5TL	CAN-CAU	4.73	1.46	1.38
4	L	701	5TL	CAT-CAU	4.71	1.46	1.38
4	K	701	5TL	CAV-NAW	4.71	1.41	1.33
4	J	701	5TL	CAT-CAU	4.68	1.46	1.38
4	I	701	5TL	CAT-CAU	4.65	1.46	1.38
4	C	701	5TL	CAT-CAU	4.65	1.46	1.38
4	B	701	5TL	CAT-CAU	4.63	1.46	1.38
4	A	701	5TL	CAT-CAU	4.57	1.46	1.38
4	E	701	5TL	CAT-CAU	4.57	1.46	1.38
4	K	701	5TL	CAT-CAU	4.55	1.46	1.38
4	C	701	5TL	CAV-NAW	4.54	1.41	1.33
4	I	701	5TL	CAV-NAW	4.54	1.41	1.33
4	J	701	5TL	CAN-CAU	4.53	1.45	1.38
4	B	701	5TL	CAN-CAU	4.53	1.45	1.38
4	A	701	5TL	CAV-NAW	4.52	1.41	1.33
4	B	701	5TL	CAV-NAW	4.52	1.41	1.33
4	L	701	5TL	CAN-CAU	4.52	1.45	1.38
4	H	701	5TL	CAT-CAU	4.50	1.45	1.38
4	F	701	5TL	CAT-CAU	4.47	1.45	1.38
4	H	701	5TL	CAN-CAU	4.44	1.45	1.38
4	D	701	5TL	CAV-NAW	4.42	1.41	1.33
4	G	701	5TL	CAV-NAW	4.41	1.41	1.33
4	H	701	5TL	CAV-NAW	4.37	1.41	1.33
4	L	701	5TL	CAV-NAW	4.36	1.41	1.33
4	F	701	5TL	CAV-NAW	4.35	1.41	1.33
4	J	701	5TL	CAV-NAW	4.35	1.41	1.33
4	K	701	5TL	CAN-CAU	4.34	1.45	1.38
4	L	701	5TL	CAU-S	4.30	1.83	1.77
4	I	701	5TL	CAN-CAU	4.30	1.45	1.38
4	A	701	5TL	CAN-CAU	4.24	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	701	5TL	CAN-CAU	4.24	1.45	1.38
4	D	701	5TL	CAU-S	4.20	1.83	1.77
4	E	701	5TL	CAN-CAU	4.20	1.45	1.38
4	G	701	5TL	CAT-CAU	4.18	1.45	1.38
4	C	701	5TL	CAN-CAU	4.17	1.45	1.38
4	B	701	5TL	CAU-S	4.14	1.83	1.77
4	G	701	5TL	CAN-CAU	4.13	1.45	1.38
4	E	701	5TL	CAU-S	4.05	1.83	1.77
4	J	701	5TL	CAU-S	4.03	1.83	1.77
4	I	701	5TL	CAU-S	4.02	1.83	1.77
4	C	701	5TL	CAU-S	3.95	1.83	1.77
4	H	701	5TL	CAU-S	3.88	1.83	1.77
4	A	701	5TL	CAU-S	3.86	1.83	1.77
4	F	701	5TL	CAU-S	3.85	1.83	1.77
4	D	701	5TL	CAR-NAY	3.75	1.49	1.37
4	F	701	5TL	CAR-NAY	3.70	1.49	1.37
4	L	701	5TL	CAR-NAY	3.69	1.49	1.37
4	A	701	5TL	CAG-CAH	-3.68	1.40	1.49
4	J	701	5TL	CAR-NAY	3.67	1.49	1.37
4	K	701	5TL	CAU-S	3.67	1.82	1.77
4	H	701	5TL	CAR-NAY	3.65	1.49	1.37
4	K	701	5TL	CAR-NAY	3.65	1.48	1.37
4	A	701	5TL	CAR-NAY	3.62	1.48	1.37
4	G	701	5TL	CAR-NAY	3.62	1.48	1.37
4	E	701	5TL	CAR-NAY	3.60	1.48	1.37
4	E	701	5TL	CAG-CAH	-3.59	1.40	1.49
4	B	701	5TL	CAR-NAY	3.56	1.48	1.37
4	L	701	5TL	CAG-CAH	-3.56	1.40	1.49
4	I	701	5TL	CAR-NAY	3.56	1.48	1.37
4	C	701	5TL	CAR-NAY	3.54	1.48	1.37
4	B	701	5TL	CAG-CAH	-3.54	1.40	1.49
4	H	701	5TL	CAG-CAH	-3.52	1.40	1.49
4	I	701	5TL	CAG-CAH	-3.51	1.40	1.49
4	G	701	5TL	CAU-S	3.47	1.82	1.77
4	K	701	5TL	CAG-CAH	-3.45	1.40	1.49
4	C	701	5TL	CAG-CAH	-3.41	1.41	1.49
4	L	701	5TL	CAS-CAL	-3.40	1.32	1.39
4	D	701	5TL	CAG-CAH	-3.38	1.41	1.49
4	J	701	5TL	CAG-CAH	-3.37	1.41	1.49
4	H	701	5TL	CAS-CAL	-3.37	1.32	1.39
4	G	701	5TL	CAG-CAH	-3.37	1.41	1.49
4	F	701	5TL	CAG-CAH	-3.26	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	5TL	CAS-CAL	-3.26	1.33	1.39
4	G	701	5TL	CAS-CAL	-3.24	1.33	1.39
4	C	701	5TL	CAS-CAL	-3.23	1.33	1.39
4	B	701	5TL	CAS-CAL	-3.17	1.33	1.39
4	D	701	5TL	CAS-CAL	-3.13	1.33	1.39
4	E	701	5TL	CAS-CAL	-3.10	1.33	1.39
4	J	701	5TL	CAS-CAL	-3.09	1.33	1.39
4	I	701	5TL	CAS-CAL	-3.08	1.33	1.39
4	F	701	5TL	CAS-CAL	-3.03	1.33	1.39
4	K	701	5TL	CAS-CAL	-2.94	1.33	1.39
4	G	701	5TL	CAQ-CAV	-2.72	1.46	1.50
4	J	701	5TL	CAQ-CAV	-2.48	1.46	1.50
4	A	701	5TL	CAI-CAJ	-2.38	1.36	1.39
4	D	701	5TL	CAQ-CAV	-2.37	1.46	1.50
4	H	701	5TL	CAS-CAT	2.32	1.42	1.38
4	H	701	5TL	CAQ-CAV	-2.30	1.46	1.50
4	B	701	5TL	CAS-CAT	2.28	1.42	1.38
4	I	701	5TL	CAI-CAJ	-2.25	1.36	1.39
4	L	701	5TL	CAQ-CAV	-2.25	1.47	1.50
4	E	701	5TL	CAI-CAJ	-2.24	1.36	1.39
4	C	701	5TL	CAI-CAJ	-2.24	1.36	1.39
4	F	701	5TL	CAI-CAJ	-2.22	1.36	1.39
4	A	701	5TL	CAS-CAT	2.21	1.42	1.38
4	B	701	5TL	CAQ-CAV	-2.14	1.47	1.50
4	K	701	5TL	CAI-CAJ	-2.14	1.36	1.39
4	G	701	5TL	CAI-CAJ	-2.14	1.36	1.39
4	C	701	5TL	CAQ-CAV	-2.11	1.47	1.50
4	B	701	5TL	CAI-CAJ	-2.09	1.36	1.39
4	J	701	5TL	CAS-CAT	2.07	1.42	1.38
4	K	701	5TL	CAS-CAT	2.07	1.42	1.38
4	A	701	5TL	CAQ-CAV	-2.04	1.47	1.50
4	L	701	5TL	CAI-CAJ	-2.02	1.36	1.39
4	H	701	5TL	CAI-CAJ	-2.02	1.36	1.39
4	J	701	5TL	CAI-CAJ	-2.01	1.36	1.39
4	A	701	5TL	CAI-CAH	-2.00	1.36	1.39
4	L	701	5TL	CAS-CAT	2.00	1.42	1.38

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	5TL	CAT-CAS-CAL	-14.75	102.19	121.12
4	D	701	5TL	CAS-CAL-CAM	14.71	144.01	117.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	701	5TL	CAT-CAS-CAL	-14.71	102.24	121.12
4	L	701	5TL	CAT-CAS-CAL	-14.67	102.29	121.12
4	J	701	5TL	CAS-CAL-CAM	14.65	143.88	117.68
4	A	701	5TL	CAT-CAS-CAL	-14.63	102.34	121.12
4	C	701	5TL	CAT-CAS-CAL	-14.59	102.40	121.12
4	L	701	5TL	CAS-CAL-CAM	14.58	143.76	117.68
4	K	701	5TL	CAT-CAS-CAL	-14.56	102.43	121.12
4	G	701	5TL	CAT-CAS-CAL	-14.51	102.50	121.12
4	E	701	5TL	CAT-CAS-CAL	-14.50	102.52	121.12
4	H	701	5TL	CAT-CAS-CAL	-14.48	102.53	121.12
4	I	701	5TL	CAT-CAS-CAL	-14.46	102.56	121.12
4	K	701	5TL	CAS-CAL-CAM	14.41	143.47	117.68
4	H	701	5TL	CAS-CAL-CAM	14.40	143.45	117.68
4	E	701	5TL	CAS-CAL-CAM	14.36	143.37	117.68
4	A	701	5TL	CAS-CAL-CAM	14.28	143.23	117.68
4	F	701	5TL	CAS-CAL-CAM	14.27	143.21	117.68
4	B	701	5TL	CAT-CAS-CAL	-14.26	102.82	121.12
4	C	701	5TL	CAS-CAL-CAM	14.24	143.16	117.68
4	I	701	5TL	CAS-CAL-CAM	14.22	143.13	117.68
4	G	701	5TL	CAS-CAL-CAM	14.22	143.12	117.68
4	B	701	5TL	CAS-CAL-CAM	14.17	143.03	117.68
4	F	701	5TL	CAT-CAS-CAL	-13.65	103.60	121.12
4	K	701	5TL	CAM-CAN-CAU	-11.76	108.00	119.44
4	C	701	5TL	CAM-CAN-CAU	-11.68	108.08	119.44
4	G	701	5TL	CAM-CAN-CAU	-11.59	108.17	119.44
4	E	701	5TL	CAM-CAN-CAU	-11.54	108.21	119.44
4	A	701	5TL	CAM-CAN-CAU	-11.51	108.25	119.44
4	I	701	5TL	CAM-CAN-CAU	-11.40	108.35	119.44
4	J	701	5TL	CAM-CAN-CAU	-11.38	108.37	119.44
4	D	701	5TL	CAM-CAN-CAU	-11.36	108.39	119.44
4	H	701	5TL	CAM-CAN-CAU	-11.28	108.47	119.44
4	B	701	5TL	CAM-CAN-CAU	-11.26	108.49	119.44
4	L	701	5TL	CAM-CAN-CAU	-11.25	108.50	119.44
4	F	701	5TL	CAN-CAU-S	-10.29	105.75	119.72
4	F	701	5TL	CAM-CAN-CAU	-10.26	109.47	119.44
4	E	701	5TL	CAN-CAU-S	-9.25	107.16	119.72
4	C	701	5TL	CAN-CAU-S	-9.18	107.25	119.72
4	K	701	5TL	CAN-CAU-S	-9.08	107.39	119.72
4	A	701	5TL	CAN-CAU-S	-9.02	107.47	119.72
4	I	701	5TL	CAN-CAU-S	-9.01	107.48	119.72
4	G	701	5TL	CAN-CAU-S	-8.98	107.53	119.72
4	D	701	5TL	CAN-CAU-S	-8.90	107.64	119.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	701	5TL	CAN-CAU-S	-8.88	107.67	119.72
4	B	701	5TL	CAN-CAU-S	-8.83	107.73	119.72
4	J	701	5TL	CAN-CAU-S	-8.73	107.87	119.72
4	H	701	5TL	CAN-CAU-S	-8.70	107.91	119.72
4	J	701	5TL	CAS-CAL-CAJ	-8.62	106.63	120.91
4	B	701	5TL	CAS-CAL-CAJ	-8.59	106.68	120.91
4	L	701	5TL	CAS-CAL-CAJ	-8.56	106.73	120.91
4	H	701	5TL	CAS-CAL-CAJ	-8.51	106.81	120.91
4	K	701	5TL	CAS-CAL-CAJ	-8.48	106.87	120.91
4	D	701	5TL	CAS-CAL-CAJ	-8.47	106.88	120.91
4	E	701	5TL	CAS-CAL-CAJ	-8.45	106.91	120.91
4	G	701	5TL	CAS-CAL-CAJ	-8.41	106.97	120.91
4	A	701	5TL	CAS-CAL-CAJ	-8.35	107.07	120.91
4	C	701	5TL	CAS-CAL-CAJ	-8.25	107.24	120.91
4	I	701	5TL	CAS-CAL-CAJ	-8.20	107.33	120.91
4	F	701	5TL	CAM-CAL-CAJ	-8.14	107.43	120.91
4	K	701	5TL	O2-S-O4	-8.00	106.49	118.80
4	J	701	5TL	O2-S-O4	-7.81	106.78	118.80
4	F	701	5TL	CAS-CAL-CAJ	-7.76	108.05	120.91
4	D	701	5TL	CAM-CAL-CAJ	-7.62	108.29	120.91
4	J	701	5TL	CAM-CAL-CAJ	-7.47	108.53	120.91
4	L	701	5TL	CAM-CAL-CAJ	-7.46	108.55	120.91
4	G	701	5TL	O2-S-O4	-7.45	107.34	118.80
4	F	701	5TL	O2-S-O4	-7.40	107.41	118.80
4	E	701	5TL	CAM-CAL-CAJ	-7.38	108.68	120.91
4	I	701	5TL	CAM-CAL-CAJ	-7.34	108.74	120.91
4	K	701	5TL	CAM-CAL-CAJ	-7.32	108.78	120.91
4	H	701	5TL	CAM-CAL-CAJ	-7.31	108.80	120.91
4	B	701	5TL	CAM-CAL-CAJ	-7.29	108.83	120.91
4	C	701	5TL	CAM-CAL-CAJ	-7.22	108.95	120.91
4	D	701	5TL	O2-S-O4	-7.20	107.73	118.80
4	G	701	5TL	CAM-CAL-CAJ	-7.15	109.06	120.91
4	A	701	5TL	CAM-CAL-CAJ	-7.14	109.08	120.91
4	C	701	5TL	O2-S-O4	-7.12	107.84	118.80
4	A	701	5TL	O2-S-O4	-7.06	107.94	118.80
4	I	701	5TL	O2-S-O4	-7.05	107.95	118.80
4	L	701	5TL	O2-S-O4	-6.82	108.30	118.80
4	B	701	5TL	O2-S-O4	-6.72	108.46	118.80
4	K	701	5TL	CAT-CAU-CAN	6.64	129.13	120.47
4	H	701	5TL	O2-S-O4	-6.62	108.61	118.80
4	E	701	5TL	O2-S-O4	-6.39	108.97	118.80
4	E	701	5TL	CAT-CAU-CAN	6.26	128.63	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	701	5TL	CAT-CAU-CAN	6.21	128.56	120.47
4	C	701	5TL	CAT-CAU-CAN	6.16	128.50	120.47
4	J	701	5TL	CAT-CAU-CAN	6.11	128.44	120.47
4	A	701	5TL	CAT-CAU-CAN	6.08	128.40	120.47
4	I	701	5TL	CAT-CAU-CAN	6.05	128.35	120.47
4	D	701	5TL	CAT-CAU-CAN	5.97	128.25	120.47
4	F	701	5TL	CAT-CAU-CAN	5.94	128.22	120.47
4	H	701	5TL	CAT-CAU-CAN	5.91	128.17	120.47
4	B	701	5TL	CAT-CAU-CAN	5.86	128.11	120.47
4	L	701	5TL	CAT-CAU-CAN	5.65	127.84	120.47
4	D	701	5TL	O4-S-CAU	5.20	113.23	107.35
4	F	701	5TL	CAN-CAM-CAL	-5.19	114.45	121.12
4	C	701	5TL	O4-S-CAU	4.97	112.97	107.35
4	D	701	5TL	CAN-CAM-CAL	-4.78	114.99	121.12
4	J	701	5TL	CAN-CAM-CAL	-4.73	115.05	121.12
4	I	701	5TL	O4-S-CAU	4.72	112.69	107.35
4	G	701	5TL	CAI-CAJ-CAL	4.70	127.23	118.63
4	E	701	5TL	OAO-CAV-NAW	-4.67	115.86	122.62
4	A	701	5TL	O4-S-CAU	4.67	112.62	107.35
4	H	701	5TL	O4-S-CAU	4.63	112.58	107.35
4	L	701	5TL	O4-S-CAU	4.62	112.58	107.35
4	F	701	5TL	CAT-CAU-S	4.59	125.96	119.72
4	K	701	5TL	O4-S-CAU	4.59	112.53	107.35
4	B	701	5TL	O4-S-CAU	4.57	112.52	107.35
4	L	701	5TL	CAN-CAM-CAL	-4.55	115.28	121.12
4	K	701	5TL	OAO-CAV-NAW	-4.52	116.09	122.62
4	H	701	5TL	CAN-CAM-CAL	-4.51	115.33	121.12
4	K	701	5TL	CAN-CAM-CAL	-4.49	115.36	121.12
4	E	701	5TL	CAN-CAM-CAL	-4.48	115.38	121.12
4	H	701	5TL	CAI-CAJ-CAL	4.45	126.78	118.63
4	J	701	5TL	O4-S-CAU	4.44	112.36	107.35
4	G	701	5TL	O4-S-CAU	4.41	112.33	107.35
4	I	701	5TL	CAN-CAM-CAL	-4.39	115.48	121.12
4	C	701	5TL	CAI-CAJ-CAL	4.39	126.67	118.63
4	D	701	5TL	CAI-CAJ-CAL	4.37	126.63	118.63
4	E	701	5TL	CAI-CAJ-CAL	4.37	126.63	118.63
4	I	701	5TL	CAI-CAJ-CAL	4.35	126.59	118.63
4	B	701	5TL	CAN-CAM-CAL	-4.35	115.54	121.12
4	G	701	5TL	CAN-CAM-CAL	-4.34	115.55	121.12
4	K	701	5TL	CAI-CAJ-CAL	4.32	126.55	118.63
4	L	701	5TL	CAI-CAJ-CAL	4.32	126.54	118.63
4	B	701	5TL	CAI-CAJ-CAL	4.32	126.53	118.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	701	5TL	CAI-CAJ-CAL	4.28	126.47	118.63
4	A	701	5TL	CAN-CAM-CAL	-4.27	115.64	121.12
4	A	701	5TL	CAI-CAJ-CAL	4.25	126.42	118.63
4	C	701	5TL	CAN-CAM-CAL	-4.25	115.67	121.12
4	I	701	5TL	OAO-CAV-NAW	-4.22	116.52	122.62
4	F	701	5TL	CAI-CAJ-CAL	4.21	126.34	118.63
4	C	701	5TL	OAO-CAV-NAW	-4.16	116.61	122.62
4	F	701	5TL	OAO-CAV-NAW	-4.04	116.78	122.62
4	E	701	5TL	O4-S-CAU	3.89	111.74	107.35
4	F	701	5TL	CAU-S-N1	3.85	113.77	108.40
4	A	701	5TL	OAO-CAV-NAW	-3.81	117.11	122.62
4	E	701	5TL	CAQ-CAV-NAW	3.81	124.21	118.29
4	L	701	5TL	OAO-CAV-NAW	-3.77	117.16	122.62
4	H	701	5TL	OAO-CAV-NAW	-3.74	117.21	122.62
4	G	701	5TL	OAO-CAV-NAW	-3.66	117.32	122.62
4	B	701	5TL	OAO-CAV-NAW	-3.62	117.38	122.62
4	J	701	5TL	OAO-CAV-NAW	-3.57	117.46	122.62
4	D	701	5TL	OAO-CAV-NAW	-3.56	117.48	122.62
4	J	701	5TL	CAU-S-N1	3.54	113.33	108.40
4	I	701	5TL	CAQ-CAV-NAW	3.50	123.72	118.29
4	L	701	5TL	CAT-CAU-S	3.47	124.43	119.72
4	F	701	5TL	O4-S-CAU	3.39	111.18	107.35
4	C	701	5TL	CAQ-CAV-NAW	3.38	123.53	118.29
4	J	701	5TL	CAQ-CAV-NAW	3.34	123.48	118.29
4	L	701	5TL	CAQ-CAV-NAW	3.34	123.47	118.29
4	K	701	5TL	CAQ-CAV-NAW	3.33	123.46	118.29
4	C	701	5TL	CAT-CAU-S	3.29	124.19	119.72
4	E	701	5TL	CAT-CAU-S	3.27	124.16	119.72
4	G	701	5TL	CAQ-CAV-NAW	3.26	123.35	118.29
4	D	701	5TL	CAQ-CAV-NAW	3.26	123.35	118.29
4	I	701	5TL	CAT-CAU-S	3.23	124.11	119.72
4	B	701	5TL	CAT-CAU-S	3.22	124.11	119.72
4	H	701	5TL	CAQ-CAV-NAW	3.20	123.25	118.29
4	A	701	5TL	O2-S-CAU	-3.19	103.75	107.35
4	A	701	5TL	CAT-CAU-S	3.18	124.05	119.72
4	D	701	5TL	CAT-CAU-S	3.18	124.04	119.72
4	F	701	5TL	CAQ-CAV-NAW	3.13	123.15	118.29
4	B	701	5TL	CAQ-CAV-NAW	3.12	123.14	118.29
4	L	701	5TL	CAU-S-N1	3.07	112.67	108.40
4	H	701	5TL	CAT-CAU-S	3.05	123.86	119.72
4	D	701	5TL	CAU-S-N1	3.04	112.64	108.40
4	G	701	5TL	CAT-CAU-S	3.03	123.84	119.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	701	5TL	CAU-S-N1	3.01	112.59	108.40
4	B	701	5TL	CAU-S-N1	2.97	112.54	108.40
4	G	701	5TL	CAI-CAJ-CAR	-2.96	115.45	119.36
4	A	701	5TL	CAU-S-N1	2.92	112.47	108.40
4	J	701	5TL	CAT-CAU-S	2.88	123.63	119.72
4	A	701	5TL	CAQ-CAV-NAW	2.84	122.69	118.29
4	K	701	5TL	O4-S-N1	2.78	111.35	107.35
4	K	701	5TL	CAT-CAU-S	2.73	123.43	119.72
4	G	701	5TL	CAU-S-N1	2.72	112.19	108.40
4	F	701	5TL	CAL-CAJ-CAR	-2.72	115.86	121.40
4	C	701	5TL	CAU-S-N1	2.70	112.16	108.40
4	I	701	5TL	CAU-S-N1	2.69	112.15	108.40
4	D	701	5TL	O2-S-CAU	-2.65	104.35	107.35
4	E	701	5TL	CAU-S-N1	2.65	112.09	108.40
4	C	701	5TL	O2-S-CAU	-2.61	104.40	107.35
4	F	701	5TL	O4-S-N1	2.60	111.10	107.35
4	K	701	5TL	CAU-S-N1	2.59	112.01	108.40
4	J	701	5TL	O2-S-CAU	-2.58	104.43	107.35
4	F	701	5TL	O2-S-CAU	-2.56	104.45	107.35
4	J	701	5TL	O4-S-N1	2.55	111.03	107.35
4	G	701	5TL	CAJ-CAR-NAY	-2.54	116.05	120.33
4	I	701	5TL	O2-S-CAU	-2.54	104.48	107.35
4	B	701	5TL	O2-S-CAU	-2.52	104.50	107.35
4	G	701	5TL	CAR-CAQ-CAV	2.45	125.41	120.88
4	C	701	5TL	CAJ-CAR-NAY	-2.45	116.21	120.33
4	A	701	5TL	CAJ-CAR-NAY	-2.44	116.22	120.33
4	K	701	5TL	CAR-CAQ-CAV	2.44	125.39	120.88
4	A	701	5TL	CAI-CAJ-CAR	-2.43	116.14	119.36
4	A	701	5TL	O4-S-N1	2.43	110.86	107.35
4	C	701	5TL	CAI-CAJ-CAR	-2.43	116.15	119.36
4	D	701	5TL	CAL-CAJ-CAR	-2.42	116.46	121.40
4	C	701	5TL	CAR-CAQ-CAV	2.42	125.36	120.88
4	H	701	5TL	CAI-CAJ-CAR	-2.40	116.19	119.36
4	K	701	5TL	CAJ-CAR-CAQ	2.38	124.88	119.38
4	G	701	5TL	CAJ-CAR-CAQ	2.36	124.83	119.38
4	K	701	5TL	CAJ-CAR-NAY	-2.35	116.37	120.33
4	L	701	5TL	CAJ-CAR-NAY	-2.35	116.37	120.33
4	I	701	5TL	CAL-CAJ-CAR	-2.34	116.63	121.40
4	K	701	5TL	CAI-CAJ-CAR	-2.34	116.27	119.36
4	E	701	5TL	CAJ-CAR-NAY	-2.33	116.40	120.33
4	E	701	5TL	CAR-CAQ-CAV	2.33	125.19	120.88
4	G	701	5TL	CAQ-CAP-CAH	-2.31	116.52	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	701	5TL	CAI-CAJ-CAR	-2.30	116.32	119.36
4	J	701	5TL	CAL-CAJ-CAR	-2.29	116.74	121.40
4	J	701	5TL	CAR-CAQ-CAV	2.29	125.11	120.88
4	H	701	5TL	CAJ-CAR-NAY	-2.28	116.48	120.33
4	H	701	5TL	CAR-CAQ-CAV	2.28	125.10	120.88
4	L	701	5TL	CAI-CAJ-CAR	-2.26	116.37	119.36
4	L	701	5TL	CAR-CAQ-CAV	2.24	125.03	120.88
4	H	701	5TL	CAL-CAJ-CAR	-2.24	116.84	121.40
4	A	701	5TL	CAJ-CAR-CAQ	2.23	124.54	119.38
4	H	701	5TL	O2-S-CAU	-2.23	104.83	107.35
4	E	701	5TL	CAJ-CAR-CAQ	2.22	124.52	119.38
4	I	701	5TL	O4-S-N1	2.22	110.55	107.35
4	H	701	5TL	CAJ-CAR-CAQ	2.21	124.50	119.38
4	B	701	5TL	CAL-CAJ-CAR	-2.21	116.90	121.40
4	B	701	5TL	CAF-CAG-CAD	2.20	121.62	117.68
4	B	701	5TL	CAJ-CAR-NAY	-2.20	116.62	120.33
4	I	701	5TL	CAJ-CAR-NAY	-2.20	116.63	120.33
4	C	701	5TL	CAL-CAJ-CAR	-2.19	116.94	121.40
4	L	701	5TL	CAL-CAJ-CAR	-2.19	116.94	121.40
4	E	701	5TL	CAL-CAJ-CAR	-2.18	116.95	121.40
4	I	701	5TL	CAR-CAQ-CAV	2.18	124.91	120.88
4	B	701	5TL	CAR-CAQ-CAV	2.17	124.90	120.88
4	F	701	5TL	CAF-CAG-CAD	2.16	121.55	117.68
4	K	701	5TL	CAL-CAJ-CAR	-2.16	117.01	121.40
4	C	701	5TL	CAJ-CAR-CAQ	2.15	124.35	119.38
4	L	701	5TL	O2-S-CAU	-2.15	104.92	107.35
4	A	701	5TL	CAQ-CAP-CAH	-2.13	116.87	120.82
4	I	701	5TL	CAI-CAJ-CAR	-2.13	116.55	119.36
4	G	701	5TL	O4-S-N1	2.13	110.42	107.35
4	B	701	5TL	CAI-CAJ-CAR	-2.12	116.55	119.36
4	H	701	5TL	CAF-CAG-CAD	2.12	121.48	117.68
4	A	701	5TL	CAR-CAQ-CAV	2.12	124.81	120.88
4	D	701	5TL	CAR-CAQ-CAV	2.12	124.80	120.88
4	J	701	5TL	CAJ-CAR-NAY	-2.11	116.77	120.33
4	G	701	5TL	CAL-CAJ-CAR	-2.11	117.10	121.40
4	G	701	5TL	CAP-CAQ-CAV	-2.10	114.67	120.93
4	I	701	5TL	CAJ-CAR-CAQ	2.10	124.23	119.38
4	C	701	5TL	O4-S-N1	2.10	110.38	107.35
4	G	701	5TL	O2-S-CAU	-2.09	104.99	107.35
4	A	701	5TL	CAL-CAJ-CAR	-2.08	117.15	121.40
4	D	701	5TL	CAJ-CAR-NAY	-2.08	116.83	120.33
4	J	701	5TL	CAJ-CAR-CAQ	2.08	124.18	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	701	5TL	CAI-CAJ-CAR	-2.07	116.62	119.36
4	B	701	5TL	O4-S-N1	2.05	110.31	107.35
4	J	701	5TL	CAF-CAG-CAD	2.05	121.34	117.68
4	L	701	5TL	CAJ-CAR-CAQ	2.05	124.12	119.38
4	B	701	5TL	CAQ-CAP-CAH	-2.05	117.01	120.82
4	E	701	5TL	CAF-CAG-CAD	2.04	121.33	117.68
4	B	701	5TL	CAJ-CAR-CAQ	2.04	124.09	119.38
4	D	701	5TL	CAI-CAJ-CAR	-2.04	116.67	119.36
4	G	701	5TL	CAF-CAG-CAD	2.00	121.26	117.68

