



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:21 AM UTC

PDB ID : 3GHG / pdb_00003ghg
Title : Crystal Structure of Human Fibrinogen
Authors : Doolittle, R.F.; Kollman, J.M.; Sawaya, M.R.; Pandi, L.; Riley, M.
Deposited on : 2009-03-03
Resolution : 2.90 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
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

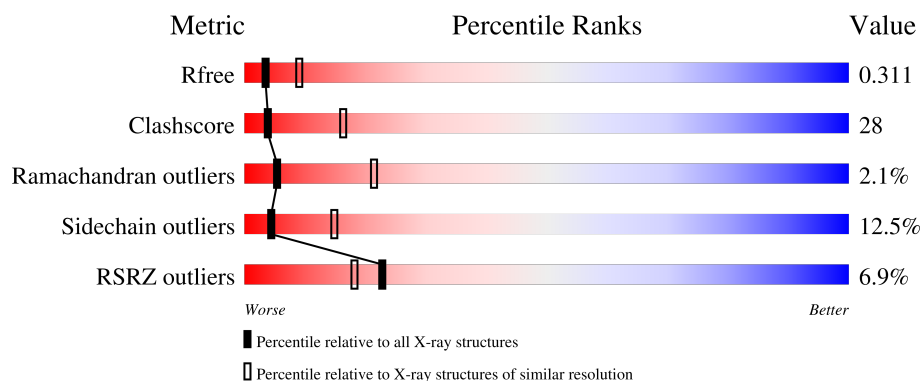
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	562	
1	D	562	
1	G	562	
1	J	562	
2	B	461	

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Mol	Chain	Length	Quality of chain
2	E	461	
2	H	461	
2	K	461	
3	C	411	
3	F	411	
3	I	411	
3	L	411	
4	M	4	
4	N	4	
4	Q	4	
4	R	4	
5	O	4	
5	P	4	
5	S	4	
5	T	4	
6	U	11	
6	V	11	
6	X	11	
7	W	5	
8	Y	2	

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
6	NAG	U	1	-	-	X	-
6	NAG	U	2	X	-	-	-
6	NAG	U	5	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GAL	U	6	X	-	-	-
6	NAG	U	9	X	-	-	-
6	NAG	V	1	X	-	-	-
6	NAG	V	2	X	-	-	-
6	NAG	V	5	X	-	-	-
6	GAL	V	6	X	-	-	-
6	NAG	V	9	X	-	-	-
6	NAG	X	1	-	-	X	-
6	NAG	X	2	X	-	X	-
6	NAG	X	5	X	-	-	-
6	GAL	X	6	X	-	-	-
6	NAG	X	9	X	-	-	-
7	NAG	W	1	X	-	-	-
7	NAG	W	2	X	-	-	-
8	NAG	Y	1	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31833 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	D	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	G	174	Total	C	N	O	S	0	0	0
			1431	876	268	278	9			
1	J	186	Total	C	N	O	S	0	0	0
			1527	941	284	292	10			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	E	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	H	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			
2	K	401	Total	C	N	O	S	0	0	0
			3209	1995	564	624	26			

- Molecule 3 is a protein called Fibrinogen gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	381	Total	C	N	O	S	0	0	0
			3050	1931	510	593	16			
3	F	382	Total	C	N	O	S	0	0	0
			3054	1933	511	594	16			
3	I	394	Total	C	N	O	S	0	0	0
			3145	1986	527	614	18			
3	L	391	Total	C	N	O	S	0	0	0
			3126	1974	524	610	18			

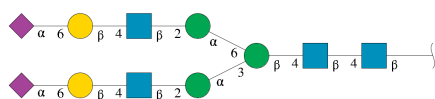
- Molecule 4 is a protein called A knob.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	N	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	Q	4	Total	C	N	O	0	0	0
			30	18	7	5			
4	R	4	Total	C	N	O	0	0	0
			30	18	7	5			

- Molecule 5 is a protein called B knob.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	P	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	S	4	Total	C	N	O	0	0	0
			33	19	9	5			
5	T	4	Total	C	N	O	0	0	0
			33	19	9	5			

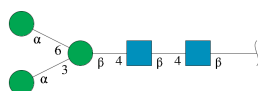
- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	11	Total	C	N	O	0	0	0
			151	84	6	61			
6	V	11	Total	C	N	O	0	0	0
			151	84	6	61			
6	X	11	Total	C	N	O	0	0	0
			151	84	6	61			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	W	5	Total	C	N	O	0	0	0
			61	34	2	25			

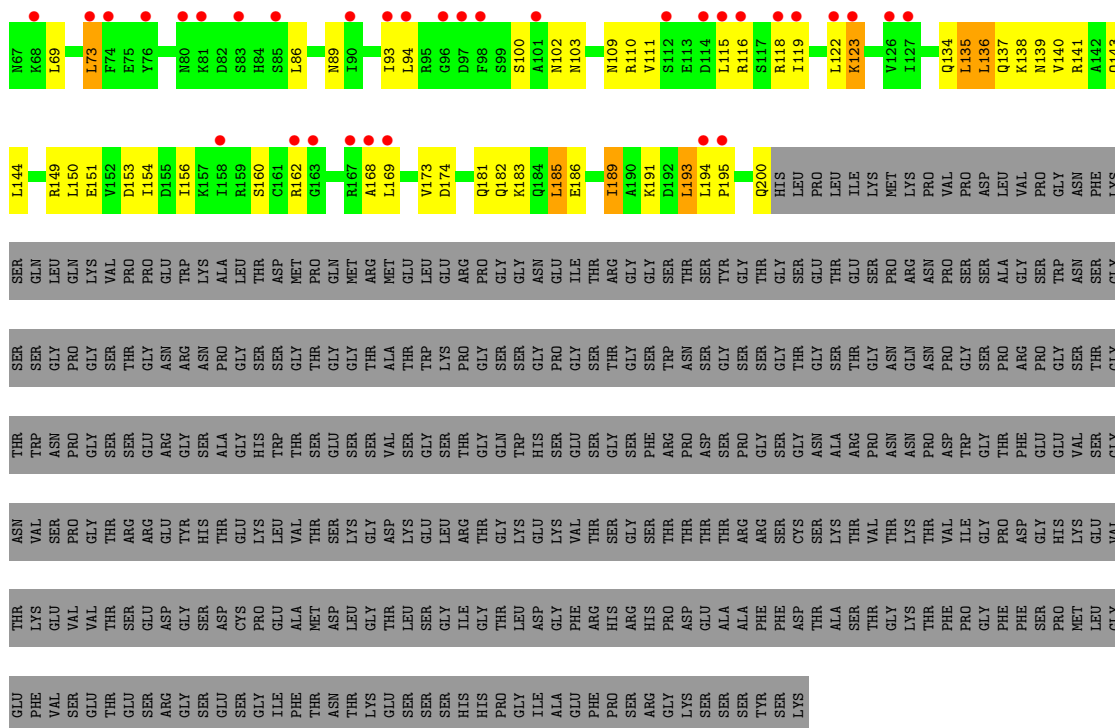
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



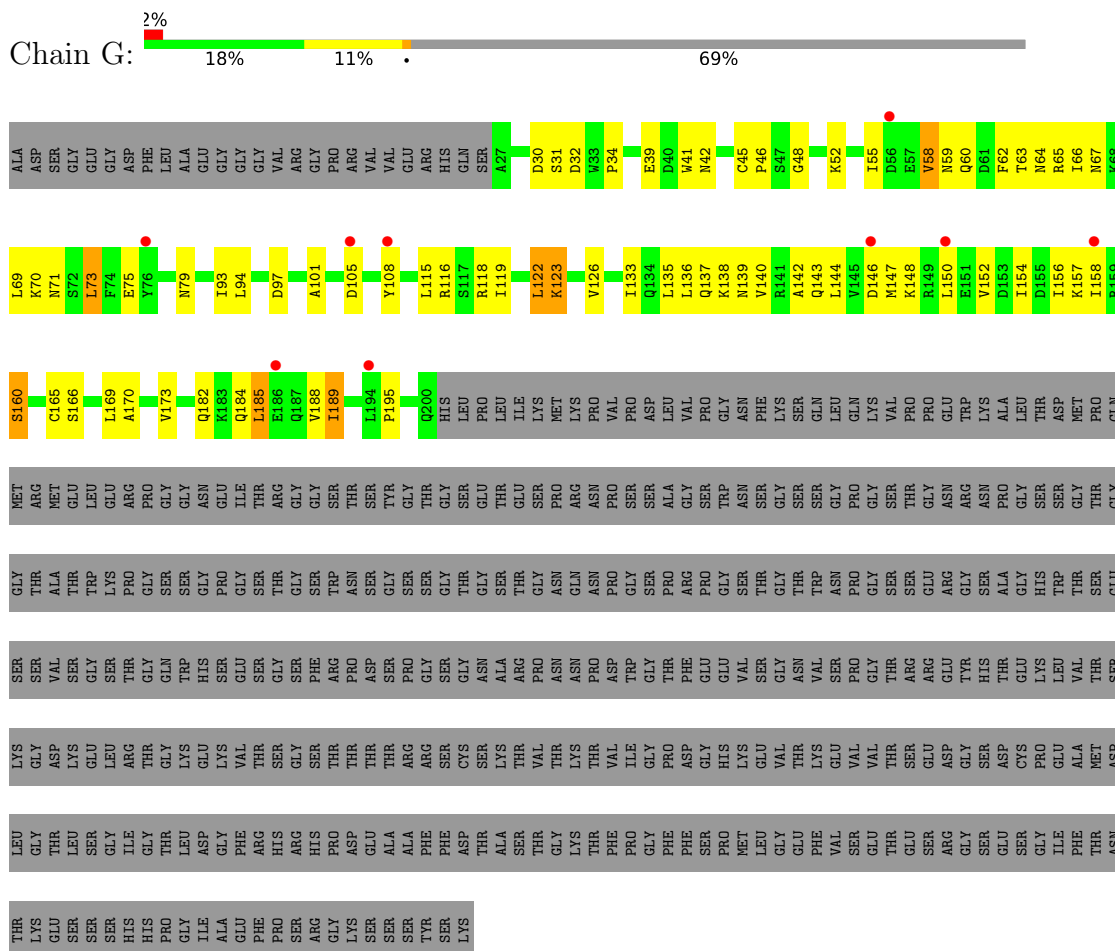
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

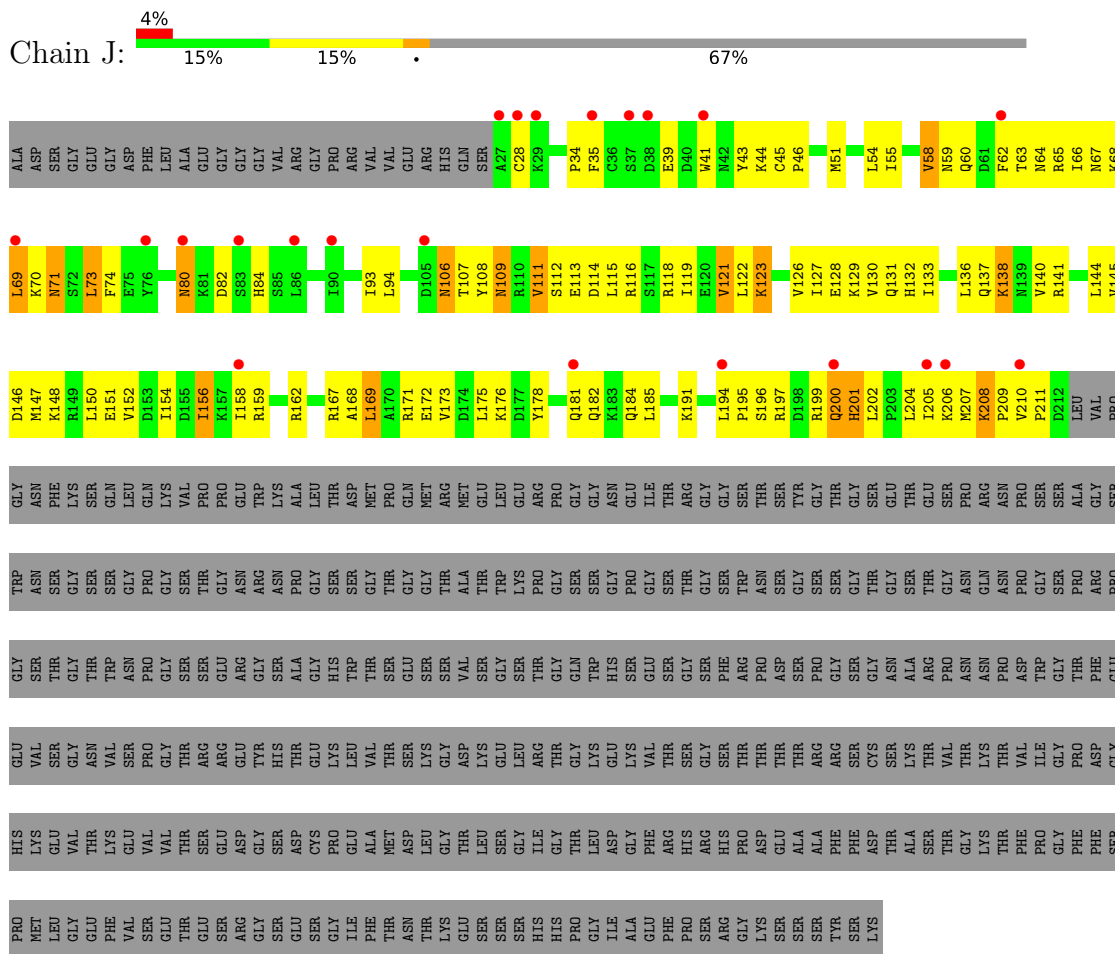
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Ca	0	0
			1	1		
9	C	1	Total	Ca	0	0
			1	1		
9	E	1	Total	Ca	0	0
			1	1		
9	F	1	Total	Ca	0	0
			1	1		
9	H	1	Total	Ca	0	0
			1	1		
9	I	1	Total	Ca	0	0
			1	1		
9	K	1	Total	Ca	0	0
			1	1		
9	L	1	Total	Ca	0	0
			1	1		



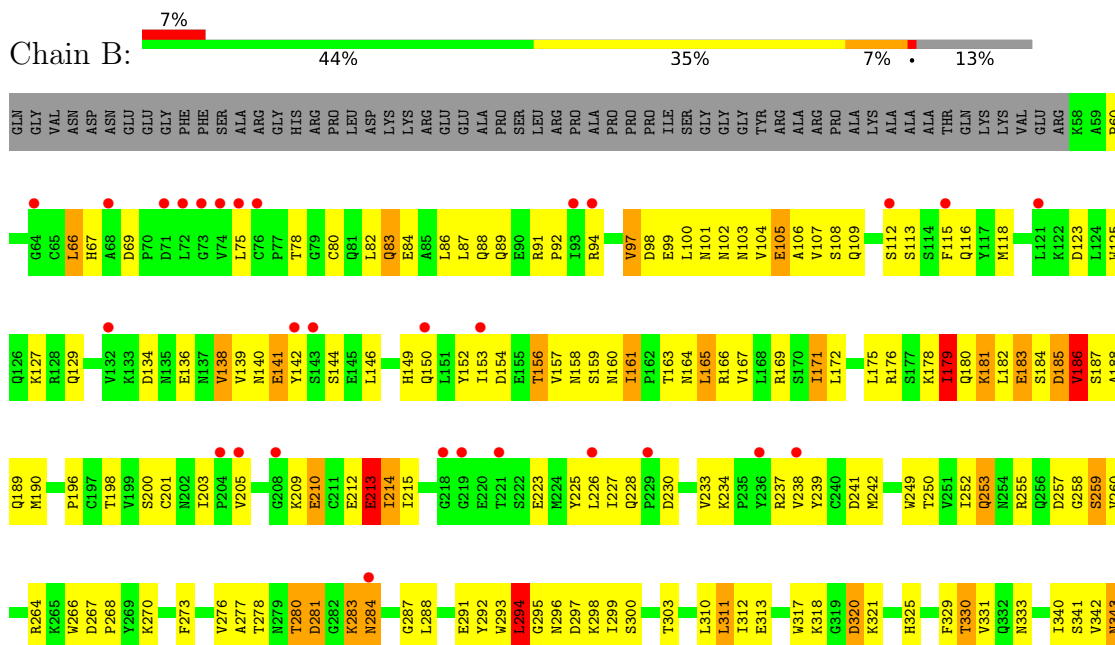
- Molecule 1: Fibrinogen alpha chain

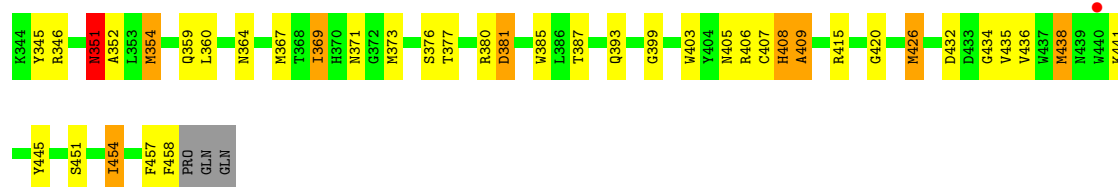


- Molecule 1: Fibrinogen alpha chain

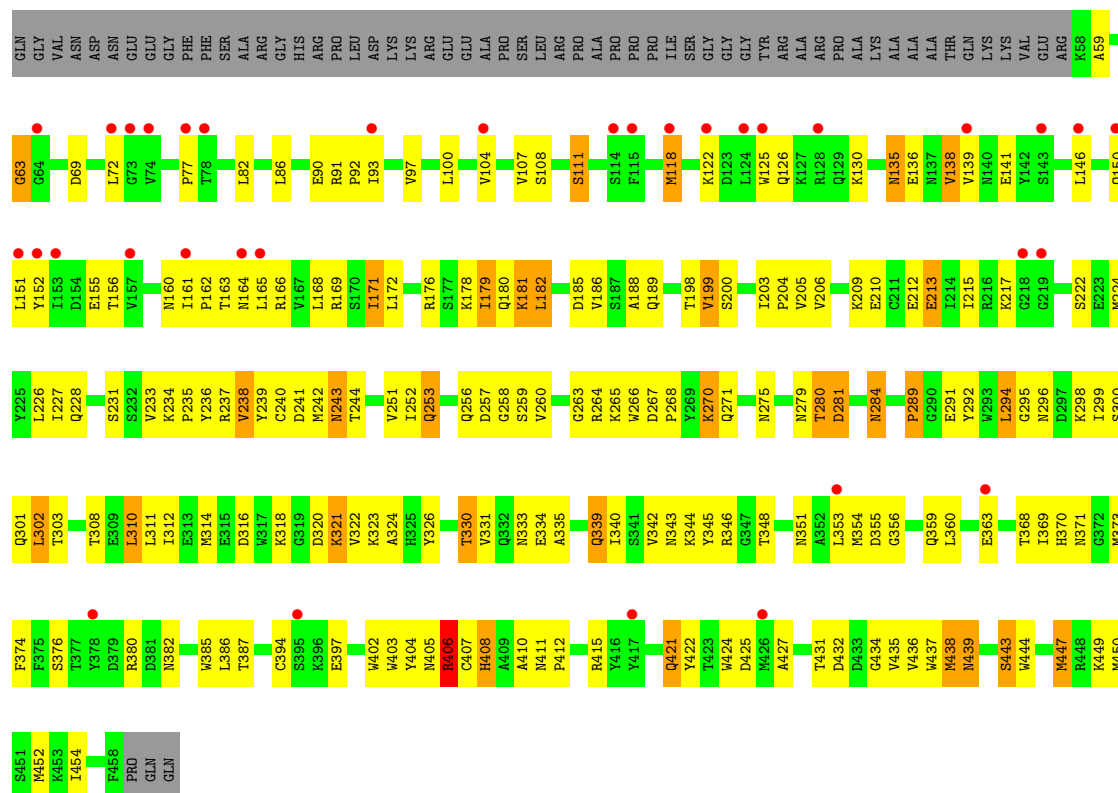
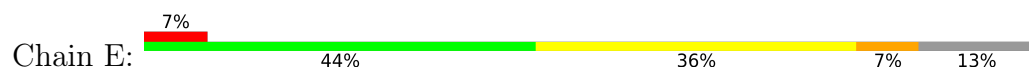