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	5TL	CAR-CAJ-CAL-CAM
4	A	701	5TL	CAR-CAJ-CAL-CAS
4	B	701	5TL	CAR-CAJ-CAL-CAM
4	C	701	5TL	CAR-CAJ-CAL-CAM
4	C	701	5TL	CAR-CAJ-CAL-CAS
4	D	701	5TL	CAR-CAJ-CAL-CAM
4	E	701	5TL	CAR-CAJ-CAL-CAM
4	F	701	5TL	CAR-CAJ-CAL-CAM
4	G	701	5TL	CAR-CAJ-CAL-CAM
4	H	701	5TL	CAR-CAJ-CAL-CAM
4	I	701	5TL	CAR-CAJ-CAL-CAM
4	J	701	5TL	CAR-CAJ-CAL-CAM
4	K	701	5TL	CAR-CAJ-CAL-CAM
4	L	701	5TL	CAR-CAJ-CAL-CAM
4	D	701	5TL	CAR-CAJ-CAL-CAS
4	E	701	5TL	CAR-CAJ-CAL-CAS
4	F	701	5TL	CAR-CAJ-CAL-CAS
4	G	701	5TL	CAR-CAJ-CAL-CAS
4	H	701	5TL	CAR-CAJ-CAL-CAS
4	I	701	5TL	CAR-CAJ-CAL-CAS
4	J	701	5TL	CAR-CAJ-CAL-CAS
4	K	701	5TL	CAR-CAJ-CAL-CAS
4	L	701	5TL	CAR-CAJ-CAL-CAS
4	B	701	5TL	CAR-CAJ-CAL-CAS
4	J	701	5TL	CAI-CAJ-CAL-CAM
4	L	701	5TL	CAI-CAJ-CAL-CAM
4	E	701	5TL	CAI-CAJ-CAL-CAM
4	G	701	5TL	CAI-CAJ-CAL-CAM

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Mol	Chain	Res	Type	Atoms
4	H	701	5TL	CAI-CAJ-CAL-CAM
4	I	701	5TL	CAI-CAJ-CAL-CAM
4	K	701	5TL	CAI-CAJ-CAL-CAM
4	A	701	5TL	CAI-CAJ-CAL-CAM
4	C	701	5TL	CAI-CAJ-CAL-CAM
4	D	701	5TL	CAI-CAJ-CAL-CAM
4	F	701	5TL	CAI-CAJ-CAL-CAM
4	B	701	5TL	CAI-CAJ-CAL-CAM
4	A	701	5TL	CAI-CAJ-CAL-CAS
4	B	701	5TL	CAI-CAJ-CAL-CAS
4	C	701	5TL	CAI-CAJ-CAL-CAS
4	D	701	5TL	CAI-CAJ-CAL-CAS
4	E	701	5TL	CAI-CAJ-CAL-CAS
4	F	701	5TL	CAI-CAJ-CAL-CAS
4	G	701	5TL	CAI-CAJ-CAL-CAS
4	H	701	5TL	CAI-CAJ-CAL-CAS
4	I	701	5TL	CAI-CAJ-CAL-CAS
4	J	701	5TL	CAI-CAJ-CAL-CAS
4	K	701	5TL	CAI-CAJ-CAL-CAS
4	L	701	5TL	CAI-CAJ-CAL-CAS
4	C	701	5TL	CAT-CAU-S-O2
4	C	701	5TL	CAT-CAU-S-N1
4	D	701	5TL	CAN-CAU-S-N1
4	J	701	5TL	CAN-CAU-S-O2
4	E	701	5TL	CAN-CAU-S-N1
4	I	701	5TL	CAT-CAU-S-O2
4	J	701	5TL	CAT-CAU-S-N1
4	C	701	5TL	CAN-CAU-S-O2
4	D	701	5TL	CAT-CAU-S-N1
4	E	701	5TL	CAT-CAU-S-N1
4	K	701	5TL	CAT-CAU-S-O2
4	J	701	5TL	CAN-CAU-S-N1
4	A	701	5TL	CAT-CAU-S-O2
4	J	701	5TL	CAT-CAU-S-O2
4	F	701	5TL	CAT-CAU-S-O2
4	I	701	5TL	CAN-CAU-S-O2
4	I	701	5TL	CAT-CAU-S-N1
4	K	701	5TL	CAN-CAU-S-O2
4	K	701	5TL	CAT-CAU-S-N1
4	C	701	5TL	CAN-CAU-S-N1
4	F	701	5TL	CAN-CAU-S-O2
4	F	701	5TL	CAT-CAU-S-N1

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Mol	Chain	Res	Type	Atoms
4	E	701	5TL	CAT-CAU-S-O4
4	A	701	5TL	CAN-CAU-S-O2
4	A	701	5TL	CAT-CAU-S-N1
4	E	701	5TL	CAN-CAU-S-O4
4	I	701	5TL	CAN-CAU-S-N1
4	K	701	5TL	CAN-CAU-S-N1
4	B	701	5TL	CAT-CAU-S-O2
4	H	701	5TL	CAT-CAU-S-O2
4	H	701	5TL	CAN-CAU-S-O2
4	B	701	5TL	CAN-CAU-S-O2
4	F	701	5TL	CAN-CAU-S-N1
4	L	701	5TL	CAN-CAU-S-O4
4	A	701	5TL	CAN-CAU-S-N1
4	G	701	5TL	CAN-CAU-S-O4
4	D	701	5TL	CAN-CAU-S-O2
4	L	701	5TL	CAT-CAU-S-O4

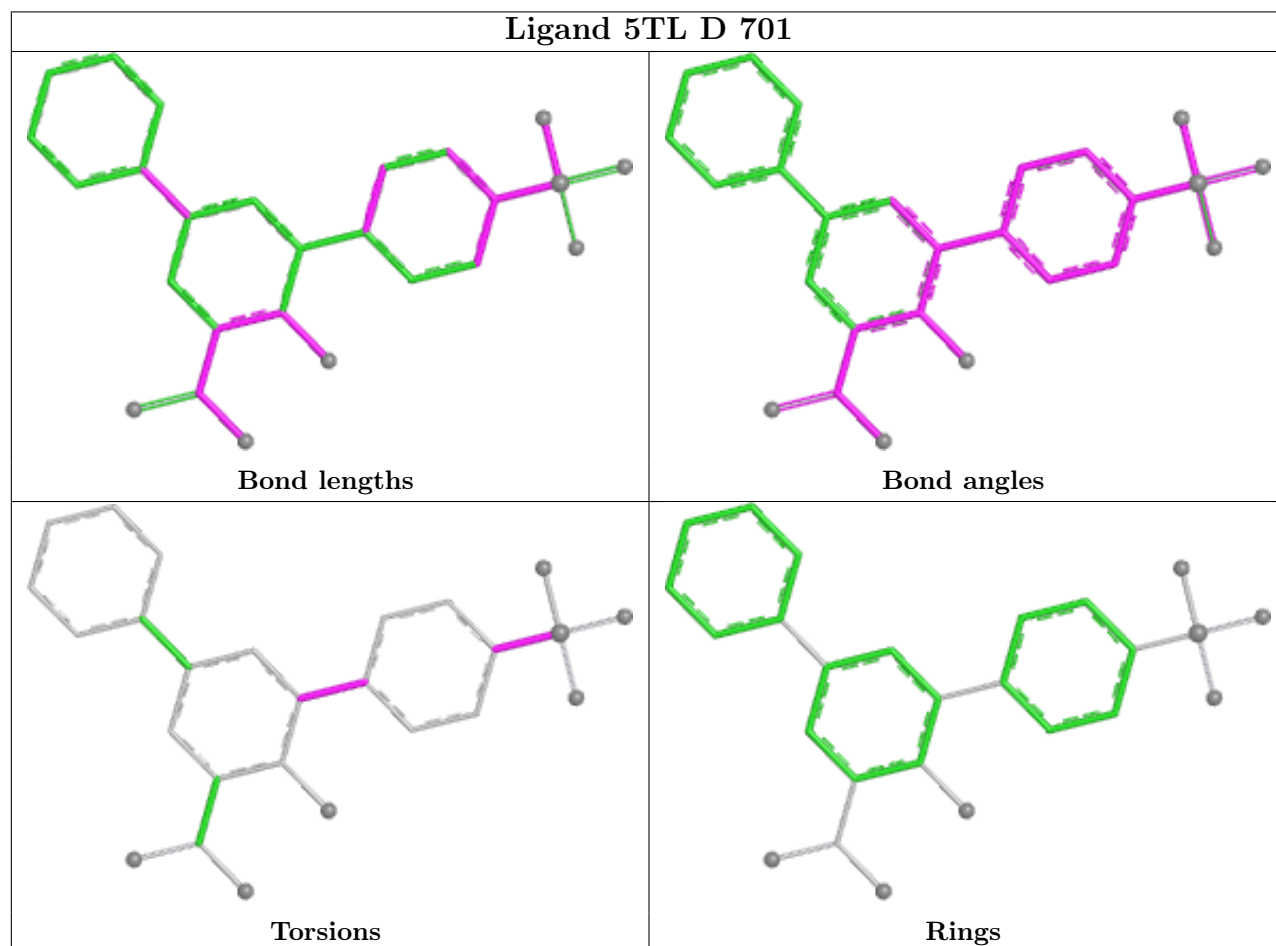
There are no ring outliers.

12 monomers are involved in 39 short contacts:

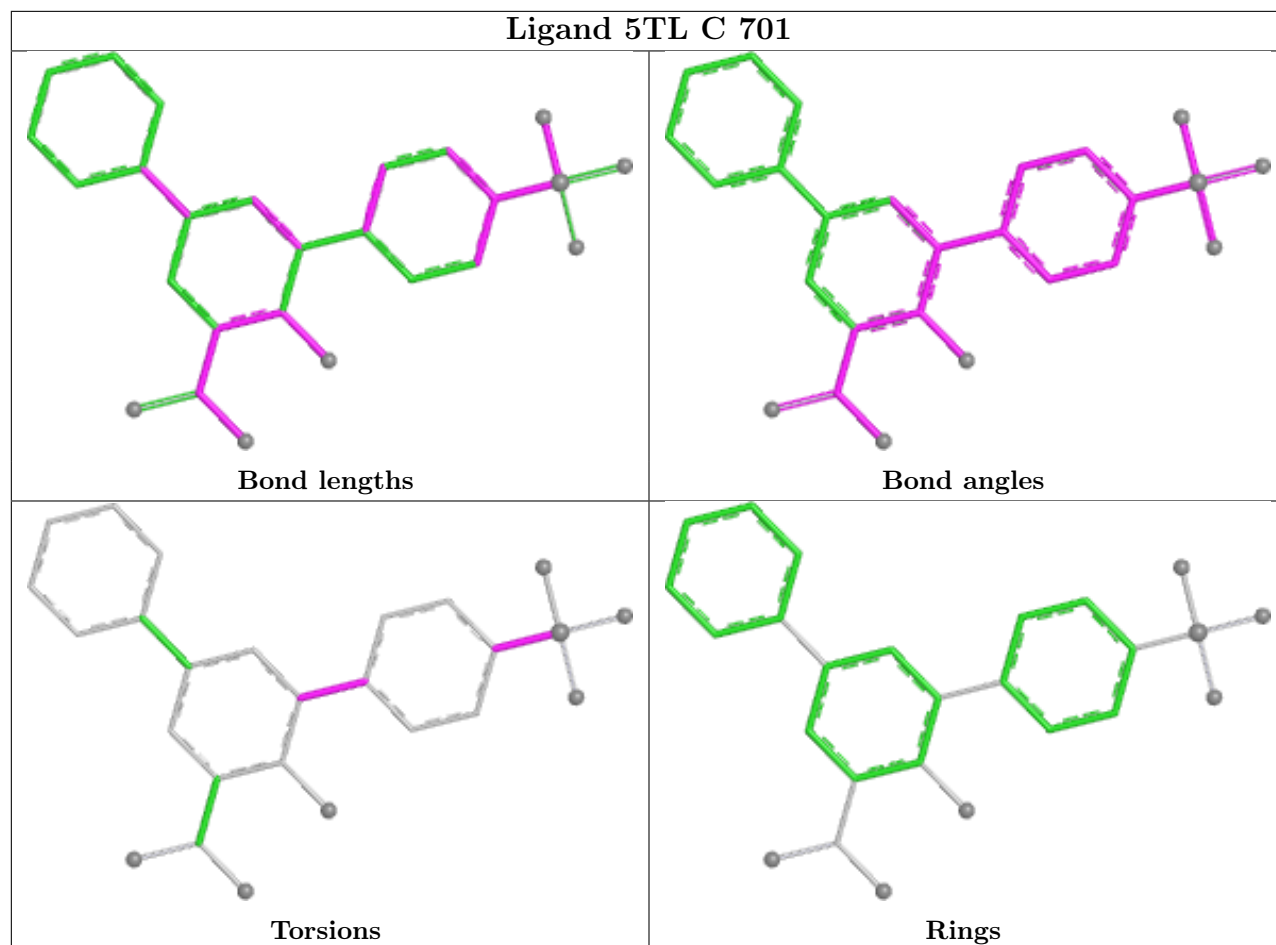
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	701	5TL	2	0
4	C	701	5TL	4	0
4	G	701	5TL	4	0
4	J	701	5TL	2	0
4	A	701	5TL	3	0
4	I	701	5TL	6	0
4	B	701	5TL	2	0
4	K	701	5TL	3	0
4	F	701	5TL	6	0
4	E	701	5TL	3	0
4	L	701	5TL	2	0
4	H	701	5TL	2	0

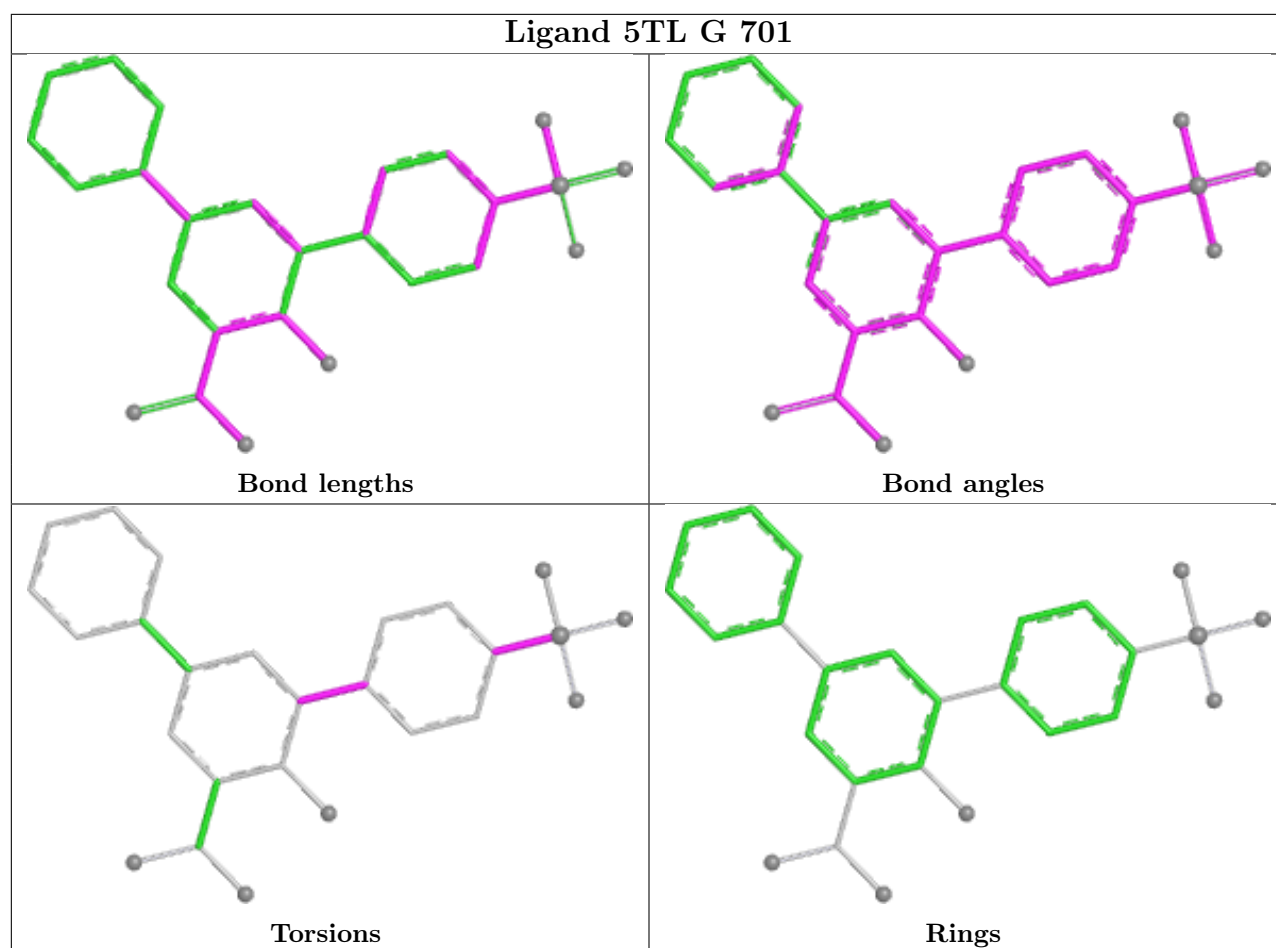
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

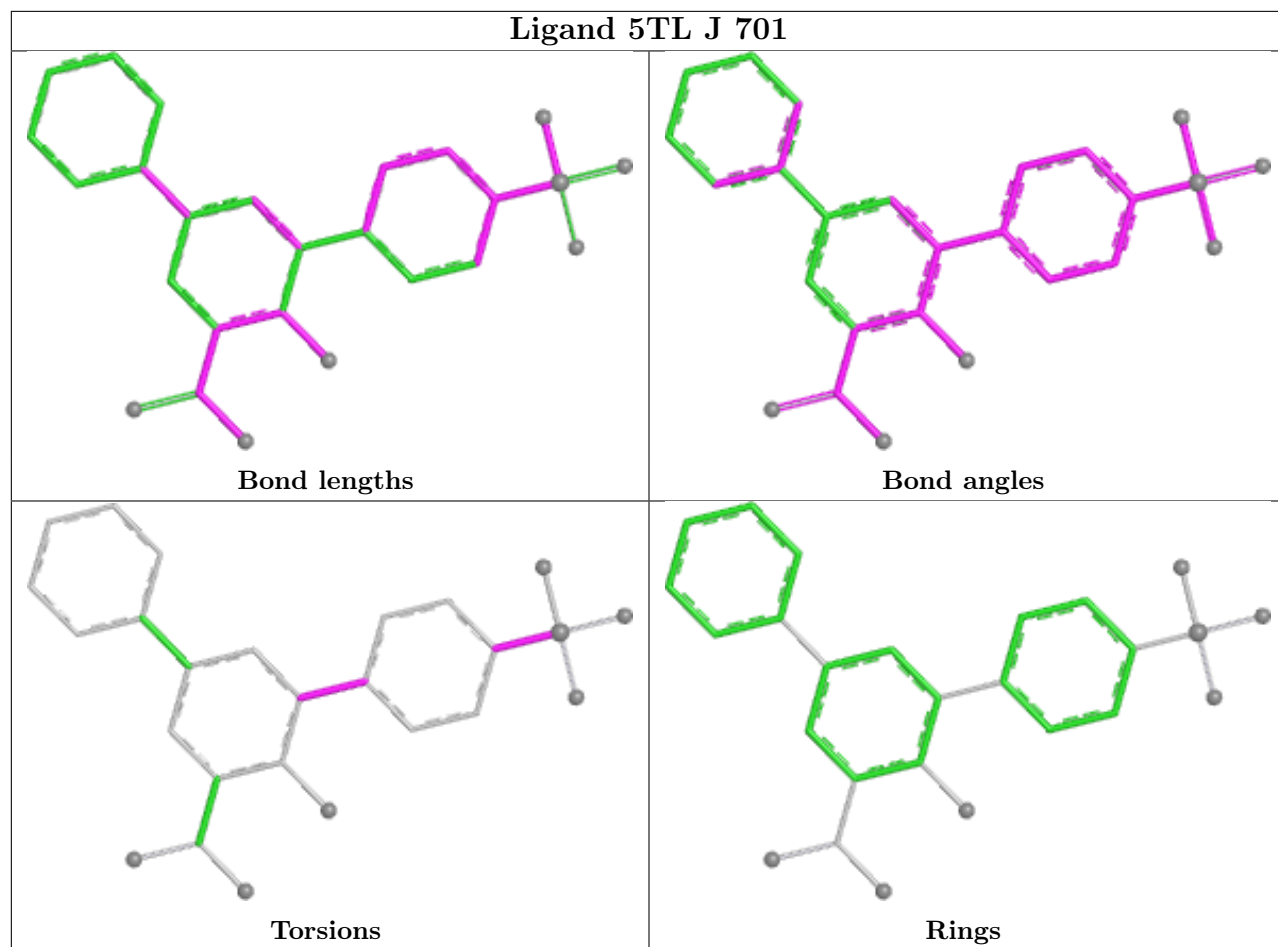
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