- Molecule 2: Fibrinogen beta chain

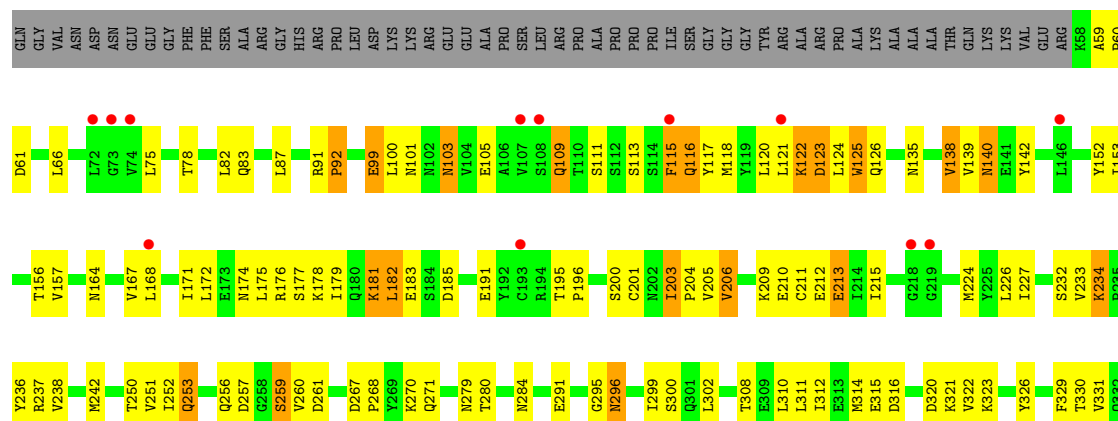


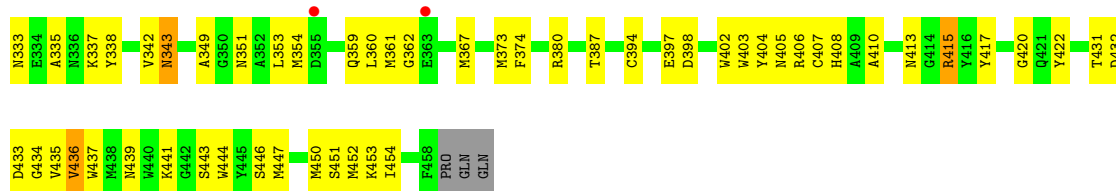


• Molecule 2: Fibrinogen beta chain

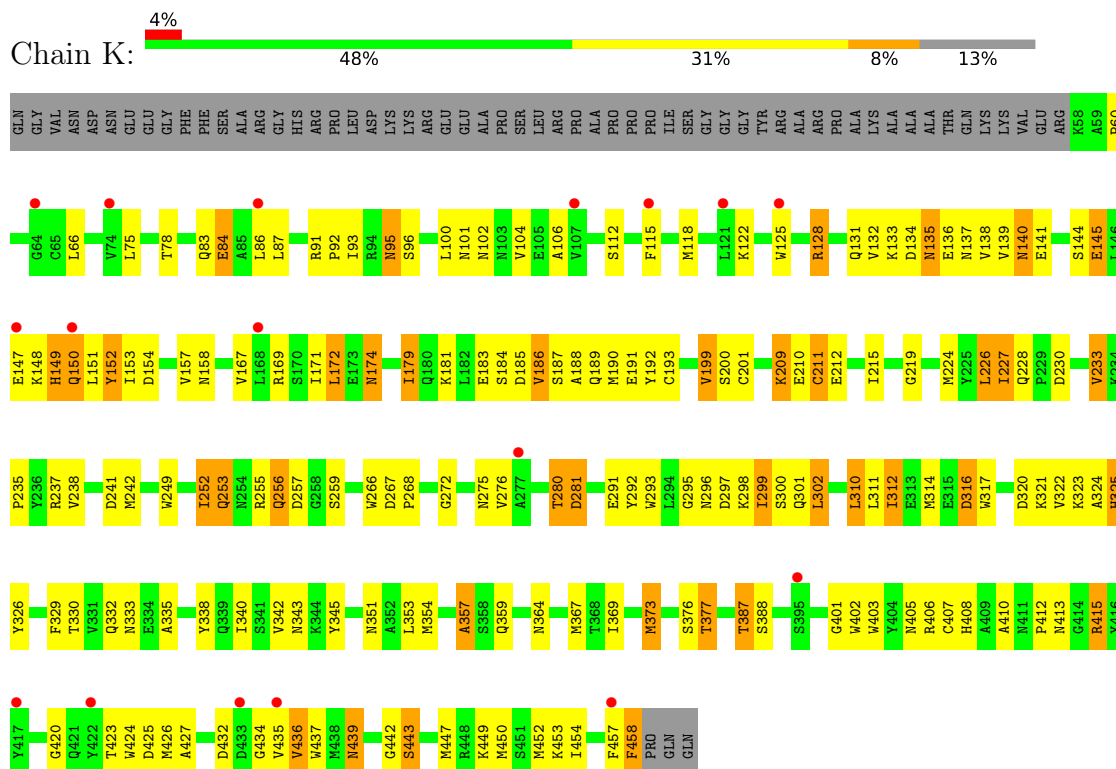


• Molecule 2: Fibrinogen beta chain

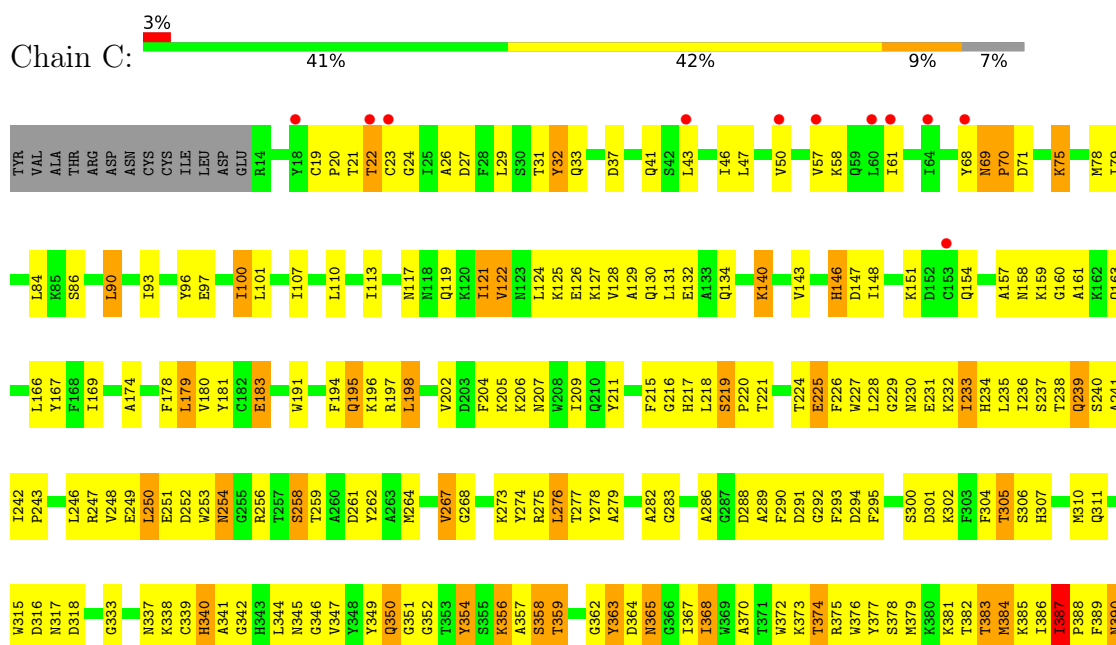


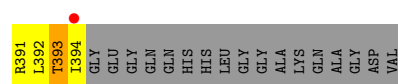


● Molecule 2: Fibrinogen beta chain

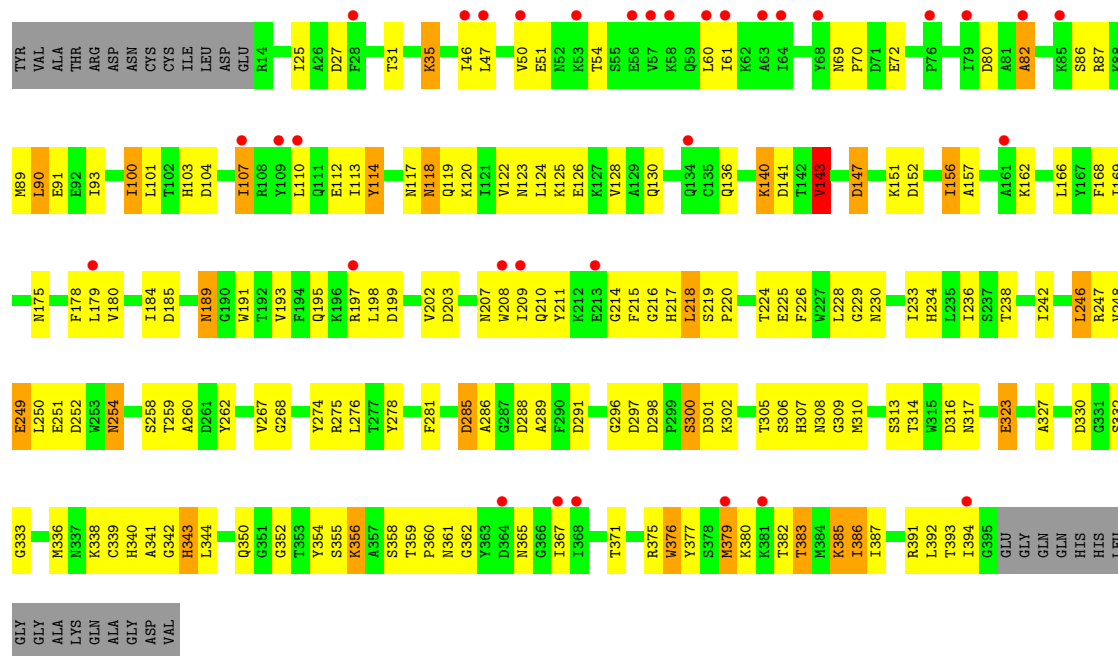


● Molecule 3: Fibrinogen gamma chain

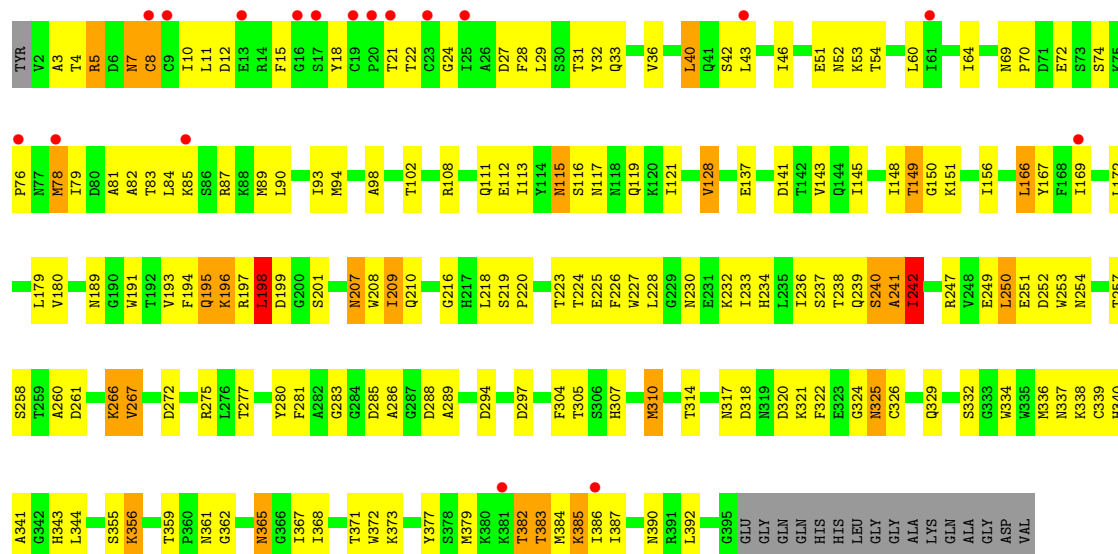




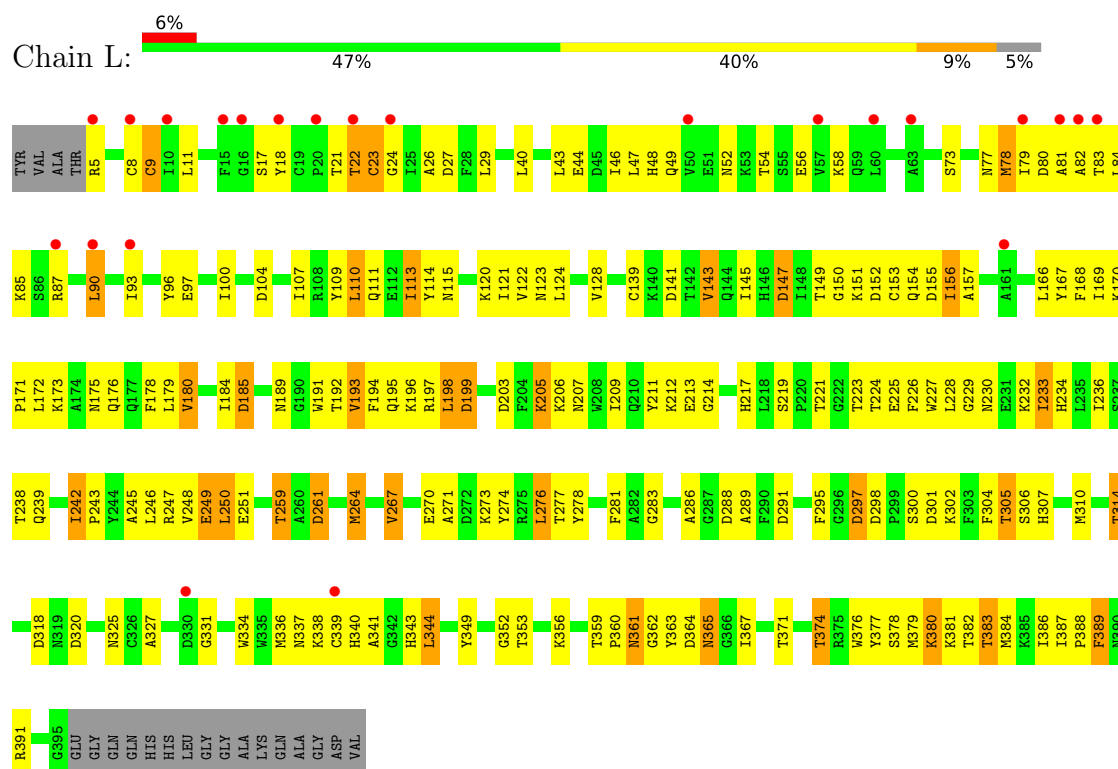
• Molecule 3: Fibrinogen gamma chain



• Molecule 3: Fibrinogen gamma chain



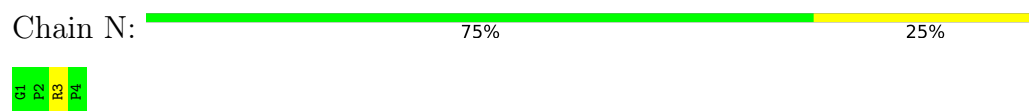
• Molecule 3: Fibrinogen gamma chain



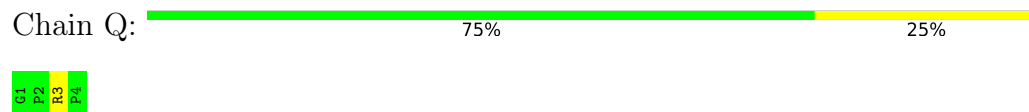
- Molecule 4: A knob



- Molecule 4: A knob



- Molecule 4: A knob



- Molecule 4: A knob



- Molecule 5: B knob





- Molecule 5: B knob



- Molecule 5: B knob



- Molecule 5: B knob



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2
BRM3
MAN4
NAG5
GAL6
STN7
MAN8
NAG9
GAL10
SIA11

- Molecule 7: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain W:  20% 20% 60%

NAG1
NAG2
BRM3
MAN4
MAN5

- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain Y:  100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.24Å 94.87Å 300.81Å 90.00° 94.81° 90.00°	Depositor
Resolution (Å)	19.95 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.90) 69.2 (19.95-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.4.0061	Depositor
R, R_{free}	0.252 , 0.309 0.259 , 0.311	Depositor DCC
R_{free} test set	5820 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31833	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.84 % 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 1.2228e-03. 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, SIA, MAN, BMA, CA, NAG

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	0.59	0/1447	0.84	0/1939
1	D	0.59	0/1447	0.77	0/1939
1	G	0.52	0/1447	0.80	0/1939
1	J	0.59	0/1547	0.90	2/2076 (0.1%)
2	B	0.76	0/3283	0.97	10/4438 (0.2%)
2	E	0.63	0/3283	0.81	1/4438 (0.0%)
2	H	0.65	0/3283	0.88	6/4438 (0.1%)
2	K	0.63	0/3283	0.88	4/4438 (0.1%)
3	C	1.00	5/3125 (0.2%)	1.12	10/4224 (0.2%)
3	F	0.58	0/3129	0.79	2/4229 (0.0%)
3	I	0.65	0/3220	0.87	2/4353 (0.0%)
3	L	0.65	0/3201	0.90	2/4326 (0.0%)
4	M	0.85	0/31	1.08	0/40
4	N	0.55	0/31	0.91	0/40
4	Q	0.80	0/31	0.92	0/40
4	R	0.75	0/31	1.05	0/40
5	O	0.74	0/34	0.90	0/43
5	P	0.59	0/34	0.76	0/43
5	S	0.61	0/34	0.66	0/43
5	T	0.62	0/34	1.04	0/43
All	All	0.68	5/31955 (0.0%)	0.89	39/43109 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	VAL	CA-CB	6.23	1.62	1.54
3	C	183	GLU	CA-C	-5.61	1.45	1.53
3	C	225	GLU	CA-C	-5.35	1.45	1.52
3	C	384	MET	CA-C	-5.30	1.46	1.52
3	C	69	ASN	C-O	5.08	1.30	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	283	GLY	N-CA-C	-8.59	102.75	111.85
3	L	193	VAL	N-CA-C	7.42	117.38	106.85
2	B	228	GLN	CA-C-N	6.99	126.69	119.56
2	B	228	GLN	C-N-CA	6.99	126.69	119.56
3	C	219	SER	CA-C-N	6.56	128.04	119.84
3	C	219	SER	C-N-CA	6.56	128.04	119.84
3	L	193	VAL	CB-CA-C	-6.39	103.22	111.53
2	H	259	SER	N-CA-C	6.22	119.97	112.38
2	B	408	HIS	N-CA-C	6.11	118.35	109.07
3	C	374	THR	N-CA-C	6.07	117.88	110.41
3	C	363	TYR	N-CA-C	-6.05	99.54	109.40
2	B	186	VAL	N-CA-C	6.04	116.10	110.42
1	J	208	LYS	CA-C-N	6.04	125.43	118.85
1	J	208	LYS	C-N-CA	6.04	125.43	118.85
3	F	226	PHE	N-CA-C	6.01	117.28	108.14
3	I	242	ILE	N-CA-C	-5.98	102.12	107.56
2	B	214	ILE	CB-CA-C	-5.79	104.23	112.22
2	K	299	ILE	CB-CA-C	-5.74	105.99	111.44
2	H	203	ILE	CA-C-N	5.74	125.64	119.85
2	H	203	ILE	C-N-CA	5.74	125.64	119.85
2	B	161	ILE	CB-CA-C	-5.73	108.26	113.70
2	B	409	ALA	N-CA-C	-5.64	102.93	111.56
2	K	211	CYS	N-CA-C	5.51	118.05	111.71
3	I	280	TYR	N-CA-C	5.49	116.61	108.60
2	B	293	TRP	N-CA-C	-5.48	99.96	108.90
2	B	294	LEU	N-CA-C	-5.46	103.17	110.55
3	F	297	ASP	N-CA-C	-5.45	106.14	112.89
2	H	436	VAL	N-CA-C	5.43	115.78	108.17
2	K	373	MET	N-CA-C	5.38	117.63	110.53
2	H	343	ASN	N-CA-C	5.32	115.39	107.88
2	K	408	HIS	N-CA-C	5.29	116.88	108.79
3	C	363	TYR	CA-CB-CG	5.26	123.38	113.90
2	H	408	HIS	N-CA-C	5.24	117.04	108.76
3	C	69	ASN	N-CA-C	5.23	121.36	109.81
2	B	333	ASN	N-CA-C	5.16	116.76	110.41
3	C	354	TYR	N-CA-C	5.10	114.88	108.45
2	E	408	HIS	N-CA-C	5.04	116.50	108.79
3	C	387	ILE	CA-C-N	-5.00	114.79	119.89
3	C	387	ILE	C-N-CA	-5.00	114.79	119.89

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	1431	0	1424	109	0
1	D	1431	0	1424	75	0
1	G	1431	0	1424	80	0
1	J	1527	0	1533	144	1
2	B	3209	0	3042	222	0
2	E	3209	0	3042	194	0
2	H	3209	0	3041	171	0
2	K	3209	0	3043	205	0
3	C	3050	0	2906	224	0
3	F	3054	0	2909	166	0
3	I	3145	0	2993	200	1
3	L	3126	0	2972	246	0
4	M	30	0	32	3	0
4	N	30	0	32	0	0
4	Q	30	0	32	0	0
4	R	30	0	32	1	0
5	O	33	0	32	3	0
5	P	33	0	32	2	0
5	S	33	0	32	4	0
5	T	33	0	32	4	0
6	U	151	0	126	24	0
6	V	151	0	126	17	0
6	X	151	0	126	19	0
7	W	61	0	52	7	0
8	Y	28	0	25	12	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
All	All	31833	0	30464	1771	1

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 28.

All (1771) 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)
2:K:364:ASN:HD21	6:X:1:NAG:C1	1.17	1.55
2:B:364:ASN:ND2	6:U:1:NAG:C1	1.70	1.52
2:K:364:ASN:ND2	6:X:1:NAG:C1	1.85	1.38
3:L:56:GLU:HB2	8:Y:1:NAG:O3	1.20	1.32
1:J:108:TYR:OH	3:L:83:THR:C	1.85	1.20
2:H:172:LEU:HD21	3:I:113:ILE:CG2	1.70	1.19
1:J:115:LEU:CD2	3:L:90:LEU:HD21	1.78	1.14
1:A:115:LEU:HD21	3:C:90:LEU:HD13	1.23	1.13
3:I:10:ILE:O	3:I:18:TYR:OH	1.65	1.12
2:K:302:LEU:HD22	2:K:454:ILE:HD11	1.31	1.11
1:G:108:TYR:CE2	3:I:82:ALA:HB1	1.86	1.11
3:I:12:ASP:HB3	3:I:15:PHE:HD1	0.99	1.09
3:I:12:ASP:CB	3:I:15:PHE:HD1	1.65	1.08
1:G:154:ILE:HD11	3:I:128:VAL:HG21	1.28	1.07
1:J:108:TYR:OH	3:L:84:LEU:N	1.87	1.07
3:I:12:ASP:HB3	3:I:15:PHE:CD1	1.90	1.06
1:A:55:ILE:HG23	2:B:86:LEU:HD21	1.35	1.06
3:I:27:ASP:O	3:I:31:THR:HG23	1.56	1.06
1:J:115:LEU:HD21	3:L:90:LEU:HD21	1.12	1.06
1:A:108:TYR:O	1:A:112:SER:OG	1.74	1.05
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.34	1.04
3:F:250:LEU:HD23	3:F:379:MET:HE2	1.35	1.03
3:L:49:GLN:NE2	8:Y:1:NAG:H81	1.72	1.02
3:L:359:THR:HG21	3:L:363:TYR:O	1.59	1.02
1:G:119:ILE:HD11	3:I:93:ILE:CD1	1.89	1.01
1:A:119:ILE:HD13	3:C:93:ILE:HD13	1.43	1.01
2:B:252:ILE:HD11	2:B:454:ILE:HD13	1.02	1.01
2:H:172:LEU:HD21	3:I:113:ILE:HG21	1.39	1.01
3:L:52:ASN:ND2	8:Y:1:NAG:C1	2.24	1.01
1:G:154:ILE:CD1	3:I:128:VAL:HG21	1.90	0.99
1:D:135:LEU:HD22	1:D:136:LEU:HD22	1.43	0.99
1:G:105:ASP:OD1	3:I:79:ILE:HD11	1.63	0.98
2:B:154:ASP:OD1	3:C:96:TYR:OH	1.79	0.98
1:J:60:GLN:O	1:J:64:ASN:OD1	1.81	0.98
1:A:115:LEU:CD2	3:C:90:LEU:HD13	1.94	0.97
1:J:108:TYR:CE1	3:L:83:THR:HB	1.99	0.97
1:J:207:MET:HB2	2:K:135:ASN:HD21	1.21	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ILE:HD12	2:H:82:LEU:HD22	1.44	0.97
2:K:412:PRO:HG3	2:K:450:MET:HE3	1.46	0.97
3:I:8:CYS:SG	3:I:18:TYR:CE2	2.58	0.97
3:I:8:CYS:SG	3:I:18:TYR:CD2	2.58	0.97
1:G:119:ILE:HD11	3:I:93:ILE:HD11	1.48	0.95
3:L:56:GLU:HB2	8:Y:1:NAG:HO3	1.21	0.95
3:L:219:SER:H	3:L:224:THR:HG21	1.29	0.95
2:B:159:SER:O	2:B:163:THR:HG23	1.67	0.95
1:J:148:LYS:HZ1	2:K:425:ASP:CG	1.75	0.94
3:L:56:GLU:CB	8:Y:1:NAG:O3	2.15	0.94
2:E:241:ASP:OD1	2:E:244:THR:OG1	1.85	0.94
1:J:115:LEU:HD13	3:L:90:LEU:HD11	1.50	0.93
2:B:252:ILE:HD11	2:B:454:ILE:CD1	1.97	0.93
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.51	0.92
2:H:310:LEU:HD12	2:H:311:LEU:N	1.85	0.92
2:E:222:SER:OG	2:E:242:MET:N	2.01	0.92
2:H:252:ILE:HD12	2:H:454:ILE:HG23	1.50	0.92
2:B:239:TYR:OH	2:B:287:GLY:O	1.85	0.91
2:B:230:ASP:O	2:B:233:VAL:HG12	1.69	0.91
3:I:12:ASP:CB	3:I:15:PHE:CD1	2.51	0.90
3:C:390:ASN:HD22	3:C:391:ARG:N	1.69	0.90
3:C:372:TRP:HZ3	3:C:379:MET:HE1	1.35	0.90
1:J:115:LEU:HD21	3:L:90:LEU:CD2	2.00	0.90
2:B:252:ILE:CD1	2:B:454:ILE:HD13	1.96	0.89
3:F:323:GLU:N	3:F:323:GLU:OE2	2.05	0.89
2:H:172:LEU:CD2	3:I:113:ILE:HG21	2.02	0.89
2:H:117:TYR:C	2:H:118:MET:HE2	1.98	0.89
3:C:307:HIS:HE1	3:C:342:GLY:H	1.21	0.88
3:L:52:ASN:ND2	8:Y:1:NAG:O5	2.07	0.88
1:A:55:ILE:HD12	2:B:82:LEU:HD22	1.53	0.88
1:A:144:LEU:HD13	2:B:175:LEU:HD11	1.54	0.88
1:J:108:TYR:HH	3:L:84:LEU:N	1.69	0.88
2:H:224:MET:HE2	2:H:237:ARG:HD3	1.56	0.87
2:B:172:LEU:HB3	3:C:113:ILE:HG21	1.57	0.87
2:H:135:ASN:O	2:H:139:VAL:HG23	1.74	0.87
2:B:364:ASN:CG	6:U:1:NAG:C1	2.46	0.87
1:J:184:GLN:HE21	2:K:167:VAL:HG23	1.37	0.87
3:L:219:SER:OG	3:L:224:THR:HG22	1.74	0.86
2:E:312:ILE:HD11	2:E:452:MET:HE3	1.58	0.86
2:K:201:CYS:O	3:L:143:VAL:HG21	1.74	0.86
1:A:55:ILE:HG23	2:B:86:LEU:CD2	2.04	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:LEU:HB2	2:K:189:GLN:HE22	1.41	0.85
2:E:222:SER:HG	2:E:242:MET:H	1.19	0.85
3:I:219:SER:OG	3:I:224:THR:HG22	1.77	0.85
3:L:49:GLN:NE2	8:Y:1:NAG:C8	2.39	0.85
2:H:210:GLU:OE2	2:H:212:GLU:N	2.09	0.84
1:J:69:LEU:HD11	2:K:100:LEU:HD13	1.56	0.84
3:C:253:TRP:C	3:C:254:ASN:HD22	1.85	0.84
1:A:122:LEU:HD11	2:B:153:ILE:HG21	1.60	0.83
1:A:73:LEU:HD23	2:B:104:VAL:HG22	1.60	0.83
3:F:246:LEU:HD11	3:F:248:VAL:HG23	1.59	0.83
2:H:172:LEU:HD21	3:I:113:ILE:CB	2.08	0.83
6:X:2:NAG:H62	6:X:5:NAG:H83	1.60	0.83
6:X:2:NAG:H62	6:X:5:NAG:C8	2.09	0.83
2:E:172:LEU:CD2	3:F:113:ILE:HG23	2.07	0.83
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.61	0.83
2:H:302:LEU:HD22	2:H:454:ILE:CD1	2.09	0.82
2:K:310:LEU:HD12	2:K:311:LEU:N	1.94	0.82
2:B:351:ASN:C	2:B:351:ASN:HD22	1.87	0.82
3:L:52:ASN:HD22	8:Y:1:NAG:C1	1.91	0.82
3:L:379:MET:HA	3:L:379:MET:HE3	1.61	0.82
3:C:194:PHE:CD1	3:C:233:ILE:CD1	2.63	0.82
1:A:59:ASN:HD21	2:B:86:LEU:HD23	1.41	0.82
2:H:252:ILE:HD11	2:H:454:ILE:HD13	1.60	0.82
1:J:207:MET:HB2	2:K:135:ASN:ND2	1.95	0.82
2:K:133:LYS:O	2:K:136:GLU:HG2	1.79	0.82
2:K:343:ASN:HA	2:K:354:MET:SD	2.21	0.81
2:H:122:LYS:HZ3	3:I:60:LEU:HB3	1.46	0.81
1:J:115:LEU:HD13	3:L:90:LEU:CD1	2.11	0.80
2:E:212:GLU:O	2:E:215:ILE:HG22	1.81	0.80
3:C:254:ASN:HD22	3:C:254:ASN:N	1.79	0.80
2:H:310:LEU:HD12	2:H:311:LEU:H	1.46	0.80
2:K:423:THR:OG1	2:K:425:ASP:OD1	1.99	0.80
1:A:123:LYS:HA	1:A:126:VAL:HG12	1.62	0.80
1:G:93:ILE:HG22	1:G:94:LEU:HD12	1.62	0.80
2:K:149:HIS:ND1	2:K:149:HIS:C	2.39	0.80
3:C:215:PHE:CE2	3:C:227:TRP:HB3	2.17	0.80
3:C:179:LEU:HD22	3:C:218:LEU:HD13	1.63	0.79
3:F:234:HIS:ND1	3:F:267:VAL:O	2.11	0.79
3:I:208:TRP:HA	3:I:314:THR:HG21	1.64	0.79
2:B:354:MET:O	2:B:369:ILE:HD13	1.81	0.79
1:D:119:ILE:HD11	3:F:93:ILE:HD13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:252:ILE:HD12	2:K:452:MET:C	2.08	0.79
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.62	0.79
2:H:252:ILE:CD1	2:H:454:ILE:HG23	2.12	0.79
2:K:295:GLY:O	2:K:299:ILE:HG13	1.83	0.79
3:F:46:ILE:O	3:F:50:VAL:HG22	1.83	0.79
1:J:69:LEU:C	1:J:69:LEU:HD13	2.08	0.79
1:A:119:ILE:HD13	3:C:93:ILE:CD1	2.14	0.78
3:C:307:HIS:CE1	3:C:342:GLY:H	2.02	0.78
1:G:58:VAL:HG21	3:I:29:LEU:HD11	1.66	0.78
2:B:179:ILE:HG23	2:B:180:GLN:N	1.98	0.78
1:J:108:TYR:CZ	3:L:83:THR:HB	2.18	0.78
1:J:205:ILE:HG13	2:K:138:VAL:HG11	1.65	0.78
2:E:343:ASN:HA	2:E:354:MET:SD	2.24	0.78
3:I:141:ASP:CG	3:I:143:VAL:HG22	2.07	0.78
1:A:69:LEU:HD12	2:B:100:LEU:HD13	1.67	0.77
2:E:326:TYR:CE1	2:E:353:LEU:HD12	2.19	0.77
2:E:165:LEU:HD21	3:F:107:ILE:HD12	1.64	0.77
1:A:71:ASN:HD22	1:A:72:SER:N	1.82	0.77
3:F:296:GLY:N	3:F:301:ASP:OD2	2.18	0.77
2:B:252:ILE:HD12	2:B:454:ILE:HG23	1.67	0.77
1:J:46:PRO:O	3:L:22:THR:HG21	1.85	0.77
2:E:203:ILE:HG22	2:E:204:PRO:O	1.85	0.77
2:H:78:THR:HG23	1:J:43:TYR:O	1.84	0.76
2:K:210:GLU:OE2	2:K:212:GLU:N	2.14	0.76
2:B:165:LEU:HD11	3:C:107:ILE:CD1	2.15	0.76
3:I:8:CYS:SG	3:I:18:TYR:HD2	2.06	0.76
1:A:55:ILE:CD1	2:B:82:LEU:HD22	2.16	0.76
3:C:246:LEU:HD21	3:C:248:VAL:CG2	2.16	0.76
3:C:364:ASP:OD1	3:C:364:ASP:O	2.04	0.76
3:I:8:CYS:SG	3:I:18:TYR:HE2	2.06	0.76
3:I:281:PHE:CE2	3:I:283:GLY:HA2	2.20	0.76
3:F:246:LEU:HD12	3:F:247:ARG:N	2.00	0.76
3:I:143:VAL:O	3:I:143:VAL:HG23	1.84	0.76
2:K:312:ILE:HB	2:K:324:ALA:HB3	1.67	0.76
1:A:122:LEU:HD11	2:B:153:ILE:CG2	2.16	0.76
1:J:148:LYS:NZ	2:K:425:ASP:CG	2.42	0.76
2:H:434:GLY:O	2:H:436:VAL:HG23	1.85	0.75
3:I:260:ALA:HB2	3:I:286:ALA:HB3	1.66	0.75
1:J:63:THR:HA	1:J:66:ILE:HG22	1.68	0.75
1:G:69:LEU:HD12	2:H:100:LEU:HD13	1.68	0.75
3:L:246:LEU:HD12	3:L:247:ARG:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASN:HD22	1:A:71:ASN:C	1.95	0.75
3:F:90:LEU:HD22	3:F:91:GLU:N	2.02	0.75
2:B:320:ASP:OD2	2:B:320:ASP:N	2.16	0.74
1:A:122:LEU:CD1	2:B:153:ILE:HG21	2.17	0.74
3:C:276:LEU:HD23	3:C:276:LEU:C	2.12	0.74
3:L:77:ASN:HA	3:L:82:ALA:HB2	1.69	0.74
2:H:367:MET:SD	2:H:406:ARG:HD3	2.28	0.74
3:L:213:GLU:O	3:L:232:LYS:NZ	2.20	0.74
3:C:90:LEU:O	3:C:93:ILE:HG22	1.87	0.74
3:I:207:ASN:HD21	3:I:209:ILE:HD13	1.51	0.74
1:J:128:GLU:O	1:J:132:HIS:ND1	2.21	0.74
2:K:439:ASN:HD22	2:K:439:ASN:N	1.86	0.74
2:B:205:VAL:O	2:B:205:VAL:HG12	1.87	0.73
2:B:253:GLN:HE21	2:B:253:GLN:C	1.96	0.73
2:E:181:LYS:O	2:E:185:ASP:HB2	1.87	0.73
3:L:198:LEU:HD13	3:L:199:ASP:N	2.02	0.73
2:K:345:TYR:HB2	2:K:354:MET:HE2	1.70	0.73
1:D:55:ILE:HG23	2:E:86:LEU:HD13	1.69	0.73
2:B:381:ASP:HB2	2:B:393:GLN:HE21	1.54	0.73
3:I:310:MET:HE1	3:I:321:LYS:NZ	2.04	0.73
2:B:169:ARG:HA	3:C:110:LEU:HD21	1.69	0.73
1:J:66:ILE:HG23	1:J:67:ASN:HD22	1.54	0.73
6:X:1:NAG:O3	6:X:2:NAG:H2	1.90	0.72
2:H:172:LEU:CD2	3:I:113:ILE:CG2	2.58	0.72
3:F:309:GLY:O	3:F:310:MET:HE2	1.89	0.72
2:H:59:ALA:HB1	2:H:60:PRO:HD2	1.70	0.72
2:H:201:CYS:O	3:I:143:VAL:HG21	1.88	0.72
3:C:368:ILE:CG2	3:C:377:TYR:O	2.37	0.72
3:F:218:LEU:N	3:F:218:LEU:HD23	2.04	0.72
3:L:314:THR:C	3:L:327:ALA:HB1	2.15	0.72
3:I:219:SER:OG	3:I:224:THR:CG2	2.37	0.72
2:K:364:ASN:CG	6:X:1:NAG:C1	2.61	0.72
3:L:203:ASP:O	3:L:206:LYS:NZ	2.23	0.72
1:D:86:LEU:HD23	3:F:61:ILE:HD12	1.71	0.72
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.72	0.71
2:K:364:ASN:ND2	6:X:1:NAG:C2	2.52	0.71
3:L:334:TRP:HH2	3:L:344:LEU:HD12	1.54	0.71
1:J:129:LYS:O	1:J:133:ILE:HD13	1.91	0.71
2:K:172:LEU:HD22	3:L:113:ILE:HG23	1.70	0.71
3:L:344:LEU:HA	3:L:367:ILE:HG23	1.72	0.71
2:B:364:ASN:HA	2:B:367:MET:HE3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:ILE:HA	1:J:130:VAL:HG12	1.70	0.71
3:L:318:ASP:OD1	3:L:325:ASN:ND2	2.22	0.71
3:C:194:PHE:CD1	3:C:233:ILE:HD13	2.25	0.71
3:C:295:PHE:CE1	3:C:305:THR:HG21	2.25	0.71
1:J:169:LEU:HB2	2:K:189:GLN:NE2	2.06	0.71
2:E:316:ASP:OD2	2:E:320:ASP:N	2.23	0.71
3:L:288:ASP:C	3:L:371:THR:HG21	2.14	0.71
2:E:406:ARG:H	2:E:407:CYS:HA	1.56	0.71
3:F:301:ASP:O	3:F:305:THR:HG23	1.89	0.71
1:J:67:ASN:HA	1:J:70:LYS:HE2	1.73	0.71
1:A:175:LEU:HD12	2:B:426:MET:CE	2.21	0.70
1:G:55:ILE:CD1	2:H:82:LEU:HD22	2.20	0.70
2:K:149:HIS:ND1	2:K:150:GLN:N	2.39	0.70
3:C:194:PHE:CG	3:C:233:ILE:HD13	2.27	0.70
3:I:3:ALA:HB2	3:L:11:LEU:HD12	1.73	0.70
3:F:147:ASP:OD1	3:F:147:ASP:N	2.23	0.70
2:H:302:LEU:HD22	2:H:454:ILE:HD11	1.73	0.70
1:A:175:LEU:HD12	2:B:426:MET:HE1	1.73	0.70
1:G:123:LYS:HA	1:G:126:VAL:HG12	1.72	0.70
3:L:195:GLN:NE2	3:L:197:ARG:HG3	2.06	0.70
2:E:169:ARG:HA	3:F:110:LEU:HD11	1.74	0.70
3:F:169:ILE:HD11	3:F:180:VAL:HG21	1.74	0.70
1:A:129:LYS:O	1:A:133:ILE:HD13	1.91	0.70
3:L:9:CYS:O	3:L:17:SER:HA	1.92	0.70
2:B:101:ASN:OD1	3:C:43:LEU:HD21	1.92	0.69
5:S:4:PRO:HB3	7:W:1:NAG:H62	1.73	0.69
1:A:119:ILE:CD1	3:C:93:ILE:HD13	2.18	0.69
2:B:364:ASN:HD22	6:U:1:NAG:C1	1.96	0.69
3:C:100:ILE:HG23	3:C:101:LEU:HD23	1.74	0.69
2:E:168:LEU:HD22	3:F:110:LEU:CD2	2.21	0.69
2:K:118:MET:O	2:K:122:LYS:HB3	1.93	0.69
3:L:219:SER:OG	3:L:224:THR:CG2	2.38	0.69
1:A:59:ASN:HD21	2:B:86:LEU:CD2	2.05	0.69
1:D:118:ARG:HH22	3:F:90:LEU:HD23	1.56	0.69
2:E:351:ASN:HD21	2:E:354:MET:H	1.39	0.69
1:J:207:MET:O	1:J:211:PRO:HD3	1.93	0.69
3:I:81:ALA:O	3:I:85:LYS:N	2.23	0.69
2:B:154:ASP:CG	3:C:96:TYR:OH	2.34	0.69
3:C:368:ILE:HG22	3:C:377:TYR:O	1.92	0.69
1:J:115:LEU:O	1:J:119:ILE:HG12	1.93	0.69
2:K:179:ILE:HD11	3:L:121:ILE:HG13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:7:SIA:O10	6:U:7:SIA:H7	1.93	0.69
1:A:111:VAL:O	1:A:115:LEU:HD12	1.93	0.69
6:U:10:GAL:H5	6:U:11:SIA:H32	1.74	0.69
3:C:372:TRP:CZ3	3:C:379:MET:HE1	2.23	0.68
3:F:246:LEU:HD11	3:F:248:VAL:CG2	2.23	0.68
3:I:194:PHE:CZ	3:I:384:MET:HE2	2.29	0.68
1:J:71:ASN:HA	1:J:74:PHE:CD2	2.28	0.68
2:B:252:ILE:CD1	2:B:454:ILE:HG23	2.23	0.68
3:C:166:LEU:HB3	3:C:179:LEU:HD21	1.75	0.68
3:C:197:ARG:NH1	3:C:367:ILE:HD11	2.08	0.68
2:H:342:VAL:HG11	2:H:353:LEU:HD13	1.74	0.68
1:J:145:VAL:HG13	1:J:146:ASP:N	2.07	0.68
2:K:212:GLU:O	2:K:215:ILE:HG22	1.92	0.68
2:K:432:ASP:OD1	2:K:443:SER:OG	2.10	0.68
3:C:248:VAL:HG12	3:C:250:LEU:HD11	1.73	0.68
1:A:115:LEU:HD21	3:C:90:LEU:CD1	2.14	0.68
2:E:436:VAL:HG11	2:E:443:SER:HA	1.75	0.68
1:G:115:LEU:HD11	3:I:89:MET:HB2	1.75	0.68
3:F:27:ASP:O	3:F:31:THR:HB	1.94	0.68
2:K:412:PRO:CG	2:K:450:MET:HE3	2.21	0.68
1:A:63:THR:HA	1:A:66:ILE:HG22	1.75	0.68
3:C:291:ASP:O	3:C:302:LYS:NZ	2.27	0.68
3:I:10:ILE:C	3:I:18:TYR:HH	1.92	0.68
3:F:260:ALA:HB2	3:F:286:ALA:CB	2.20	0.67
2:H:172:LEU:HD21	3:I:113:ILE:HB	1.75	0.67
1:J:144:LEU:HD22	2:K:171:ILE:HD11	1.75	0.67
1:J:69:LEU:HD11	2:K:100:LEU:CD1	2.24	0.67
1:J:121:VAL:HG12	1:J:122:LEU:HD22	1.74	0.67
2:K:102:ASN:O	2:K:106:ALA:HB3	1.94	0.67
2:B:406:ARG:N	2:B:407:CYS:HA	2.08	0.67
1:D:55:ILE:CG2	2:E:86:LEU:HD13	2.24	0.67
3:L:310:MET:HE2	3:L:310:MET:HA	1.77	0.67
2:B:408:HIS:O	5:O:1:GLY:N	2.24	0.67
3:C:350:GLN:O	3:C:352:GLY:N	2.21	0.67
1:A:115:LEU:HD11	3:C:90:LEU:HB2	1.76	0.67
3:C:181:TYR:HE1	3:C:220:PRO:O	1.77	0.67
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.77	0.67
1:J:207:MET:HE2	2:K:131:GLN:HE22	1.58	0.67
2:H:135:ASN:HA	2:H:138:VAL:HG12	1.77	0.67
3:I:79:ILE:HA	3:I:82:ALA:HB3	1.76	0.67
2:H:373:MET:HA	2:H:373:MET:HE3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:194:PHE:HZ	3:I:384:MET:HE2	1.59	0.66
3:I:199:ASP:OD1	3:I:201:SER:N	2.27	0.66
2:K:351:ASN:HD21	2:K:354:MET:HG3	1.59	0.66
1:J:106:ASN:ND2	1:J:106:ASN:C	2.54	0.66
2:B:367:MET:SD	2:B:406:ARG:HD3	2.35	0.66
3:C:225:GLU:O	3:C:226:PHE:HB3	1.96	0.66
2:H:360:LEU:HD11	5:S:2:HIS:ND1	2.10	0.66
2:H:361:MET:HB2	7:W:1:NAG:H81	1.78	0.66
3:L:185:ASP:OD2	3:L:189:ASN:N	2.25	0.66
3:I:11:LEU:HD23	3:I:12:ASP:N	2.11	0.66
3:C:276:LEU:HD21	3:C:278:TYR:CD2	2.31	0.66
2:E:406:ARG:N	2:E:407:CYS:HA	2.10	0.66
3:L:242:ILE:HG23	3:L:243:PRO:HD2	1.76	0.66
6:U:5:NAG:H4	6:U:6:GAL:O2	1.95	0.66
3:C:365:ASN:HD22	3:C:365:ASN:H	1.43	0.66
6:U:2:NAG:O6	6:U:5:NAG:H2	1.94	0.66
3:C:194:PHE:CD1	3:C:233:ILE:HD11	2.29	0.66
1:J:51:MET:HG3	3:L:22:THR:HG22	1.77	0.66
1:J:208:LYS:HB2	1:J:209:PRO:HD3	1.78	0.66
3:L:11:LEU:HB3	3:L:18:TYR:CE1	2.31	0.66
3:C:179:LEU:HD23	3:C:180:VAL:N	2.10	0.66
3:C:364:ASP:OD2	4:M:1:GLY:N	2.28	0.66
1:G:119:ILE:HD11	3:I:93:ILE:HD13	1.78	0.66
2:H:253:GLN:HE21	2:H:253:GLN:C	2.03	0.66
1:D:109:ASN:OD1	1:D:110:ARG:N	2.29	0.65
2:H:182:LEU:O	2:H:185:ASP:N	2.29	0.65
2:B:294:LEU:HD12	2:B:295:GLY:H	1.62	0.65
2:H:257:ASP:OD1	2:H:259:SER:OG	2.10	0.65
3:F:27:ASP:O	3:F:31:THR:CB	2.45	0.65
1:G:123:LYS:NZ	2:H:153:ILE:HG21	2.10	0.65
2:K:314:MET:HE2	2:K:450:MET:SD	2.35	0.65
2:B:354:MET:O	2:B:369:ILE:HG23	1.96	0.65
3:C:197:ARG:HD2	3:C:344:LEU:O	1.97	0.65
2:E:340:ILE:HD12	2:E:403:TRP:CZ3	2.31	0.65
2:H:302:LEU:HD22	2:H:454:ILE:HD12	1.77	0.65
3:I:42:SER:O	3:I:46:ILE:HD13	1.96	0.65
3:L:236:ILE:HG21	3:L:386:ILE:HD11	1.77	0.65
3:L:264:MET:O	3:L:278:TYR:HA	1.96	0.65
8:Y:1:NAG:H62	8:Y:2:NAG:H61	1.77	0.65
2:K:276:VAL:HA	2:K:292:TYR:CD2	2.32	0.65
6:U:8:MAN:H4	6:U:9:NAG:N2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:205:VAL:HG22	3:F:218:LEU:HD21	1.78	0.65
3:I:193:VAL:HG22	3:I:385:LYS:HB3	1.77	0.65
3:C:146:HIS:HD2	3:C:167:TYR:CZ	2.14	0.64
1:D:144:LEU:HD21	1:D:182:GLN:HA	1.78	0.64
3:L:169:ILE:CD1	3:L:180:VAL:HG11	2.27	0.64
1:A:134:GLN:NE2	1:A:193:LEU:HD23	2.12	0.64
2:E:296:ASN:O	2:E:299:ILE:N	2.28	0.64
2:H:252:ILE:CD1	2:H:454:ILE:CG2	2.75	0.64
2:E:253:GLN:HE21	2:E:253:GLN:C	2.06	0.64
2:E:227:ILE:HD11	2:E:236:TYR:CE2	2.33	0.64
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.31	0.64
2:H:316:ASP:OD2	2:H:320:ASP:N	2.20	0.64
3:L:246:LEU:HD12	3:L:247:ARG:H	1.63	0.64
3:L:219:SER:N	3:L:224:THR:HG21	2.09	0.64
2:B:171:ILE:HG22	2:B:172:LEU:HD13	1.80	0.64
2:B:205:VAL:HG22	3:C:218:LEU:HG	1.79	0.64
3:C:390:ASN:HD22	3:C:390:ASN:C	2.05	0.64
2:E:160:ASN:O	2:E:164:ASN:N	2.20	0.64
2:H:66:LEU:N	1:J:34:PRO:O	2.31	0.64
1:J:71:ASN:HA	1:J:74:PHE:CE2	2.33	0.64
6:U:1:NAG:O3	6:U:2:NAG:H2	1.98	0.64
7:W:2:NAG:O7	7:W:2:NAG:H3	1.98	0.64
3:L:152:ASP:OD1	3:L:155:ASP:N	2.30	0.64
1:G:97:ASP:O	1:G:101:ALA:CB	2.46	0.64
1:A:104:ARG:HH22	3:C:78:MET:HE2	1.63	0.64
2:B:165:LEU:HD11	3:C:107:ILE:HD12	1.79	0.64
3:C:365:ASN:HD22	3:C:365:ASN:N	1.96	0.64
3:C:174:ALA:HB2	3:C:235:LEU:HD13	1.79	0.63
3:C:340:HIS:ND1	3:C:340:HIS:O	2.30	0.63
2:E:199:VAL:O	3:F:141:ASP:OD2	2.16	0.63
3:L:209:ILE:H	3:L:209:ILE:HD12	1.63	0.63
3:I:189:ASN:HB3	3:I:387:ILE:HD11	1.78	0.63
1:J:69:LEU:HD13	1:J:70:LYS:N	2.13	0.63
1:A:134:GLN:HE22	1:A:193:LEU:HD23	1.63	0.63
1:A:169:LEU:HD23	1:A:171:ARG:HD2	1.80	0.63
3:I:5:ARG:HB2	3:I:11:LEU:HD13	1.80	0.63
2:K:199:VAL:HG23	3:L:141:ASP:HA	1.80	0.63
3:I:12:ASP:OD2	3:I:15:PHE:CD1	2.52	0.63
1:J:132:HIS:CB	3:L:107:ILE:HD11	2.28	0.63
2:K:332:GLN:O	2:K:338:TYR:HA	1.98	0.63
3:L:197:ARG:NH1	3:L:367:ILE:HD11	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:VAL:HG11	2:B:250:THR:HG23	1.81	0.63
3:C:121:ILE:HG22	3:C:122:VAL:N	2.12	0.63
3:C:261:ASP:HB3	3:C:282:ALA:HB3	1.81	0.63
2:E:172:LEU:HD21	3:F:113:ILE:HG23	1.79	0.63
2:E:314:MET:CG	2:E:322:VAL:HG23	2.28	0.63
2:K:436:VAL:HG11	2:K:442:GLY:O	1.99	0.63
2:B:172:LEU:HB3	3:C:113:ILE:CG2	2.27	0.63
1:D:50:ARG:HD3	2:E:59:ALA:HB1	1.81	0.63
2:H:153:ILE:O	2:H:153:ILE:HG22	1.97	0.63
1:G:118:ARG:NH2	3:I:90:LEU:HD21	2.14	0.63
3:I:356:LYS:HA	3:I:359:THR:HG23	1.80	0.63
1:G:184:GLN:HE21	2:H:167:VAL:HG23	1.64	0.62
3:I:242:ILE:HD12	3:I:242:ILE:O	1.98	0.62
1:J:73:LEU:HD13	1:J:73:LEU:C	2.24	0.62
2:B:281:ASP:O	2:B:281:ASP:OD2	2.18	0.62
2:E:226:LEU:HD11	2:E:235:PRO:HB2	1.80	0.62
2:E:385:TRP:O	2:E:387:THR:N	2.29	0.62
1:J:115:LEU:CD2	3:L:90:LEU:CD2	2.66	0.62
2:K:172:LEU:CD2	3:L:113:ILE:HG23	2.29	0.62
3:F:90:LEU:HD22	3:F:90:LEU:C	2.24	0.62
3:C:250:LEU:HB3	3:C:379:MET:HE2	1.82	0.62
3:C:246:LEU:HA	3:C:386:ILE:HG22	1.80	0.62
3:C:349:TYR:CE1	3:C:354:TYR:CE1	2.88	0.62
2:H:87:LEU:HD23	2:H:87:LEU:O	2.00	0.62
1:G:62:PHE:CE1	3:I:36:VAL:HG12	2.35	0.62
1:J:137:GLN:O	1:J:140:VAL:HG22	1.99	0.62
1:J:156:ILE:O	1:J:159:ARG:N	2.32	0.62
2:K:373:MET:SD	2:K:405:ASN:HB2	2.38	0.62
2:K:406:ARG:N	2:K:407:CYS:HA	2.13	0.62
1:D:86:LEU:CD2	3:F:61:ILE:HG21	2.30	0.62
1:D:118:ARG:NH2	3:F:90:LEU:HD23	2.13	0.62
2:E:171:ILE:CG2	2:E:172:LEU:N	2.62	0.62
2:E:205:VAL:HG23	3:F:216:GLY:O	1.98	0.62
3:I:169:ILE:HD11	3:I:180:VAL:HG11	1.80	0.62
2:K:376:SER:O	2:K:401:GLY:HA2	1.99	0.62
3:C:248:VAL:HG12	3:C:250:LEU:CD1	2.29	0.62
3:C:261:ASP:CB	3:C:282:ALA:HB3	2.30	0.61
2:H:171:ILE:HG23	2:H:172:LEU:N	2.15	0.61
2:K:345:TYR:CB	2:K:354:MET:HE2	2.30	0.61
3:C:333:GLY:O	3:C:345:ASN:ND2	2.32	0.61
2:E:340:ILE:HD12	2:E:403:TRP:CE3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:441:LYS:HG3	2:H:447:MET:HE1	1.82	0.61
1:J:154:ILE:HD11	3:L:128:VAL:HG21	1.80	0.61
3:C:295:PHE:HE1	3:C:305:THR:HG21	1.63	0.61
3:C:307:HIS:HE2	3:C:340:HIS:HB2	1.65	0.61
2:E:165:LEU:HD21	3:F:107:ILE:CD1	2.30	0.61
3:F:250:LEU:CD2	3:F:379:MET:HE2	2.23	0.61
2:K:326:TYR:CE1	2:K:353:LEU:HD12	2.35	0.61
3:C:310:MET:HE2	3:C:310:MET:HA	1.82	0.61
1:D:137:GLN:O	1:D:140:VAL:HG22	1.99	0.61
2:B:102:ASN:O	2:B:106:ALA:HB3	2.00	0.61
3:F:124:LEU:O	3:F:128:VAL:HG23	1.99	0.61
2:K:137:ASN:HA	2:K:140:ASN:HD21	1.64	0.61
3:C:240:SER:O	3:C:242:ILE:N	2.28	0.61
2:B:154:ASP:CG	3:C:96:TYR:HH	2.01	0.61
3:F:217:HIS:C	3:F:218:LEU:HD23	2.26	0.61
1:G:185:LEU:HD11	1:G:189:ILE:HD11	1.82	0.61
2:B:172:LEU:HD22	3:C:110:LEU:HD22	1.81	0.61
2:E:176:ARG:O	2:E:179:ILE:HG22	2.01	0.61
3:L:56:GLU:CB	8:Y:1:NAG:HO3	2.03	0.61
1:D:135:LEU:HD22	1:D:136:LEU:CD2	2.24	0.61
3:I:116:SER:O	3:I:119:GLN:N	2.33	0.61
2:K:410:ALA:HB1	2:K:437:TRP:CE3	2.36	0.61
1:J:118:ARG:O	1:J:122:LEU:HD23	2.01	0.61
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.82	0.60
2:E:226:LEU:HD11	2:E:235:PRO:CB	2.30	0.60
3:F:249:GLU:C	3:F:250:LEU:HD12	2.26	0.60
2:H:75:LEU:HD22	1:J:46:PRO:N	2.16	0.60
1:J:63:THR:HA	1:J:66:ILE:CG2	2.31	0.60
2:B:260:VAL:HG21	2:B:291:GLU:O	2.01	0.60
2:E:312:ILE:CD1	2:E:452:MET:HE3	2.31	0.60
3:F:191:TRP:CE3	3:F:385:LYS:HG3	2.35	0.60
1:G:154:ILE:HD11	3:I:128:VAL:CG2	2.19	0.60
3:L:21:THR:HG23	3:L:24:GLY:H	1.66	0.60
3:L:143:VAL:HG23	3:L:143:VAL:O	2.00	0.60
3:L:236:ILE:CG2	3:L:386:ILE:HD11	2.30	0.60
3:C:367:ILE:O	3:C:378:SER:HA	2.01	0.60
2:H:172:LEU:HD21	3:I:113:ILE:HG22	1.78	0.60
3:I:141:ASP:OD2	3:I:143:VAL:HG22	2.01	0.60
3:I:209:ILE:H	3:I:209:ILE:HD12	1.66	0.60
1:A:122:LEU:C	1:A:122:LEU:HD13	2.26	0.60
3:C:359:THR:HG21	3:C:363:TYR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.82	0.60
3:C:191:TRP:CH2	3:C:387:ILE:HG21	2.37	0.60
2:H:406:ARG:N	2:H:407:CYS:HA	2.16	0.60
3:L:153:CYS:HB2	3:L:192:THR:OG1	2.02	0.60
1:A:139:ASN:O	1:A:142:ALA:HB3	2.00	0.60
2:B:75:LEU:HD13	1:D:44:LYS:O	2.00	0.60
2:B:179:ILE:C	2:B:179:ILE:HD13	2.26	0.60
2:B:238:VAL:HG11	2:B:250:THR:CG2	2.32	0.60
3:F:246:LEU:CD1	3:F:248:VAL:HG23	2.30	0.60
2:H:312:ILE:HG23	2:H:451:SER:O	2.02	0.60
3:F:298:ASP:OD2	3:F:300:SER:N	2.35	0.60
2:H:374:PHE:O	2:H:403:TRP:HA	2.02	0.60
2:K:157:VAL:C	2:K:158:ASN:HD22	2.10	0.60
1:G:58:VAL:HG12	1:G:59:ASN:N	2.16	0.60
3:I:387:ILE:HG23	3:I:387:ILE:O	2.02	0.60
2:K:139:VAL:HG21	3:L:79:ILE:HG21	1.84	0.60
2:K:169:ARG:HA	3:L:110:LEU:HD11	1.84	0.60
2:K:199:VAL:HG23	3:L:141:ASP:CA	2.31	0.60
2:E:126:GLN:O	2:E:130:LYS:N	2.31	0.60
1:J:132:HIS:HB3	3:L:107:ILE:HD11	1.83	0.60
3:C:293:PHE:CD1	3:C:370:ALA:HB1	2.37	0.59
3:I:79:ILE:O	3:I:83:THR:N	2.25	0.59
6:V:5:NAG:H62	6:V:6:GAL:C1	2.32	0.59
2:B:179:ILE:CG2	2:B:180:GLN:N	2.64	0.59
2:E:405:ASN:O	2:E:406:ARG:CB	2.50	0.59
2:E:412:PRO:HB3	2:E:450:MET:HE3	1.84	0.59
1:G:166:SER:HB3	2:H:195:THR:OG1	2.02	0.59
3:I:98:ALA:O	3:I:102:THR:HG23	2.02	0.59
2:K:266:TRP:HA	2:K:377:THR:HG21	1.84	0.59
3:L:349:TYR:OH	3:L:365:ASN:ND2	2.32	0.59
3:I:51:GLU:O	3:I:54:THR:OG1	2.16	0.59
2:K:171:ILE:HG23	2:K:172:LEU:N	2.17	0.59
6:X:11:SIA:O10	6:X:11:SIA:H7	2.01	0.59
3:F:197:ARG:NH2	3:F:367:ILE:HD11	2.18	0.59
3:I:227:TRP:HE1	3:I:230:ASN:HD22	1.50	0.59
2:B:210:GLU:OE2	2:B:212:GLU:N	2.31	0.59
2:E:238:VAL:HG13	2:E:239:TYR:O	2.02	0.59
1:G:188:VAL:HG11	2:H:164:ASN:ND2	2.18	0.59
2:K:139:VAL:HG21	3:L:79:ILE:CG2	2.33	0.59
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.03	0.59
2:E:146:LEU:O	2:E:150:GLN:N	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:333:ASN:OD1	2:H:335:ALA:HB3	2.03	0.59
1:A:185:LEU:O	1:A:185:LEU:HD22	2.01	0.59
2:H:211:CYS:SG	2:H:250:THR:HG23	2.43	0.59
3:I:11:LEU:HA	3:I:18:TYR:OH	2.02	0.59
3:C:121:ILE:O	3:C:122:VAL:C	2.46	0.59
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.51	0.59
1:G:30:ASP:O	1:G:32:ASP:N	2.35	0.59
3:I:310:MET:HE1	3:I:321:LYS:HZ1	1.67	0.59
1:G:75:GLU:O	1:G:79:ASN:HB2	2.03	0.59
2:B:351:ASN:HD21	2:B:354:MET:H	1.50	0.59
3:C:126:GLU:O	3:C:129:ALA:HB3	2.03	0.59
1:D:55:ILE:HG23	2:E:86:LEU:CD1	2.32	0.59
1:J:127:ILE:O	1:J:130:VAL:HG12	2.03	0.59
2:B:434:GLY:O	2:B:436:VAL:N	2.36	0.58
3:C:246:LEU:HG	3:C:247:ARG:N	2.17	0.58
3:L:44:GLU:O	3:L:48:HIS:HB2	2.03	0.58
3:L:224:THR:HG23	3:L:224:THR:O	2.02	0.58
3:C:367:ILE:HG21	3:C:382:THR:HG21	1.85	0.58
1:A:169:LEU:HD21	2:B:185:ASP:OD2	2.04	0.58
3:C:206:LYS:HB2	3:C:211:TYR:CE1	2.38	0.58
2:E:171:ILE:HG22	2:E:172:LEU:N	2.19	0.58
1:G:115:LEU:HD11	3:I:89:MET:CB	2.33	0.58
1:A:147:MET:SD	3:C:121:ILE:HD11	2.43	0.58
2:H:176:ARG:NH1	3:I:113:ILE:HG23	2.18	0.58
3:I:84:LEU:HD12	3:I:87:ARG:HD2	1.84	0.58
1:A:119:ILE:O	1:A:122:LEU:HB3	2.04	0.58
2:E:185:ASP:O	2:E:188:ALA:HB3	2.03	0.58
3:I:166:LEU:HD23	3:I:218:LEU:HB3	1.85	0.58
2:K:141:GLU:O	2:K:145:GLU:HB2	2.04	0.58
3:L:84:LEU:HD23	3:L:84:LEU:C	2.28	0.58
2:H:351:ASN:C	2:H:351:ASN:HD22	2.10	0.58
3:L:314:THR:C	3:L:327:ALA:CB	2.76	0.58
3:L:367:ILE:HG21	3:L:382:THR:HG21	1.85	0.58
1:A:115:LEU:CD1	3:C:90:LEU:HB2	2.33	0.58
2:B:257:ASP:N	2:B:257:ASP:OD1	2.35	0.58
3:C:179:LEU:HD23	3:C:180:VAL:H	1.69	0.58
3:F:236:ILE:HG21	3:F:386:ILE:HD11	1.86	0.58
1:J:123:LYS:HA	1:J:126:VAL:HG12	1.85	0.58
1:J:207:MET:HA	1:J:210:VAL:HG12	1.86	0.58
3:C:249:GLU:C	3:C:250:LEU:HD12	2.29	0.58
3:F:393:THR:HG23	3:F:394:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:215:ILE:HD12	2:K:219:GLY:O	2.04	0.58
1:A:71:ASN:C	1:A:71:ASN:ND2	2.62	0.58
2:B:66:LEU:HD12	1:D:31:SER:HB3	1.86	0.58
2:E:270:LYS:NZ	2:E:334:GLU:OE1	2.24	0.58
3:I:336:MET:HE1	3:I:343:HIS:NE2	2.19	0.58
2:B:325:HIS:HB3	2:B:346:ARG:HG2	1.85	0.58
3:C:121:ILE:O	3:C:124:LEU:N	2.37	0.58
1:D:64:ASN:C	1:D:64:ASN:HD22	2.12	0.58
2:E:213:GLU:OE2	2:E:217:LYS:HE3	2.03	0.58
3:F:288:ASP:C	3:F:371:THR:HG21	2.29	0.58
1:G:105:ASP:OD1	3:I:79:ILE:CD1	2.46	0.58
1:G:122:LEU:HB3	1:G:123:LYS:HZ2	1.69	0.58
3:L:169:ILE:HD13	3:L:180:VAL:HG11	1.85	0.58
1:A:91:MET:O	1:A:95:ARG:N	2.37	0.57
2:B:142:TYR:O	2:B:146:LEU:HG	2.04	0.57
2:H:178:LYS:O	2:H:181:LYS:HG3	2.03	0.57
2:H:205:VAL:HG23	3:I:216:GLY:O	2.04	0.57
2:K:351:ASN:C	2:K:351:ASN:HD22	2.11	0.57
1:A:149:ARG:O	1:A:152:VAL:CG1	2.52	0.57
1:J:133:ILE:O	1:J:137:GLN:HG3	2.04	0.57
2:H:415:ARG:O	2:H:434:GLY:HA2	2.05	0.57
1:J:184:GLN:HE21	2:K:167:VAL:CG2	2.14	0.57
2:B:186:VAL:HG12	2:B:187:SER:N	2.18	0.57
1:J:210:VAL:HG21	2:K:131:GLN:HG3	1.86	0.57
3:C:97:GLU:O	3:C:100:ILE:HG22	2.05	0.57
3:C:340:HIS:C	3:C:340:HIS:HD1	2.13	0.57
2:E:394:CYS:SG	2:E:406:ARG:HA	2.45	0.57
3:I:289:ALA:HA	3:I:371:THR:HG23	1.87	0.57
1:J:106:ASN:C	1:J:106:ASN:HD22	2.12	0.57
2:B:205:VAL:O	2:B:205:VAL:CG1	2.53	0.57
1:D:122:LEU:HD12	1:D:123:LYS:HE3	1.86	0.57
3:F:197:ARG:CZ	3:F:367:ILE:HD11	2.35	0.57
1:G:150:LEU:O	1:G:154:ILE:HD13	2.04	0.57
2:H:251:VAL:HG22	2:H:453:LYS:HE2	1.86	0.57
2:B:87:LEU:HD23	2:B:87:LEU:C	2.29	0.57
1:G:108:TYR:CZ	3:I:82:ALA:HB1	2.38	0.57
3:I:334:TRP:HB3	3:I:336:MET:HE2	1.86	0.57
1:J:58:VAL:HG22	1:J:62:PHE:CE1	2.39	0.57
1:A:70:LYS:HG2	2:B:100:LEU:HD21	1.86	0.57
2:B:179:ILE:HG23	2:B:180:GLN:H	1.70	0.57
1:D:111:VAL:HG11	3:F:87:ARG:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:210:GLU:OE1	2:E:213:GLU:N	2.30	0.57
2:E:310:LEU:HD12	2:E:311:LEU:N	2.19	0.57
3:F:189:ASN:HD22	3:F:391:ARG:HE	1.53	0.57
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.85	0.57
1:J:136:LEU:O	1:J:140:VAL:HG13	2.05	0.57
2:K:140:ASN:N	2:K:140:ASN:OD1	2.38	0.57
2:K:312:ILE:HD13	2:K:452:MET:HG2	1.86	0.57
2:K:333:ASN:ND2	2:K:335:ALA:HB3	2.20	0.57
2:B:311:LEU:HD12	2:B:312:ILE:N	2.20	0.57
1:D:94:LEU:HD13	2:E:125:TRP:CD1	2.40	0.57
3:L:143:VAL:O	3:L:143:VAL:CG2	2.53	0.57
2:B:153:ILE:O	2:B:153:ILE:HG22	2.05	0.56
3:I:10:ILE:O	3:I:18:TYR:CZ	2.57	0.56
6:X:8:MAN:C1	6:X:9:NAG:O5	2.53	0.56
2:B:115:PHE:CE2	3:C:50:VAL:HG13	2.40	0.56
2:B:296:ASN:O	2:B:299:ILE:N	2.34	0.56
6:V:8:MAN:H62	6:V:10:GAL:H2	1.86	0.56
6:X:6:GAL:H5	6:X:7:SIA:O6	2.04	0.56
2:B:212:GLU:O	2:B:213:GLU:C	2.48	0.56
3:C:228:LEU:HD11	3:C:232:LYS:HD2	1.85	0.56
2:E:340:ILE:HG22	2:E:373:MET:O	2.05	0.56
3:I:338:LYS:N	3:I:339:CYS:HA	2.20	0.56
1:J:138:LYS:C	1:J:138:LYS:HD3	2.30	0.56
1:J:209:PRO:C	1:J:211:PRO:HD2	2.30	0.56