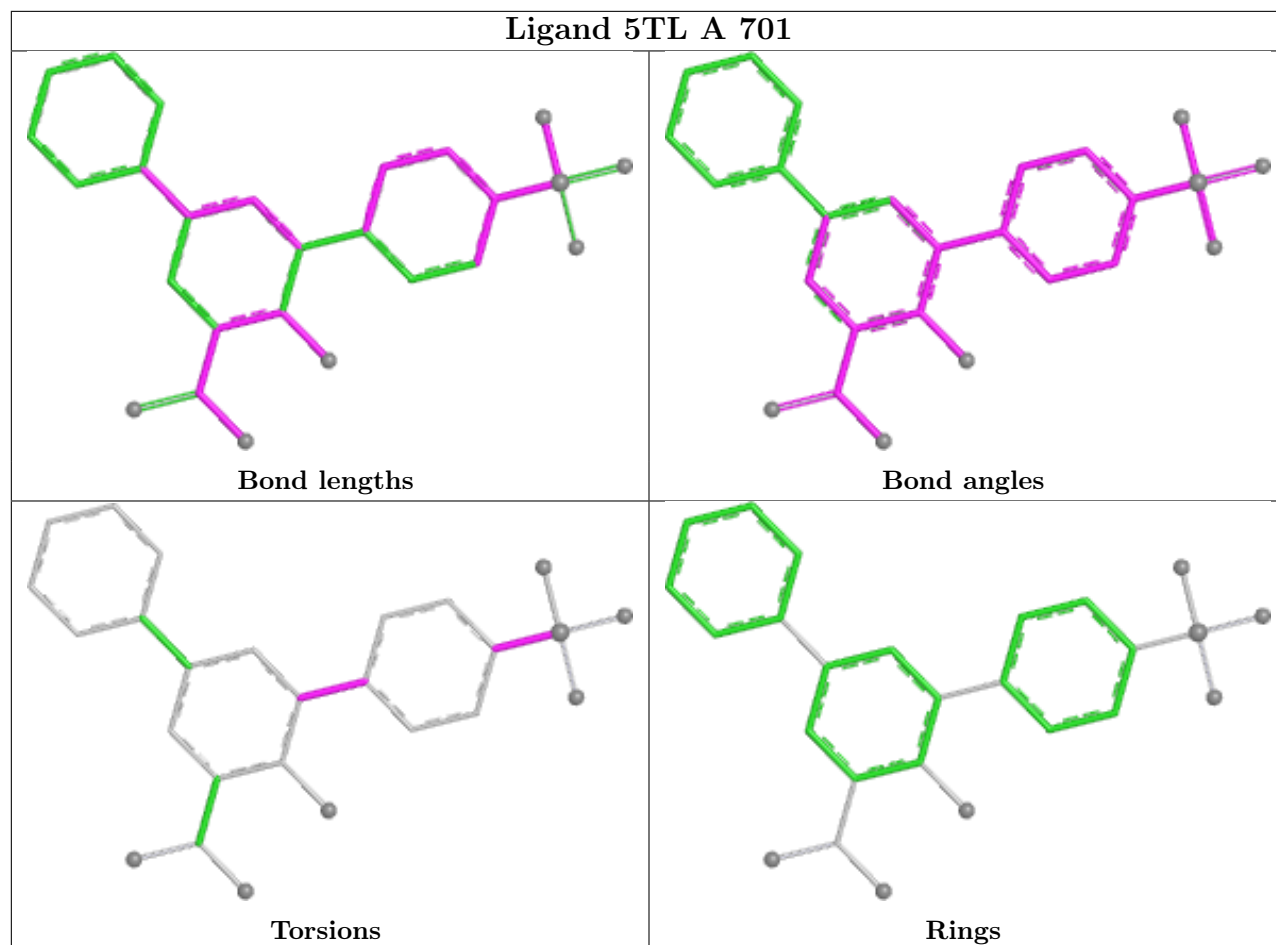
Ligand 5TL C 701

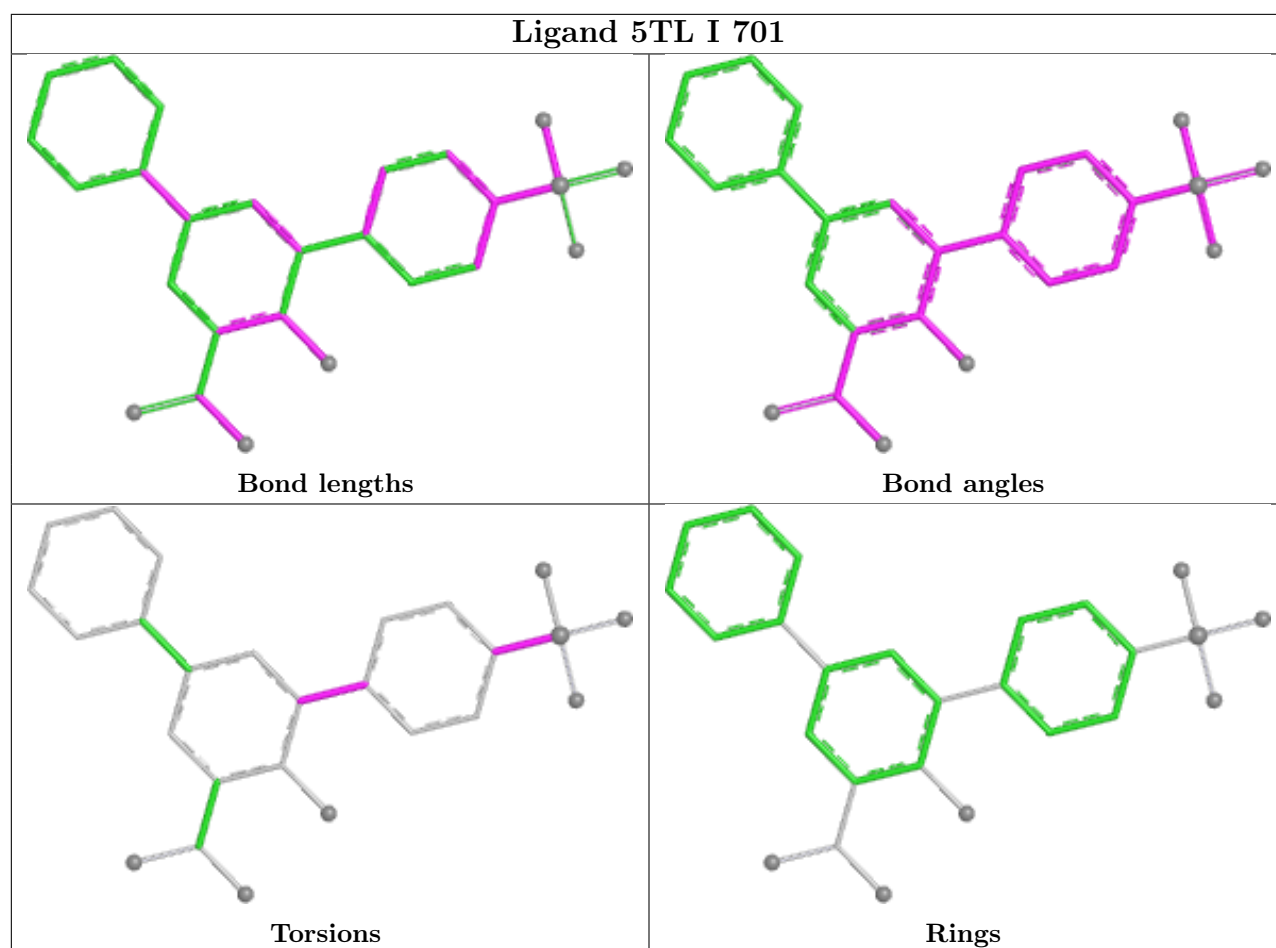


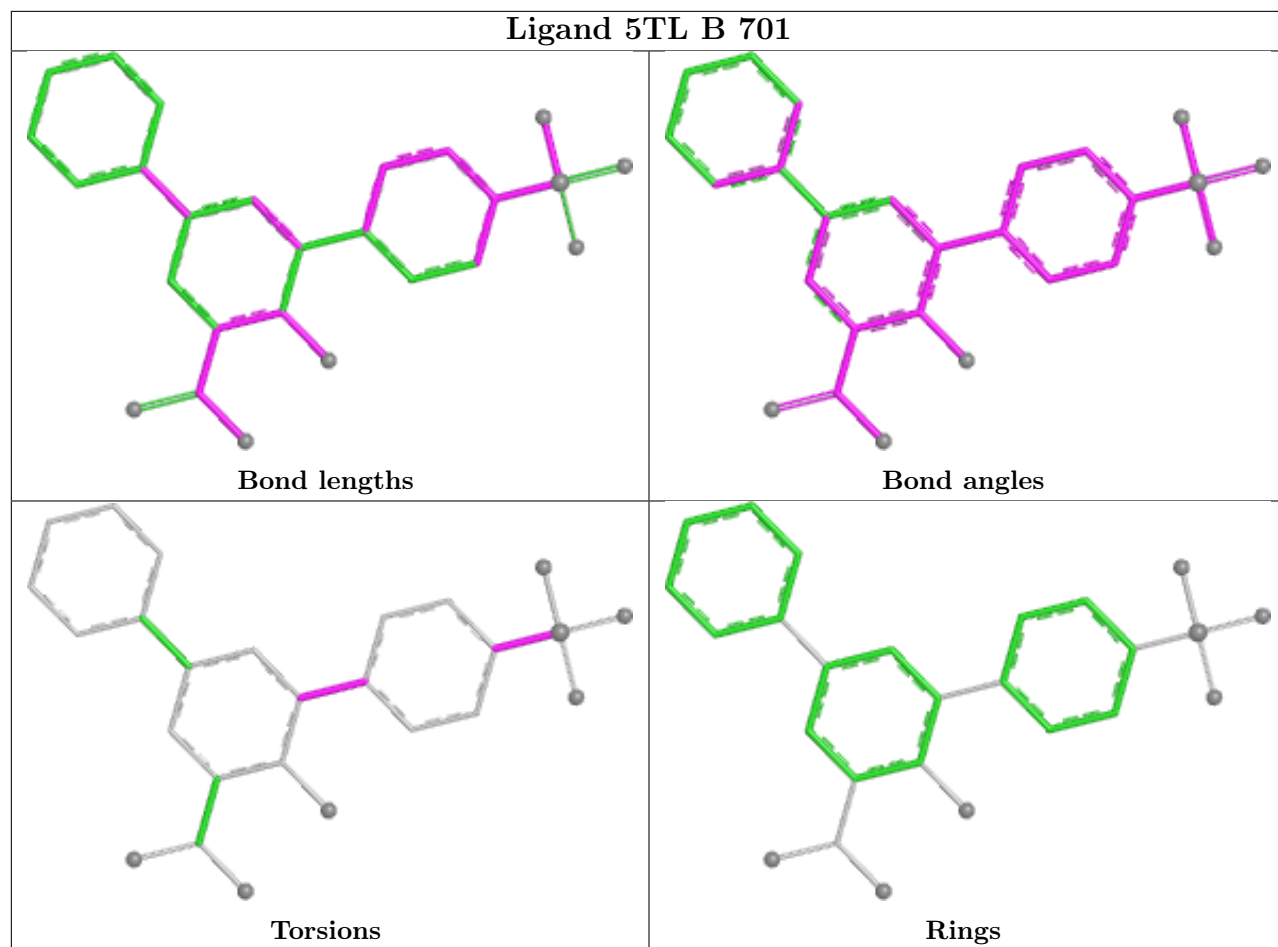


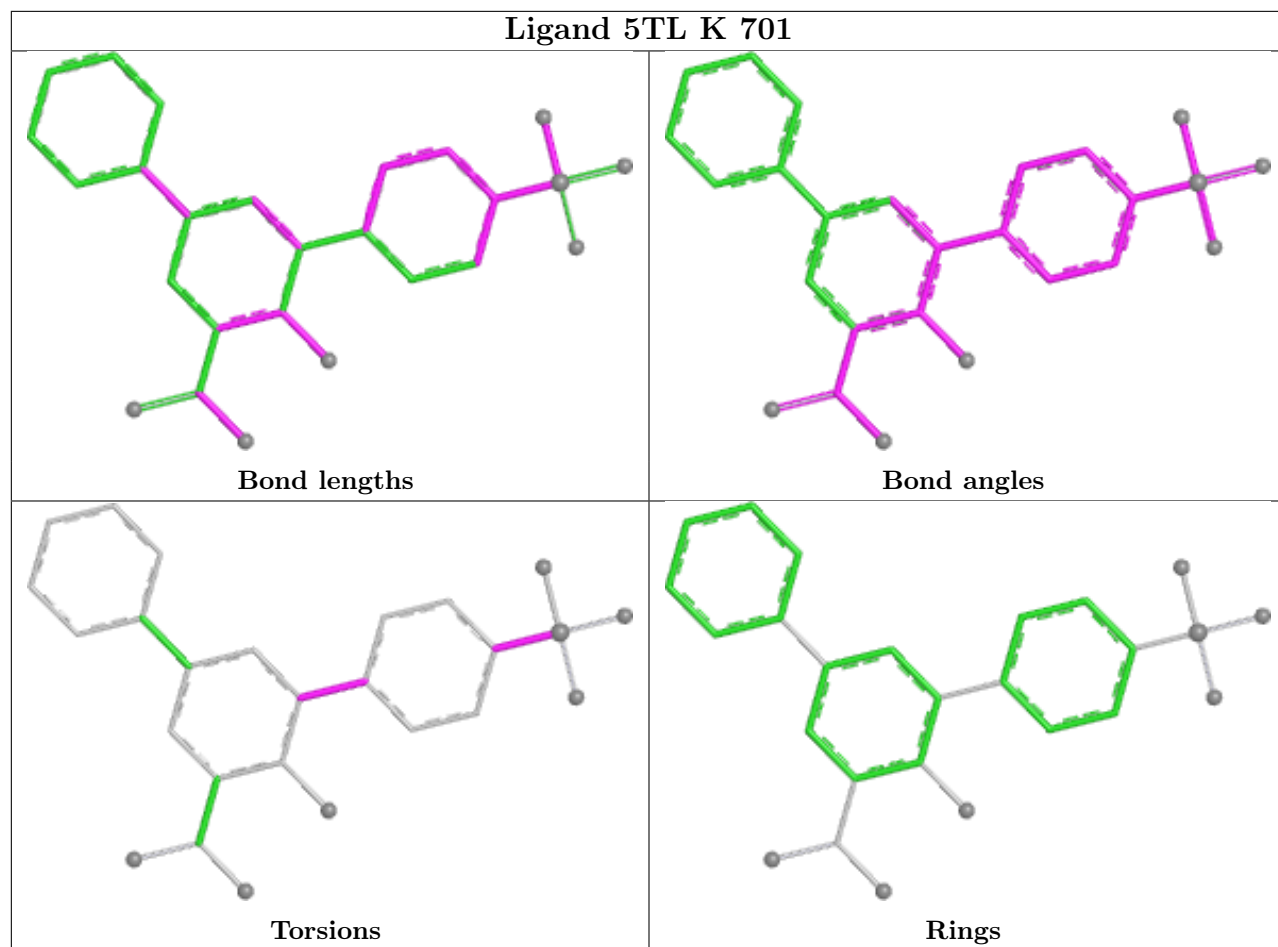


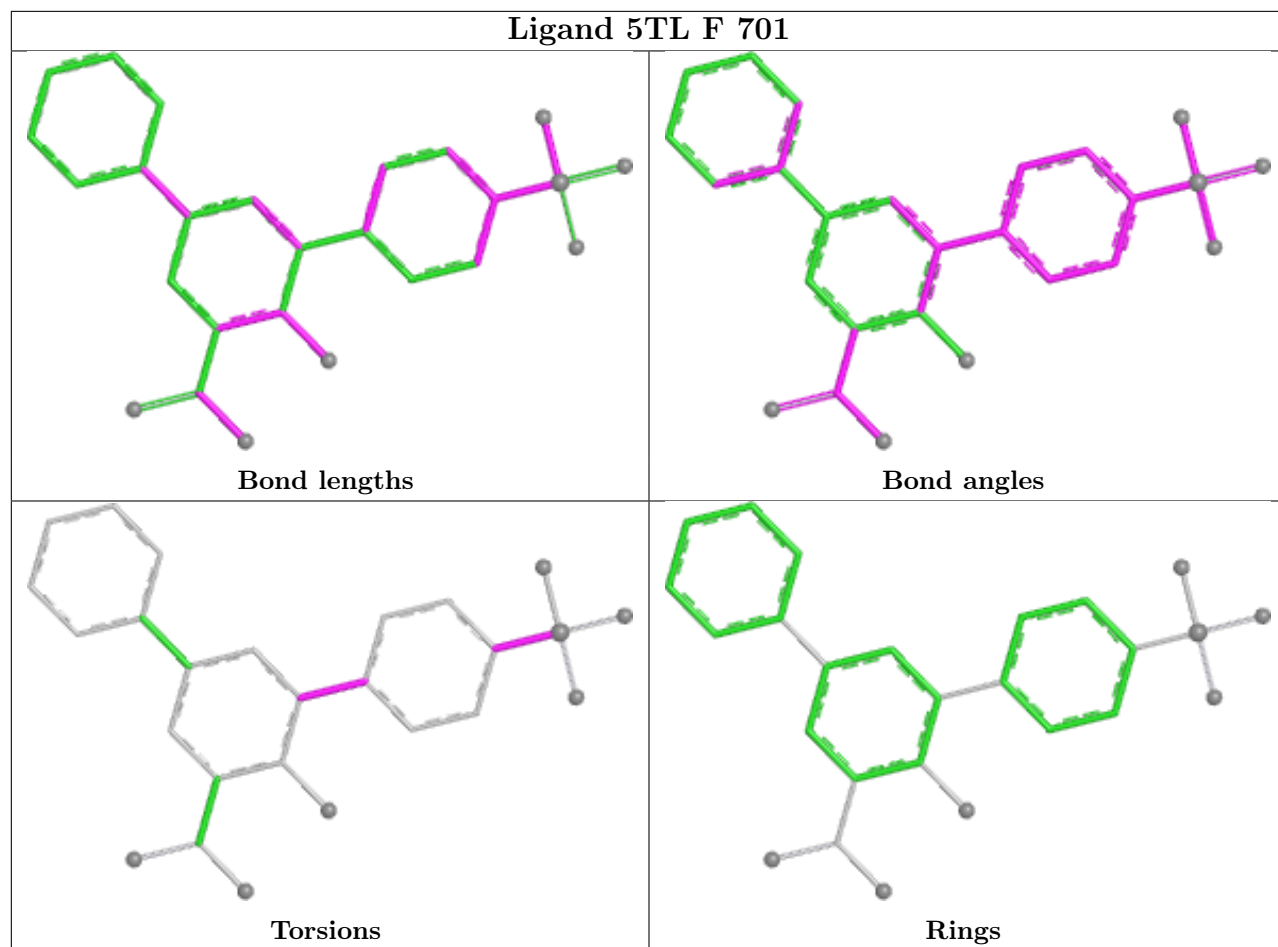
Ligand 5TL A 701

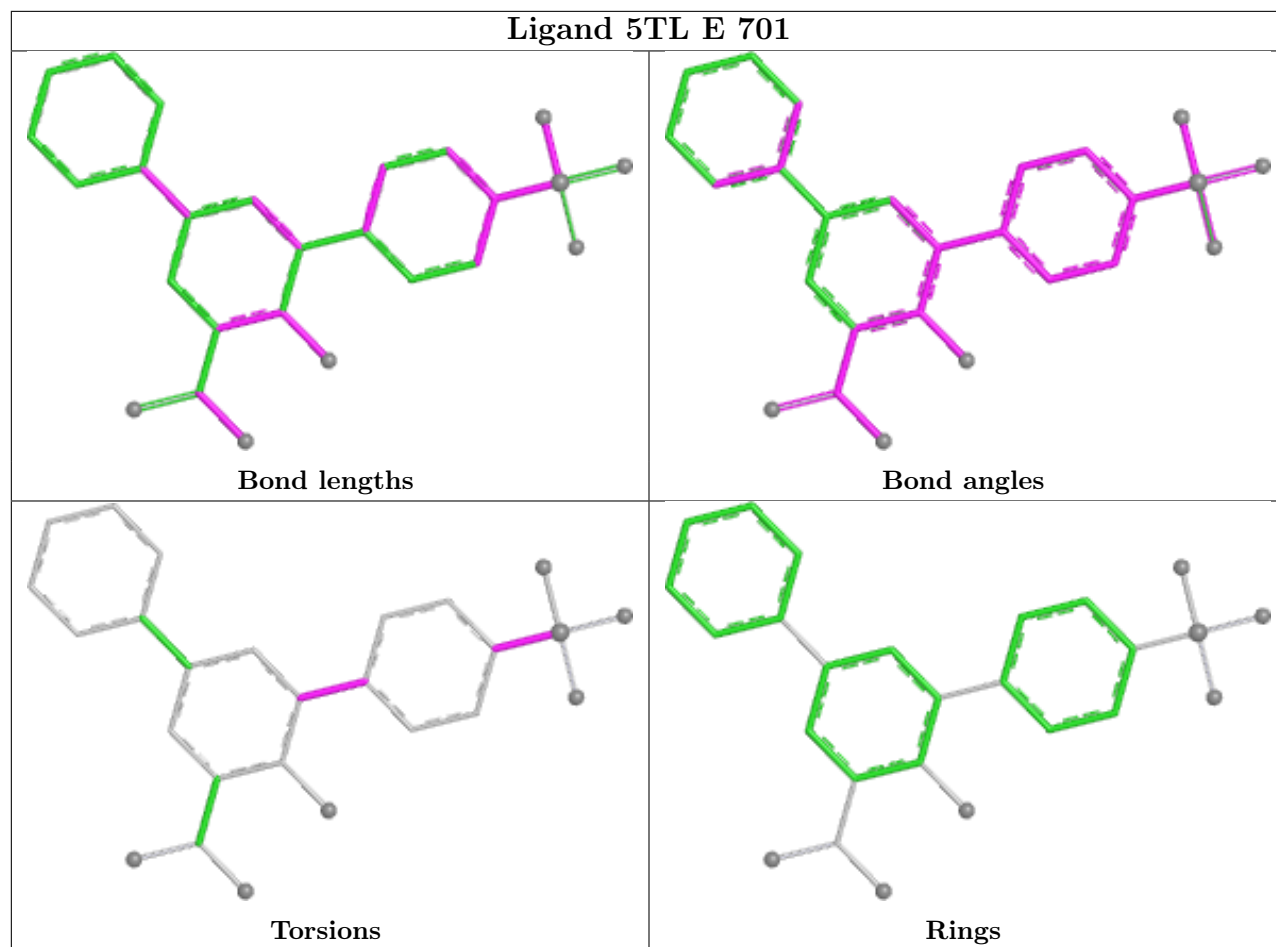


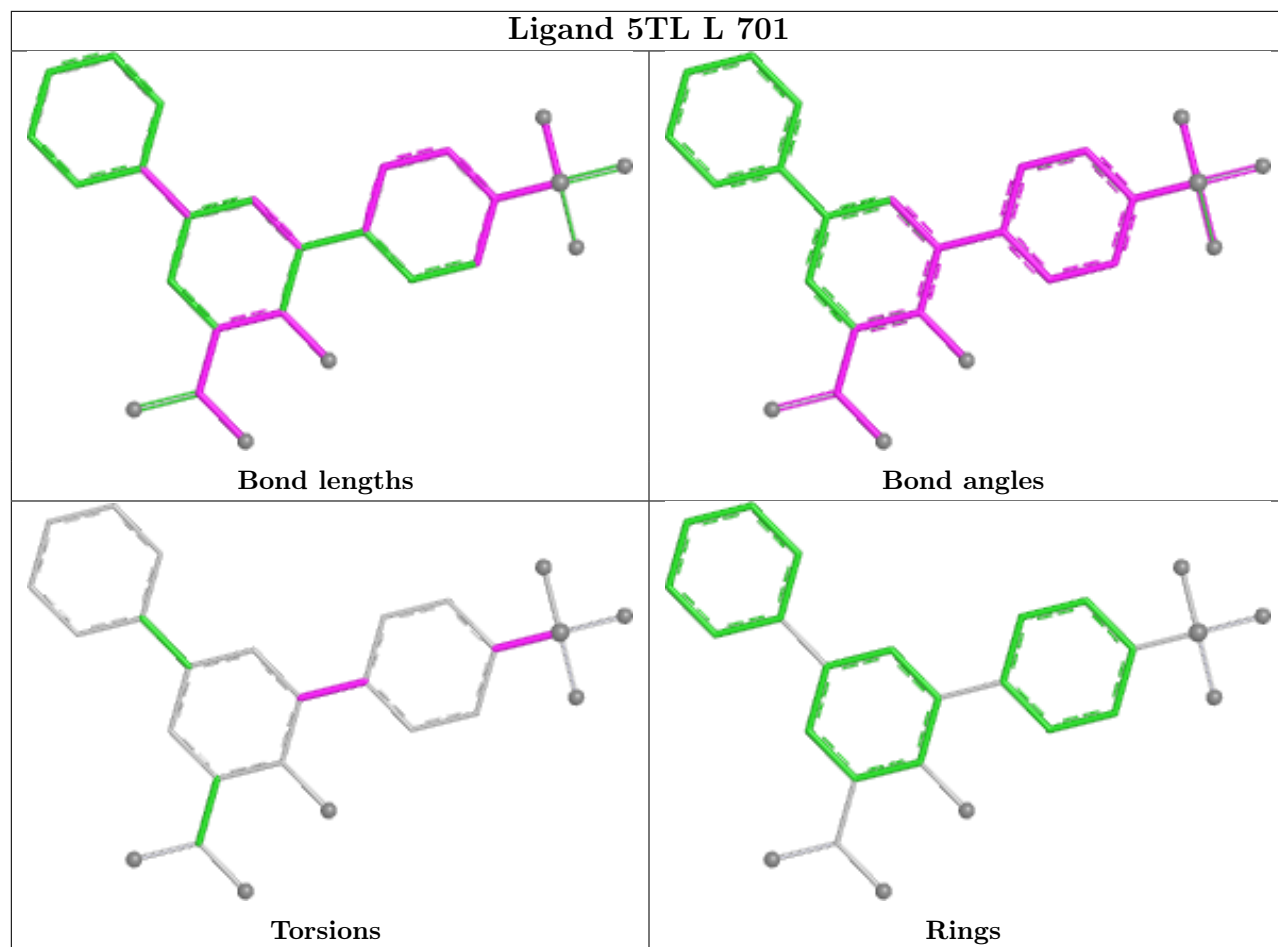


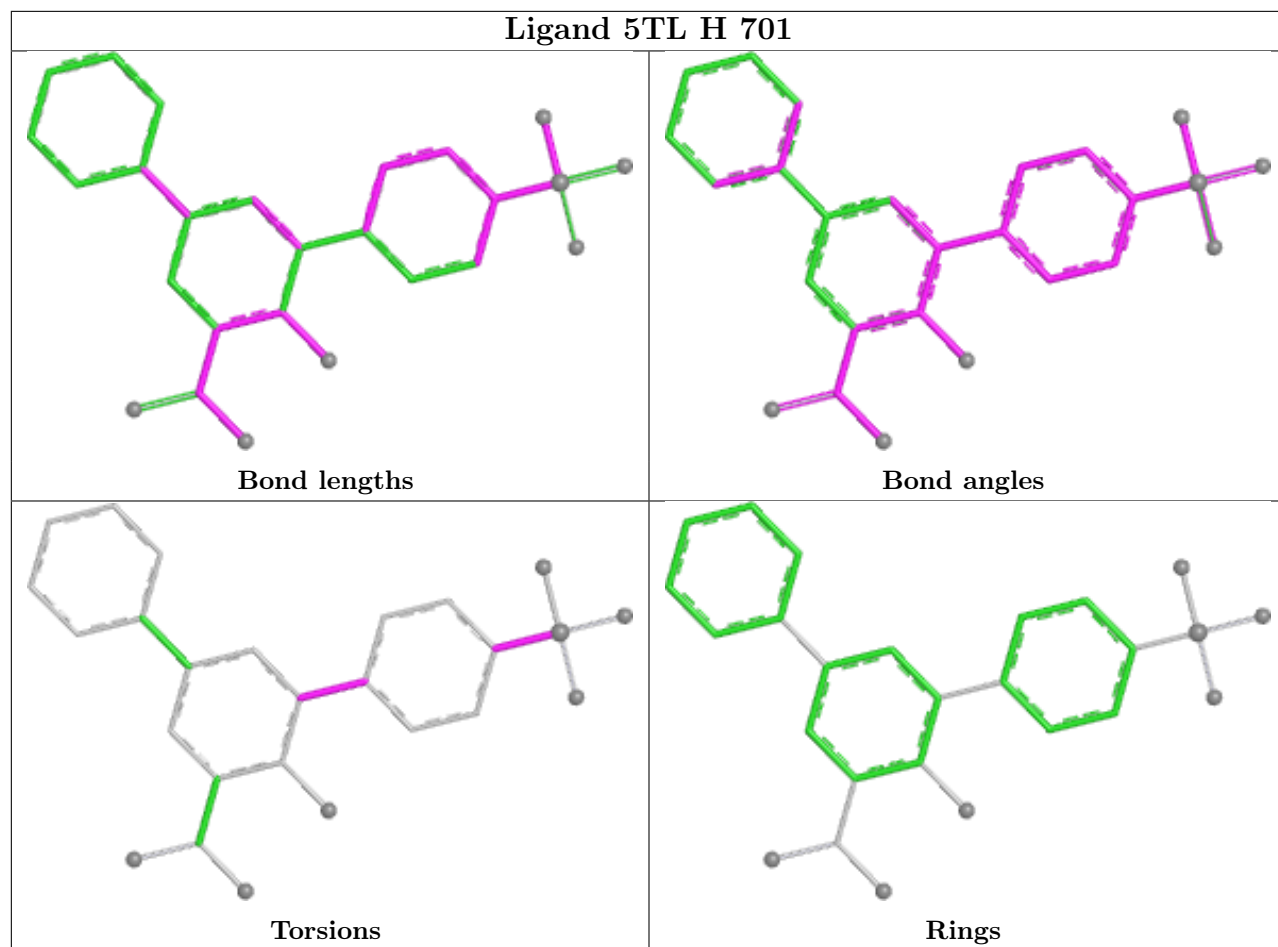












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	655/655 (100%)	-0.00	13 (1%)	65 51	124, 249, 346, 440	0
1	B	655/655 (100%)	-0.11	11 (1%)	69 55	166, 260, 355, 433	0
1	C	655/655 (100%)	-0.05	11 (1%)	69 55	148, 254, 349, 435	0
1	D	655/655 (100%)	-0.05	18 (2%)	56 44	164, 262, 366, 442	0
1	E	655/655 (100%)	0.01	13 (1%)	65 51	132, 252, 350, 465	0
1	F	655/655 (100%)	-0.11	9 (1%)	73 58	164, 262, 370, 469	0
1	G	655/655 (100%)	0.04	10 (1%)	72 57	67, 249, 345, 479	0
1	H	655/655 (100%)	-0.13	6 (0%)	81 67	149, 261, 356, 419	0
1	I	655/655 (100%)	-0.12	8 (1%)	76 62	130, 257, 355, 440	0
1	J	655/655 (100%)	-0.02	12 (1%)	67 53	162, 264, 366, 440	0
1	K	655/655 (100%)	0.05	12 (1%)	67 53	128, 252, 347, 450	0
1	L	655/655 (100%)	0.01	13 (1%)	65 51	165, 263, 370, 484	0
All	All	7860/7860 (100%)	-0.04	136 (1%)	69 55	67, 257, 357, 484	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	LYS	6.0
1	L	653	LEU	4.8
1	K	93	LEU	4.6
1	A	656	ILE	4.5
1	D	65	MET	4.3
1	F	653	LEU	4.3
1	K	282	TRP	4.2
1	L	553	GLN	4.2
1	G	448	GLN	4.1
1	B	573	HIS	4.0
1	D	321	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	653	LEU	3.8
1	J	542	MET	3.7
1	B	550	GLY	3.7
1	J	361	SER	3.7
1	C	573	HIS	3.7
1	C	379	CYS	3.6
1	E	93	LEU	3.6
1	K	653	LEU	3.5
1	K	550	GLY	3.5
1	E	410	ILE	3.5
1	I	573	HIS	3.4
1	F	23	THR	3.4
1	B	335	HIS	3.4
1	H	573	HIS	3.4
1	B	636	ASP	3.3
1	L	477	LYS	3.3
1	E	541	ILE	3.3
1	E	550	GLY	3.3
1	B	572	LYS	3.1
1	F	78	ASP	3.1
1	D	361	SER	3.0
1	B	476	LEU	3.0
1	C	192	LEU	3.0
1	I	91	PRO	3.0
1	D	22	GLY	2.9
1	B	491	LEU	2.9
1	J	507	MET	2.9
1	A	289	GLY	2.9
1	C	27	GLY	2.9
1	G	93	LEU	2.9
1	J	22	GLY	2.9
1	F	193	PHE	2.8
1	L	19	GLU	2.8
1	A	126	SER	2.8
1	L	417	GLN	2.8
1	G	23	THR	2.8
1	L	550	GLY	2.8
1	H	479	LYS	2.8
1	H	415	LYS	2.8
1	G	653	LEU	2.7
1	G	112	ASN	2.7
1	G	452	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	258	LEU	2.7
1	K	352	GLN	2.7
1	K	410	ILE	2.7
1	E	557	MET	2.7
1	J	93	LEU	2.6
1	B	113	CYS	2.6
1	I	248	MET	2.6
1	L	217	GLY	2.6
1	K	57	ARG	2.6
1	A	184	THR	2.6
1	L	524	VAL	2.6
1	E	542	MET	2.6
1	D	95	MET	2.6
1	D	481	GLU	2.5
1	A	224	HIS	2.5
1	L	125	LEU	2.5
1	D	9	PHE	2.5
1	D	93	LEU	2.5
1	A	318	MET	2.5
1	D	54	ASN	2.5
1	E	415	LYS	2.5
1	E	573	HIS	2.5
1	D	444	LEU	2.4
1	D	479	LYS	2.4
1	K	235	LYS	2.4
1	D	23	THR	2.4
1	G	126	SER	2.4
1	A	654	LEU	2.4
1	C	93	LEU	2.4
1	B	424	ARG	2.4
1	C	571	LEU	2.3
1	K	59	CYS	2.3
1	B	635	ALA	2.3
1	D	653	LEU	2.3
1	H	550	GLY	2.3
1	E	212	PHE	2.3
1	D	10	GLY	2.3
1	E	22	GLY	2.3
1	F	15	TRP	2.3
1	A	128	ILE	2.3
1	D	341	ILE	2.3
1	J	89	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	19	GLU	2.3
1	K	335	HIS	2.3
1	C	31	LEU	2.2
1	L	554	GLY	2.2
1	C	248	MET	2.2
1	J	65	MET	2.2
1	I	27	GLY	2.2
1	L	193	PHE	2.2
1	K	468	THR	2.2
1	H	491	LEU	2.2
1	I	297	GLN	2.2
1	D	106	LEU	2.2
1	J	7	PRO	2.2
1	G	467	ASN	2.2
1	C	312	ILE	2.2
1	C	65	MET	2.2
1	E	272	MET	2.2
1	I	217	GLY	2.1
1	J	506	LYS	2.1
1	K	601	LEU	2.1
1	L	324	ILE	2.1
1	A	421	ILE	2.1
1	F	650	ILE	2.1
1	G	242	ILE	2.1
1	J	541	ILE	2.1
1	F	378	GLY	2.1
1	J	352	GLN	2.1
1	J	23	THR	2.1
1	G	155	VAL	2.1
1	I	379	CYS	2.1
1	D	52	THR	2.1
1	L	101	GLY	2.1
1	B	400	SER	2.1
1	I	40	LYS	2.1
1	D	520	HIS	2.1
1	A	422	GLN	2.1
1	E	352	GLN	2.1
1	H	413	ASP	2.0
1	C	515	GLU	2.0
1	F	39	LEU	2.0
1	F	22	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	5TH	T	7	17/18	0.01	0.11	286,465,514,523	0
3	5TK	T	6	13/14	0.18	0.11	498,545,563,567	0
2	5LS	Z	1	20/20	0.18	0.09	404,467,489,501	0
2	GLC	U	2	11/12	0.22	0.14	419,441,472,478	0
3	Z4K	O	5	15/16	0.23	0.10	441,493,519,523	0
2	GLC	W	2	11/12	0.25	0.12	347,378,409,472	0
2	PDX	S	3	19/20	0.31	0.10	242,541,570,575	0
2	GLC	R	2	11/12	0.35	0.14	358,404,431,439	0
3	5TH	O	7	17/18	0.35	0.08	382,454,506,522	0
3	5TJ	O	2	17/18	0.36	0.09	520,543,568,570	0
3	5TM	T	3	17/18	0.36	0.12	479,506,524,529	0
3	5LS	T	1	20/20	0.38	0.11	390,510,562,568	0
2	PDX	X	3	19/20	0.40	0.14	120,485,579,583	0
2	PDX	P	3	19/20	0.42	0.11	246,460,539,547	0
2	5LS	Y	1	20/20	0.44	0.08	275,459,474,500	0
3	5TM	O	3	17/18	0.44	0.11	442,503,540,543	0
2	PDX	W	3	19/20	0.50	0.14	366,456,485,489	0
2	PDX	M	3	19/20	0.54	0.06	294,542,568,576	0
3	5TJ	T	4	17/18	0.55	0.09	291,502,575,583	0
3	5TJ	O	4	17/18	0.60	0.08	394,528,538,539	0
2	GLC	X	2	11/12	0.62	0.09	335,392,442,495	0
3	5LS	O	1	20/20	0.62	0.12	410,470,536,552	0
2	5LS	V	1	20/20	0.63	0.08	368,431,456,471	0
2	GLC	P	2	11/12	0.64	0.13	259,379,417,450	0
3	5TK	O	6	13/14	0.66	0.07	377,494,522,528	0
2	5LS	S	1	20/20	0.67	0.11	318,398,444,472	0
2	5LS	U	1	20/20	0.70	0.09	340,440,517,518	0
2	5LS	N	1	20/20	0.72	0.07	320,445,483,493	0
2	PDX	V	3	19/20	0.72	0.08	373,430,480,492	0
2	PDX	R	3	19/20	0.73	0.11	382,434,463,471	0
2	5LS	Q	1	20/20	0.74	0.07	356,421,481,498	0
2	5LS	M	1	20/20	0.77	0.10	337,376,407,435	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PDX	Q	3	19/20	0.77	0.07	309,489,529,530	0
2	GLC	V	2	11/12	0.78	0.12	380,397,417,446	0
2	5LS	W	1	20/20	0.79	0.11	406,436,450,462	0
2	5LS	X	1	20/20	0.79	0.08	384,414,438,442	0
2	5LS	a	1	20/20	-	-	282,367,436,438	0
2	GLC	a	2	11/12	-	-	370,394,435,475	0
2	PDX	a	3	19/20	-	-	394,475,502,529	0
2	5LS	b	1	20/20	-	-	361,462,493,495	0
2	GLC	b	2	11/12	-	-	263,307,356,360	0
2	PDX	b	3	19/20	-	-	241,384,434,436	0
2	5LS	d	1	20/20	-	-	291,429,473,484	0
2	GLC	d	2	11/12	-	-	220,288,388,445	0
2	PDX	d	3	19/20	-	-	266,436,468,474	0
2	5LS	e	1	20/20	-	-	402,453,485,501	0
2	GLC	e	2	11/12	-	-	394,429,498,537	0
2	PDX	e	3	19/20	-	-	404,488,531,532	0
2	5LS	f	1	20/20	-	-	414,473,550,553	0
2	GLC	f	2	11/12	-	-	361,408,422,461	0
2	PDX	f	3	19/20	-	-	291,428,471,474	0
2	5LS	g	1	20/20	-	-	388,452,499,510	0
2	GLC	g	2	11/12	-	-	216,358,388,409	0
2	PDX	g	3	19/20	-	-	247,401,449,453	0
2	5LS	h	1	20/20	-	-	255,515,567,577	0
2	GLC	h	2	11/12	-	-	197,292,365,403	0
2	PDX	h	3	19/20	-	-	270,404,472,478	0
2	5LS	j	1	20/20	-	-	308,429,475,496	0
2	GLC	j	2	11/12	-	-	329,361,377,405	0
2	PDX	j	3	19/20	-	-	321,419,508,517	0
2	5LS	k	1	20/20	-	-	363,425,467,471	0
2	GLC	k	2	11/12	-	-	360,413,466,537	0
2	PDX	k	3	19/20	-	-	442,555,569,571	0
2	5LS	l	1	20/20	-	-	347,522,574,579	0
2	GLC	l	2	11/12	-	-	321,350,440,452	0
2	PDX	l	3	19/20	-	-	257,458,487,488	0
2	5LS	m	1	20/20	-	-	358,404,444,460	0
2	GLC	m	2	11/12	-	-	330,367,393,433	0
2	PDX	m	3	19/20	-	-	373,474,502,503	0
2	5LS	n	1	20/20	-	-	442,520,539,550	0
2	GLC	n	2	11/12	-	-	315,385,428,432	0
2	PDX	n	3	19/20	-	-	302,421,476,480	0
2	PDX	U	3	19/20	0.80	0.12	395,433,465,466	0
2	GLC	N	2	11/12	0.80	0.08	357,383,424,432	0