2:K:209:LYS:HA	2:K:228:GLN:O	2.04	0.56
3:L:228:LEU:HD11	3:L:232:LYS:HD2	1.87	0.56
6:U:8:MAN:C3	6:U:9:NAG:HN2	2.17	0.56
1:A:169:LEU:H	2:B:189:GLN:NE2	2.04	0.56
2:B:253:GLN:C	2:B:253:GLN:NE2	2.62	0.56
3:C:75:LYS:HB3	3:C:78:MET:HE3	1.87	0.56
3:C:246:LEU:HD21	3:C:248:VAL:HG22	1.88	0.56
1:D:94:LEU:HD22	2:E:125:TRP:NE1	2.20	0.56
2:K:151:LEU:HD23	2:K:151:LEU:C	2.30	0.56
3:L:259:THR:O	3:L:286:ALA:HB3	2.06	0.56
2:H:351:ASN:HD21	2:H:354:MET:HG3	1.70	0.56
1:J:69:LEU:CD1	2:K:100:LEU:CD1	2.83	0.56
3:L:78:MET:O	3:L:81:ALA:N	2.38	0.56
6:V:7:SIA:H112	6:V:7:SIA:H7	1.88	0.56
6:V:9:NAG:H83	6:V:9:NAG:O3	2.06	0.56
1:A:70:LYS:HG3	2:B:100:LEU:HD11	1.87	0.56
1:D:169:LEU:HB2	2:E:189:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:LEU:C	2:E:168:LEU:HD23	2.31	0.56
2:E:345:TYR:CG	2:E:351:ASN:HB2	2.40	0.56
3:F:289:ALA:HA	3:F:371:THR:HG23	1.87	0.56
1:G:58:VAL:HG13	1:G:62:PHE:CE2	2.40	0.56
3:I:209:ILE:HD12	3:I:209:ILE:N	2.21	0.56
2:K:101:ASN:OD1	3:L:43:LEU:HD13	2.06	0.56
1:J:162:ARG:HA	1:J:168:ALA:HB2	1.85	0.56
2:B:112:SER:HA	2:B:115:PHE:CD2	2.41	0.56
2:E:402:TRP:CZ3	2:E:412:PRO:HG2	2.41	0.56
3:I:297:ASP:OD1	3:I:297:ASP:N	2.38	0.56
1:J:196:SER:C	1:J:197:ARG:HD3	2.31	0.56
3:L:389:PHE:CD1	3:L:389:PHE:C	2.83	0.56
2:E:402:TRP:CH2	2:E:412:PRO:HG3	2.41	0.56
3:I:143:VAL:O	3:I:143:VAL:CG2	2.53	0.56
3:I:344:LEU:HA	3:I:367:ILE:HG23	1.86	0.56
1:J:108:TYR:CE1	3:L:83:THR:CB	2.84	0.56
2:E:432:ASP:OD1	2:E:443:SER:OG	2.19	0.56
1:J:69:LEU:C	1:J:69:LEU:CD1	2.79	0.56
2:K:185:ASP:O	2:K:188:ALA:HB3	2.05	0.56
2:K:314:MET:HE1	2:K:437:TRP:CE3	2.41	0.56
2:B:104:VAL:HG12	2:B:105:GLU:OE2	2.06	0.55
2:K:171:ILE:CG2	2:K:172:LEU:N	2.69	0.55
3:C:197:ARG:HH11	3:C:367:ILE:HD11	1.70	0.55
1:D:135:LEU:HD23	1:D:135:LEU:C	2.32	0.55
2:E:303:THR:HG22	2:E:308:THR:HG21	1.88	0.55
2:H:252:ILE:HD11	2:H:454:ILE:CG2	2.36	0.55
3:I:7:ASN:O	3:L:9:CYS:HA	2.07	0.55
3:I:11:LEU:HD23	3:I:11:LEU:C	2.32	0.55
1:J:108:TYR:OH	3:L:83:THR:CA	2.53	0.55
3:C:158:ASN:C	3:C:160:GLY:H	2.12	0.55
2:E:437:TRP:O	2:E:438:MET:C	2.49	0.55
2:H:402:TRP:HB3	2:H:404:TYR:CE2	2.41	0.55
1:A:137:GLN:HB3	1:A:189:ILE:HD13	1.89	0.55
2:B:373:MET:HA	2:B:373:MET:HE3	1.89	0.55
3:C:295:PHE:HB3	3:C:375:ARG:NH2	2.22	0.55
1:G:123:LYS:HZ3	2:H:153:ILE:HG21	1.70	0.55
1:J:66:ILE:O	1:J:70:LYS:HG3	2.07	0.55
2:K:415:ARG:O	2:K:434:GLY:HA2	2.06	0.55
1:A:105:ASP:O	1:A:109:ASN:N	2.35	0.55
1:A:184:GLN:NE2	2:B:167:VAL:HG23	2.21	0.55
2:E:227:ILE:HD11	2:E:236:TYR:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:336:MET:HE1	3:F:343:HIS:CD2	2.42	0.55
3:I:179:LEU:HD23	3:I:218:LEU:HD12	1.89	0.55
3:I:387:ILE:O	3:I:387:ILE:CG2	2.55	0.55
6:X:2:NAG:H5	6:X:3:BMA:C2	2.37	0.55
2:B:156:THR:HG22	2:B:157:VAL:N	2.22	0.55
3:C:276:LEU:HD21	3:C:278:TYR:HD2	1.68	0.55
3:I:151:LYS:HE2	3:I:172:LEU:HD13	1.89	0.55
3:F:218:LEU:N	3:F:218:LEU:CD2	2.70	0.55
3:L:189:ASN:HD22	3:L:391:ARG:HE	1.54	0.55
2:H:117:TYR:CD1	2:H:120:LEU:HD12	2.42	0.55
3:L:251:GLU:CD	3:L:381:LYS:NZ	2.65	0.55
3:L:334:TRP:CH2	3:L:344:LEU:HD12	2.40	0.55
3:C:390:ASN:ND2	3:C:391:ARG:N	2.48	0.54
3:F:191:TRP:CH2	3:F:247:ARG:HB2	2.42	0.54
1:A:149:ARG:O	1:A:152:VAL:HG12	2.08	0.54
2:K:340:ILE:HG22	2:K:403:TRP:CD1	2.42	0.54
2:B:123:ASP:O	2:B:127:LYS:N	2.40	0.54
2:B:176:ARG:O	2:B:179:ILE:HG22	2.07	0.54
1:D:169:LEU:HB2	2:E:189:GLN:NE2	2.23	0.54
2:E:182:LEU:O	2:E:185:ASP:N	2.40	0.54
3:F:289:ALA:HB1	3:F:341:ALA:O	2.08	0.54
3:L:79:ILE:HD12	3:L:79:ILE:H	1.73	0.54
3:L:338:LYS:N	3:L:339:CYS:HA	2.21	0.54
2:B:311:LEU:HD11	2:B:313:GLU:HG2	1.88	0.54
3:C:23:CYS:O	3:C:26:ALA:N	2.40	0.54
1:G:46:PRO:O	3:I:22:THR:CB	2.56	0.54
2:B:190:MET:HE1	3:C:130:GLN:HB3	1.89	0.54
2:E:376:SER:OG	2:E:382:ASN:N	2.34	0.54
2:H:315:GLU:HA	2:H:320:ASP:O	2.06	0.54
3:I:310:MET:CE	3:I:321:LYS:HZ1	2.19	0.54
3:L:110:LEU:HA	3:L:113:ILE:CG2	2.36	0.54
3:L:276:LEU:HD23	3:L:277:THR:N	2.22	0.54
2:B:300:SER:HB2	2:B:331:VAL:O	2.07	0.54
3:C:148:ILE:HD12	3:C:161:ALA:HB2	1.90	0.54
2:E:373:MET:HE3	2:E:374:PHE:H	1.71	0.54
3:F:189:ASN:HB3	3:F:387:ILE:HD11	1.90	0.54
3:I:310:MET:HE1	3:I:321:LYS:HZ2	1.72	0.54
1:J:129:LYS:HE2	3:L:104:ASP:HB3	1.89	0.54
3:F:233:ILE:CG2	3:F:267:VAL:HG21	2.37	0.54
1:G:46:PRO:O	3:I:22:THR:OG1	2.21	0.54
3:L:234:HIS:HB2	3:L:267:VAL:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:352:GLY:O	3:L:377:TYR:HA	2.08	0.54
3:C:364:ASP:OD2	3:C:375:ARG:HG3	2.07	0.54
1:D:89:ASN:O	1:D:93:ILE:HG23	2.06	0.54
2:H:59:ALA:HB1	2:H:60:PRO:CD	2.36	0.54
2:H:398:ASP:OD1	5:S:3:ARG:NH1	2.40	0.54
3:I:253:TRP:C	3:I:254:ASN:HD22	2.16	0.54
1:J:132:HIS:CG	3:L:107:ILE:HD11	2.43	0.54
1:J:140:VAL:HG23	1:J:141:ARG:N	2.23	0.54
1:A:181:GLN:HB3	2:B:171:ILE:HD11	1.90	0.54
2:B:299:ILE:O	2:B:303:THR:HG23	2.07	0.54
3:C:304:PHE:O	3:C:337:ASN:CG	2.51	0.54
2:E:312:ILE:HD11	2:E:452:MET:CE	2.35	0.54
2:E:424:TRP:CH2	6:V:7:SIA:H31	2.43	0.54
3:F:246:LEU:HD12	3:F:246:LEU:C	2.33	0.54
3:I:238:THR:HG22	3:I:266:LYS:HG3	1.88	0.54
2:K:135:ASN:O	2:K:139:VAL:HG23	2.08	0.54
3:I:288:ASP:C	3:I:371:THR:HG21	2.33	0.54
1:J:115:LEU:CD1	3:L:90:LEU:HD11	2.30	0.54
2:K:252:ILE:HG21	2:K:299:ILE:HG23	1.89	0.54
1:A:94:LEU:HD13	2:B:125:TRP:CZ3	2.43	0.53
3:C:349:TYR:CE1	3:C:354:TYR:CD1	2.96	0.53
2:E:275:ASN:N	2:E:291:GLU:O	2.41	0.53
3:L:152:ASP:OD1	3:L:154:GLN:N	2.40	0.53
6:U:7:SIA:H7	6:U:7:SIA:C10	2.39	0.53
1:A:188:VAL:CG1	2:B:164:ASN:ND2	2.71	0.53
1:G:73:LEU:O	1:G:73:LEU:HD22	2.08	0.53
1:J:65:ARG:NH2	3:L:44:GLU:OE2	2.38	0.53
1:A:135:LEU:CD2	1:A:136:LEU:HD22	2.38	0.53
2:E:351:ASN:C	2:E:351:ASN:HD22	2.16	0.53
2:E:405:ASN:O	2:E:406:ARG:HB3	2.07	0.53
1:J:127:ILE:O	1:J:131:GLN:N	2.34	0.53
3:L:150:GLY:HA3	3:L:155:ASP:OD1	2.09	0.53
6:X:2:NAG:H5	6:X:3:BMA:H2	1.90	0.53
2:B:317:TRP:HB2	2:B:445:TYR:OH	2.08	0.53
2:E:135:ASN:HA	2:E:138:VAL:HG12	1.91	0.53
1:G:166:SER:CB	2:H:195:THR:OG1	2.56	0.53
2:H:326:TYR:OH	2:H:351:ASN:ND2	2.41	0.53
2:K:310:LEU:HD22	2:K:329:PHE:CE2	2.43	0.53
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.90	0.53
2:E:435:VAL:O	2:E:435:VAL:HG12	2.09	0.53
2:H:118:MET:O	2:H:123:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:191:TRP:CE3	3:I:385:LYS:HD2	2.43	0.53
3:I:249:GLU:HB2	3:I:383:THR:HG23	1.89	0.53
1:J:145:VAL:CG1	1:J:146:ASP:N	2.71	0.53
1:J:210:VAL:N	1:J:211:PRO:CD	2.72	0.53
2:K:252:ILE:HG21	2:K:299:ILE:CG2	2.37	0.53
3:L:23:CYS:O	3:L:26:ALA:N	2.37	0.53
3:C:217:HIS:O	3:C:224:THR:CG2	2.56	0.53
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.90	0.53
3:F:193:VAL:CG1	3:F:195:GLN:O	2.56	0.53
3:F:233:ILE:HG22	3:F:267:VAL:HG21	1.91	0.53
3:F:314:THR:OG1	3:F:316:ASP:OD1	2.26	0.53
1:G:97:ASP:O	1:G:101:ALA:HB3	2.08	0.53
3:C:340:HIS:ND1	3:C:340:HIS:C	2.67	0.53
3:L:120:LYS:O	3:L:123:ASN:HB2	2.09	0.53
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.90	0.53
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.91	0.53
3:L:229:GLY:O	3:L:233:ILE:HG13	2.08	0.53
2:E:369:ILE:H	2:E:405:ASN:HD22	1.55	0.53
2:H:314:MET:HE2	2:H:450:MET:SD	2.49	0.53
1:J:138:LYS:C	1:J:138:LYS:CD	2.82	0.53
2:K:137:ASN:HA	2:K:140:ASN:ND2	2.24	0.53
3:L:207:ASN:C	3:L:207:ASN:OD1	2.52	0.53
2:B:178:LYS:O	2:B:179:ILE:C	2.52	0.53
3:C:354:TYR:CE2	3:C:376:TRP:HA	2.44	0.53
2:E:421:GLN:HE21	2:E:421:GLN:HA	1.74	0.53
2:H:115:PHE:CZ	3:I:54:THR:HG22	2.43	0.53
2:B:101:ASN:CG	3:C:43:LEU:HD11	2.34	0.52
2:B:373:MET:CG	2:B:405:ASN:HB2	2.35	0.52
3:C:251:GLU:HA	3:C:256:ARG:O	2.09	0.52
3:I:191:TRP:CE3	3:I:387:ILE:HB	2.44	0.52
4:M:3:ARG:HG3	4:M:4:PRO:O	2.08	0.52
6:X:8:MAN:H4	6:X:9:NAG:HN2	1.72	0.52
3:C:46:ILE:HG22	3:C:46:ILE:O	2.10	0.52
3:C:191:TRP:CZ3	3:C:387:ILE:CG2	2.92	0.52
3:F:189:ASN:ND2	3:F:391:ARG:HE	2.07	0.52
3:L:167:TYR:O	3:L:179:LEU:HD12	2.09	0.52
2:B:187:SER:OG	3:C:127:LYS:NZ	2.39	0.52
2:E:168:LEU:HD22	3:F:110:LEU:HD23	1.90	0.52
3:F:285:ASP:OD1	3:F:285:ASP:N	2.26	0.52
2:K:354:MET:O	2:K:369:ILE:HD13	2.10	0.52
1:A:73:LEU:HD22	1:A:73:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:GLU:OE2	2:B:210:GLU:C	2.52	0.52
2:K:280:THR:HG22	2:K:281:ASP:H	1.75	0.52
3:L:195:GLN:OE1	3:L:384:MET:HG3	2.09	0.52
2:B:342:VAL:C	2:B:343:ASN:HD22	2.17	0.52
2:E:172:LEU:HD23	3:F:113:ILE:HG23	1.88	0.52
2:E:280:THR:HG22	2:E:281:ASP:OD2	2.08	0.52
3:F:268:GLY:N	3:F:275:ARG:O	2.39	0.52
3:F:355:SER:O	3:F:359:THR:HG23	2.10	0.52
2:H:75:LEU:HD13	1:J:44:LYS:O	2.10	0.52
2:K:325:HIS:O	2:K:345:TYR:HA	2.09	0.52
3:L:90:LEU:HD23	3:L:90:LEU:C	2.35	0.52
3:L:246:LEU:HA	3:L:386:ILE:HG22	1.91	0.52
1:A:55:ILE:HG12	2:B:86:LEU:HD11	1.91	0.52
3:F:340:HIS:ND1	3:F:343:HIS:HB2	2.24	0.52
1:G:59:ASN:O	1:G:63:THR:HG23	2.09	0.52
2:H:226:LEU:HD12	2:H:236:TYR:C	2.35	0.52
2:H:342:VAL:HG23	2:H:354:MET:HG2	1.91	0.52
2:K:136:GLU:HB2	3:L:79:ILE:HD11	1.92	0.52
2:B:317:TRP:CD1	2:B:420:GLY:HA3	2.45	0.52
3:I:209:ILE:H	3:I:209:ILE:CD1	2.23	0.52
1:J:59:ASN:OD1	2:K:93:ILE:HD12	2.10	0.52
6:V:2:NAG:H5	6:V:3:BMA:O2	2.10	0.52
2:B:203:ILE:HD12	2:B:203:ILE:N	2.25	0.52
3:F:209:ILE:H	3:F:209:ILE:HD12	1.74	0.52
2:H:174:ASN:O	2:H:177:SER:OG	2.24	0.52
2:K:200:SER:HA	3:L:141:ASP:OD2	2.10	0.52
3:L:389:PHE:C	3:L:389:PHE:HD1	2.16	0.52
6:V:11:SIA:H7	6:V:11:SIA:C10	2.39	0.52
2:B:94:ARG:O	2:B:97:VAL:HG12	2.09	0.52
1:D:48:GLY:HA2	2:E:82:LEU:HD11	1.92	0.52
2:E:264:ARG:HG2	3:F:136:GLN:HE22	1.73	0.52
3:I:325:ASN:C	3:I:325:ASN:HD22	2.18	0.52
3:L:288:ASP:O	3:L:371:THR:HG21	2.09	0.52
2:E:82:LEU:CB	3:F:25:ILE:HD13	2.40	0.51
2:E:251:VAL:HB	2:E:292:TYR:OH	2.10	0.51
2:E:260:VAL:HG23	2:E:291:GLU:HB2	1.92	0.51
3:F:268:GLY:O	3:F:274:TYR:HA	2.10	0.51
3:L:261:ASP:OD2	3:L:261:ASP:N	2.43	0.51
3:L:356:LYS:HG2	3:L:362:GLY:O	2.09	0.51
2:B:171:ILE:CG2	2:B:172:LEU:N	2.74	0.51
1:D:181:GLN:HB3	2:E:171:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:110:LEU:HD12	3:F:113:ILE:HG21	1.91	0.51
3:F:156:ILE:HG22	3:F:157:ALA:N	2.25	0.51
3:I:115:ASN:HD22	3:I:115:ASN:C	2.18	0.51
3:I:233:ILE:HA	3:I:236:ILE:HD12	1.92	0.51
2:K:252:ILE:HD11	2:K:454:ILE:HG23	1.93	0.51
6:U:6:GAL:H4	6:U:7:SIA:O6	2.10	0.51
6:V:6:GAL:H4	6:V:7:SIA:O4	2.11	0.51
1:A:48:GLY:CA	2:B:82:LEU:HD11	2.40	0.51
1:A:147:MET:O	1:A:148:LYS:C	2.53	0.51
1:D:86:LEU:HD23	3:F:61:ILE:HG21	1.91	0.51
2:E:252:ILE:HG21	2:E:299:ILE:HG23	1.92	0.51
2:E:340:ILE:CD1	2:E:403:TRP:CE3	2.93	0.51
2:H:432:ASP:OD1	2:H:443:SER:OG	2.28	0.51
3:I:179:LEU:HD23	3:I:218:LEU:CD1	2.39	0.51
2:K:302:LEU:HD22	2:K:454:ILE:CD1	2.22	0.51
2:B:150:GLN:O	2:B:153:ILE:N	2.43	0.51
2:E:82:LEU:HB2	3:F:25:ILE:HD13	1.92	0.51
2:E:168:LEU:HD22	3:F:110:LEU:HD21	1.93	0.51
2:H:99:GLU:O	2:H:103:ASN:N	2.43	0.51
3:I:196:LYS:HG3	3:I:197:ARG:N	2.25	0.51
1:J:63:THR:CA	1:J:66:ILE:HG22	2.37	0.51
2:K:314:MET:CG	2:K:322:VAL:HG23	2.40	0.51
1:A:175:LEU:HD23	1:A:176:LYS:H	1.76	0.51
2:B:360:LEU:HD22	5:O:2:HIS:CE1	2.46	0.51
1:D:63:THR:CG2	2:E:93:ILE:HD11	2.40	0.51
1:D:69:LEU:HD13	3:F:47:LEU:CD1	2.41	0.51
3:F:141:ASP:OD2	3:F:143:VAL:HG13	2.10	0.51
2:H:252:ILE:HD11	2:H:454:ILE:CD1	2.35	0.51
1:A:70:LYS:CG	2:B:100:LEU:HD11	2.40	0.51
2:B:441:LYS:HB3	2:B:445:TYR:HB3	1.92	0.51
2:H:140:ASN:C	2:H:140:ASN:HD22	2.19	0.51
2:H:397:GLU:HG3	2:H:431:THR:HG21	1.93	0.51
2:H:405:ASN:O	2:H:406:ARG:HB3	2.09	0.51
3:L:81:ALA:O	3:L:85:LYS:HG2	2.10	0.51
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.46	0.51
2:B:146:LEU:HA	2:B:149:HIS:HB3	1.93	0.51
2:B:340:ILE:HB	2:B:403:TRP:CD1	2.45	0.51
3:C:207:ASN:OD1	3:C:209:ILE:N	2.44	0.51
1:D:86:LEU:HD23	3:F:61:ILE:CD1	2.40	0.51
1:G:52:LYS:HB2	2:H:82:LEU:HD21	1.92	0.51
3:L:124:LEU:O	3:L:128:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:MET:HE2	2:B:118:MET:HA	1.93	0.51
1:G:184:GLN:NE2	2:H:167:VAL:HG23	2.26	0.51
2:H:122:LYS:NZ	3:I:60:LEU:HB3	2.23	0.51
2:H:296:ASN:O	2:H:299:ILE:N	2.44	0.51
3:I:238:THR:O	3:I:238:THR:OG1	2.28	0.51
3:I:365:ASN:HD22	3:I:365:ASN:H	1.57	0.51
1:J:207:MET:HE1	2:K:131:GLN:OE1	2.10	0.51
2:K:257:ASP:O	2:K:291:GLU:OE2	2.29	0.51
1:A:48:GLY:O	1:A:52:LYS:N	2.28	0.51
1:A:104:ARG:HD3	3:C:79:ILE:HG21	1.92	0.51
1:A:175:LEU:HD12	2:B:426:MET:HE2	1.93	0.51
2:B:78:THR:HG23	1:D:43:TYR:O	2.11	0.51
2:B:364:ASN:ND2	6:U:1:NAG:C2	2.66	0.51
3:C:356:LYS:HG3	3:C:362:GLY:O	2.11	0.51
2:E:314:MET:HA	2:E:449:LYS:O	2.11	0.51
3:I:5:ARG:CB	3:I:11:LEU:HD13	2.40	0.51
1:J:70:LYS:HB3	1:J:74:PHE:CZ	2.46	0.51
2:K:104:VAL:HG11	3:L:47:LEU:HB2	1.93	0.51
3:L:172:LEU:HB2	3:L:239:GLN:HB2	1.92	0.50
6:X:11:SIA:H7	6:X:11:SIA:C10	2.41	0.50
1:A:111:VAL:O	1:A:115:LEU:CD1	2.60	0.50
1:A:136:LEU:O	1:A:140:VAL:HG13	2.10	0.50
2:B:104:VAL:O	2:B:108:SER:HB3	2.11	0.50
3:C:132:GLU:C	3:C:134:GLN:H	2.19	0.50
3:C:228:LEU:CD1	3:C:232:LYS:HD2	2.41	0.50
2:E:226:LEU:HD12	2:E:236:TYR:C	2.37	0.50
1:G:64:ASN:OD1	1:G:65:ARG:N	2.44	0.50
3:I:240:SER:O	3:I:241:ALA:C	2.54	0.50
2:K:145:GLU:HA	2:K:145:GLU:OE2	2.12	0.50
2:B:171:ILE:HG22	2:B:172:LEU:N	2.26	0.50
2:B:345:TYR:C	2:B:345:TYR:CD2	2.90	0.50
3:C:246:LEU:HD12	3:C:386:ILE:HG22	1.93	0.50
3:I:272:ASP:OD1	3:I:275:ARG:NH1	2.45	0.50
1:J:167:ARG:HB3	2:K:192:TYR:HB3	1.92	0.50
2:K:169:ARG:HE	3:L:110:LEU:HD21	1.76	0.50
2:K:412:PRO:HG3	2:K:450:MET:CE	2.31	0.50
3:I:27:ASP:O	3:I:31:THR:CG2	2.43	0.50
1:A:94:LEU:HD22	2:B:125:TRP:CZ3	2.47	0.50
2:B:223:GLU:HG2	2:B:225:TYR:CE2	2.46	0.50
3:C:69:ASN:O	3:C:71:ASP:N	2.44	0.50
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:CYS:CB	2:E:242:MET:HE2	2.41	0.50
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.46	0.50
1:G:147:MET:SD	3:I:121:ILE:HD11	2.52	0.50
3:I:251:GLU:HB2	3:I:257:THR:HG22	1.94	0.50
3:L:219:SER:CB	3:L:224:THR:HG21	2.42	0.50
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.92	0.50
1:D:115:LEU:HD13	3:F:86:SER:HA	1.93	0.50
2:E:253:GLN:C	2:E:253:GLN:NE2	2.69	0.50
3:F:89:MET:HE3	3:F:93:ILE:CG1	2.41	0.50
3:F:224:THR:HG23	3:F:224:THR:O	2.12	0.50
1:J:108:TYR:HH	3:L:84:LEU:H	1.55	0.50
2:K:230:ASP:O	2:K:233:VAL:HG12	2.11	0.50
2:K:252:ILE:HD12	2:K:452:MET:O	2.12	0.50
2:K:257:ASP:OD1	2:K:259:SER:CB	2.60	0.50
6:X:2:NAG:C6	6:X:5:NAG:H83	2.36	0.50
1:A:48:GLY:HA2	2:B:82:LEU:HD11	1.94	0.50
2:B:329:PHE:C	2:B:330:THR:CG2	2.85	0.50
2:E:360:LEU:HD13	5:P:2:HIS:ND1	2.26	0.50
2:K:257:ASP:OD1	2:K:259:SER:OG	2.23	0.50
2:E:295:GLY:O	2:E:298:LYS:HB2	2.12	0.50
3:F:330:ASP:OD2	3:F:340:HIS:NE2	2.44	0.50
3:I:5:ARG:HG2	3:I:11:LEU:HB3	1.93	0.50
3:I:195:GLN:OE1	3:I:382:THR:HG22	2.11	0.50
3:I:250:LEU:N	3:I:250:LEU:CD1	2.74	0.50
2:B:284:ASN:H	2:B:284:ASN:HD22	1.59	0.50
1:D:111:VAL:HG11	3:F:87:ARG:CB	2.42	0.50
3:F:69:ASN:HB2	3:F:70:PRO:HD2	1.93	0.50
3:F:80:ASP:O	3:F:82:ALA:N	2.45	0.50
3:F:218:LEU:C	3:F:224:THR:HG21	2.37	0.50
3:I:252:ASP:HB2	3:I:377:TYR:OH	2.12	0.50
3:I:356:LYS:HA	3:I:359:THR:CG2	2.41	0.50
1:J:208:LYS:HB2	1:J:209:PRO:CD	2.41	0.50
1:J:210:VAL:N	1:J:211:PRO:HD2	2.27	0.50
3:L:152:ASP:OD1	3:L:152:ASP:C	2.54	0.50
1:A:59:ASN:ND2	2:B:86:LEU:HD23	2.20	0.49
2:B:87:LEU:HD23	2:B:87:LEU:O	2.12	0.49
2:B:351:ASN:C	2:B:351:ASN:ND2	2.56	0.49
3:C:262:TYR:CE2	3:C:290:PHE:HB2	2.47	0.49
1:D:63:THR:HG23	2:E:93:ILE:HD11	1.94	0.49
1:D:143:GLN:NE2	3:F:118:ASN:OD1	2.45	0.49
3:I:3:ALA:HB2	3:L:11:LEU:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:2:HIS:CD2	5:T:4:PRO:HD3	2.47	0.49
2:B:171:ILE:HG22	2:B:172:LEU:CD1	2.42	0.49
2:H:326:TYR:CE1	2:H:353:LEU:HD12	2.48	0.49
2:K:351:ASN:ND2	2:K:354:MET:H	2.09	0.49
3:L:291:ASP:OD1	3:L:302:LYS:NZ	2.44	0.49
3:L:297:ASP:N	3:L:297:ASP:OD1	2.45	0.49
1:A:136:LEU:HD13	1:A:139:ASN:HD22	1.76	0.49
3:C:276:LEU:HD23	3:C:276:LEU:O	2.13	0.49
3:L:194:PHE:CD1	3:L:233:ILE:HD13	2.47	0.49
3:C:97:GLU:C	3:C:100:ILE:HG22	2.36	0.49
3:C:289:ALA:O	3:C:292:GLY:N	2.35	0.49
2:E:314:MET:HG3	2:E:322:VAL:HG23	1.95	0.49
3:L:193:VAL:O	3:L:226:PHE:HZ	1.95	0.49
3:L:248:VAL:HG12	3:L:249:GLU:N	2.27	0.49
3:F:166:LEU:HD11	3:F:220:PRO:N	2.28	0.49
2:H:402:TRP:CE3	2:H:413:ASN:ND2	2.81	0.49
3:I:208:TRP:CE3	3:I:317:ASN:HB3	2.48	0.49
1:J:115:LEU:CD1	3:L:90:LEU:HD21	2.42	0.49
3:L:295:PHE:HE1	3:L:305:THR:HG21	1.77	0.49
2:E:257:ASP:OD1	2:E:259:SER:OG	2.24	0.49
3:I:281:PHE:CD2	3:I:283:GLY:HA2	2.46	0.49
1:J:93:ILE:HD12	1:J:94:LEU:HD23	1.93	0.49
2:K:215:ILE:CD1	2:K:242:MET:HB3	2.42	0.49
2:K:255:ARG:NH1	2:K:412:PRO:O	2.43	0.49
3:L:264:MET:SD	3:L:264:MET:N	2.86	0.49
2:B:385:TRP:CD1	2:B:406:ARG:HG3	2.48	0.49
1:D:86:LEU:HD21	3:F:61:ILE:HG21	1.93	0.49
2:E:108:SER:HA	2:E:111:SER:HB3	1.95	0.49
2:E:205:VAL:HG22	3:F:218:LEU:CD2	2.43	0.49
3:F:375:ARG:HG3	3:F:376:TRP:N	2.27	0.49
1:G:97:ASP:O	1:G:101:ALA:HB2	2.13	0.49
3:I:12:ASP:CG	3:I:15:PHE:CD1	2.90	0.49
1:J:127:ILE:CA	1:J:130:VAL:HG12	2.39	0.49
3:L:197:ARG:O	3:L:381:LYS:HA	2.13	0.49
3:C:207:ASN:OD1	3:C:207:ASN:C	2.56	0.49
3:C:258:SER:HB2	3:C:286:ALA:HB2	1.94	0.49
1:D:115:LEU:HD13	3:F:86:SER:HB2	1.94	0.49
2:E:212:GLU:O	2:E:213:GLU:C	2.56	0.49
2:H:210:GLU:OE1	2:H:213:GLU:N	2.45	0.49
2:H:329:PHE:HE2	2:H:454:ILE:HG21	1.77	0.49
1:J:152:VAL:HG11	2:K:426:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:225:GLU:O	3:L:226:PHE:HB3	2.12	0.49
1:A:133:ILE:HD11	3:C:107:ILE:CG1	2.42	0.49
1:A:200:GLN:NE2	2:B:149:HIS:NE2	2.61	0.49
2:E:178:LYS:O	2:E:181:LYS:HG3	2.13	0.49
2:E:439:ASN:HD22	2:E:439:ASN:H	1.59	0.49
2:H:337:LYS:O	2:H:338:TYR:C	2.55	0.49
1:J:129:LYS:CE	3:L:104:ASP:HB3	2.43	0.49
3:L:367:ILE:O	3:L:378:SER:HA	2.13	0.49
2:B:179:ILE:CG2	2:B:180:GLN:H	2.26	0.49
2:E:179:ILE:HD12	3:F:120:LYS:HD3	1.95	0.49
3:F:90:LEU:C	3:F:90:LEU:CD2	2.85	0.49
2:H:308:THR:CG2	2:H:454:ILE:HB	2.43	0.49
2:H:326:TYR:CZ	2:H:353:LEU:HD12	2.48	0.49
3:C:301:ASP:O	3:C:305:THR:OG1	2.30	0.48
1:D:149:ARG:NE	2:E:427:ALA:O	2.45	0.48
2:E:161:ILE:HG21	3:F:103:HIS:CG	2.47	0.48
2:E:330:THR:O	2:E:331:VAL:HG22	2.12	0.48
2:H:343:ASN:HA	2:H:354:MET:SD	2.53	0.48
2:K:95:ASN:C	2:K:95:ASN:ND2	2.70	0.48
2:K:410:ALA:CB	2:K:437:TRP:CE3	2.96	0.48
3:L:214:GLY:HA3	3:L:228:LEU:O	2.13	0.48
2:E:199:VAL:HG23	3:F:141:ASP:CA	2.42	0.48
3:F:166:LEU:CD2	3:F:218:LEU:HB2	2.43	0.48
3:F:191:TRP:CE3	3:F:385:LYS:CG	2.96	0.48
1:G:46:PRO:O	3:I:22:THR:HG21	2.13	0.48
1:G:116:ARG:HD3	2:H:142:TYR:OH	2.13	0.48
2:H:314:MET:HE1	2:H:437:TRP:CE3	2.48	0.48
1:J:145:VAL:HG13	1:J:146:ASP:H	1.76	0.48
1:A:46:PRO:O	3:C:22:THR:HG21	2.13	0.48
1:D:65:ARG:O	1:D:69:LEU:HD23	2.13	0.48
3:F:352:GLY:O	3:F:354:TYR:HD2	1.95	0.48
3:I:305:THR:HB	3:I:341:ALA:HB2	1.96	0.48
3:I:355:SER:O	3:I:359:THR:HG23	2.14	0.48
2:K:122:LYS:O	2:K:125:TRP:HB3	2.13	0.48
3:C:288:ASP:O	3:C:289:ALA:C	2.54	0.48
2:E:152:TYR:O	2:E:156:THR:HG22	2.13	0.48
1:J:63:THR:C	1:J:66:ILE:HG22	2.37	0.48
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.95	0.48
3:L:46:ILE:HG22	3:L:46:ILE:O	2.12	0.48
2:B:252:ILE:HD11	2:B:454:ILE:CG2	2.43	0.48
3:C:246:LEU:HD12	3:C:386:ILE:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:292:GLY:HA2	3:C:341:ALA:CB	2.43	0.48
2:E:321:LYS:O	2:E:322:VAL:HG13	2.13	0.48
3:F:169:ILE:HD11	3:F:180:VAL:CG2	2.41	0.48
2:K:144:SER:HB3	2:K:148:LYS:HZ1	1.79	0.48
6:U:2:NAG:H5	6:U:3:BMA:C2	2.43	0.48
6:V:7:SIA:O1A	6:V:7:SIA:H6	2.13	0.48
2:B:281:ASP:O	2:B:283:LYS:NZ	2.46	0.48
2:B:405:ASN:CG	2:B:405:ASN:O	2.55	0.48
3:C:246:LEU:CD2	3:C:248:VAL:CG2	2.89	0.48
3:C:387:ILE:O	3:C:387:ILE:HG23	2.13	0.48
2:E:205:VAL:HG21	3:F:215:PHE:O	2.14	0.48
2:E:373:MET:HE2	2:E:404:TYR:O	2.14	0.48
2:E:422:TYR:CE1	2:E:444:TRP:HA	2.48	0.48
2:H:314:MET:HE2	2:H:450:MET:HE1	1.95	0.48
3:I:365:ASN:HD22	3:I:365:ASN:N	2.12	0.48
2:K:148:LYS:HD3	2:K:148:LYS:N	2.28	0.48
3:L:172:LEU:H	3:L:239:GLN:HE21	1.61	0.48
3:L:300:SER:O	3:L:301:ASP:C	2.56	0.48
6:U:2:NAG:H3	6:U:3:BMA:O2	2.13	0.48
3:C:347:VAL:CG2	3:C:349:TYR:CE1	2.97	0.48
2:E:330:THR:C	2:E:331:VAL:CG2	2.87	0.48
2:E:351:ASN:ND2	2:E:351:ASN:C	2.68	0.48
3:F:327:ALA:HB1	3:F:332:SER:O	2.13	0.48
2:H:224:MET:CE	2:H:237:ARG:HD3	2.36	0.48
3:I:236:ILE:HA	3:I:239:GLN:HE21	1.78	0.48
2:K:310:LEU:HD12	2:K:310:LEU:C	2.38	0.48
3:L:259:THR:N	3:L:286:ALA:HB2	2.29	0.48
3:L:307:HIS:CE1	3:L:341:ALA:H	2.31	0.48
1:A:165:CYS:HA	2:B:196:PRO:HA	1.96	0.48
1:A:185:LEU:HD11	1:A:189:ILE:HD11	1.95	0.48
2:B:352:ALA:HB1	2:B:409:ALA:HB3	1.95	0.48
3:C:300:SER:O	3:C:301:ASP:C	2.56	0.48
1:J:169:LEU:HD22	1:J:171:ARG:HG2	1.96	0.48
2:K:212:GLU:HA	2:K:215:ILE:HG22	1.95	0.48
2:K:300:SER:OG	2:K:301:GLN:N	2.46	0.48
2:B:115:PHE:HE2	3:C:50:VAL:HG13	1.78	0.48
2:E:266:TRP:CD1	2:E:380:ARG:NH2	2.82	0.48
3:I:15:PHE:O	3:L:24:GLY:HA3	2.14	0.48
1:J:62:PHE:O	1:J:66:ILE:HB	2.13	0.48
2:K:353:LEU:O	2:K:369:ILE:HG23	2.14	0.48
3:L:110:LEU:HA	3:L:113:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:382:THR:C	3:L:383:THR:HG22	2.39	0.48
6:U:8:MAN:O5	6:U:9:NAG:H3	2.13	0.48
6:V:3:BMA:H3	6:V:4:MAN:O2	2.13	0.48
1:A:175:LEU:CD1	2:B:426:MET:HE1	2.42	0.48
2:B:101:ASN:OD1	3:C:43:LEU:CD2	2.61	0.48
2:B:125:TRP:O	2:B:129:GLN:HB3	2.13	0.48
3:C:252:ASP:HB2	3:C:373:LYS:NZ	2.29	0.48
1:D:100:SER:HB3	3:F:80:ASP:CG	2.39	0.48
2:E:322:VAL:HG12	2:E:348:THR:HB	1.95	0.48
2:E:370:HIS:O	2:E:373:MET:N	2.36	0.48
2:E:424:TRP:CZ2	6:V:7:SIA:H31	2.49	0.48
1:G:123:LYS:HA	1:G:123:LYS:HE3	1.96	0.48
1:G:157:LYS:HD2	3:I:128:VAL:HG13	1.96	0.48
3:I:234:HIS:HB2	3:I:267:VAL:HG12	1.95	0.48
3:I:247:ARG:NE	3:I:261:ASP:OD1	2.47	0.48
1:J:111:VAL:HG11	3:L:87:ARG:HD2	1.95	0.48
2:K:435:VAL:HG12	2:K:435:VAL:O	2.12	0.48
3:L:154:GLN:O	3:L:157:ALA:HB3	2.14	0.48
2:B:113:SER:O	2:B:116:GLN:NE2	2.46	0.47
3:C:238:THR:O	3:C:238:THR:OG1	2.24	0.47
2:E:228:GLN:NE2	2:E:231:SER:HA	2.29	0.47
1:G:63:THR:O	1:G:66:ILE:HG22	2.14	0.47
3:I:169:ILE:CD1	3:I:180:VAL:HG11	2.43	0.47
1:J:194:LEU:HD12	2:K:152:TYR:CD2	2.49	0.47
2:K:457:PHE:C	2:K:458:PHE:CG	2.92	0.47
1:A:135:LEU:HD22	1:A:136:LEU:HD22	1.97	0.47
2:B:295:GLY:O	2:B:299:ILE:HG13	2.13	0.47
2:K:249:TRP:HB3	2:K:453:LYS:HD3	1.96	0.47
2:B:345:TYR:HB3	2:B:354:MET:HE2	1.97	0.47
3:C:90:LEU:O	3:C:90:LEU:HD12	2.12	0.47
3:C:215:PHE:CE2	3:C:227:TRP:CB	2.95	0.47
3:C:387:ILE:O	3:C:388:PRO:C	2.56	0.47
1:D:86:LEU:HD23	3:F:61:ILE:CG2	2.44	0.47
3:F:31:THR:HG22	3:F:35:LYS:NZ	2.28	0.47
1:G:169:LEU:HD23	1:G:170:ALA:N	2.29	0.47
3:I:116:SER:O	3:I:117:ASN:C	2.57	0.47
2:K:199:VAL:HG23	3:L:141:ASP:CB	2.44	0.47
3:L:298:ASP:OD2	3:L:300:SER:N	2.44	0.47
6:X:2:NAG:H62	6:X:5:NAG:H81	1.95	0.47
2:B:67:HIS:CD2	2:B:69:ASP:HB3	2.50	0.47
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:ALA:O	2:B:438:MET:HB2	2.14	0.47
3:C:216:GLY:HA3	3:C:226:PHE:CB	2.44	0.47
3:F:262:TYR:OH	3:F:288:ASP:OD1	2.16	0.47
3:L:247:ARG:HG3	3:L:248:VAL:O	2.14	0.47
2:B:255:ARG:HA	2:B:291:GLU:HG2	1.96	0.47
3:C:47:LEU:HD23	3:C:47:LEU:C	2.39	0.47
3:C:252:ASP:OD2	3:C:256:ARG:NH1	2.47	0.47
1:D:73:LEU:C	1:D:73:LEU:HD13	2.40	0.47
3:F:281:PHE:HB2	3:F:288:ASP:OD2	2.14	0.47
2:K:112:SER:HA	2:K:115:PHE:HD2	1.79	0.47
2:K:179:ILE:O	2:K:183:GLU:HB2	2.14	0.47
2:K:257:ASP:OD1	2:K:259:SER:HB3	2.15	0.47
1:A:188:VAL:HG12	2:B:164:ASN:ND2	2.29	0.47
2:B:80:CYS:O	2:B:84:GLU:N	2.30	0.47
3:F:291:ASP:C	3:F:302:LYS:HZ2	2.21	0.47
3:L:289:ALA:HA	3:L:371:THR:HG23	1.96	0.47
1:A:58:VAL:CG1	1:A:59:ASN:N	2.78	0.47
2:B:280:THR:O	2:B:281:ASP:C	2.57	0.47
3:C:27:ASP:O	3:C:31:THR:HG23	2.15	0.47
3:C:276:LEU:C	3:C:276:LEU:CD2	2.82	0.47
1:D:160:SER:HA	2:E:258:GLY:O	2.15	0.47
2:E:284:ASN:C	2:E:284:ASN:HD22	2.21	0.47
1:G:60:GLN:HE22	1:G:64:ASN:HD22	1.61	0.47
2:H:415:ARG:N	2:H:434:GLY:HA2	2.30	0.47
3:I:228:LEU:O	3:I:232:LYS:HD2	2.15	0.47
3:L:147:ASP:OD1	3:L:147:ASP:N	2.47	0.47
3:L:304:PHE:O	3:L:306:SER:N	2.48	0.47
5:T:4:PRO:CG	6:X:1:NAG:H62	2.45	0.47
1:A:148:LYS:O	1:A:152:VAL:HG12	2.15	0.47
2:B:381:ASP:C	2:B:381:ASP:OD2	2.58	0.47
1:D:59:ASN:O	1:D:63:THR:HG23	2.14	0.47
2:E:402:TRP:CZ3	2:E:412:PRO:CG	2.98	0.47
2:H:253:GLN:C	2:H:253:GLN:NE2	2.73	0.47
2:K:147:GLU:O	2:K:150:GLN:HG3	2.15	0.47
3:L:153:CYS:O	3:L:156:ILE:HB	2.15	0.47
3:C:178:PHE:CD1	3:C:232:LYS:HD3	2.50	0.47
3:C:350:GLN:C	3:C:352:GLY:H	2.19	0.47
1:D:162:ARG:HA	1:D:168:ALA:HB2	1.96	0.47
2:H:342:VAL:CG2	2:H:354:MET:HG2	2.45	0.47
3:I:286:ALA:O	3:I:372:TRP:HB2	2.14	0.47
1:J:123:LYS:HA	1:J:123:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:172:LEU:HD11	3:L:114:TYR:HB2	1.96	0.47
5:T:4:PRO:HG3	6:X:1:NAG:H62	1.97	0.47
2:B:163:THR:HG22	2:B:166:ARG:HH22	1.80	0.47
2:B:212:GLU:HA	2:B:215:ILE:HG22	1.96	0.47
3:C:206:LYS:HB2	3:C:211:TYR:HE1	1.78	0.47
2:E:233:VAL:HG22	2:E:234:LYS:O	2.14	0.47
2:E:376:SER:HG	2:E:382:ASN:H	1.61	0.47
2:E:402:TRP:CH2	2:E:412:PRO:CG	2.97	0.47
2:H:101:ASN:OD1	3:I:43:LEU:HD11	2.14	0.47
3:L:169:ILE:HD11	3:L:180:VAL:HG11	1.97	0.47
3:L:219:SER:CB	3:L:224:THR:CG2	2.93	0.47
3:C:179:LEU:CD2	3:C:180:VAL:O	2.63	0.46
1:D:134:GLN:OE1	1:D:193:LEU:HD22	2.15	0.46
2:E:410:ALA:HB2	2:E:437:TRP:CE3	2.49	0.46
3:F:51:GLU:HA	3:F:54:THR:HG22	1.97	0.46
1:J:108:TYR:HE1	3:L:83:THR:CG2	2.28	0.46
2:B:343:ASN:HA	2:B:354:MET:SD	2.55	0.46
3:C:163:GLN:O	3:C:167:TYR:OH	2.30	0.46
3:C:183:GLU:O	3:C:191:TRP:HB2	2.16	0.46
3:C:374:THR:OG1	3:C:375:ARG:N	2.48	0.46
2:E:435:VAL:O	2:E:447:MET:HG2	2.14	0.46
2:H:200:SER:O	2:H:279:ASN:ND2	2.48	0.46
2:H:260:VAL:HG12	2:H:261:ASP:O	2.14	0.46
2:H:329:PHE:CE2	2:H:454:ILE:HG21	2.51	0.46
2:K:312:ILE:CB	2:K:324:ALA:HB3	2.41	0.46
3:L:270:GLU:O	3:L:271:ALA:C	2.57	0.46
2:B:329:PHE:HD1	2:B:342:VAL:HG12	1.79	0.46
3:C:205:LYS:HZ1	3:C:315:TRP:CD1	2.34	0.46
3:C:264:MET:HB2	3:C:279:ALA:CB	2.45	0.46
3:F:211:TYR:CE1	3:F:333:GLY:HA3	2.50	0.46
3:F:332:SER:CB	3:F:343:HIS:NE2	2.78	0.46
2:H:171:ILE:HG23	2:H:172:LEU:H	1.78	0.46
2:H:420:GLY:HA2	2:H:446:SER:O	2.16	0.46
2:E:91:ARG:N	2:E:92:PRO:HD2	2.30	0.46
3:I:304:PHE:CG	3:I:338:LYS:HE3	2.51	0.46
2:K:144:SER:HA	2:K:148:LYS:HZ3	1.80	0.46
3:L:96:TYR:O	3:L:100:ILE:HD13	2.15	0.46
1:A:41:TRP:O	1:A:42:ASN:HB2	2.15	0.46
2:B:252:ILE:CD1	2:B:454:ILE:CG2	2.91	0.46
3:C:179:LEU:HD23	3:C:180:VAL:O	2.16	0.46
2:E:295:GLY:O	2:E:296:ASN:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:122:VAL:HG13	3:F:123:ASN:ND2	2.30	0.46
3:F:307:HIS:O	3:F:308:ASN:C	2.56	0.46
1:G:135:LEU:HD23	1:G:136:LEU:HD22	1.98	0.46
2:H:302:LEU:HD13	2:H:454:ILE:HD11	1.98	0.46
1:J:111:VAL:HG21	3:L:87:ARG:CZ	2.45	0.46
1:J:140:VAL:CG2	1:J:141:ARG:N	2.78	0.46
2:K:172:LEU:HD22	3:L:113:ILE:CG2	2.41	0.46
2:K:329:PHE:CD1	2:K:329:PHE:C	2.92	0.46
2:K:340:ILE:HG21	2:K:403:TRP:CG	2.50	0.46
3:L:109:TYR:O	3:L:113:ILE:HG22	2.15	0.46
2:B:253:GLN:NE2	2:B:451:SER:HA	2.30	0.46
3:C:113:ILE:O	3:C:117:ASN:HB2	2.15	0.46
3:F:143:VAL:O	3:F:143:VAL:HG22	2.16	0.46
2:H:210:GLU:OE2	2:H:212:GLU:HB3	2.15	0.46
2:K:436:VAL:HG12	2:K:437:TRP:N	2.30	0.46
3:L:379:MET:HA	3:L:379:MET:CE	2.41	0.46
2:B:184:SER:O	2:B:185:ASP:C	2.58	0.46
1:D:151:GLU:CG	1:D:173:VAL:HG11	2.45	0.46
1:J:159:ARG:HB2	1:J:159:ARG:CZ	2.45	0.46
1:J:206:LYS:O	1:J:210:VAL:N	2.47	0.46
2:K:424:TRP:CG	2:K:425:ASP:N	2.84	0.46
3:L:194:PHE:HZ	3:L:384:MET:HE2	1.81	0.46
2:B:160:ASN:O	2:B:163:THR:OG1	2.19	0.46
3:C:21:THR:HG23	3:C:24:GLY:H	1.81	0.46
3:C:219:SER:H	3:C:224:THR:HG21	1.81	0.46
3:C:264:MET:HB2	3:C:279:ALA:HB2	1.98	0.46
3:C:304:PHE:O	3:C:337:ASN:ND2	2.49	0.46
3:F:246:LEU:HD12	3:F:247:ARG:C	2.40	0.46
1:G:122:LEU:HD12	1:G:123:LYS:NZ	2.31	0.46
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.98	0.46
2:H:314:MET:HE2	2:H:450:MET:CE	2.45	0.46
3:I:29:LEU:HD12	3:I:33:GLN:HB2	1.97	0.46
3:I:60:LEU:O	3:I:64:ILE:HD13	2.16	0.46
1:J:210:VAL:HG21	2:K:131:GLN:CD	2.41	0.46
3:L:205:LYS:HD2	3:L:331:GLY:CA	2.46	0.46
2:B:172:LEU:CD2	3:C:110:LEU:HD22	2.46	0.46
2:B:181:LYS:HD3	2:B:182:LEU:HD12	1.97	0.46
2:B:364:ASN:ND2	6:U:1:NAG:N2	2.64	0.46
3:C:75:LYS:HB3	3:C:78:MET:CE	2.46	0.46
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	2.13	0.46
2:E:435:VAL:HG12	2:E:447:MET:CG	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:210:GLN:O	3:F:214:GLY:N	2.43	0.46
1:G:188:VAL:O	1:G:189:ILE:C	2.59	0.46
2:H:122:LYS:HZ3	3:I:60:LEU:CB	2.21	0.46
3:L:49:GLN:HE21	8:Y:1:NAG:C8	2.28	0.46
3:L:198:LEU:HD13	3:L:199:ASP:HB3	1.98	0.46
1:A:96:GLY:O	1:A:99:SER:N	2.44	0.46
1:A:160:SER:O	2:B:259:SER:O	2.33	0.46
3:C:246:LEU:CD2	3:C:248:VAL:HG23	2.45	0.46
3:F:254:ASN:HD22	3:F:254:ASN:N	2.15	0.46
1:G:73:LEU:HD11	2:H:103:ASN:OD1	2.16	0.46
3:L:304:PHE:C	3:L:306:SER:H	2.23	0.46
6:U:8:MAN:H4	6:U:9:NAG:HN2	1.79	0.46
2:B:136:GLU:O	2:B:140:ASN:O	2.34	0.45
3:C:169:ILE:HD13	3:C:180:VAL:HG21	1.98	0.45
2:E:298:LYS:O	2:E:302:LEU:HB2	2.16	0.45
3:F:168:PHE:CE2	3:F:179:LEU:HD13	2.51	0.45
1:G:65:ARG:CD	3:I:40:LEU:HD23	2.47	0.45
1:G:185:LEU:CD1	1:G:189:ILE:HD11	2.44	0.45
2:H:105:GLU:OE2	3:I:46:ILE:HG21	2.16	0.45
3:I:225:GLU:O	3:I:226:PHE:HB3	2.16	0.45
2:K:259:SER:OG	2:K:291:GLU:HG3	2.16	0.45
6:V:3:BMA:H5	6:V:5:NAG:H82	1.97	0.45
1:A:149:ARG:O	1:A:152:VAL:HG13	2.16	0.45
1:A:169:LEU:H	2:B:189:GLN:HE22	1.63	0.45
1:A:188:VAL:HG12	2:B:164:ASN:HD21	1.81	0.45
2:B:134:ASP:O	2:B:138:VAL:HG12	2.16	0.45
1:D:55:ILE:HD11	3:F:25:ILE:CG2	2.46	0.45
2:E:432:ASP:CG	2:E:432:ASP:O	2.59	0.45
2:H:66:LEU:HD22	1:J:35:PHE:CE1	2.51	0.45
2:H:167:VAL:HG13	2:H:168:LEU:N	2.31	0.45
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.98	0.45
3:I:148:ILE:HG22	3:I:149:THR:N	2.32	0.45
2:K:436:VAL:HG21	2:K:443:SER:O	2.16	0.45
2:B:364:ASN:ND2	6:U:1:NAG:O5	2.42	0.45
1:J:73:LEU:HD13	1:J:74:PHE:N	2.31	0.45
1:J:80:ASN:C	1:J:80:ASN:OD1	2.59	0.45
2:K:84:GLU:OE1	3:L:5:ARG:NH1	2.50	0.45
2:K:150:GLN:O	2:K:153:ILE:N	2.47	0.45
3:L:227:TRP:CD1	3:L:227:TRP:C	2.93	0.45
3:L:295:PHE:CE1	3:L:305:THR:HG21	2.50	0.45
3:L:343:HIS:O	3:L:343:HIS:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:NH2	3:C:78:MET:HE2	2.31	0.45
2:B:118:MET:HG3	3:C:57:VAL:HG13	1.99	0.45
2:B:198:THR:HG22	3:C:140:LYS:HB2	1.97	0.45
3:C:231:GLU:OE1	3:C:274:TYR:OH	2.16	0.45
1:D:41:TRP:O	1:D:42:ASN:CB	2.65	0.45
1:D:52:LYS:HB2	2:E:82:LEU:HD21	1.97	0.45
1:G:66:ILE:HG23	1:G:70:LYS:HE2	1.98	0.45
3:I:5:ARG:HD3	3:I:5:ARG:O	2.17	0.45
3:I:108:ARG:O	3:I:111:GLN:HG2	2.16	0.45
3:L:305:THR:HB	3:L:341:ALA:HB2	1.98	0.45
1:A:73:LEU:CD2	2:B:104:VAL:HG22	2.40	0.45
2:B:345:TYR:CG	2:B:346:ARG:N	2.82	0.45
3:C:216:GLY:HA3	3:C:226:PHE:HB2	1.97	0.45
1:G:143:GLN:O	1:G:144:LEU:C	2.59	0.45
2:H:367:MET:SD	2:H:406:ARG:CD	3.00	0.45
1:J:69:LEU:HD12	2:K:100:LEU:HD11	1.99	0.45
1:A:73:LEU:C	1:A:73:LEU:HD13	2.41	0.45
2:B:267:ASP:HB3	2:B:268:PRO:HD3	1.99	0.45
3:C:181:TYR:CE1	3:C:220:PRO:O	2.64	0.45
2:E:163:THR:HG23	2:E:166:ARG:HH12	1.81	0.45
2:E:300:SER:HB2	2:E:331:VAL:O	2.16	0.45
3:F:342:GLY:O	3:F:344:LEU:N	2.48	0.45
1:G:185:LEU:O	1:G:185:LEU:HD22	2.17	0.45
3:I:21:THR:HG23	3:I:24:GLY:H	1.82	0.45
2:K:230:ASP:O	2:K:233:VAL:CG1	2.64	0.45
1:A:94:LEU:HD22	2:B:125:TRP:HZ3	1.80	0.45
3:C:166:LEU:HD21	3:C:218:LEU:HB3	1.99	0.45
1:D:29:LYS:O	1:D:31:SER:N	2.50	0.45
3:F:251:GLU:O	3:F:380:LYS:HB3	2.17	0.45
2:K:256:GLN:O	2:K:449:LYS:NZ	2.44	0.45
2:K:326:TYR:CZ	2:K:353:LEU:HD12	2.52	0.45
5:P:4:PRO:HB3	6:V:1:NAG:H62	1.99	0.45
1:A:150:LEU:HD22	3:C:125:LYS:HE3	1.99	0.45
2:E:435:VAL:HG12	2:E:447:MET:HG2	1.99	0.45
2:H:402:TRP:HB3	2:H:404:TYR:CD2	2.52	0.45
3:I:10:ILE:C	3:I:18:TYR:OH	2.52	0.45
3:L:340:HIS:ND1	3:L:343:HIS:HB3	2.32	0.45
1:A:58:VAL:HG12	1:A:59:ASN:N	2.32	0.45
3:I:10:ILE:HG13	2:K:83:GLN:HE22	1.82	0.45
3:I:224:THR:HG23	3:I:224:THR:O	2.17	0.45
3:L:291:ASP:OD1	3:L:302:LYS:CE	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HH22	3:C:78:MET:CE	2.30	0.45
1:D:45:CYS:HB3	1:D:46:PRO:HD2	1.98	0.45
1:G:116:ARG:NE	2:H:142:TYR:OH	2.50	0.45
3:I:166:LEU:HD11	3:I:220:PRO:N	2.31	0.45
1:J:115:LEU:HD11	3:L:90:LEU:HD21	1.99	0.45
1:J:151:GLU:HG2	1:J:173:VAL:HG13	1.99	0.45
2:K:128:ARG:O	2:K:132:VAL:HG22	2.17	0.45
2:K:140:ASN:O	2:K:144:SER:OG	2.22	0.45
2:K:357:ALA:HA	2:K:439:ASN:HD21	1.82	0.45
2:B:253:GLN:HE22	2:B:451:SER:HA	1.81	0.44
1:D:63:THR:O	1:D:66:ILE:HG22	2.16	0.44
1:D:150:LEU:HD11	3:F:125:LYS:NZ	2.32	0.44
2:E:415:ARG:O	2:E:434:GLY:HA2	2.17	0.44
1:J:147:MET:HE1	2:K:179:ILE:HG13	1.99	0.44
2:K:272:GLY:HA3	2:K:295:GLY:N	2.32	0.44
3:L:221:THR:OG1	3:L:223:THR:CG2	2.64	0.44
5:S:4:PRO:HB3	7:W:1:NAG:C6	2.46	0.44
3:C:183:GLU:HB3	3:C:191:TRP:HB2	1.99	0.44
1:D:122:LEU:HD12	1:D:123:LYS:CE	2.47	0.44
2:E:104:VAL:O	2:E:104:VAL:HG12	2.17	0.44
2:E:424:TRP:CG	2:E:425:ASP:N	2.85	0.44
3:F:202:VAL:HG12	3:F:203:ASP:O	2.17	0.44
1:G:135:LEU:HD23	1:G:139:ASN:HD22	1.82	0.44
2:K:401:GLY:O	2:K:413:ASN:ND2	2.51	0.44
3:L:11:LEU:HB3	3:L:18:TYR:CZ	2.52	0.44
3:C:158:ASN:C	3:C:160:GLY:N	2.74	0.44
1:D:135:LEU:C	1:D:135:LEU:CD2	2.90	0.44
3:F:246:LEU:HD12	3:F:247:ARG:CA	2.46	0.44
3:I:156:ILE:HD13	3:I:167:TYR:CD2	2.53	0.44
3:I:208:TRP:HB3	3:I:209:ILE:HD12	1.99	0.44
1:J:55:ILE:HG23	2:K:86:LEU:CD2	2.47	0.44
1:J:55:ILE:O	1:J:58:VAL:HG12	2.18	0.44
2:B:156:THR:HG22	2:B:157:VAL:HG23	2.00	0.44
2:B:266:TRP:O	2:B:267:ASP:C	2.60	0.44
3:C:273:LYS:O	3:C:274:TYR:C	2.61	0.44
1:D:69:LEU:HD13	3:F:47:LEU:HD11	2.00	0.44
1:D:122:LEU:HD12	1:D:123:LYS:HZ1	1.81	0.44
2:E:63:GLY:O	2:E:77:PRO:HD3	2.18	0.44
2:H:121:LEU:HD23	2:H:124:LEU:HD23	1.99	0.44
1:J:66:ILE:HD11	2:K:100:LEU:HD12	1.99	0.44
3:L:173:LYS:NZ	3:L:238:THR:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:10:GAL:H4	6:X:11:SIA:H31	1.98	0.44
2:B:258:GLY:O	2:B:260:VAL:N	2.51	0.44
3:C:68:TYR:O	3:C:69:ASN:HB2	2.18	0.44
2:E:161:ILE:HB	2:E:162:PRO:HD3	2.00	0.44
2:H:295:GLY:O	2:H:299:ILE:HG13	2.17	0.44
2:H:351:ASN:C	2:H:351:ASN:ND2	2.76	0.44
3:L:318:ASP:OD1	3:L:320:ASP:OD1	2.36	0.44
6:U:2:NAG:H5	6:U:3:BMA:H2	1.99	0.44
6:V:2:NAG:H5	6:V:3:BMA:C2	2.48	0.44
1:A:99:SER:HA	1:A:102:ASN:HD22	1.83	0.44
2:B:294:LEU:HD12	2:B:295:GLY:N	2.29	0.44
1:D:30:ASP:O	1:D:32:ASP:N	2.51	0.44
1:D:134:GLN:CD	1:D:193:LEU:HD22	2.43	0.44
2:E:291:GLU:O	2:E:292:TYR:HB3	2.16	0.44
3:F:236:ILE:CG2	3:F:386:ILE:HD11	2.46	0.44
2:H:314:MET:HG3	2:H:322:VAL:CG2	2.48	0.44
3:I:251:GLU:CB	3:I:257:THR:HG22	2.48	0.44
1:A:105:ASP:O	1:A:108:TYR:N	2.51	0.44
1:A:194:LEU:HG	2:B:152:TYR:CD2	2.52	0.44
3:C:275:ARG:HA	3:C:311:GLN:HA	1.99	0.44
1:D:115:LEU:HD13	3:F:86:SER:CA	2.48	0.44
2:E:271:GLN:C	2:E:295:GLY:HA3	2.42	0.44
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.33	0.44
3:F:289:ALA:CA	3:F:371:THR:HG23	2.46	0.44
1:G:166:SER:N	2:H:195:THR:O	2.40	0.44
2:H:233:VAL:HG22	2:H:234:LYS:O	2.18	0.44
3:I:10:ILE:CD1	2:K:83:GLN:HE22	2.30	0.44
1:J:69:LEU:CD1	2:K:100:LEU:HD11	2.47	0.44
1:J:201:HIS:CE1	1:J:202:LEU:HD23	2.53	0.44
2:K:412:PRO:CB	2:K:450:MET:HE3	2.48	0.44
3:L:193:VAL:O	3:L:226:PHE:CZ	2.71	0.44
3:L:226:PHE:CD1	3:L:226:PHE:C	2.94	0.44
1:D:119:ILE:HD11	3:F:93:ILE:CD1	2.40	0.44
1:D:151:GLU:HG3	1:D:173:VAL:HG11	1.98	0.44
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.99	0.44
3:F:254:ASN:N	3:F:254:ASN:ND2	2.65	0.44
3:I:151:LYS:CE	3:I:172:LEU:HD13	2.47	0.44
3:I:166:LEU:HD23	3:I:218:LEU:CB	2.47	0.44
2:K:364:ASN:HA	2:K:367:MET:HE3	2.00	0.44
3:L:80:ASP:N	3:L:80:ASP:OD1	2.51	0.44
3:L:217:HIS:O	3:L:224:THR:OG1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:248:VAL:HG12	3:L:250:LEU:HD13	2.00	0.44
6:V:2:NAG:H3	6:V:2:NAG:O7	2.17	0.44
3:C:167:TYR:CD1	3:C:167:TYR:N	2.86	0.44
3:C:195:GLN:OE1	3:C:196:LYS:C	2.60	0.44
3:C:344:LEU:HA	3:C:367:ILE:HG23	1.99	0.44
2:H:75:LEU:HD22	1:J:46:PRO:CD	2.48	0.44
2:H:135:ASN:O	2:H:139:VAL:N	2.50	0.44
2:H:181:LYS:O	2:H:182:LEU:C	2.59	0.44
3:I:240:SER:HB2	3:I:242:ILE:HG13	1.99	0.44
2:K:151:LEU:HA	2:K:154:ASP:HB3	2.00	0.44
2:K:373:MET:HG3	2:K:405:ASN:HB2	2.00	0.44
3:L:156:ILE:HG22	3:L:157:ALA:N	2.32	0.44
3:L:197:ARG:CZ	3:L:367:ILE:HD11	2.48	0.44
3:L:198:LEU:CD1	3:L:199:ASP:N	2.75	0.44
3:L:367:ILE:CG2	3:L:382:THR:HG21	2.48	0.44
3:C:197:ARG:NH2	3:C:204:PHE:CD2	2.83	0.43
1:D:115:LEU:HD13	3:F:86:SER:CB	2.48	0.43
2:E:410:ALA:HA	2:E:436:VAL:O	2.18	0.43
3:F:100:ILE:HG22	3:F:101:LEU:HD12	1.99	0.43
2:H:99:GLU:O	2:H:103:ASN:HB2	2.17	0.43
2:B:203:ILE:HD12	2:B:203:ILE:H	1.82	0.43
3:C:338:LYS:N	3:C:339:CYS:HA	2.32	0.43
2:E:241:ASP:OD2	2:E:243:ASN:N	2.42	0.43
2:E:351:ASN:ND2	2:E:354:MET:H	2.12	0.43
3:F:281:PHE:CB	3:F:288:ASP:OD2	2.66	0.43
3:L:380:LYS:HG2	3:L:381:LYS:HE2	2.00	0.43
2:B:163:THR:HG22	2:B:166:ARG:HH12	1.82	0.43
2:E:212:GLU:HA	2:E:215:ILE:HG22	2.00	0.43
2:E:302:LEU:HD22	2:E:454:ILE:HD11	1.99	0.43
3:F:50:VAL:O	3:F:54:THR:HB	2.18	0.43
3:F:193:VAL:HA	3:F:385:LYS:HB3	2.00	0.43
1:G:143:GLN:O	1:G:146:ASP:N	2.51	0.43
2:H:252:ILE:HG23	2:H:299:ILE:HD13	2.01	0.43
2:H:434:GLY:O	2:H:436:VAL:N	2.51	0.43
1:J:154:ILE:HD11	3:L:128:VAL:CG2	2.46	0.43
1:J:175:LEU:O	1:J:178:TYR:N	2.52	0.43
3:L:196:LYS:O	3:L:225:GLU:HA	2.18	0.43
3:L:207:ASN:OD1	3:L:209:ILE:N	2.51	0.43
3:L:318:ASP:CG	3:L:325:ASN:ND2	2.76	0.43
5:O:4:PRO:HG3	6:U:1:NAG:H62	2.00	0.43
2:B:105:GLU:O	2:B:109:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:HD2	2:B:273:PHE:CD2	2.54	0.43
2:B:294:LEU:HD11	2:B:298:LYS:HD3	1.99	0.43
2:B:329:PHE:C	2:B:330:THR:HG22	2.44	0.43
3:C:174:ALA:CB	3:C:235:LEU:HD13	2.47	0.43
3:F:119:GLN:O	3:F:122:VAL:HG12	2.18	0.43
3:I:145:ILE:HD13	3:I:179:LEU:HD13	2.00	0.43
3:I:199:ASP:OD1	3:I:201:SER:CB	2.66	0.43
3:I:209:ILE:O	3:I:210:GLN:C	2.60	0.43
3:I:320:ASP:C	3:I:320:ASP:OD2	2.61	0.43
1:J:145:VAL:CG1	1:J:146:ASP:H	2.31	0.43
2:K:91:ARG:N	2:K:92:PRO:HD2	2.34	0.43
2:K:100:LEU:O	2:K:104:VAL:HG23	2.18	0.43
2:K:139:VAL:HG11	3:L:79:ILE:HG23	2.01	0.43
2:K:338:TYR:O	2:K:403:TRP:NE1	2.46	0.43
3:L:281:PHE:CZ	3:L:283:GLY:HA2	2.54	0.43
3:L:307:HIS:HE1	3:L:341:ALA:H	1.64	0.43
1:A:63:THR:HA	1:A:66:ILE:CG2	2.47	0.43
2:B:214:ILE:HG22	2:B:242:MET:HE1	2.00	0.43
1:G:60:GLN:NE2	1:G:64:ASN:HD22	2.16	0.43
2:H:115:PHE:CZ	3:I:54:THR:CG2	3.02	0.43
3:I:289:ALA:HA	3:I:371:THR:CG2	2.48	0.43
3:I:372:TRP:HZ3	3:I:379:MET:CE	2.32	0.43
2:K:228:GLN:CD	2:K:235:PRO:HG3	2.43	0.43
3:L:228:LEU:CD1	3:L:232:LYS:HD2	2.48	0.43
3:C:267:VAL:HG13	3:C:268:GLY:N	2.34	0.43
3:C:295:PHE:HZ	3:C:341:ALA:HA	1.84	0.43
2:E:226:LEU:HD12	2:E:236:TYR:O	2.19	0.43
2:E:240:CYS:HB2	2:E:242:MET:HE2	2.01	0.43
2:E:257:ASP:OD1	2:E:259:SER:CB	2.66	0.43
2:E:330:THR:O	2:E:331:VAL:CG2	2.66	0.43
2:H:394:CYS:SG	2:H:406:ARG:HA	2.59	0.43
1:J:169:LEU:HD12	2:K:188:ALA:HB3	2.00	0.43
3:L:156:ILE:HD13	3:L:167:TYR:CD2	2.53	0.43
3:L:172:LEU:H	3:L:239:GLN:NE2	2.17	0.43
3:L:359:THR:HG22	3:L:365:ASN:ND2	2.33	0.43
2:B:80:CYS:HA	2:B:83:GLN:HG3	1.99	0.43
3:C:31:THR:OG1	3:C:32:TYR:N	2.52	0.43
3:C:191:TRP:CD2	3:C:385:LYS:HE3	2.54	0.43
1:D:156:ILE:HD13	2:E:415:ARG:NH1	2.34	0.43
3:F:234:HIS:CE1	3:F:238:THR:HG21	2.54	0.43
3:I:5:ARG:HA	3:I:11:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:211:TYR:O	3:L:230:ASN:OD1	2.36	0.43
7:W:1:NAG:O3	7:W:2:NAG:H2	2.17	0.43
3:C:69:ASN:O	3:C:70:PRO:C	2.62	0.43
3:F:89:MET:HE3	3:F:93:ILE:HG12	2.01	0.43
2:H:211:CYS:HB2	2:H:250:THR:OG1	2.18	0.43
2:H:314:MET:CE	2:H:450:MET:HE1	2.48	0.43
3:I:5:ARG:HA	3:I:11:LEU:HD12	2.01	0.43
3:L:387:ILE:HG23	3:L:388:PRO:O	2.19	0.43
3:C:166:LEU:CD2	3:C:218:LEU:HB3	2.49	0.43
2:E:210:GLU:OE1	2:E:213:GLU:HB2	2.18	0.43
2:E:410:ALA:CB	2:E:437:TRP:CE3	3.02	0.43
3:F:275:ARG:HA	3:F:310:MET:O	2.18	0.43
2:H:236:TYR:C	2:H:236:TYR:CD2	2.96	0.43
3:I:195:GLN:OE1	3:I:382:THR:CG2	2.67	0.43
3:I:326:CYS:HB2	3:I:336:MET:HG3	2.00	0.43
3:I:382:THR:CG2	3:I:383:THR:N	2.82	0.43
1:J:69:LEU:CD1	2:K:100:LEU:HD13	2.36	0.43
2:K:134:ASP:O	2:K:138:VAL:HG23	2.18	0.43
3:L:49:GLN:HE21	8:Y:1:NAG:H81	1.73	0.43
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.53	0.43
3:L:270:GLU:O	3:L:273:LYS:N	2.40	0.43
2:B:352:ALA:HB1	2:B:409:ALA:CB	2.48	0.43
3:C:364:ASP:CG	4:M:1:GLY:N	2.77	0.43
3:F:168:PHE:O	3:F:169:ILE:HG23	2.19	0.43
1:G:67:ASN:O	1:G:71:ASN:HB2	2.19	0.43
1:G:156:ILE:O	1:G:160:SER:N	2.42	0.43
2:H:361:MET:CB	7:W:1:NAG:H81	2.47	0.43
1:J:112:SER:HB3	1:J:116:ARG:NH2	2.34	0.43
1:J:205:ILE:CG1	2:K:138:VAL:HG11	2.42	0.43
2:K:183:GLU:OE1	3:L:120:LYS:NZ	2.27	0.43
7:W:2:NAG:H3	7:W:3:BMA:O2	2.19	0.43
1:A:130:VAL:O	1:A:131:GLN:C	2.61	0.42
2:B:185:ASP:O	2:B:188:ALA:HB3	2.19	0.42
3:C:100:ILE:HG23	3:C:101:LEU:CD2	2.44	0.42
3:C:236:ILE:O	3:C:239:GLN:HG2	2.19	0.42
2:E:135:ASN:O	2:E:139:VAL:HG12	2.18	0.42
3:I:27:ASP:OD1	3:I:28:PHE:N	2.51	0.42
3:I:329:GLN:HA	3:I:361:ASN:HD21	1.83	0.42
1:J:147:MET:O	1:J:148:LYS:C	2.62	0.42
2:K:137:ASN:O	2:K:141:GLU:HG2	2.19	0.42
2:K:435:VAL:HG12	2:K:447:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:100:ILE:O	3:L:104:ASP:HB2	2.18	0.42
3:L:150:GLY:CA	3:L:155:ASP:OD1	2.66	0.42
2:E:303:THR:HB	2:E:330:THR:HA	2.01	0.42
2:E:355:ASP:O	2:E:369:ILE:HD11	2.19	0.42
3:F:242:ILE:H	3:F:242:ILE:HD12	1.83	0.42
1:G:42:ASN:O	2:K:78:THR:HG21	2.18	0.42
2:H:203:ILE:HG22	2:H:204:PRO:O	2.19	0.42
2:H:260:VAL:CG2	2:H:291:GLU:HB2	2.49	0.42
2:K:174:ASN:OD1	2:K:174:ASN:C	2.62	0.42
2:K:215:ILE:HD13	2:K:242:MET:HB3	2.01	0.42
2:K:373:MET:HA	2:K:373:MET:HE3	2.01	0.42
2:K:439:ASN:N	2:K:439:ASN:ND2	2.57	0.42
3:L:361:ASN:H	3:L:361:ASN:HD22	1.68	0.42
2:B:276:VAL:HA	2:B:292:TYR:CD2	2.54	0.42
2:B:342:VAL:O	2:B:371:ASN:ND2	2.52	0.42
1:D:66:ILE:HG13	2:E:100:LEU:HD11	2.00	0.42
2:E:330:THR:C	2:E:331:VAL:HG23	2.44	0.42
3:F:166:LEU:HD11	3:F:219:SER:C	2.44	0.42
3:I:253:TRP:C	3:I:254:ASN:ND2	2.76	0.42
1:J:184:GLN:NE2	2:K:167:VAL:HG23	2.18	0.42
1:J:210:VAL:HG11	2:K:131:GLN:NE2	2.34	0.42
3:L:145:ILE:CD1	3:L:179:LEU:HD22	2.49	0.42
6:V:4:MAN:O3	6:V:5:NAG:C1	2.67	0.42
2:B:226:LEU:HA	2:B:226:LEU:HD12	1.71	0.42
3:C:247:ARG:HB2	3:C:261:ASP:OD2	2.19	0.42
2:H:139:VAL:HG11	3:I:78:MET:HG2	2.01	0.42
2:H:210:GLU:CD	2:H:213:GLU:H	2.27	0.42
3:I:307:HIS:CE1	3:I:341:ALA:H	2.37	0.42
3:I:318:ASP:OD1	3:I:318:ASP:C	2.62	0.42
1:J:144:LEU:HD23	1:J:182:GLN:HG3	2.01	0.42
2:K:211:CYS:O	2:K:242:MET:HE1	2.18	0.42
2:K:293:TRP:HZ2	2:K:296:ASN:HD21	1.66	0.42
3:L:229:GLY:O	3:L:233:ILE:N	2.43	0.42
3:C:243:PRO:HG2	3:C:389:PHE:HB3	2.02	0.42
3:C:393:THR:O	3:C:394:ILE:HD13	2.20	0.42
2:E:345:TYR:CG	2:E:346:ARG:N	2.88	0.42
2:H:267:ASP:HB3	2:H:268:PRO:HD3	2.00	0.42
1:J:115:LEU:HD11	3:L:90:LEU:CD2	2.49	0.42
2:K:181:LYS:O	2:K:184:SER:OG	2.29	0.42
3:C:390:ASN:C	3:C:390:ASN:ND2	2.74	0.42
2:E:179:ILE:HD11	3:F:120:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:249:GLU:O	3:F:250:LEU:HD12	2.18	0.42
3:I:304:PHE:C	3:I:337:ASN:ND2	2.78	0.42
2:K:172:LEU:HD23	3:L:113:ILE:HD13	2.00	0.42
3:L:178:PHE:CE1	3:L:180:VAL:HG12	2.54	0.42
3:L:194:PHE:CZ	3:L:384:MET:HB3	2.55	0.42
3:L:379:MET:HE3	3:L:379:MET:CA	2.38	0.42
6:U:6:GAL:H62	6:U:7:SIA:H32	1.87	0.42
2:E:356:GLY:HA2	2:E:368:THR:O	2.19	0.42
2:H:167:VAL:CG1	2:H:168:LEU:N	2.83	0.42
2:H:373:MET:SD	2:H:405:ASN:CG	3.03	0.42
3:I:12:ASP:OD2	3:I:15:PHE:CE1	2.73	0.42
3:I:334:TRP:HB3	3:I:336:MET:CE	2.50	0.42
1:J:109:ASN:OD1	1:J:109:ASN:C	2.62	0.42
1:J:175:LEU:O	1:J:176:LYS:C	2.62	0.42
2:K:275:ASN:OD1	3:L:139:CYS:N	2.47	0.42
2:K:367:MET:SD	5:T:2:HIS:HB2	2.60	0.42
2:K:426:MET:O	2:K:427:ALA:C	2.63	0.42
2:E:303:THR:HA	2:E:308:THR:OG1	2.19	0.42
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.20	0.42
3:F:262:TYR:HD2	3:F:278:TYR:CD1	2.37	0.42
3:F:338:LYS:N	3:F:339:CYS:HA	2.35	0.42
2:H:171:ILE:CG2	2:H:172:LEU:N	2.81	0.42
2:H:410:ALA:HA	2:H:436:VAL:O	2.19	0.42
3:I:3:ALA:CB	3:L:11:LEU:HD12	2.45	0.42
3:I:332:SER:HG	3:I:343:HIS:CE1	2.30	0.42
2:K:172:LEU:HD23	3:L:113:ILE:CD1	2.50	0.42
2:K:402:TRP:CG	2:K:403:TRP:N	2.88	0.42
3:L:367:ILE:HG21	3:L:382:THR:CG2	2.47	0.42
6:U:1:NAG:O3	6:U:2:NAG:C2	2.66	0.42
1:A:135:LEU:HD23	1:A:136:LEU:HD22	2.00	0.42
3:F:307:HIS:O	3:F:310:MET:HG2	2.19	0.42
1:G:66:ILE:HD11	2:H:100:LEU:HD12	2.02	0.42
1:G:93:ILE:HG22	1:G:94:LEU:CD1	2.42	0.42
1:G:144:LEU:HD21	1:G:182:GLN:HA	2.02	0.42
3:I:10:ILE:HD11	2:K:83:GLN:NE2	2.34	0.42
3:I:197:ARG:C	3:I:198:LEU:HD23	2.45	0.42
1:J:108:TYR:CE2	3:L:80:ASP:O	2.73	0.42
1:J:200:GLN:NE2	2:K:145:GLU:HB3	2.35	0.42
1:A:104:ARG:HD3	3:C:79:ILE:CG2	2.49	0.42
2:B:405:ASN:O	2:B:406:ARG:CB	2.68	0.42
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:GLY:HA3	3:C:367:ILE:HG13	2.02	0.42
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.55	0.42
1:G:45:CYS:HB2	2:K:78:THR:HG22	2.02	0.42
2:H:91:ARG:N	2:H:92:PRO:HD2	2.35	0.42
2:H:109:GLN:O	2:H:113:SER:N	2.50	0.42
3:I:191:TRP:CD2	3:I:385:LYS:HD2	2.55	0.42
3:I:322:PHE:HB2	3:I:338:LYS:HG3	2.02	0.42
3:I:336:MET:HE1	3:I:343:HIS:CD2	2.55	0.42
2:K:316:ASP:OD2	2:K:320:ASP:N	2.53	0.42
1:A:107:THR:O	1:A:111:VAL:HB	2.20	0.41
2:B:201:CYS:O	3:C:143:VAL:HG21	2.18	0.41
3:C:237:SER:OG	3:C:238:THR:HG23	2.20	0.41
3:F:193:VAL:HG13	3:F:195:GLN:O	2.19	0.41
1:G:48:GLY:HA2	2:H:82:LEU:HD11	2.02	0.41
1:G:188:VAL:HG11	2:H:164:ASN:HD21	1.85	0.41
2:H:267:ASP:O	2:H:271:GLN:HG2	2.20	0.41
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.55	0.41
1:J:210:VAL:HG21	2:K:131:GLN:CG	2.49	0.41
3:L:212:LYS:HE3	3:L:274:TYR:OH	2.20	0.41
3:L:221:THR:C	3:L:223:THR:HG23	2.45	0.41
3:L:281:PHE:CE2	3:L:283:GLY:HA2	2.55	0.41
6:U:6:GAL:H3	6:U:7:SIA:O7	2.19	0.41
1:A:185:LEU:HD22	1:A:185:LEU:C	2.45	0.41
2:B:189:GLN:O	2:B:190:MET:C	2.63	0.41
2:B:223:GLU:HA	2:B:287:GLY:HA2	2.02	0.41
2:B:354:MET:O	2:B:369:ILE:CG2	2.66	0.41
2:B:415:ARG:O	2:B:434:GLY:HA2	2.20	0.41
3:C:316:ASP:OD1	3:C:316:ASP:N	2.52	0.41
3:F:90:LEU:HD22	3:F:91:GLU:CA	2.50	0.41
3:F:228:LEU:HD12	3:F:228:LEU:O	2.20	0.41
2:H:253:GLN:NE2	2:H:452:MET:HG3	2.35	0.41
2:H:405:ASN:O	2:H:405:ASN:CG	2.62	0.41
1:J:54:LEU:HD23	2:K:60:PRO:HG2	2.02	0.41
2:K:226:LEU:HD12	2:K:227:ILE:H	1.84	0.41
2:K:317:TRP:CD1	2:K:420:GLY:HA3	2.55	0.41
2:B:457:PHE:O	2:B:458:PHE:HB2	2.21	0.41
1:G:45:CYS:C	2:K:75:LEU:HD22	2.45	0.41
2:H:125:TRP:CD1	2:H:126:GLN:N	2.88	0.41
2:H:175:LEU:O	2:H:178:LYS:N	2.54	0.41
3:I:5:ARG:C	3:I:5:ARG:CD	2.93	0.41
2:K:186:VAL:CG1	2:K:187:SER:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:1:NAG:O3	6:V:2:NAG:N2	2.54	0.41
2:B:277:ALA:C	2:B:278:THR:HG23	2.45	0.41
3:C:19:CYS:HB3	3:C:20:PRO:HD2	2.02	0.41
3:C:119:GLN:HA	3:C:119:GLN:NE2	2.34	0.41
3:C:267:VAL:CG1	3:C:268:GLY:N	2.80	0.41
3:C:356:LYS:C	3:C:358:SER:H	2.28	0.41
2:E:69:ASP:HB3	2:E:72:LEU:HB2	2.02	0.41
3:F:31:THR:HG22	3:F:35:LYS:HZ2	1.86	0.41
3:F:141:ASP:CG	3:F:143:VAL:HG13	2.45	0.41
2:H:211:CYS:O	2:H:242:MET:HE1	2.21	0.41
2:K:224:MET:SD	2:K:237:ARG:HB3	2.60	0.41
3:L:221:THR:O	3:L:223:THR:HG23	2.20	0.41
1:A:200:GLN:HB3	2:B:146:LEU:HD11	2.03	0.41
3:C:154:GLN:O	3:C:157:ALA:HB3	2.20	0.41
3:C:278:TYR:CD1	3:C:278:TYR:C	2.98	0.41
1:D:185:LEU:HD22	1:D:189:ILE:HG13	2.02	0.41
1:G:139:ASN:O	1:G:142:ALA:HB3	2.21	0.41
3:L:205:LYS:HD2	3:L:331:GLY:HA2	2.01	0.41
3:L:288:ASP:C	3:L:288:ASP:OD1	2.63	0.41
3:L:364:ASP:OD1	4:R:1:GLY:N	2.53	0.41
1:A:86:LEU:HD12	1:A:89:ASN:HD22	1.85	0.41
1:A:156:ILE:HD13	2:B:415:ARG:CZ	2.50	0.41
2:B:91:ARG:HB3	2:B:92:PRO:HD3	2.03	0.41
2:E:118:MET:O	2:E:122:LYS:CB	2.68	0.41
2:E:210:GLU:C	2:E:210:GLU:CD	2.88	0.41
3:F:184:ILE:HG22	3:F:185:ASP:O	2.21	0.41
3:I:108:ARG:O	3:I:112:GLU:HG2	2.19	0.41
3:I:340:HIS:ND1	3:I:343:HIS:HB2	2.35	0.41
3:I:372:TRP:HZ3	3:I:379:MET:HE1	1.85	0.41
1:J:148:LYS:NZ	2:K:425:ASP:OD1	2.53	0.41
3:L:93:ILE:C	3:L:93:ILE:HD12	2.45	0.41
1:A:137:GLN:O	1:A:140:VAL:HG22	2.21	0.41
3:C:191:TRP:CE3	3:C:387:ILE:HB	2.56	0.41
3:C:206:LYS:HB2	3:C:211:TYR:CD1	2.55	0.41
3:C:356:LYS:O	3:C:362:GLY:HA2	2.20	0.41
1:D:116:ARG:NH2	2:E:146:LEU:HD21	2.35	0.41
2:E:294:LEU:O	2:E:299:ILE:HD11	2.21	0.41
3:L:245:ALA:HB3	3:L:387:ILE:CG2	2.51	0.41
2:B:160:ASN:HA	2:B:163:THR:OG1	2.21	0.41
2:B:329:PHE:O	2:B:330:THR:HG22	2.21	0.41
3:C:194:PHE:CZ	3:C:384:MET:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:MET:SD	3:F:60:LEU:HD23	2.60	0.41
2:E:198:THR:HG22	3:F:140:LYS:O	2.21	0.41
2:E:301:GLN:CD	2:E:301:GLN:C	2.88	0.41
1:J:127:ILE:HA	1:J:130:VAL:CG1	2.46	0.41
2:K:199:VAL:HG23	3:L:141:ASP:HB2	2.02	0.41
2:K:340:ILE:HB	2:K:403:TRP:CE2	2.56	0.41
3:L:54:THR:O	3:L:58:LYS:HB2	2.21	0.41
3:L:168:PHE:CD2	3:L:179:LEU:HD13	2.56	0.41
2:B:78:THR:HG22	1:D:45:CYS:SG	2.60	0.41
2:B:103:ASN:HA	2:B:107:VAL:HG23	2.03	0.41
2:B:141:GLU:HG3	2:B:144:SER:OG	2.21	0.41
2:B:163:THR:O	2:B:167:VAL:HG12	2.21	0.41
2:B:212:GLU:O	2:B:215:ILE:N	2.53	0.41
2:B:340:ILE:CG1	2:B:341:SER:N	2.84	0.41
3:C:229:GLY:O	3:C:230:ASN:C	2.63	0.41
3:C:234:HIS:O	3:C:238:THR:HG23	2.21	0.41
3:C:292:GLY:HA2	3:C:341:ALA:HB2	2.02	0.41
2:E:172:LEU:HD23	3:F:113:ILE:CG2	2.51	0.41
2:E:284:ASN:C	2:E:284:ASN:ND2	2.79	0.41
1:G:133:ILE:HG21	2:H:164:ASN:OD1	2.21	0.41
1:G:147:MET:O	1:G:148:LYS:C	2.62	0.41
2:H:116:GLN:C	2:H:118:MET:H	2.29	0.41
2:H:405:ASN:O	2:H:406:ARG:CB	2.68	0.41
2:H:439:ASN:HD22	2:H:439:ASN:N	2.19	0.41
3:I:69:ASN:N	3:I:70:PRO:CD	2.84	0.41
3:I:207:ASN:ND2	3:I:209:ILE:HD13	2.26	0.41
3:I:372:TRP:CE3	3:I:373:LYS:HG2	2.56	0.41
2:K:151:LEU:HD23	2:K:151:LEU:O	2.20	0.41
2:K:458:PHE:CD1	2:K:458:PHE:N	2.87	0.41
3:L:73:SER:O	3:L:78:MET:HE3	2.20	0.41
3:L:229:GLY:O	3:L:232:LYS:N	2.53	0.41
3:L:251:GLU:OE1	3:L:381:LYS:HE3	2.21	0.41
2:B:100:LEU:O	2:B:104:VAL:HG23	2.21	0.41
3:C:294:ASP:OD2	3:C:302:LYS:HB2	2.21	0.41
1:D:64:ASN:C	1:D:64:ASN:ND2	2.78	0.41
1:G:165:CYS:HA	2:H:196:PRO:HA	2.02	0.41
3:L:115:ASN:HD22	3:L:115:ASN:HA	1.76	0.41
1:A:46:PRO:O	3:C:22:THR:CG2	2.70	0.40
2:B:432:ASP:OD2	2:B:432:ASP:N	2.54	0.40
3:C:124:LEU:O	3:C:128:VAL:HG12	2.21	0.40
3:C:305:THR:HB	3:C:341:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ASN:OD1	1:D:103:ASN:N	2.54	0.40
1:D:139:ASN:HB3	3:F:114:TYR:CE1	2.56	0.40
1:D:141:ARG:NH1	1:D:186:GLU:OE2	2.54	0.40
1:D:193:LEU:N	1:D:193:LEU:HD23	2.36	0.40
2:E:200:SER:O	2:E:279:ASN:ND2	2.54	0.40
2:E:205:VAL:CG2	3:F:215:PHE:O	2.69	0.40
2:E:227:ILE:O	2:E:235:PRO:HA	2.21	0.40
2:E:256:GLN:NE2	2:E:289:PRO:O	2.54	0.40
3:F:252:ASP:HB2	3:F:377:TYR:OH	2.22	0.40
1:G:136:LEU:O	1:G:137:GLN:C	2.64	0.40
2:H:349:ALA:HB1	2:H:437:TRP:NE1	2.36	0.40
3:I:194:PHE:HA	3:I:228:LEU:HB2	2.03	0.40
3:I:226:PHE:CD1	3:I:226:PHE:C	2.99	0.40
3:I:340:HIS:CE1	3:I:368:ILE:HD11	2.56	0.40
3:L:334:TRP:HB3	3:L:336:MET:SD	2.61	0.40
1:A:140:VAL:O	1:A:141:ARG:C	2.64	0.40
2:B:159:SER:O	2:B:163:THR:CG2	2.55	0.40
3:C:254:ASN:N	3:C:254:ASN:ND2	2.50	0.40
3:F:356:LYS:HZ3	3:F:362:GLY:C	2.28	0.40
2:H:152:TYR:O	2:H:153:ILE:HD13	2.22	0.40
3:I:5:ARG:CA	3:I:11:LEU:HD13	2.51	0.40
3:I:230:ASN:HA	3:I:233:ILE:HD12	2.01	0.40
1:J:111:VAL:HG21	3:L:87:ARG:NH1	2.36	0.40
2:K:191:GLU:C	2:K:193:CYS:H	2.30	0.40
2:K:387:THR:HG22	2:K:388:SER:H	1.86	0.40
3:L:249:GLU:O	3:L:383:THR:HG23	2.20	0.40
3:L:337:ASN:C	3:L:337:ASN:OD1	2.64	0.40
1:A:184:GLN:HE21	2:B:167:VAL:HG23	1.85	0.40
2:B:266:TRP:HA	2:B:377:THR:HG21	2.02	0.40
2:H:157:VAL:HG12	2:H:157:VAL:O	2.21	0.40
3:I:149:THR:CG2	3:I:150:GLY:N	2.84	0.40
1:J:115:LEU:HD22	3:L:90:LEU:HD11	2.03	0.40
1:J:194:LEU:N	1:J:195:PRO:HD3	2.37	0.40
2:K:253:GLN:C	2:K:253:GLN:HE21	2.29	0.40
2:E:151:LEU:O	2:E:155:GLU:HB2	2.21	0.40
2:E:224:MET:HE2	2:E:237:ARG:HD3	2.03	0.40
3:F:207:ASN:O	3:F:208:TRP:C	2.64	0.40
3:F:211:TYR:O	3:F:229:GLY:HA2	2.22	0.40
2:H:410:ALA:CB	2:H:437:TRP:CE3	3.04	0.40
3:I:166:LEU:C	3:I:167:TYR:CD1	3.00	0.40
1:J:45:CYS:HB3	1:J:46:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:168:PHE:CE2	3:L:179:LEU:HB2	2.55	0.40
1:A:76:TYR:HA	1:A:79:ASN:HB3	2.03	0.40
2:B:138:VAL:CG1	2:B:139:VAL:N	2.84	0.40
2:B:182:LEU:O	2:B:183:GLU:C	2.64	0.40
2:B:405:ASN:O	2:B:406:ARG:HB3	2.22	0.40
3:C:382:THR:C	3:C:383:THR:HG22	2.46	0.40
2:E:107:VAL:O	2:E:107:VAL:HG12	2.22	0.40
3:F:202:VAL:HG23	3:F:225:GLU:HB2	2.03	0.40
2:H:300:SER:HB2	2:H:331:VAL:O	2.21	0.40
2:K:241:ASP:HB3	2:K:249:TRP:HB2	2.04	0.40
2:K:340:ILE:CG2	2:K:403:TRP:CG	3.05	0.40
3:L:84:LEU:C	3:L:84:LEU:CD2	2.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:72:GLU:OE2	1:J:84:HIS:NE2[1_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	172/562 (31%)	150 (87%)	20 (12%)	2 (1%)	10	34
1	D	172/562 (31%)	158 (92%)	8 (5%)	6 (4%)	3	12
1	G	172/562 (31%)	150 (87%)	18 (10%)	4 (2%)	5	19
1	J	184/562 (33%)	164 (89%)	18 (10%)	2 (1%)	11	36
2	B	399/461 (87%)	344 (86%)	46 (12%)	9 (2%)	5	19
2	E	399/461 (87%)	337 (84%)	48 (12%)	14 (4%)	3	12
2	H	399/461 (87%)	354 (89%)	38 (10%)	7 (2%)	6	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	399/461 (87%)	348 (87%)	45 (11%)	6 (2%)	8	28
3	C	379/411 (92%)	322 (85%)	48 (13%)	9 (2%)	4	18
3	F	380/411 (92%)	320 (84%)	54 (14%)	6 (2%)	7	27
3	I	392/411 (95%)	347 (88%)	39 (10%)	6 (2%)	8	28
3	L	389/411 (95%)	338 (87%)	42 (11%)	9 (2%)	5	19
4	M	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	N	2/4 (50%)	2 (100%)	0	0	100	100
4	Q	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	R	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
5	O	2/4 (50%)	2 (100%)	0	0	100	100
5	P	2/4 (50%)	2 (100%)	0	0	100	100
5	S	2/4 (50%)	2 (100%)	0	0	100	100
5	T	2/4 (50%)	2 (100%)	0	0	100	100
All	All	3852/5768 (67%)	3345 (87%)	427 (11%)	80 (2%)	5	21