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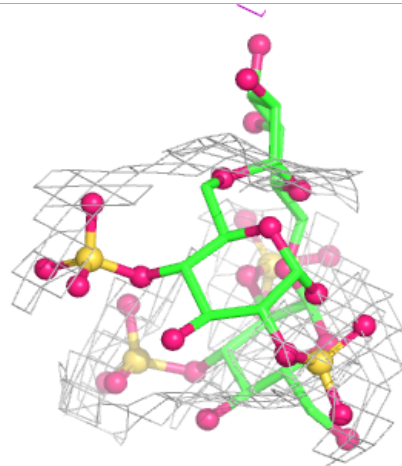
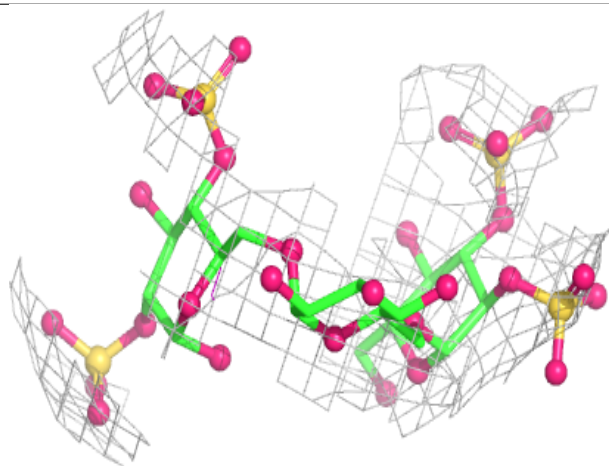
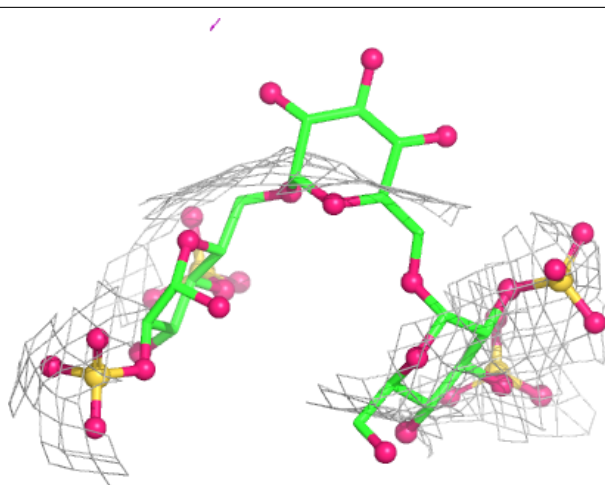
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PDX	Y	3	19/20	0.80	0.08	330,398,456,471	0
2	5LS	P	1	20/20	0.80	0.07	348,474,507,510	0
2	PDX	Z	3	19/20	0.81	0.09	366,469,493,510	0
2	5LS	R	1	20/20	0.84	0.11	412,438,452,452	0
2	GLC	S	2	11/12	0.84	0.07	287,335,428,484	0
2	GLC	Y	2	11/12	0.84	0.06	275,289,341,375	0
3	5TJ	T	2	17/18	0.85	0.07	487,535,554,557	0
2	GLC	Z	2	11/12	0.86	0.10	267,377,431,435	0
2	PDX	N	3	19/20	0.87	0.06	218,410,475,496	0
2	GLC	M	2	11/12	0.88	0.08	366,443,481,495	0
3	Z4K	T	5	15/16	0.89	0.08	512,546,562,567	0
2	GLC	Q	2	11/12	0.96	0.07	333,423,476,483	0
3	5LS	c	1	20/20	-	-	430,502,561,583	0
3	5TJ	c	2	17/18	-	-	305,465,516,533	0
3	5TM	c	3	17/18	-	-	462,507,517,524	0
3	5TJ	c	4	17/18	-	-	452,494,530,541	0
3	Z4K	c	5	15/16	-	-	442,503,528,534	0
3	5TK	c	6	13/14	-	-	431,547,571,574	0
3	5TH	c	7	17/18	-	-	386,527,562,566	0
3	5LS	i	1	20/20	-	-	472,553,561,566	0
3	5TJ	i	2	17/18	-	-	468,554,566,566	0
3	5TM	i	3	17/18	-	-	429,491,543,555	0
3	5TJ	i	4	17/18	-	-	385,519,554,575	0
3	Z4K	i	5	15/16	-	-	437,501,519,520	0
3	5TK	i	6	13/14	-	-	409,452,467,476	0
3	5TH	i	7	17/18	-	-	384,477,520,526	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

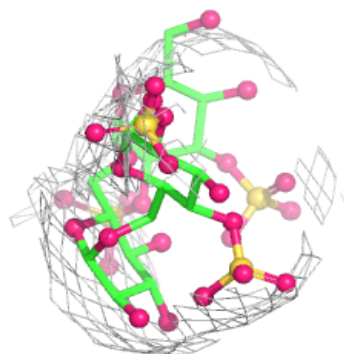
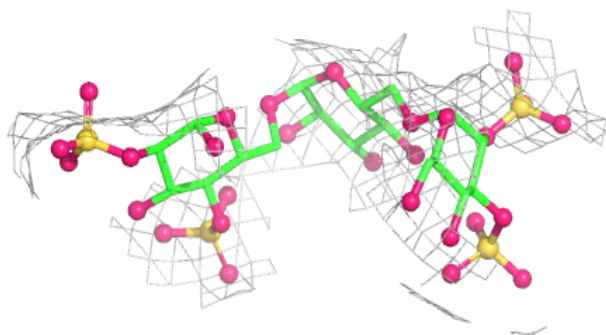
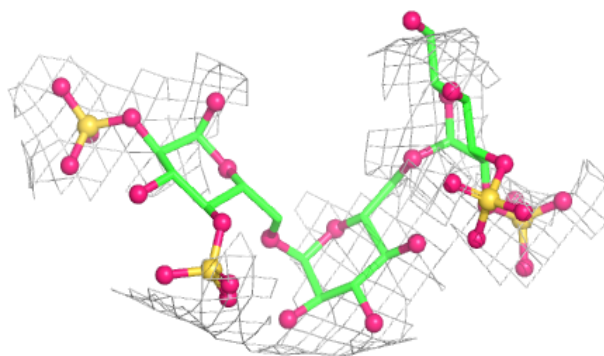
Electron density around Chain M:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

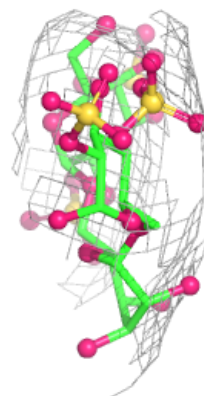
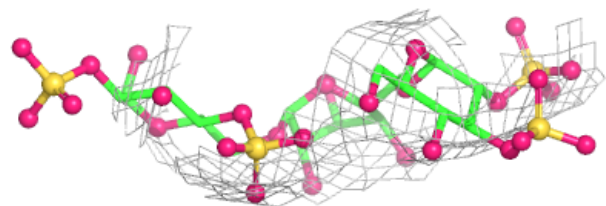
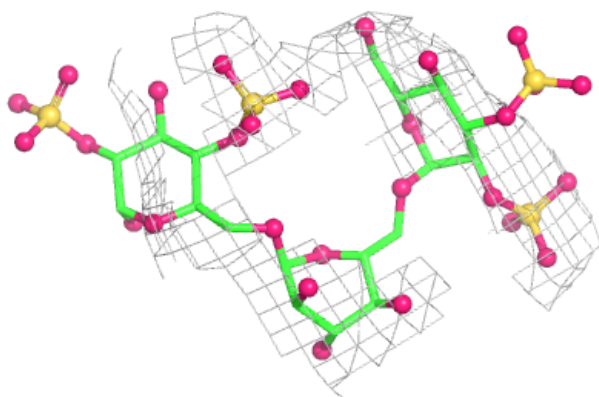


Electron density around Chain N:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

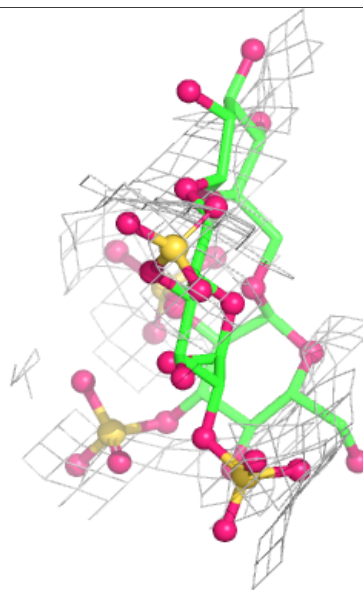
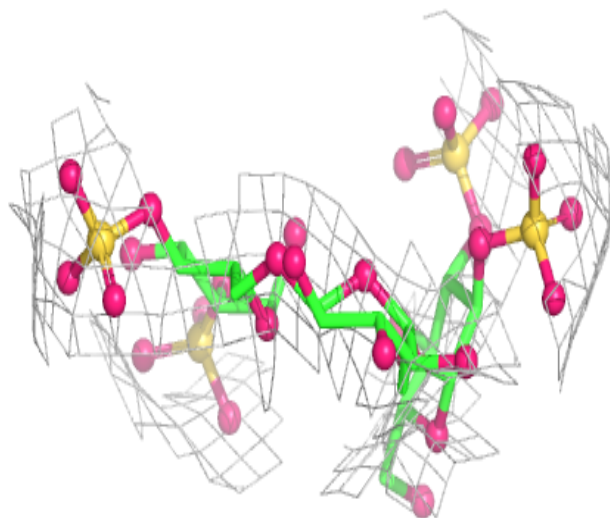
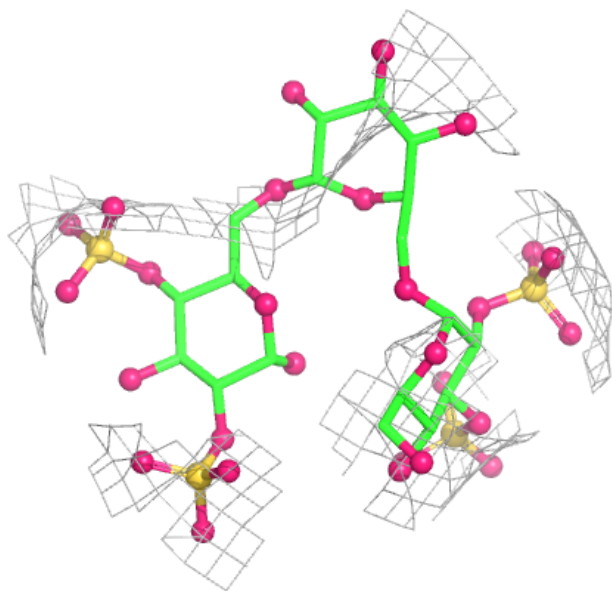
**Electron density around Chain P:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



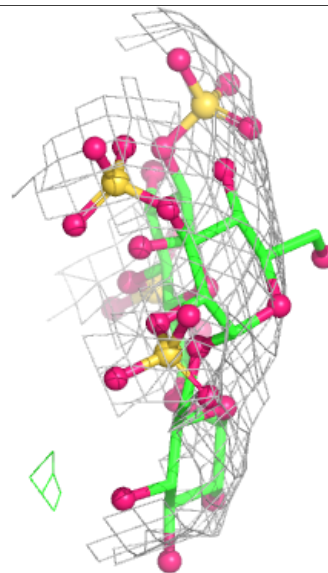
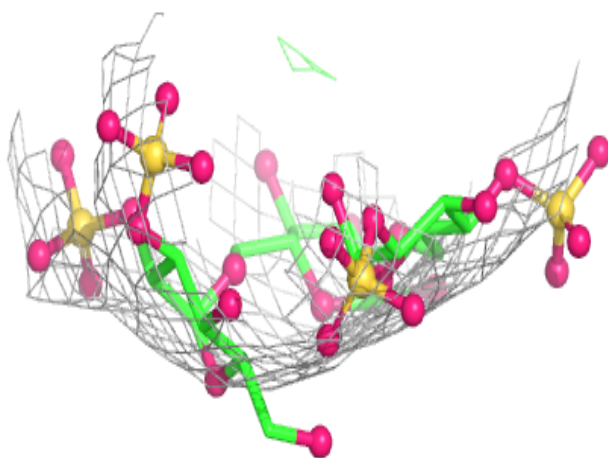
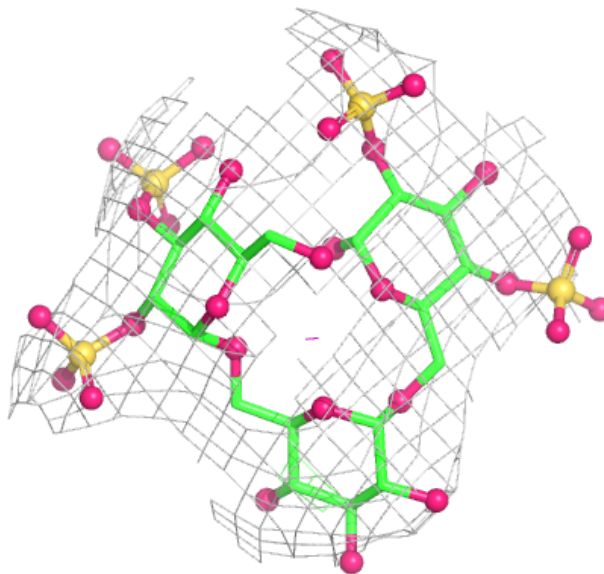
Electron density around Chain Q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



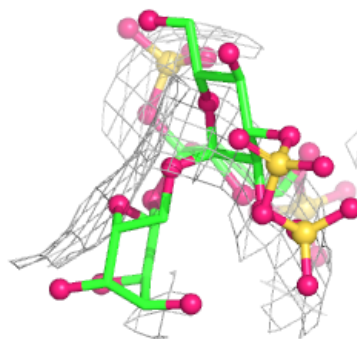
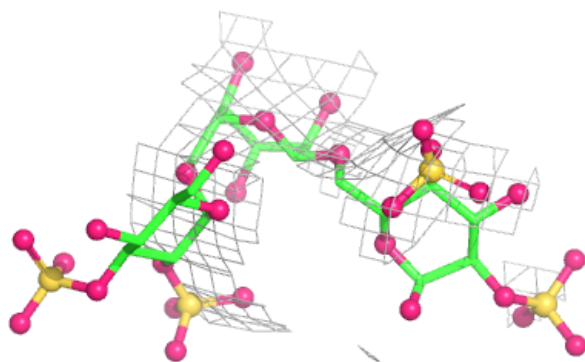
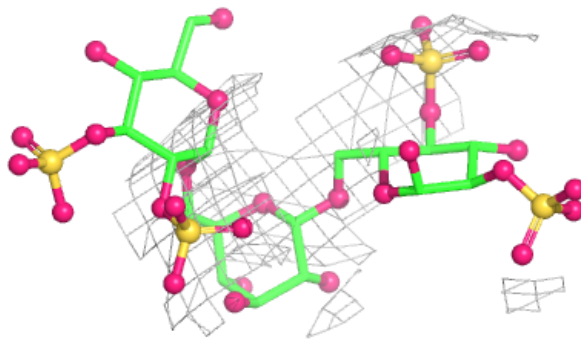
Electron density around Chain R:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



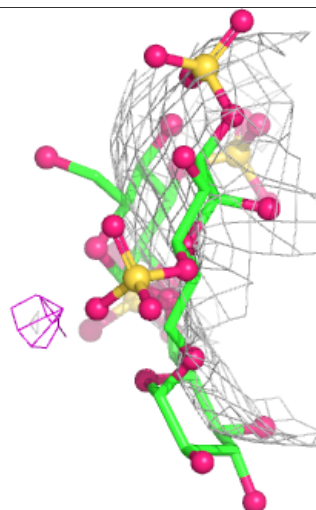
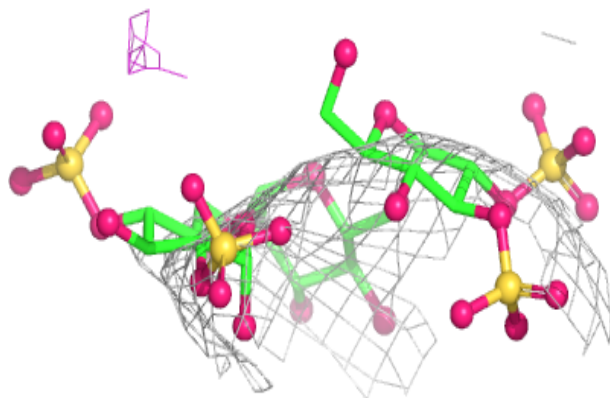
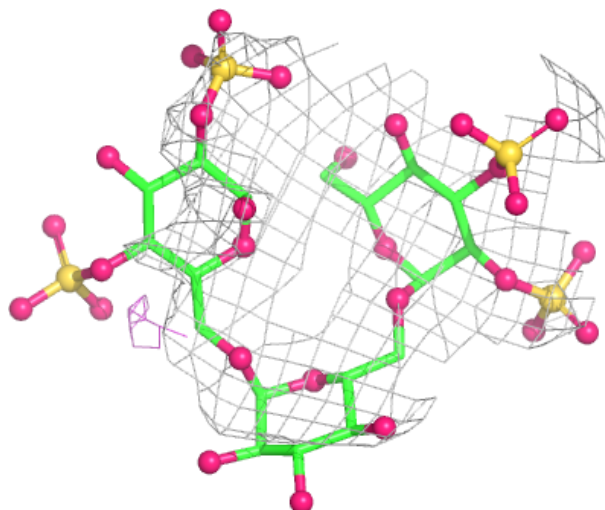
Electron density around Chain S:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