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	195	PRO
2	B	259	SER
3	C	70	PRO
3	C	350	GLN
3	C	357	ALA
1	D	30	ASP
2	E	265	LYS
2	E	406	ARG
1	G	31	SER
1	G	189	ILE
1	J	199	ARG
2	K	233	VAL
3	L	360	PRO
3	L	374	THR
2	B	281	ASP
2	B	351	ASN
2	B	399	GLY
3	C	198	LEU

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Mol	Chain	Res	Type
3	C	351	GLY
1	D	42	ASN
2	E	263	GLY
2	E	339	GLN
2	E	443	SER
2	E	447	MET
3	F	198	LEU
3	F	199	ASP
2	H	362	GLY
3	I	74	SER
1	J	200	GLN
2	K	316	ASP
3	L	9	CYS
3	L	305	THR
2	B	435	VAL
1	D	195	PRO
2	E	111	SER
2	E	371	ASN
2	E	386	LEU
3	F	82	ALA
3	F	360	PRO
2	H	183	GLU
2	H	206	VAL
2	H	256	GLN
3	I	241	ALA
2	K	281	ASP
3	L	23	CYS
3	L	205	LYS
3	L	365	ASN
2	B	213	GLU
3	C	159	LYS
2	E	281	ASP
2	E	344	LYS
2	E	363	GLU
2	H	435	VAL
3	I	198	LEU
2	K	357	ALA
2	B	60	PRO
2	B	185	ASP
3	C	146	HIS
1	D	31	SER
1	D	34	PRO