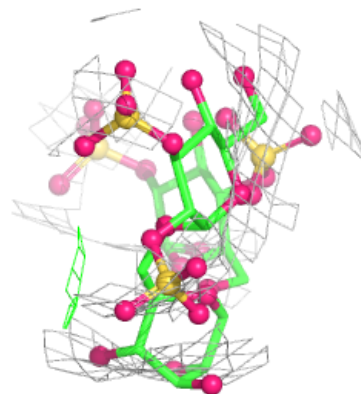
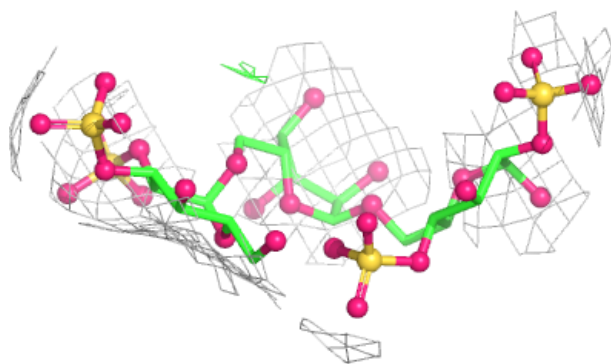
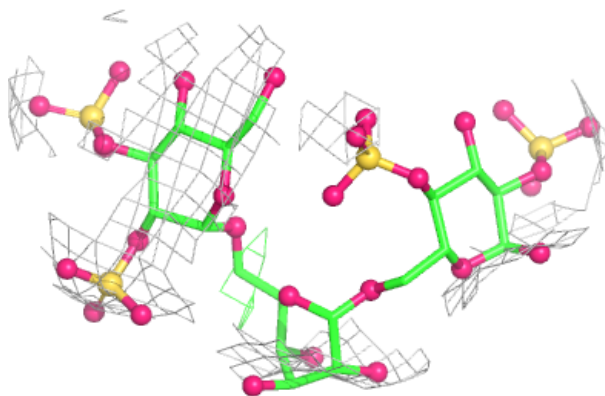
Electron density around Chain U:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



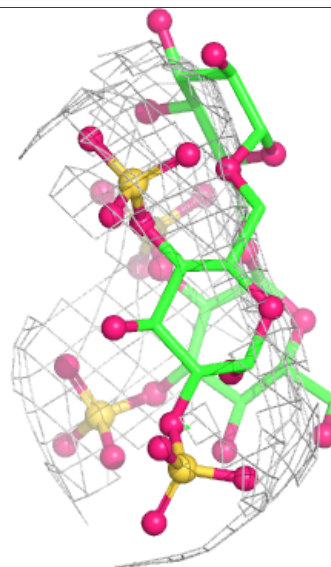
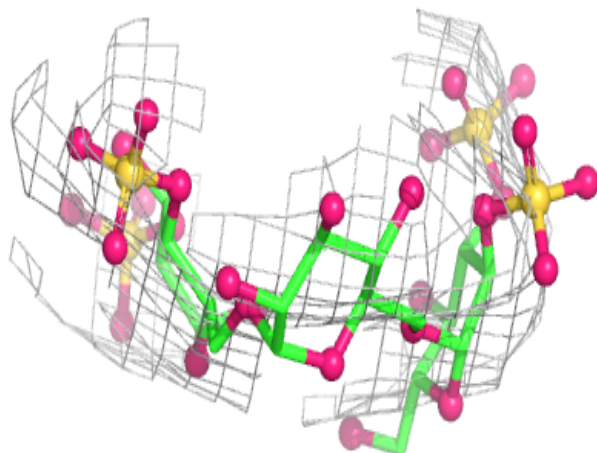
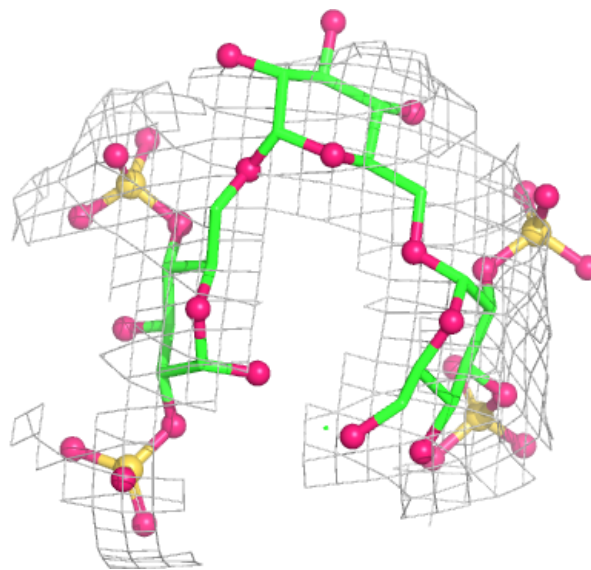
Electron density around Chain V:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



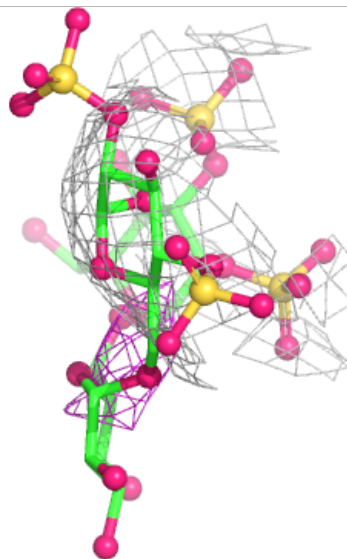
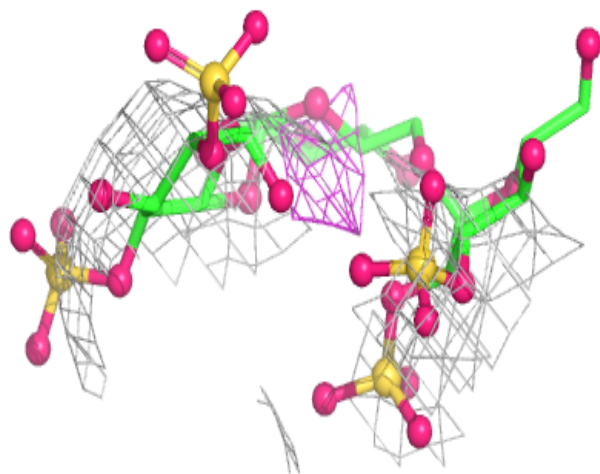
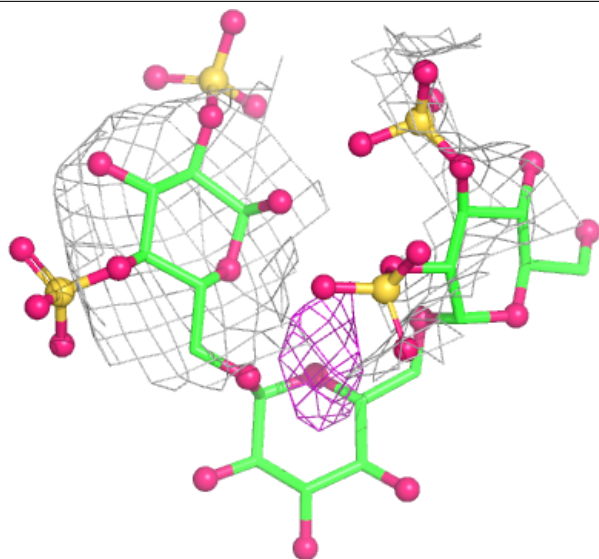
Electron density around Chain W:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



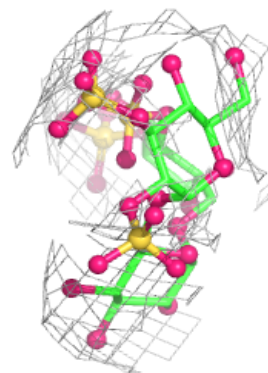
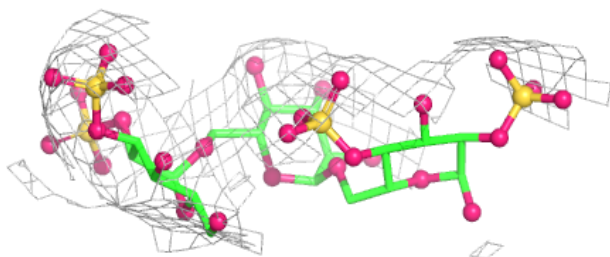
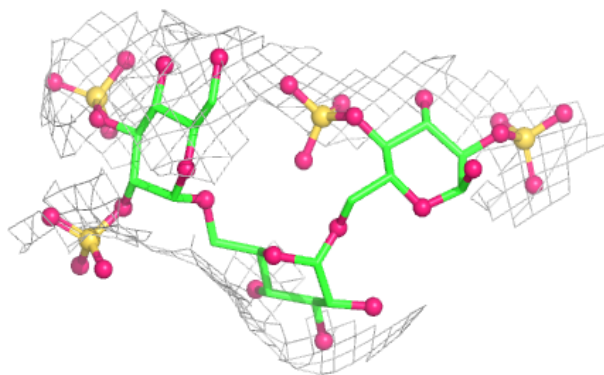
Electron density around Chain X:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

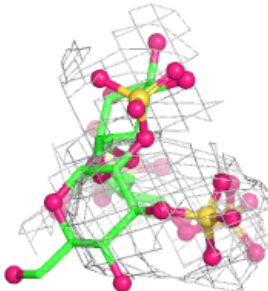
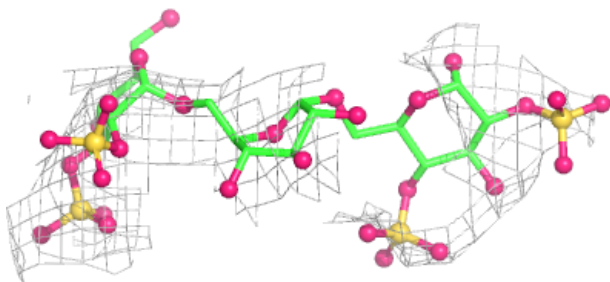
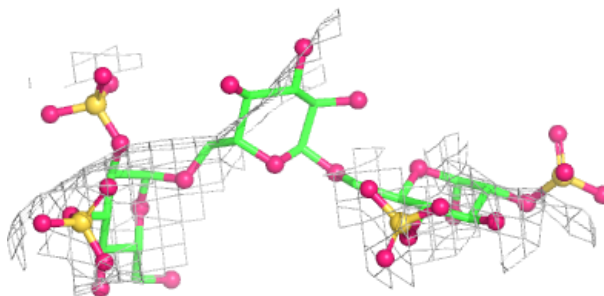


Electron density around Chain Y:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

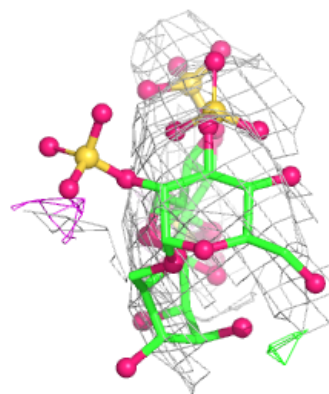
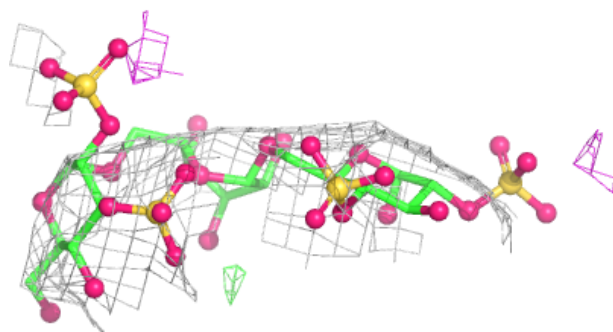
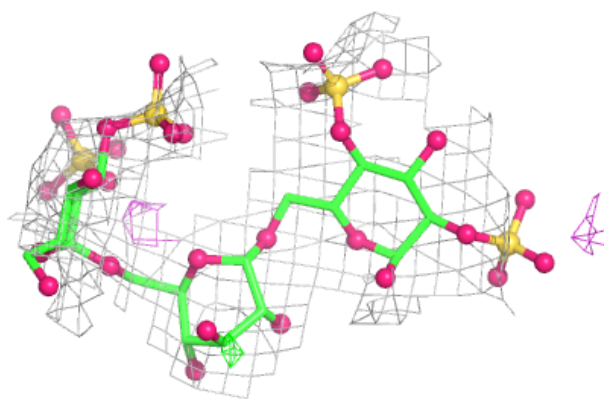
**Electron density around Chain Z:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

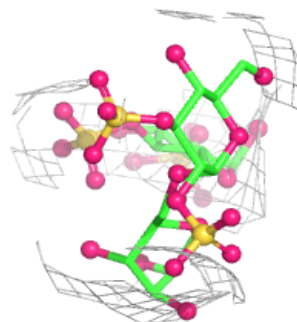
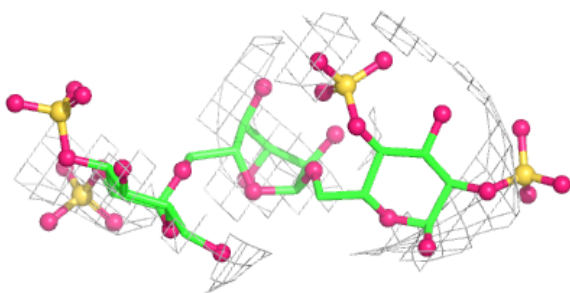
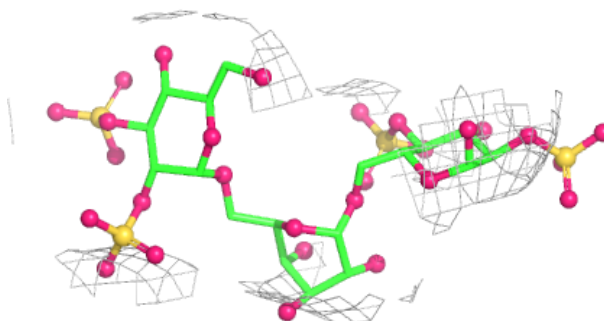


Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

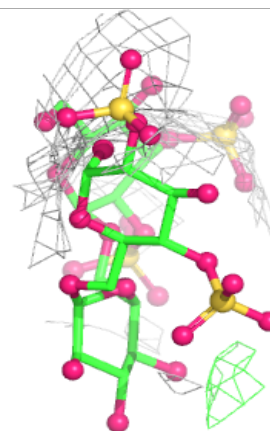
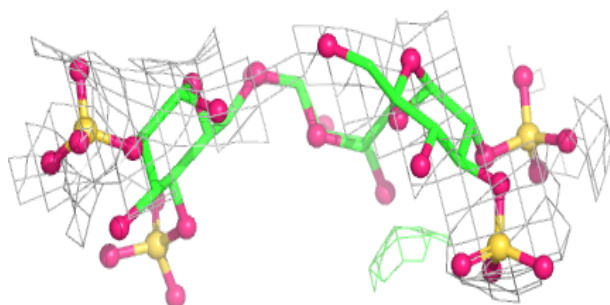
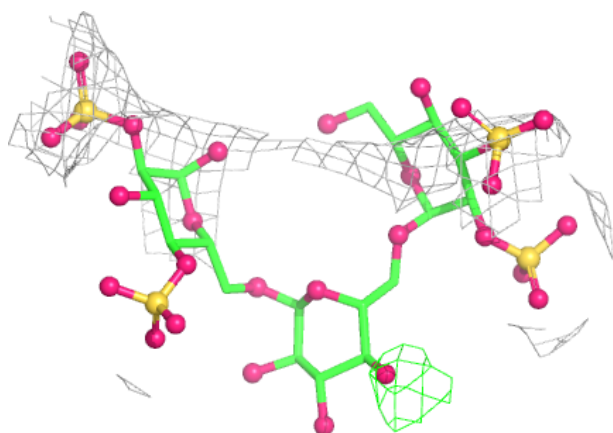
**Electron density around Chain b:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



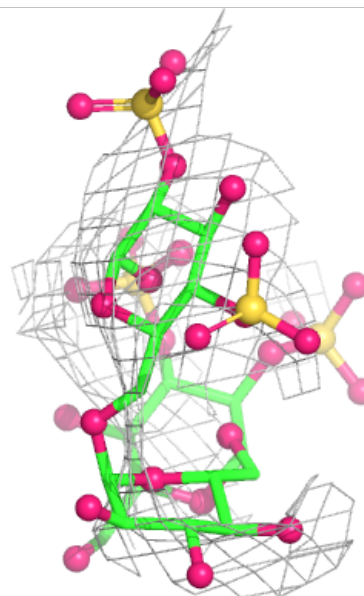
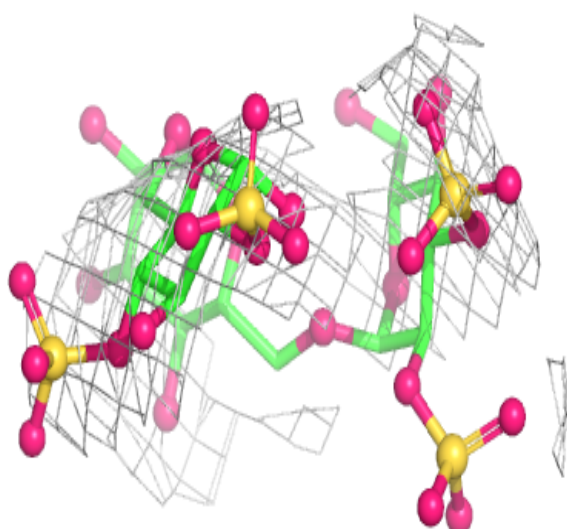
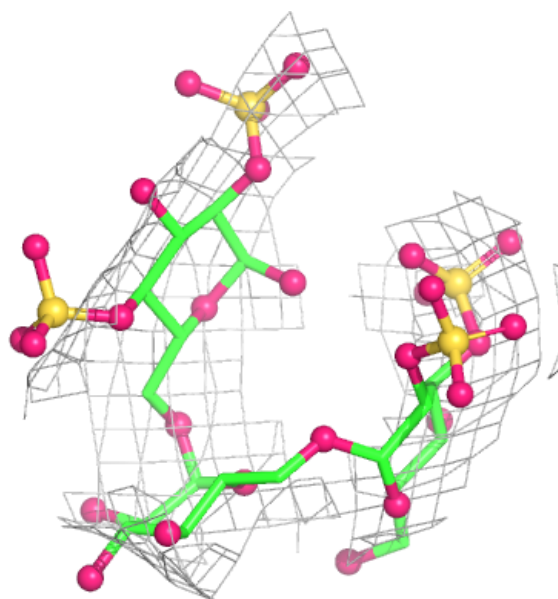
Electron density around Chain d:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



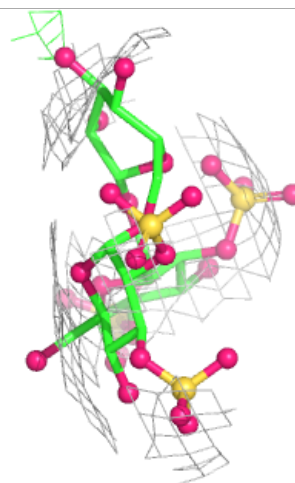
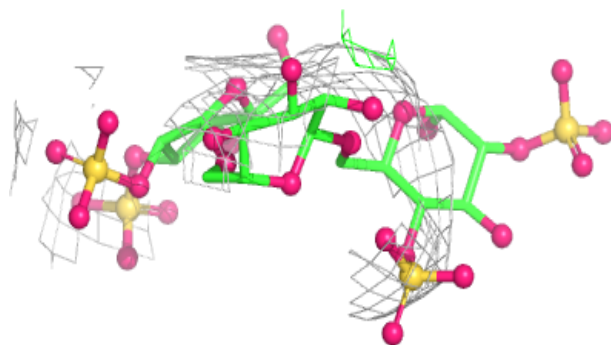
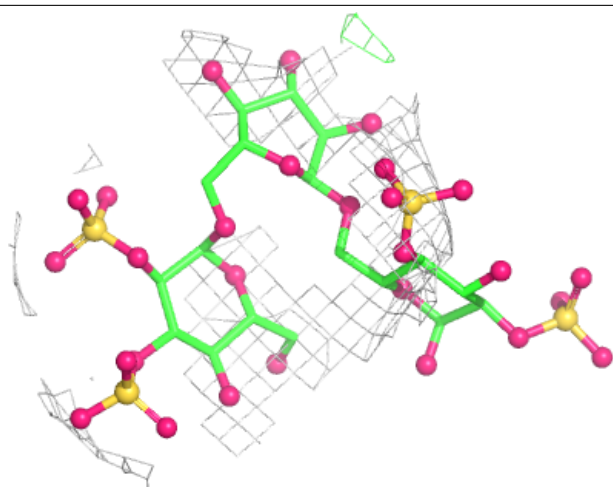
Electron density around Chain e:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



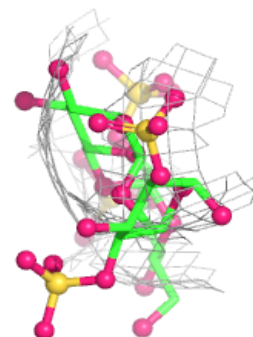
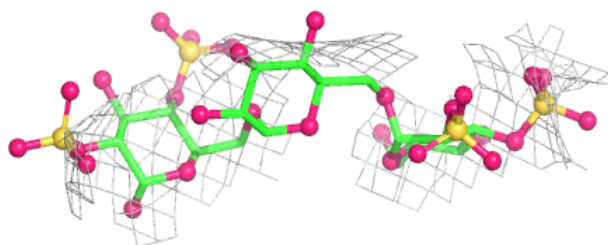
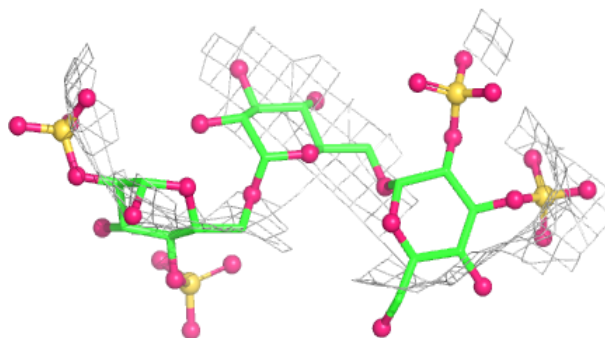
Electron density around Chain f:

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and green (positive)

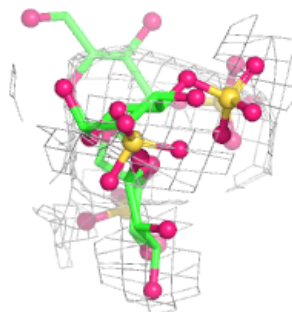
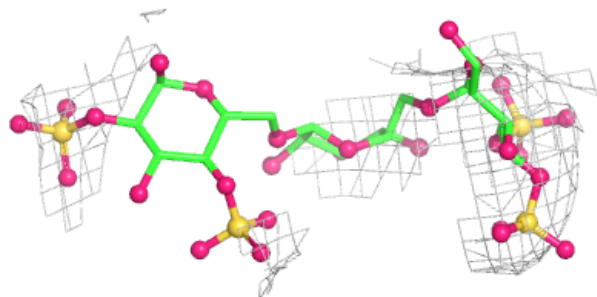
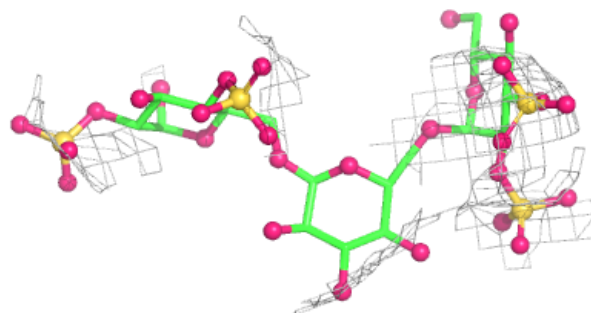


Electron density around Chain g:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

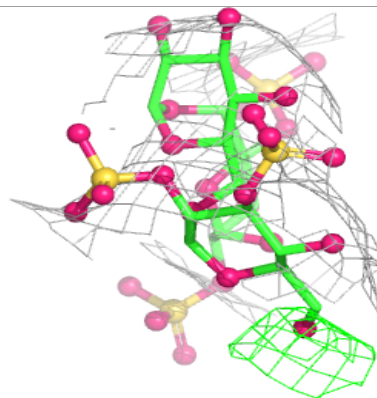
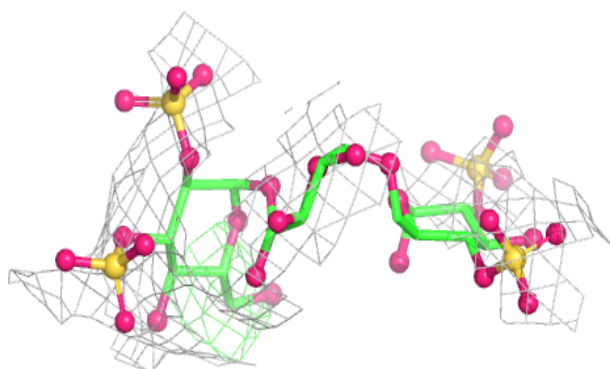
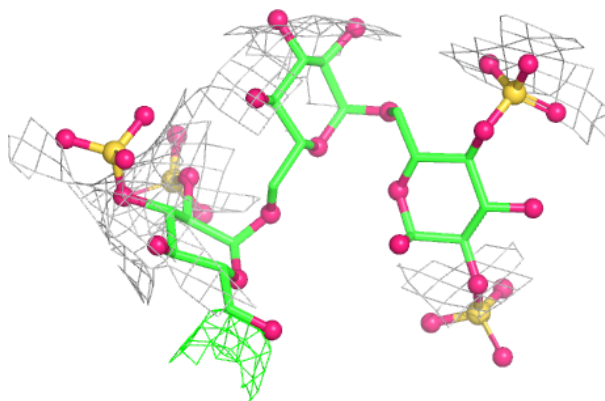
**Electron density around Chain h:**

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

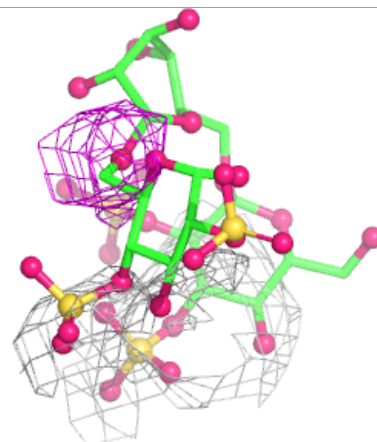
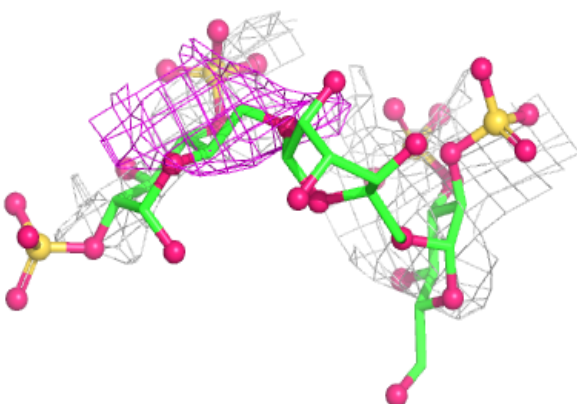
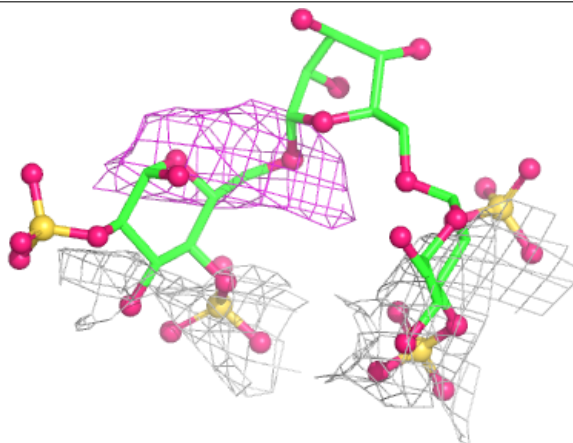


Electron density around Chain j:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)

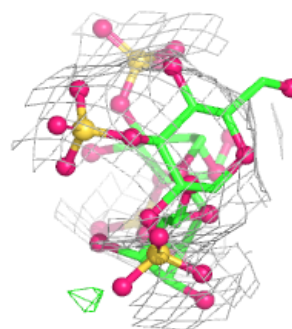
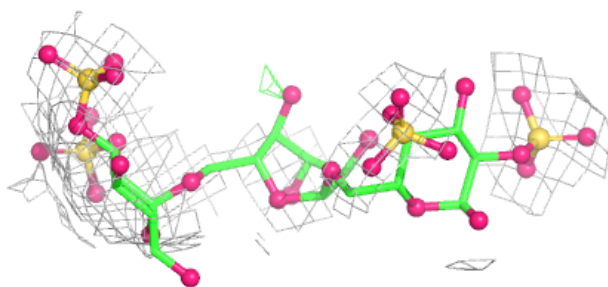
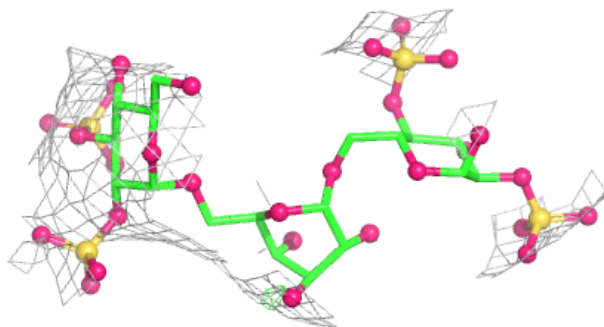
**Electron density around Chain k:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

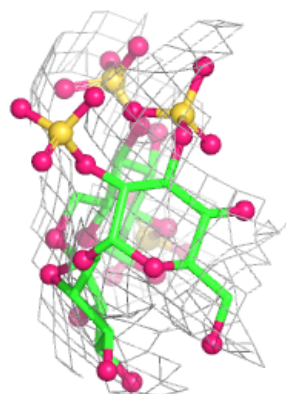
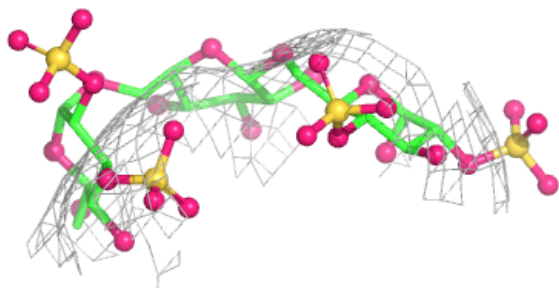
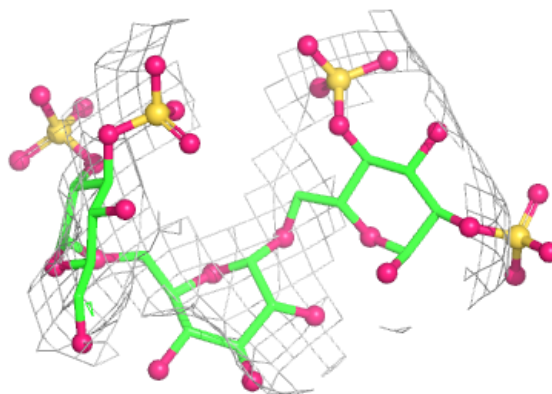


Electron density around Chain l:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

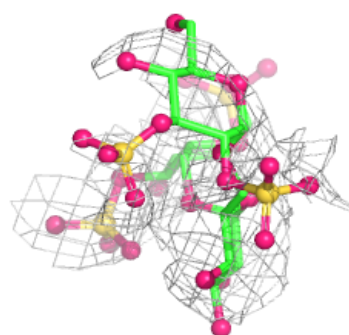
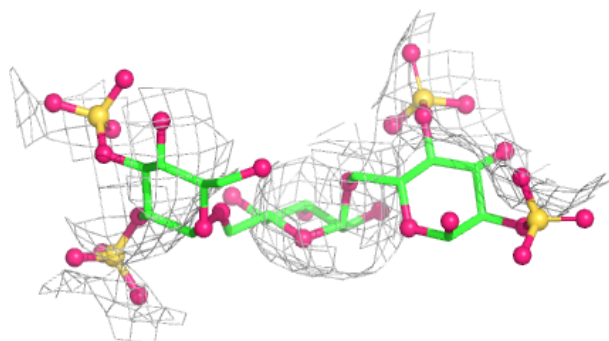
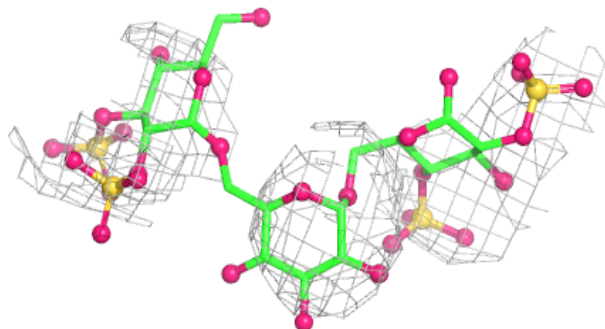
**Electron density around Chain m:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

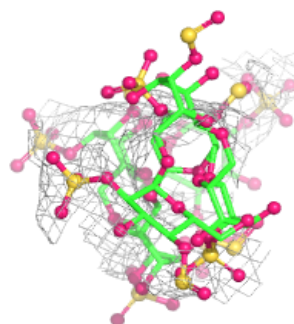
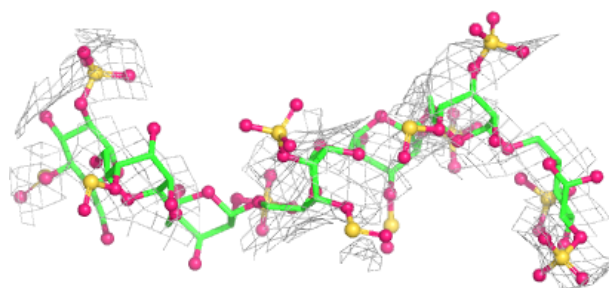
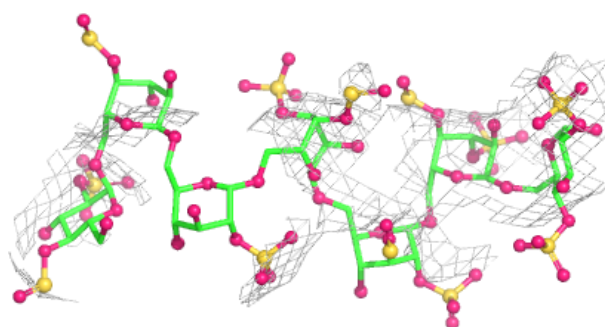


Electron density around Chain n:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

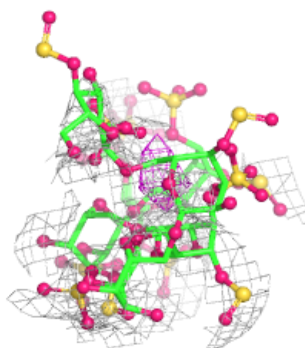
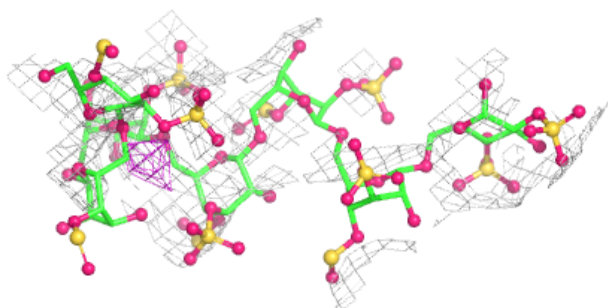
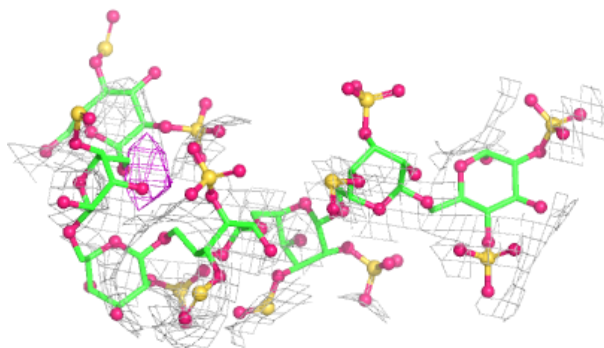
**Electron density around Chain O:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

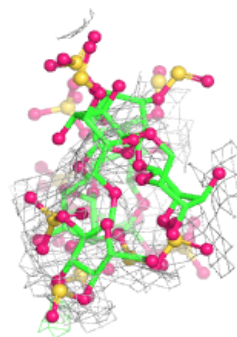
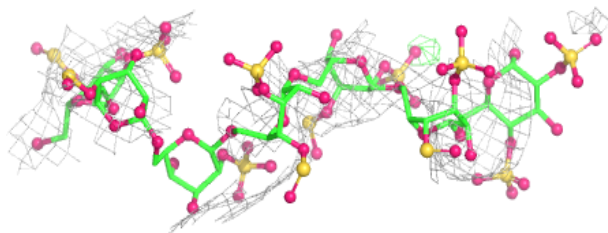
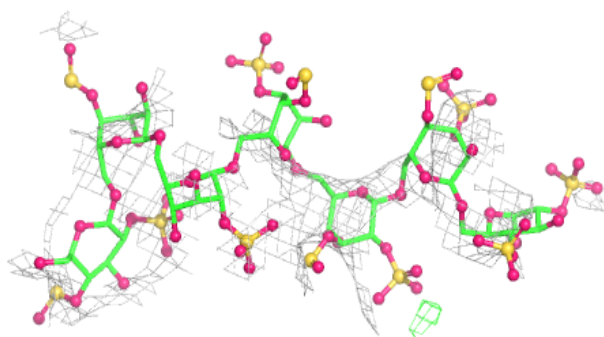


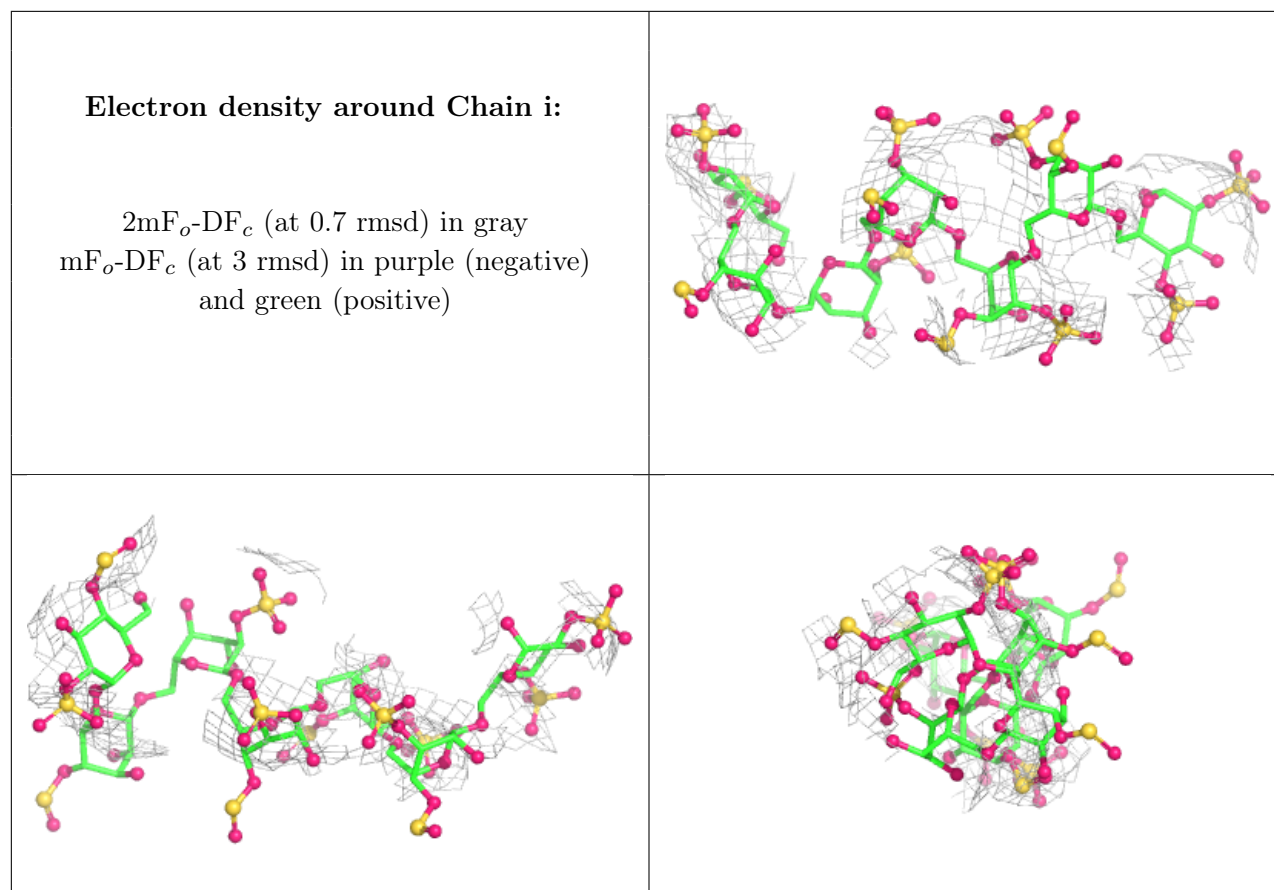
Electron density around Chain T:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain c:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

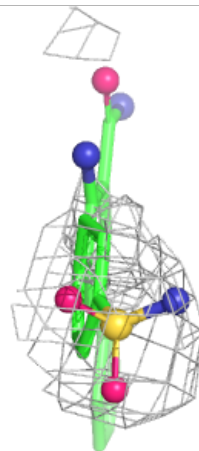
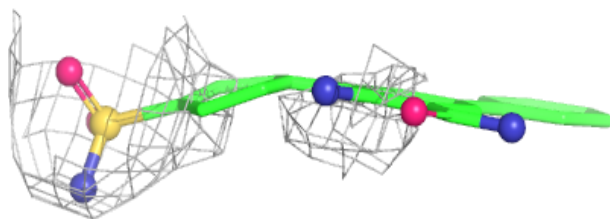
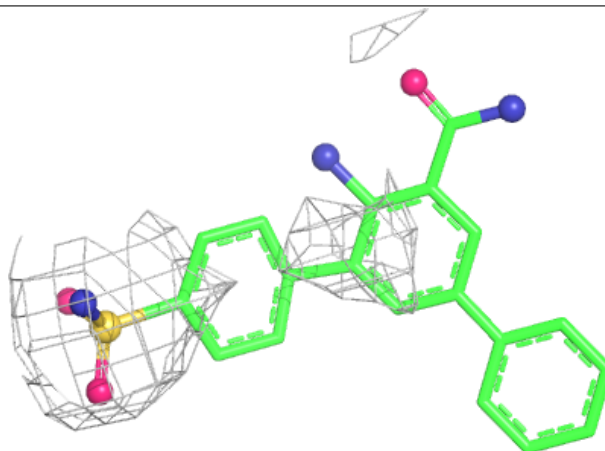
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	5TL	B	701	26/26	0.74	0.15	149,237,280,287	0
4	5TL	F	701	26/26	0.75	0.24	157,307,408,431	0
4	5TL	H	701	26/26	0.76	0.17	226,257,279,282	0
4	5TL	L	701	26/26	0.76	0.18	158,266,335,350	0
4	5TL	D	701	26/26	0.81	0.19	197,297,320,332	0
4	5TL	E	701	26/26	0.83	0.17	127,197,233,277	0
4	5TL	J	701	26/26	0.83	0.18	179,264,307,319	0
4	5TL	A	701	26/26	0.83	0.16	121,206,278,306	0
4	5TL	G	701	26/26	0.86	0.14	108,200,280,288	0
4	5TL	I	701	26/26	0.87	0.14	152,242,284,323	0
4	5TL	K	701	26/26	0.89	0.13	131,202,237,288	0
4	5TL	C	701	26/26	0.89	0.14	150,234,279,291	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