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Mol	Chain	Res	Type
2	H	92	PRO
3	I	362	GLY
2	K	256	GLN
2	K	298	LYS
3	L	78	MET
3	C	122	VAL
3	C	241	ALA
3	F	343	HIS
1	G	34	PRO
2	H	280	THR
2	B	179	ILE
1	G	195	PRO
3	F	143	VAL
3	I	324	GLY
1	D	194	LEU
2	E	63	GLY
3	I	76	PRO
2	E	289	PRO
3	L	171	PRO

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	164/479 (34%)	141 (86%)	23 (14%)	3	11
1	D	164/479 (34%)	146 (89%)	18 (11%)	6	20
1	G	164/479 (34%)	151 (92%)	13 (8%)	11	34
1	J	176/479 (37%)	147 (84%)	29 (16%)	2	8
2	B	350/396 (88%)	299 (85%)	51 (15%)	3	10
2	E	350/396 (88%)	313 (89%)	37 (11%)	6	22
2	H	350/396 (88%)	314 (90%)	36 (10%)	7	23
2	K	350/396 (88%)	308 (88%)	42 (12%)	5	16
3	C	328/350 (94%)	282 (86%)	46 (14%)	3	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	328/350 (94%)	282 (86%)	46 (14%)	3	11
3	I	339/350 (97%)	298 (88%)	41 (12%)	5	16
3	L	337/350 (96%)	294 (87%)	43 (13%)	4	14
4	M	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	N	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	Q	3/3 (100%)	2 (67%)	1 (33%)	0	0
4	R	3/3 (100%)	2 (67%)	1 (33%)	0	0
5	O	3/3 (100%)	3 (100%)	0	100	100
5	P	3/3 (100%)	3 (100%)	0	100	100
5	S	3/3 (100%)	3 (100%)	0	100	100
5	T	3/3 (100%)	3 (100%)	0	100	100
All	All	3424/4924 (70%)	2995 (88%)	429 (12%)	4	15

All (429) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	41	TRP
1	A	58	VAL
1	A	64	ASN
1	A	66	ILE
1	A	68	LYS
1	A	71	ASN
1	A	73	LEU
1	A	90	ILE
1	A	102	ASN
1	A	122	LEU
1	A	126	VAL
1	A	129	LYS
1	A	135	LEU
1	A	136	LEU
1	A	138	LYS
1	A	145	VAL
1	A	149	ARG
1	A	162	ARG
1	A	175	LEU
1	A	185	LEU
1	A	192	ASP

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Mol	Chain	Res	Type
1	A	197	ARG
2	B	66	LEU
2	B	83	GLN
2	B	88	GLN
2	B	89	GLN
2	B	97	VAL
2	B	98	ASP
2	B	99	GLU
2	B	105	GLU
2	B	138	VAL
2	B	141	GLU
2	B	156	THR
2	B	158	ASN
2	B	161	ILE
2	B	165	LEU
2	B	171	ILE
2	B	179	ILE
2	B	181	LYS
2	B	183	GLU
2	B	186	VAL
2	B	200	SER
2	B	209	LYS
2	B	210	GLU
2	B	213	GLU
2	B	227	ILE
2	B	234	LYS
2	B	237	ARG
2	B	253	GLN
2	B	280	THR
2	B	283	LYS
2	B	284	ASN
2	B	288	LEU
2	B	294	LEU
2	B	297	ASP
2	B	310	LEU
2	B	311	LEU
2	B	318	LYS
2	B	320	ASP
2	B	321	LYS
2	B	330	THR
2	B	343	ASN
2	B	351	ASN

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Mol	Chain	Res	Type
2	B	354	MET
2	B	359	GLN
2	B	369	ILE
2	B	376	SER
2	B	380	ARG
2	B	381	ASP
2	B	387	THR
2	B	426	MET
2	B	438	MET
2	B	454	ILE
3	C	22	THR
3	C	29	LEU
3	C	32	TYR
3	C	33	GLN
3	C	37	ASP
3	C	41	GLN
3	C	58	LYS
3	C	61	ILE
3	C	75	LYS
3	C	84	LEU
3	C	86	SER
3	C	90	LEU
3	C	100	ILE
3	C	121	ILE
3	C	131	LEU
3	C	140	LYS
3	C	147	ASP
3	C	151	LYS
3	C	179	LEU
3	C	195	GLN
3	C	198	LEU
3	C	221	THR
3	C	233	ILE
3	C	239	GLN
3	C	250	LEU
3	C	254	ASN
3	C	258	SER
3	C	259	THR
3	C	267	VAL
3	C	276	LEU
3	C	277	THR
3	C	305	THR

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Mol	Chain	Res	Type
3	C	306	SER
3	C	317	ASN
3	C	318	ASP
3	C	340	HIS
3	C	356	LYS
3	C	358	SER
3	C	359	THR
3	C	365	ASN
3	C	368	ILE
3	C	383	THR
3	C	387	ILE
3	C	390	ASN
3	C	392	LEU
3	C	393	THR
1	D	37	SER
1	D	47	SER
1	D	64	ASN
1	D	66	ILE
1	D	73	LEU
1	D	123	LYS
1	D	135	LEU
1	D	136	LEU
1	D	138	LYS
1	D	153	ASP
1	D	154	ILE
1	D	174	ASP
1	D	183	LYS
1	D	185	LEU
1	D	189	ILE
1	D	191	LYS
1	D	193	LEU
1	D	200	GLN
2	E	90	GLU
2	E	97	VAL
2	E	118	MET
2	E	135	ASN
2	E	136	GLU
2	E	138	VAL
2	E	141	GLU
2	E	171	ILE
2	E	179	ILE
2	E	180	GLN

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Mol	Chain	Res	Type
2	E	181	LYS
2	E	182	LEU
2	E	186	VAL
2	E	199	VAL
2	E	206	VAL
2	E	209	LYS
2	E	213	GLU
2	E	238	VAL
2	E	243	ASN
2	E	253	GLN
2	E	270	LYS
2	E	280	THR
2	E	284	ASN
2	E	294	LEU
2	E	302	LEU
2	E	310	LEU
2	E	318	LYS
2	E	321	LYS
2	E	323	LYS
2	E	330	THR
2	E	339	GLN
2	E	342	VAL
2	E	359	GLN
2	E	406	ARG
2	E	421	GLN
2	E	438	MET
2	E	439	ASN
3	F	35	LYS
3	F	72	GLU
3	F	90	LEU
3	F	100	ILE
3	F	104	ASP
3	F	107	ILE
3	F	112	GLU
3	F	114	TYR
3	F	117	ASN
3	F	118	ASN
3	F	126	GLU
3	F	130	GLN
3	F	140	LYS
3	F	143	VAL
3	F	147	ASP

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Mol	Chain	Res	Type
3	F	151	LYS
3	F	152	ASP
3	F	156	ILE
3	F	162	LYS
3	F	175	ASN
3	F	178	PHE
3	F	189	ASN
3	F	218	LEU
3	F	246	LEU
3	F	249	GLU
3	F	254	ASN
3	F	258	SER
3	F	259	THR
3	F	276	LEU
3	F	285	ASP
3	F	300	SER
3	F	306	SER
3	F	313	SER
3	F	317	ASN
3	F	323	GLU
3	F	350	GLN
3	F	356	LYS
3	F	358	SER
3	F	361	ASN
3	F	365	ASN
3	F	376	TRP
3	F	379	MET
3	F	383	THR
3	F	385	LYS
3	F	386	ILE
3	F	392	LEU
1	G	39	GLU
1	G	41	TRP
1	G	58	VAL
1	G	73	LEU
1	G	122	LEU
1	G	123	LYS
1	G	138	LYS
1	G	140	VAL
1	G	152	VAL
1	G	158	ILE
1	G	160	SER

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Mol	Chain	Res	Type
1	G	173	VAL
1	G	185	LEU
2	H	61	ASP
2	H	83	GLN
2	H	99	GLU
2	H	103	ASN
2	H	109	GLN
2	H	111	SER
2	H	115	PHE
2	H	116	GLN
2	H	122	LYS
2	H	123	ASP
2	H	125	TRP
2	H	138	VAL
2	H	140	ASN
2	H	156	THR
2	H	179	ILE
2	H	181	LYS
2	H	182	LEU
2	H	191	GLU
2	H	206	VAL
2	H	209	LYS
2	H	213	GLU
2	H	215	ILE
2	H	227	ILE
2	H	232	SER
2	H	234	LYS
2	H	238	VAL
2	H	253	GLN
2	H	284	ASN
2	H	296	ASN
2	H	321	LYS
2	H	323	LYS
2	H	330	THR
2	H	359	GLN
2	H	380	ARG
2	H	387	THR
2	H	415	ARG
3	I	4	THR
3	I	5	ARG
3	I	7	ASN
3	I	8	CYS

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Mol	Chain	Res	Type
3	I	32	TYR
3	I	40	LEU
3	I	52	ASN
3	I	53	LYS
3	I	78	MET
3	I	94	MET
3	I	115	ASN
3	I	128	VAL
3	I	137	GLU
3	I	149	THR
3	I	166	LEU
3	I	195	GLN
3	I	196	LYS
3	I	198	LEU
3	I	207	ASN
3	I	209	ILE
3	I	223	THR
3	I	237	SER
3	I	240	SER
3	I	242	ILE
3	I	250	LEU
3	I	258	SER
3	I	266	LYS
3	I	267	VAL
3	I	277	THR
3	I	285	ASP
3	I	294	ASP
3	I	310	MET
3	I	325	ASN
3	I	356	LYS
3	I	365	ASN
3	I	382	THR
3	I	383	THR
3	I	385	LYS
3	I	386	ILE
3	I	390	ASN
3	I	392	LEU
1	J	28	CYS
1	J	39	GLU
1	J	41	TRP
1	J	58	VAL
1	J	68	LYS

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Mol	Chain	Res	Type
1	J	69	LEU
1	J	71	ASN
1	J	73	LEU
1	J	80	ASN
1	J	82	ASP
1	J	106	ASN
1	J	107	THR
1	J	109	ASN
1	J	111	VAL
1	J	113	GLU
1	J	114	ASP
1	J	121	VAL
1	J	123	LYS
1	J	138	LYS
1	J	150	LEU
1	J	156	ILE
1	J	158	ILE
1	J	169	LEU
1	J	172	GLU
1	J	181	GLN
1	J	185	LEU
1	J	191	LYS
1	J	201	HIS
1	J	204	LEU
2	K	66	LEU
2	K	84	GLU
2	K	87	LEU
2	K	95	ASN
2	K	96	SER
2	K	128	ARG
2	K	135	ASN
2	K	140	ASN
2	K	145	GLU
2	K	149	HIS
2	K	150	GLN
2	K	152	TYR
2	K	172	LEU
2	K	174	ASN
2	K	179	ILE
2	K	186	VAL
2	K	190	MET
2	K	199	VAL

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Mol	Chain	Res	Type
2	K	209	LYS
2	K	226	LEU
2	K	227	ILE
2	K	238	VAL
2	K	252	ILE
2	K	253	GLN
2	K	280	THR
2	K	297	ASP
2	K	302	LEU
2	K	310	LEU
2	K	312	ILE
2	K	321	LYS
2	K	323	LYS
2	K	325	HIS
2	K	330	THR
2	K	342	VAL
2	K	359	GLN
2	K	377	THR
2	K	387	THR
2	K	415	ARG
2	K	436	VAL
2	K	439	ASN
2	K	443	SER
2	K	458	PHE
3	L	8	CYS
3	L	22	THR
3	L	27	ASP
3	L	29	LEU
3	L	40	LEU
3	L	90	LEU
3	L	97	GLU
3	L	110	LEU
3	L	111	GLN
3	L	113	ILE
3	L	122	VAL
3	L	143	VAL
3	L	147	ASP
3	L	149	THR
3	L	151	LYS
3	L	156	ILE
3	L	170	LYS
3	L	175	ASN

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Mol	Chain	Res	Type
3	L	176	GLN
3	L	180	VAL
3	L	184	ILE
3	L	185	ASP
3	L	198	LEU
3	L	199	ASP
3	L	233	ILE
3	L	242	ILE
3	L	249	GLU
3	L	250	LEU
3	L	259	THR
3	L	261	ASP
3	L	264	MET
3	L	267	VAL
3	L	276	LEU
3	L	297	ASP
3	L	314	THR
3	L	344	LEU
3	L	353	THR
3	L	361	ASN
3	L	374	THR
3	L	376	TRP
3	L	380	LYS
3	L	383	THR
3	L	389	PHE
4	M	3	ARG
4	N	3	ARG
4	Q	3	ARG
4	R	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	71	ASN
1	A	79	ASN
1	A	80	ASN
1	A	84	HIS
1	A	89	ASN
1	A	103	ASN
1	A	134	GLN
1	A	139	ASN

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Mol	Chain	Res	Type
1	A	184	GLN
1	A	200	GLN
2	B	67	HIS
2	B	88	GLN
2	B	89	GLN
2	B	95	ASN
2	B	129	GLN
2	B	137	ASN
2	B	160	ASN
2	B	164	ASN
2	B	189	GLN
2	B	243	ASN
2	B	253	GLN
2	B	256	GLN
2	B	271	GLN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	343	ASN
2	B	351	ASN
2	B	393	GLN
2	B	408	HIS
2	B	421	GLN
3	C	41	GLN
3	C	69	ASN
3	C	103	HIS
3	C	117	ASN
3	C	119	GLN
3	C	123	ASN
3	C	136	GLN
3	C	144	GLN
3	C	146	HIS
3	C	230	ASN
3	C	239	GLN
3	C	254	ASN
3	C	307	HIS
3	C	325	ASN
3	C	329	GLN
3	C	365	ASN
3	C	390	ASN
1	D	42	ASN
1	D	64	ASN

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Mol	Chain	Res	Type
1	D	131	GLN
1	D	143	GLN
1	D	182	GLN
1	D	187	GLN
1	D	200	GLN
2	E	67	HIS
2	E	83	GLN
2	E	88	GLN
2	E	89	GLN
2	E	129	GLN
2	E	164	ASN
2	E	228	GLN
2	E	253	GLN
2	E	256	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	332	GLN
2	E	339	GLN
2	E	351	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	33	GLN
3	F	48	HIS
3	F	118	ASN
3	F	123	ASN
3	F	130	GLN
3	F	136	GLN
3	F	176	GLN
3	F	189	ASN
3	F	210	GLN
3	F	230	ASN
3	F	254	ASN
3	F	317	ASN
3	F	365	ASN
1	G	59	ASN
1	G	60	GLN
1	G	71	ASN
1	G	77	GLN
1	G	84	HIS
1	G	134	GLN

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Mol	Chain	Res	Type
1	G	139	ASN
1	G	181	GLN
1	G	182	GLN
1	G	184	GLN
2	H	88	GLN
2	H	95	ASN
2	H	140	ASN
2	H	150	GLN
2	H	158	ASN
2	H	160	ASN
2	H	180	GLN
2	H	253	GLN
2	H	256	GLN
2	H	296	ASN
2	H	301	GLN
2	H	325	HIS
2	H	351	ASN
2	H	359	GLN
2	H	408	HIS
2	H	413	ASN
2	H	421	GLN
2	H	439	ASN
3	I	59	GLN
3	I	115	ASN
3	I	123	ASN
3	I	134	GLN
3	I	136	GLN
3	I	144	GLN
3	I	207	ASN
3	I	230	ASN
3	I	239	GLN
3	I	254	ASN
3	I	325	ASN
3	I	337	ASN
3	I	365	ASN
3	I	390	ASN
1	J	67	ASN
1	J	84	HIS
1	J	106	ASN
1	J	131	GLN
1	J	182	GLN
1	J	184	GLN

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Mol	Chain	Res	Type
2	K	83	GLN
2	K	95	ASN
2	K	135	ASN
2	K	158	ASN
2	K	160	ASN
2	K	189	GLN
2	K	243	ASN
2	K	253	GLN
2	K	256	GLN
2	K	296	ASN
2	K	301	GLN
2	K	351	ASN
2	K	364	ASN
2	K	421	GLN
2	K	439	ASN
3	L	7	ASN
3	L	33	GLN
3	L	49	GLN
3	L	52	ASN
3	L	59	GLN
3	L	115	ASN
3	L	136	GLN
3	L	144	GLN
3	L	177	GLN
3	L	189	ASN
3	L	239	GLN
3	L	317	ASN
3	L	325	ASN
3	L	350	GLN
3	L	361	ASN
3	L	365	ASN