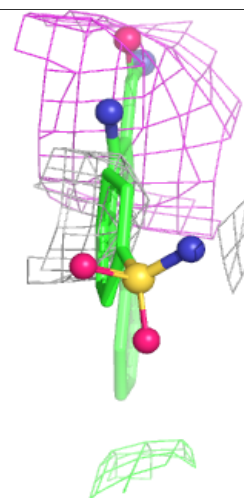
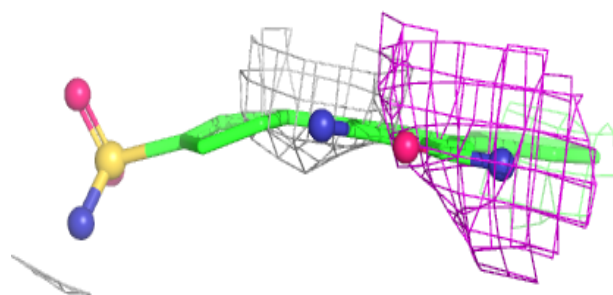
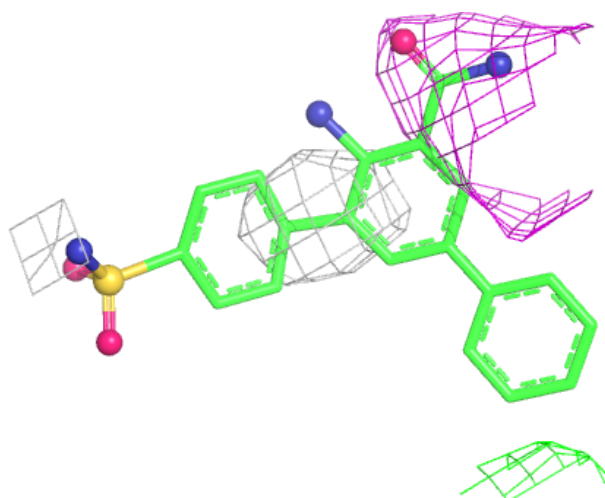
Electron density around 5TL B 701:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



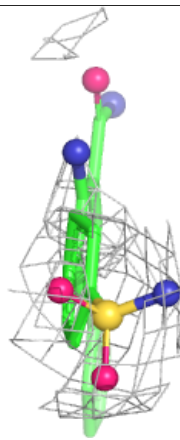
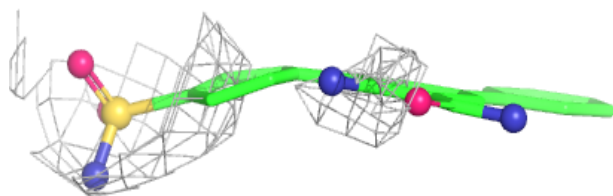
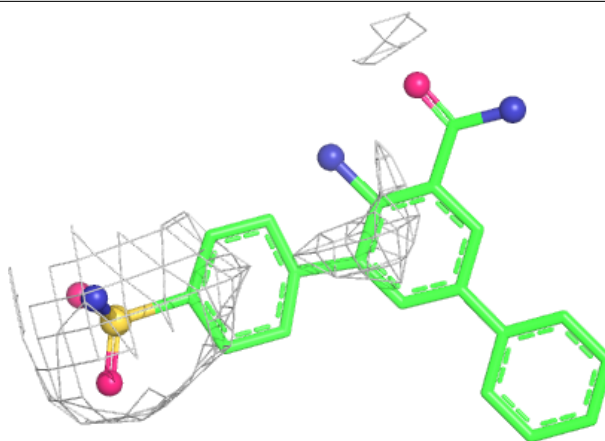
Electron density around 5TL F 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



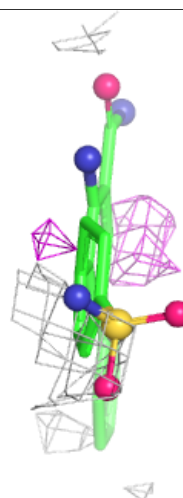
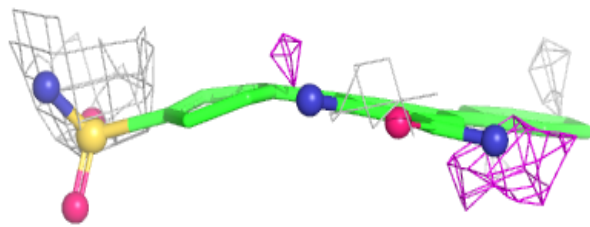
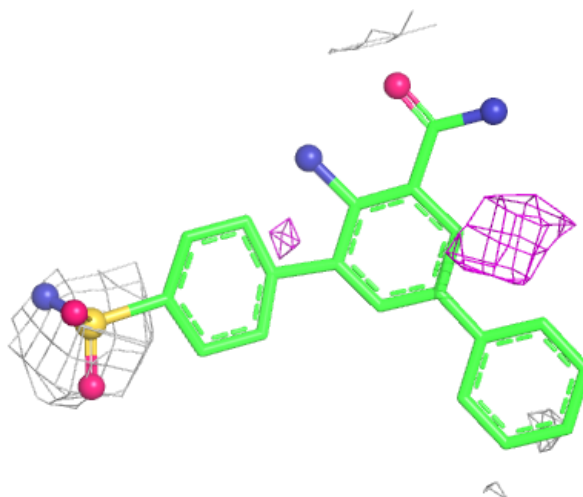
Electron density around 5TL H 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



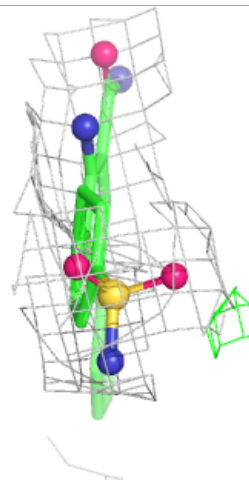
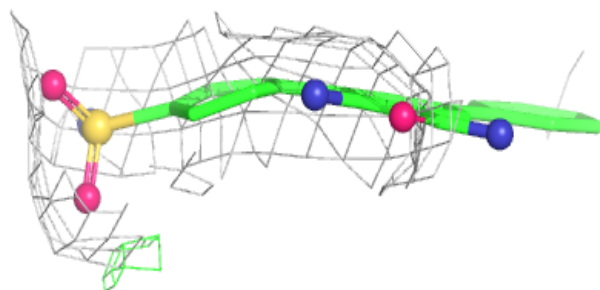
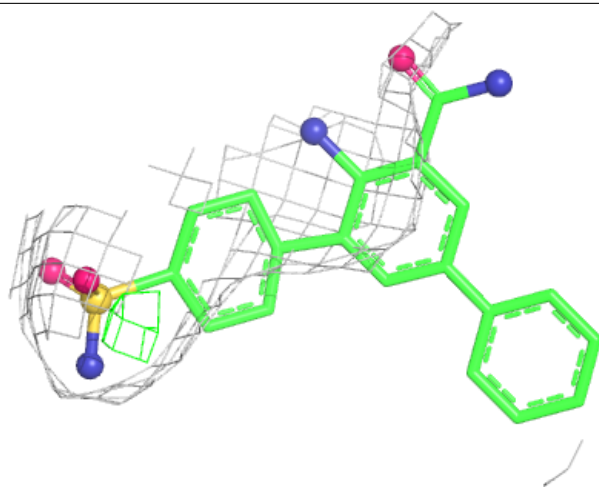
Electron density around 5TL L 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



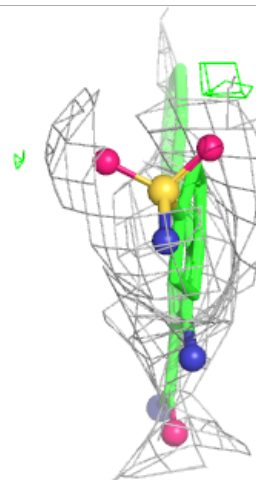
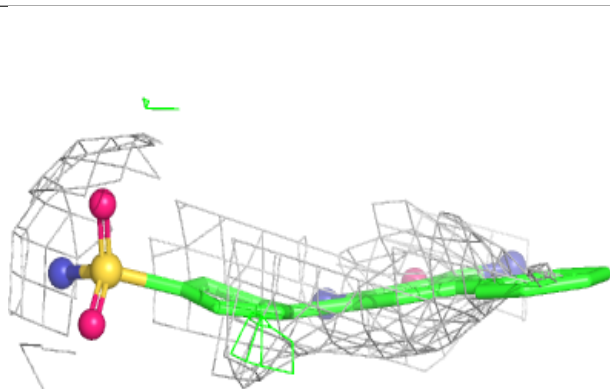
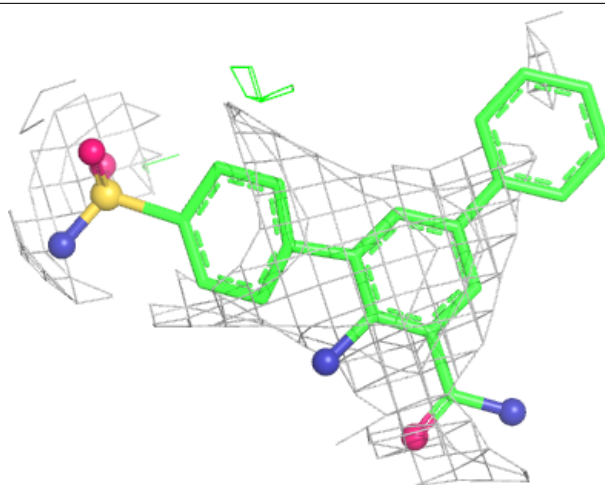
Electron density around 5TL D 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



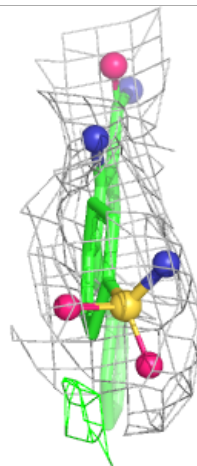
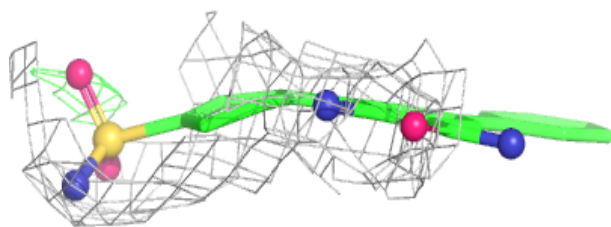
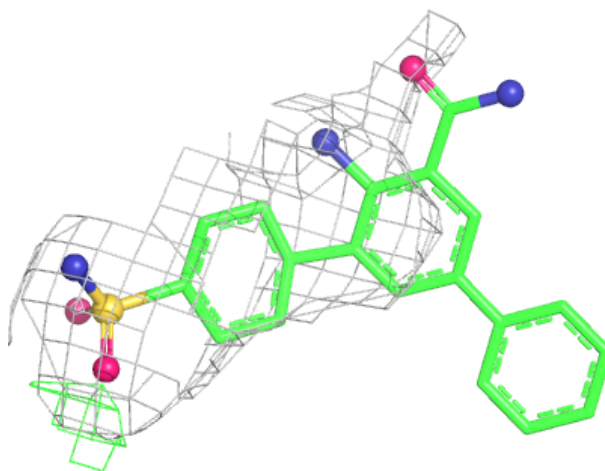
Electron density around 5TL E 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



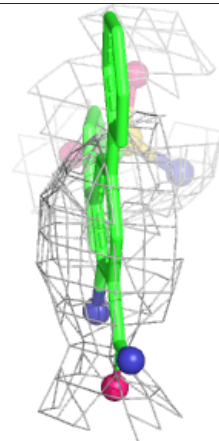
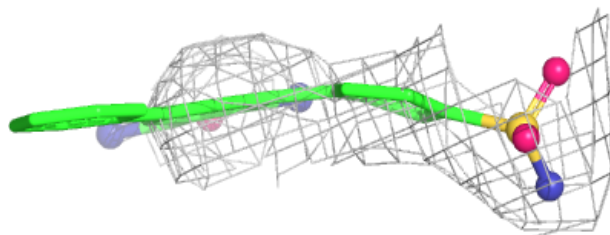
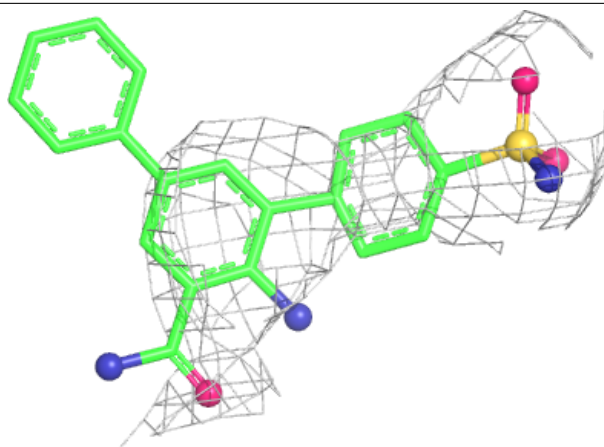
Electron density around 5TL J 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



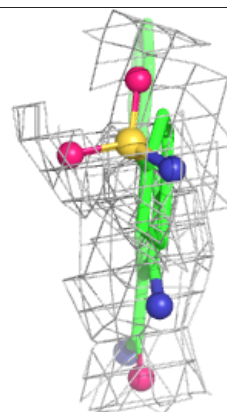
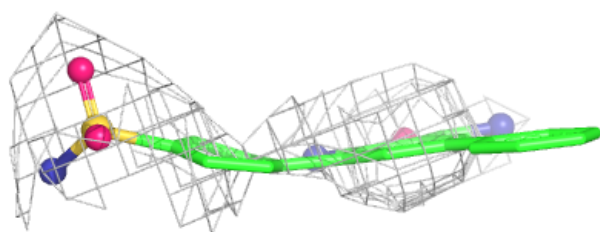
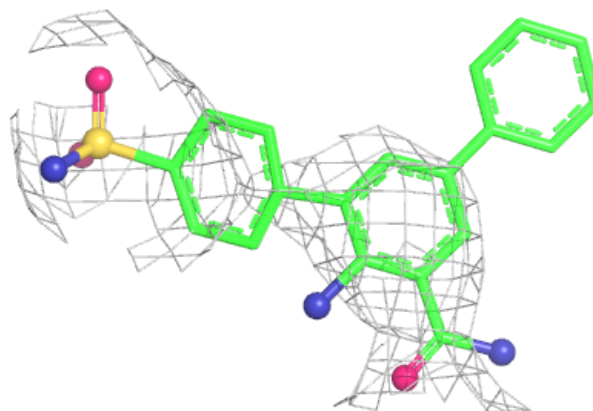
Electron density around 5TL A 701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



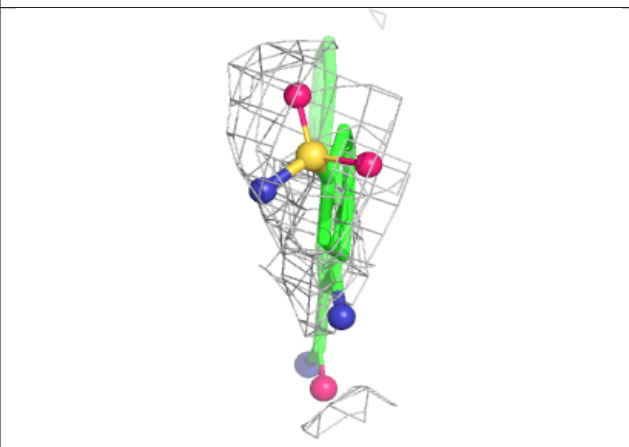
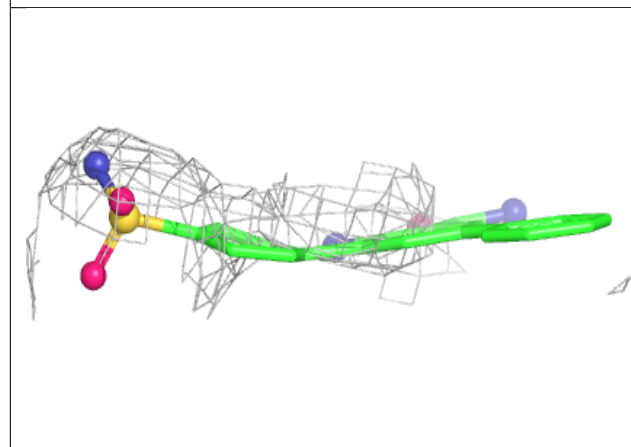
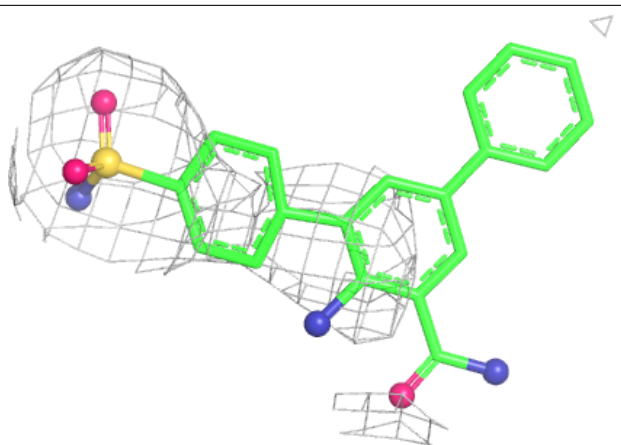
Electron density around 5TL G 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



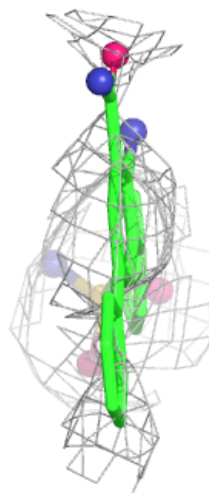
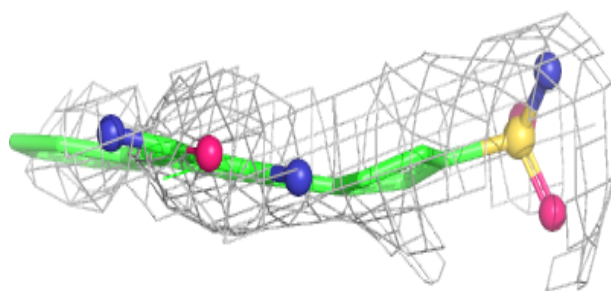
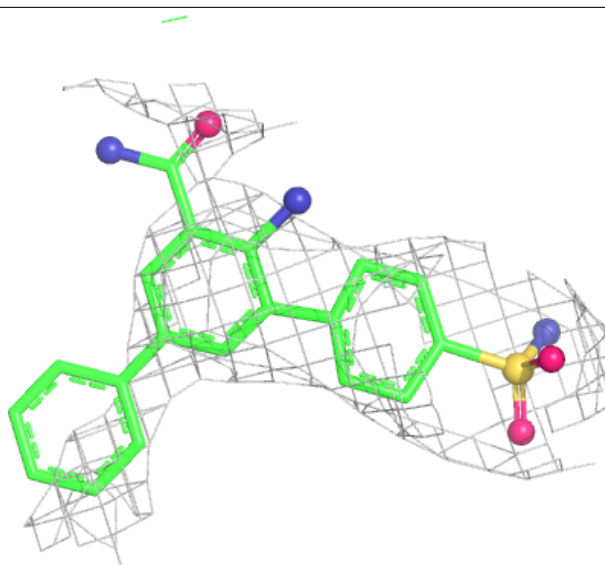
Electron density around 5TL I 701:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



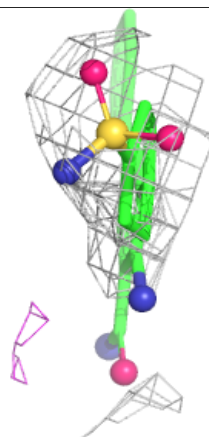
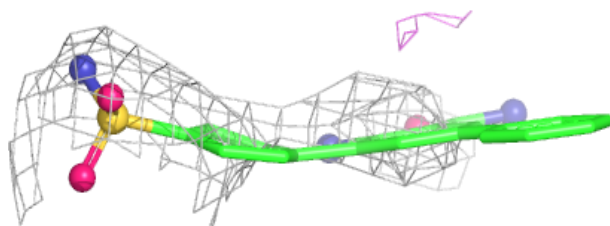
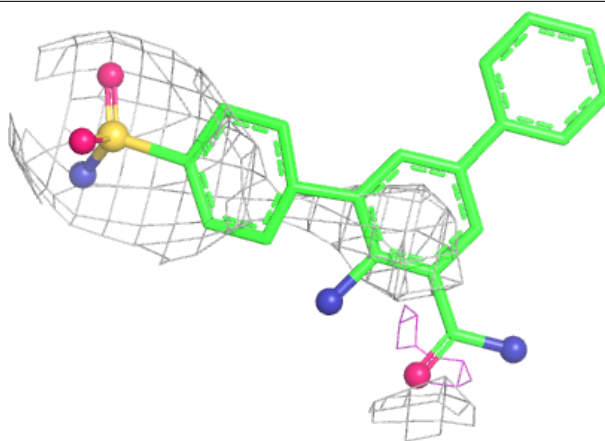
Electron density around 5TL K 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 5TL C 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.