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 ⓘ

40 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$
6	NAG	U	1	6	14,14,15	0.94	0	17,19,21	1.51	1 (5%)
6	GAL	U	10	6	11,11,12	0.96	0	15,15,17	0.72	0
6	SIA	U	11	6	20,20,21	1.63	3 (15%)	21,28,31	0.98	1 (4%)
6	NAG	U	2	6	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
6	BMA	U	3	6	11,11,12	1.06	1 (9%)	15,15,17	1.15	1 (6%)
6	MAN	U	4	6	11,11,12	1.16	0	15,15,17	0.92	1 (6%)
6	NAG	U	5	6	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
6	GAL	U	6	6	11,11,12	0.62	0	15,15,17	0.52	0
6	SIA	U	7	6	20,20,21	1.73	7 (35%)	21,28,31	0.97	1 (4%)
6	MAN	U	8	6	11,11,12	1.61	3 (27%)	15,15,17	1.23	1 (6%)
6	NAG	U	9	6	14,14,15	1.10	1 (7%)	17,19,21	0.87	0
6	NAG	V	1	2,6	14,14,15	0.79	0	17,19,21	1.20	3 (17%)
6	GAL	V	10	6	11,11,12	0.96	1 (9%)	15,15,17	0.80	1 (6%)
6	SIA	V	11	6	20,20,21	1.32	2 (10%)	21,28,31	0.92	1 (4%)
6	NAG	V	2	6	14,14,15	0.96	1 (7%)	17,19,21	0.98	0
6	BMA	V	3	6	11,11,12	1.09	1 (9%)	15,15,17	1.24	1 (6%)
6	MAN	V	4	6	11,11,12	1.42	2 (18%)	15,15,17	1.12	1 (6%)
6	NAG	V	5	6	14,14,15	1.25	2 (14%)	17,19,21	0.86	0
6	GAL	V	6	6	11,11,12	1.18	1 (9%)	15,15,17	0.72	0
6	SIA	V	7	6	20,20,21	0.96	1 (5%)	21,28,31	1.02	2 (9%)
6	MAN	V	8	6	11,11,12	0.95	0	15,15,17	1.47	3 (20%)
6	NAG	V	9	6	14,14,15	1.14	1 (7%)	17,19,21	0.91	1 (5%)
7	NAG	W	1	2,7	14,14,15	0.68	0	17,19,21	1.17	2 (11%)
7	NAG	W	2	7	14,14,15	0.82	1 (7%)	17,19,21	1.02	1 (5%)
7	BMA	W	3	7	11,11,12	0.76	0	15,15,17	1.02	1 (6%)
7	MAN	W	4	7	11,11,12	1.17	2 (18%)	15,15,17	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	W	5	7	11,11,12	0.63	0	15,15,17	0.63	0
6	NAG	X	1	6	14,14,15	0.97	0	17,19,21	1.30	3 (17%)
6	GAL	X	10	6	11,11,12	1.26	1 (9%)	15,15,17	0.68	0
6	SIA	X	11	6	20,20,21	1.22	1 (5%)	21,28,31	1.06	1 (4%)
6	NAG	X	2	6	14,14,15	1.27	2 (14%)	17,19,21	1.01	0
6	BMA	X	3	6	11,11,12	1.28	1 (9%)	15,15,17	0.97	1 (6%)
6	MAN	X	4	6	11,11,12	1.04	0	15,15,17	1.28	2 (13%)
6	NAG	X	5	6	14,14,15	1.11	2 (14%)	17,19,21	0.95	0
6	GAL	X	6	6	11,11,12	1.03	0	15,15,17	0.88	0
6	SIA	X	7	6	20,20,21	1.33	3 (15%)	21,28,31	1.27	3 (14%)
6	MAN	X	8	6	11,11,12	1.12	2 (18%)	15,15,17	1.24	3 (20%)
6	NAG	X	9	6	14,14,15	1.13	1 (7%)	17,19,21	1.13	2 (11%)
8	NAG	Y	1	8	14,14,15	1.01	0	17,19,21	1.05	2 (11%)
8	NAG	Y	2	8	14,14,15	1.24	2 (14%)	17,19,21	0.87	1 (5%)

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
6	NAG	U	1	6	-	2/6/23/26	0/1/1/1
6	GAL	U	10	6	-	2/2/19/22	0/1/1/1
6	SIA	U	11	6	-	2/18/34/38	0/1/1/1
6	NAG	U	2	6	1/1/5/7	5/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	2/2/19/22	0/1/1/1
6	NAG	U	5	6	1/1/5/7	2/6/23/26	0/1/1/1
6	GAL	U	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	U	7	6	-	11/18/34/38	0/1/1/1
6	MAN	U	8	6	-	1/2/19/22	0/1/1/1
6	NAG	U	9	6	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	V	1	2,6	1/1/5/7	4/6/23/26	0/1/1/1
6	GAL	V	10	6	-	1/2/19/22	0/1/1/1
6	SIA	V	11	6	-	6/18/34/38	0/1/1/1
6	NAG	V	2	6	1/1/5/7	6/6/23/26	0/1/1/1
6	BMA	V	3	6	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	V	4	6	-	1/2/19/22	0/1/1/1
6	NAG	V	5	6	1/1/5/7	3/6/23/26	0/1/1/1
6	GAL	V	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	V	7	6	-	11/18/34/38	0/1/1/1
6	MAN	V	8	6	-	2/2/19/22	0/1/1/1
6	NAG	V	9	6	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	W	1	2,7	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	W	2	7	1/1/5/7	5/6/23/26	0/1/1/1
7	BMA	W	3	7	-	1/2/19/22	0/1/1/1
7	MAN	W	4	7	-	1/2/19/22	0/1/1/1
7	MAN	W	5	7	-	2/2/19/22	0/1/1/1
6	NAG	X	1	6	-	4/6/23/26	0/1/1/1
6	GAL	X	10	6	-	2/2/19/22	0/1/1/1
6	SIA	X	11	6	-	11/18/34/38	0/1/1/1
6	NAG	X	2	6	1/1/5/7	3/6/23/26	0/1/1/1
6	BMA	X	3	6	-	2/2/19/22	0/1/1/1
6	MAN	X	4	6	-	2/2/19/22	0/1/1/1
6	NAG	X	5	6	1/1/5/7	4/6/23/26	0/1/1/1
6	GAL	X	6	6	1/1/4/5	2/2/19/22	0/1/1/1
6	SIA	X	7	6	-	12/18/34/38	0/1/1/1
6	MAN	X	8	6	-	2/2/19/22	0/1/1/1
6	NAG	X	9	6	1/1/5/7	2/6/23/26	0/1/1/1
8	NAG	Y	1	8	-	5/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	6/6/23/26	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	11	SIA	C3-C2	4.67	1.60	1.52
6	U	8	MAN	C2-C3	3.93	1.58	1.52
6	X	7	SIA	C4-C5	3.55	1.56	1.53
6	U	7	SIA	C2-C1	3.43	1.56	1.52
6	X	11	SIA	C2-C1	3.42	1.56	1.52
6	U	7	SIA	C4-C5	3.31	1.56	1.53
8	Y	2	NAG	C1-C2	3.24	1.56	1.52
6	V	11	SIA	C2-C1	3.15	1.56	1.52
6	U	11	SIA	C2-C1	3.14	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	3	BMA	C2-C3	3.13	1.57	1.52
6	V	9	NAG	C1-C2	2.94	1.56	1.52
6	V	4	MAN	C4-C5	2.90	1.59	1.53
6	V	2	NAG	C1-C2	2.79	1.56	1.52
6	X	2	NAG	C1-C2	2.69	1.56	1.52
6	U	5	NAG	C1-C2	2.67	1.56	1.52
6	X	5	NAG	C1-C2	2.63	1.55	1.52
7	W	4	MAN	C4-C3	2.62	1.59	1.52
6	U	7	SIA	C7-C6	2.54	1.56	1.52
6	V	5	NAG	O5-C5	2.53	1.48	1.43
6	X	2	NAG	O5-C5	2.49	1.48	1.43
6	U	7	SIA	C3-C2	2.43	1.56	1.52
7	W	4	MAN	C4-C5	2.42	1.58	1.53
6	V	10	GAL	C1-C2	2.41	1.58	1.52
6	X	9	NAG	C1-C2	2.39	1.55	1.52
6	V	11	SIA	C4-C5	2.38	1.55	1.53
7	W	2	NAG	C1-C2	2.35	1.55	1.52
6	V	4	MAN	C2-C3	2.33	1.56	1.52
6	U	9	NAG	C1-C2	2.32	1.55	1.52
6	X	7	SIA	C3-C2	2.32	1.56	1.52
6	U	8	MAN	O2-C2	2.25	1.48	1.43
6	X	7	SIA	C3-C4	2.22	1.56	1.52
6	X	8	MAN	C1-C2	2.18	1.57	1.52
6	X	8	MAN	C2-C3	2.16	1.55	1.52
8	Y	2	NAG	O5-C5	2.15	1.47	1.43
6	U	7	SIA	O6-C2	2.14	1.47	1.43
6	X	10	GAL	C1-C2	2.13	1.57	1.52
6	U	7	SIA	C6-C5	2.12	1.56	1.53
6	V	7	SIA	C4-C5	2.11	1.55	1.53
6	U	11	SIA	O6-C6	2.08	1.47	1.44
6	V	6	GAL	O5-C5	2.08	1.47	1.43
6	U	7	SIA	O6-C6	2.04	1.47	1.44
6	X	3	BMA	C2-C3	2.02	1.55	1.52
6	U	3	BMA	O3-C3	2.02	1.47	1.43
6	V	5	NAG	C4-C5	2.01	1.57	1.53
6	X	5	NAG	O5-C5	2.01	1.47	1.43
6	U	8	MAN	C1-C2	2.01	1.57	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	1	NAG	C2-N2-C7	-5.42	115.64	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	8	MAN	C1-C2-C3	3.92	115.36	109.64
6	X	4	MAN	C3-C4-C5	3.58	116.73	110.23
6	V	3	BMA	C1-C2-C3	-3.52	104.52	109.64
7	W	4	MAN	C3-C4-C5	3.41	116.41	110.23
6	U	8	MAN	C1-C2-C3	3.37	114.56	109.64
7	W	3	BMA	C1-C2-C3	-3.32	104.81	109.64
7	W	1	NAG	C2-N2-C7	-3.25	118.55	122.90
6	X	9	NAG	C2-N2-C7	-3.25	118.55	122.90
6	X	1	NAG	C2-N2-C7	-3.09	118.76	122.90
6	X	8	MAN	C1-C2-C3	2.94	113.92	109.64
6	X	4	MAN	C2-C3-C4	2.91	115.97	110.86
6	V	1	NAG	C1-O5-C5	2.89	116.06	112.19
6	U	3	BMA	C3-C4-C5	2.79	115.30	110.23
8	Y	1	NAG	C4-C3-C2	2.74	115.04	111.02
6	X	7	SIA	C8-C7-C6	-2.72	107.95	113.05
7	W	2	NAG	C2-N2-C7	-2.65	119.35	122.90
6	X	11	SIA	O1B-C1-C2	2.63	119.55	112.71
6	X	1	NAG	C1-O5-C5	2.60	115.67	112.19
6	X	8	MAN	C6-C5-C4	2.57	119.34	113.02
6	V	1	NAG	C4-C3-C2	-2.56	107.27	111.02
6	U	11	SIA	O1B-C1-C2	2.50	119.22	112.71
6	U	5	NAG	C3-C4-C5	2.48	114.73	110.23
8	Y	2	NAG	C1-O5-C5	2.47	115.50	112.19
6	V	11	SIA	O1B-C1-C2	2.46	119.12	112.71
6	V	1	NAG	C2-N2-C7	-2.45	119.61	122.90
6	U	2	NAG	C2-N2-C7	-2.42	119.66	122.90
6	X	7	SIA	C5-N5-C10	-2.39	117.52	123.11
6	V	8	MAN	C2-C3-C4	2.36	115.02	110.86
6	V	8	MAN	O2-C2-C1	2.36	114.63	109.22
6	V	10	GAL	C1-C2-C3	2.34	113.05	109.64
6	U	4	MAN	C2-C3-C4	2.34	114.97	110.86
6	U	7	SIA	O1B-C1-C2	2.30	118.68	112.71
6	V	4	MAN	C1-O5-C5	2.30	115.26	112.19
6	X	3	BMA	C2-C3-C4	-2.25	106.90	110.86
6	X	1	NAG	C6-C5-C4	2.13	118.25	113.02
6	V	7	SIA	O1B-C1-C2	2.09	118.15	112.71
8	Y	1	NAG	C2-N2-C7	-2.05	120.15	122.90
6	V	9	NAG	C2-N2-C7	-2.05	120.16	122.90
7	W	1	NAG	C1-C2-N2	-2.04	107.21	110.43
6	V	7	SIA	O1A-C1-C2	-2.04	118.44	122.85
6	X	9	NAG	C6-C5-C4	2.02	117.98	113.02
6	X	8	MAN	O2-C2-C1	2.01	113.82	109.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	7	SIA	C11-C10-N5	2.00	119.44	116.12

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	U	2	NAG	C1
6	U	5	NAG	C1
6	U	6	GAL	C1
6	U	9	NAG	C1
6	V	1	NAG	C1
6	V	2	NAG	C1
6	V	5	NAG	C1
6	V	6	GAL	C1
6	V	9	NAG	C1
6	X	2	NAG	C1
6	X	5	NAG	C1
6	X	6	GAL	C1
6	X	9	NAG	C1
7	W	1	NAG	C1
7	W	2	NAG	C1

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	U	1	NAG	C8-C7-N2-C2
6	U	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C1-C2-N2-C7
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	U	5	NAG	C8-C7-N2-C2
6	U	5	NAG	O7-C7-N2-C2
6	U	7	SIA	C5-C6-C7-C8
6	U	7	SIA	C5-C6-C7-O7
6	U	7	SIA	O6-C6-C7-C8
6	U	7	SIA	O6-C6-C7-O7
6	U	7	SIA	C11-C10-N5-C5
6	U	7	SIA	O10-C10-N5-C5
6	U	9	NAG	C8-C7-N2-C2
6	U	9	NAG	O7-C7-N2-C2
6	U	11	SIA	C11-C10-N5-C5
6	U	11	SIA	O10-C10-N5-C5
6	V	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	V	1	NAG	O7-C7-N2-C2
6	V	7	SIA	C5-C6-C7-O7
6	V	7	SIA	O6-C6-C7-O7
6	V	7	SIA	C6-C7-C8-C9
6	V	7	SIA	C6-C7-C8-O8
6	V	7	SIA	O7-C7-C8-C9
6	V	7	SIA	O7-C7-C8-O8
6	V	7	SIA	C11-C10-N5-C5
6	V	7	SIA	O10-C10-N5-C5
6	V	9	NAG	C8-C7-N2-C2
6	V	9	NAG	O7-C7-N2-C2
6	V	11	SIA	C5-C6-C7-C8
6	V	11	SIA	C5-C6-C7-O7
6	V	11	SIA	O6-C6-C7-C8
6	V	11	SIA	O6-C6-C7-O7
6	V	11	SIA	C7-C8-C9-O9
6	X	1	NAG	C8-C7-N2-C2
6	X	1	NAG	O7-C7-N2-C2
6	X	2	NAG	C1-C2-N2-C7
6	X	2	NAG	C8-C7-N2-C2
6	X	2	NAG	O7-C7-N2-C2
6	X	5	NAG	C8-C7-N2-C2
6	X	5	NAG	O7-C7-N2-C2
6	X	7	SIA	O1A-C1-C2-O6
6	X	7	SIA	C5-C6-C7-O7
6	X	7	SIA	O6-C6-C7-O7
6	X	7	SIA	C11-C10-N5-C5
6	X	7	SIA	O10-C10-N5-C5
6	X	9	NAG	C8-C7-N2-C2
6	X	9	NAG	O7-C7-N2-C2
6	X	11	SIA	O1A-C1-C2-O6
6	X	11	SIA	C5-C6-C7-C8
6	X	11	SIA	C5-C6-C7-O7
6	X	11	SIA	O6-C6-C7-C8
6	X	11	SIA	O6-C6-C7-O7
6	X	11	SIA	O8-C8-C9-O9
6	X	11	SIA	C11-C10-N5-C5
6	X	11	SIA	O10-C10-N5-C5
7	W	1	NAG	C8-C7-N2-C2
7	W	1	NAG	O7-C7-N2-C2
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	Y	2	NAG	C8-C7-N2-C2
8	Y	2	NAG	O7-C7-N2-C2
7	W	2	NAG	C8-C7-N2-C2
7	W	2	NAG	O7-C7-N2-C2
6	X	4	MAN	C4-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	V	11	SIA	O8-C8-C9-O9
6	X	4	MAN	O5-C5-C6-O6
6	X	11	SIA	C7-C8-C9-O9
6	U	9	NAG	C4-C5-C6-O6
6	V	6	GAL	O5-C5-C6-O6
6	X	3	BMA	O5-C5-C6-O6
6	V	6	GAL	C4-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
6	X	10	GAL	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
6	V	2	NAG	C8-C7-N2-C2
6	U	9	NAG	O5-C5-C6-O6
6	X	5	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	U	6	GAL	O5-C5-C6-O6
6	U	10	GAL	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6
6	X	6	GAL	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	X	5	NAG	C4-C5-C6-O6
6	X	8	MAN	C4-C5-C6-O6
6	X	10	GAL	C4-C5-C6-O6
6	U	6	GAL	C4-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
6	U	10	GAL	O5-C5-C6-O6
6	X	6	GAL	O5-C5-C6-O6
6	V	2	NAG	O7-C7-N2-C2
6	V	5	NAG	C8-C7-N2-C2
6	V	5	NAG	O7-C7-N2-C2
6	V	1	NAG	O5-C5-C6-O6
6	V	8	MAN	O5-C5-C6-O6
8	Y	2	NAG	C4-C5-C6-O6
6	X	8	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	X	3	BMA	C4-C5-C6-O6
6	U	4	MAN	C4-C5-C6-O6
7	W	4	MAN	O5-C5-C6-O6
6	U	7	SIA	C6-C7-C8-O8
7	W	1	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
6	U	7	SIA	O7-C7-C8-O8
6	X	1	NAG	O5-C5-C6-O6
6	X	7	SIA	O7-C7-C8-C9
6	V	10	GAL	O5-C5-C6-O6
6	V	9	NAG	O5-C5-C6-O6
7	W	3	BMA	O5-C5-C6-O6
7	W	5	MAN	C4-C5-C6-O6
6	V	3	BMA	O5-C5-C6-O6
6	V	5	NAG	C4-C5-C6-O6
6	U	7	SIA	C6-C7-C8-C9
6	U	8	MAN	O5-C5-C6-O6
7	W	1	NAG	C4-C5-C6-O6
8	Y	2	NAG	C3-C2-N2-C7
6	V	7	SIA	O1A-C1-C2-O6
8	Y	2	NAG	O5-C5-C6-O6
6	X	7	SIA	C6-C7-C8-C9
6	X	7	SIA	O7-C7-C8-O8
6	V	2	NAG	C1-C2-N2-C7
7	W	2	NAG	C1-C2-N2-C7
6	X	7	SIA	C6-C7-C8-O8
6	X	11	SIA	O1A-C1-C2-C3
6	X	11	SIA	O1B-C1-C2-C3
6	V	7	SIA	O6-C6-C7-C8
6	X	7	SIA	O6-C6-C7-C8
7	W	5	MAN	O5-C5-C6-O6
6	V	7	SIA	C5-C6-C7-C8
6	X	7	SIA	C5-C6-C7-C8
7	W	2	NAG	C3-C2-N2-C7
6	U	7	SIA	O1A-C1-C2-O6
6	X	1	NAG	C4-C5-C6-O6
6	U	7	SIA	O7-C7-C8-C9
6	X	7	SIA	O1B-C1-C2-O6
8	Y	1	NAG	C1-C2-N2-C7
8	Y	2	NAG	C1-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	V	8	MAN	C4-C5-C6-O6

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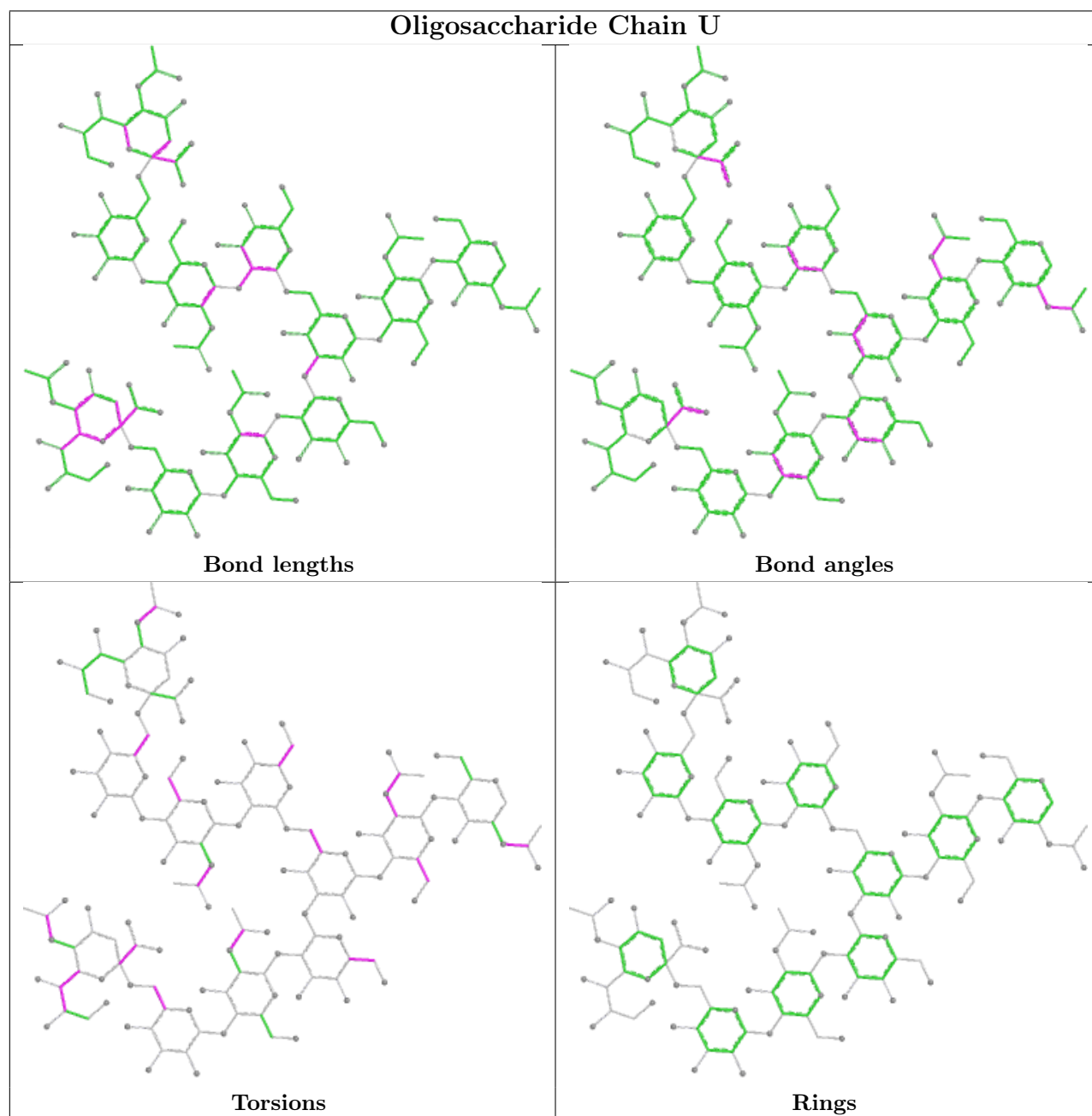
Mol	Chain	Res	Type	Atoms
6	V	4	MAN	O5-C5-C6-O6

There are no ring outliers.

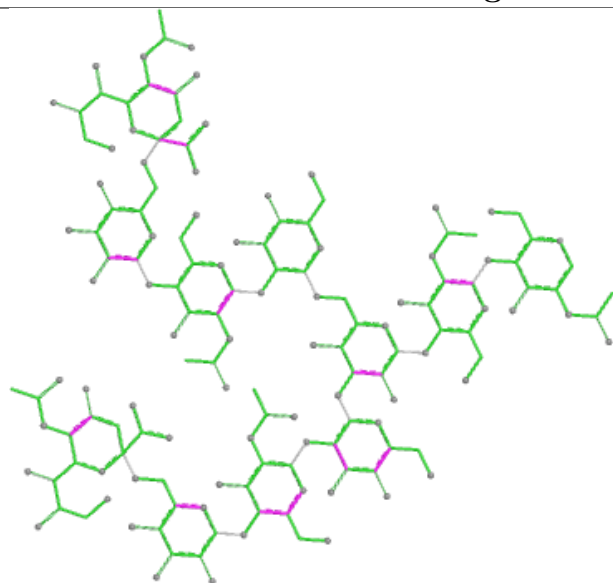
36 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	6	GAL	2	0
7	W	2	NAG	3	0
6	V	4	MAN	2	0
6	U	1	NAG	9	0
6	X	3	BMA	2	0
6	V	10	GAL	1	0
6	U	10	GAL	1	0
6	U	3	BMA	3	0
6	X	8	MAN	2	0
7	W	1	NAG	5	0
6	V	7	SIA	5	0
6	V	5	NAG	3	0
6	X	10	GAL	1	0
6	V	3	BMA	4	0
6	X	6	GAL	1	0
6	U	7	SIA	5	0
6	X	5	NAG	4	0
6	U	8	MAN	4	0
6	X	1	NAG	7	0
6	X	2	NAG	7	0
6	V	11	SIA	1	0
7	W	3	BMA	1	0
6	X	7	SIA	1	0
6	V	9	NAG	1	0
6	X	9	NAG	2	0
6	X	11	SIA	3	0
6	U	2	NAG	6	0
6	U	6	GAL	4	0
6	V	8	MAN	1	0
6	U	5	NAG	2	0
6	U	9	NAG	4	0
8	Y	1	NAG	12	0
8	Y	2	NAG	1	0
6	V	1	NAG	2	0
6	V	2	NAG	4	0
6	U	11	SIA	1	0

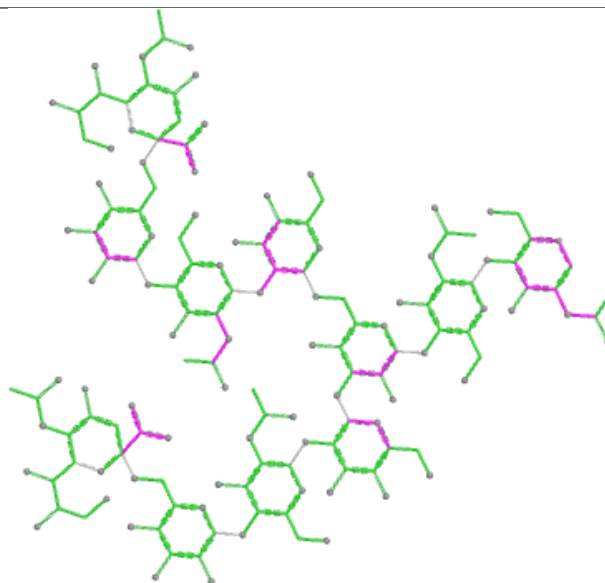
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



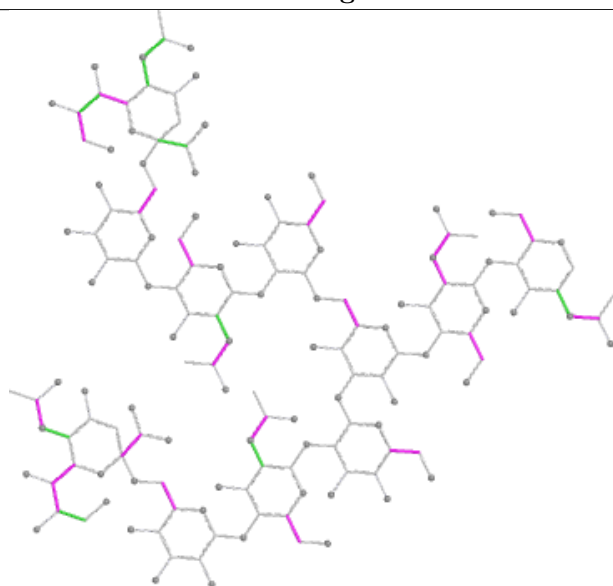
Oligosaccharide Chain V



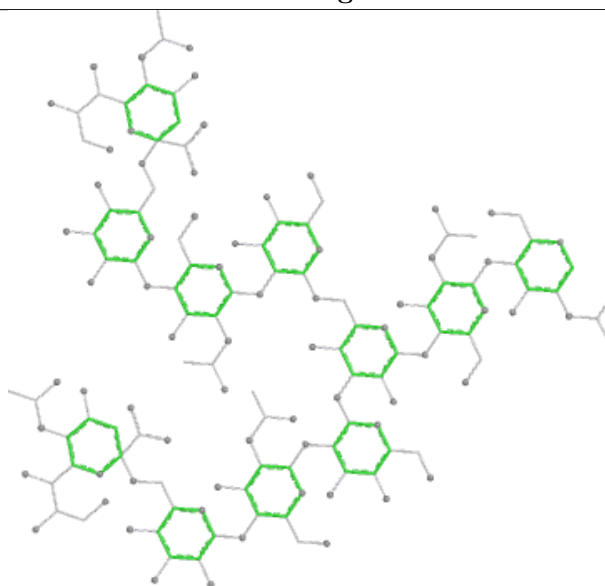
Bond lengths



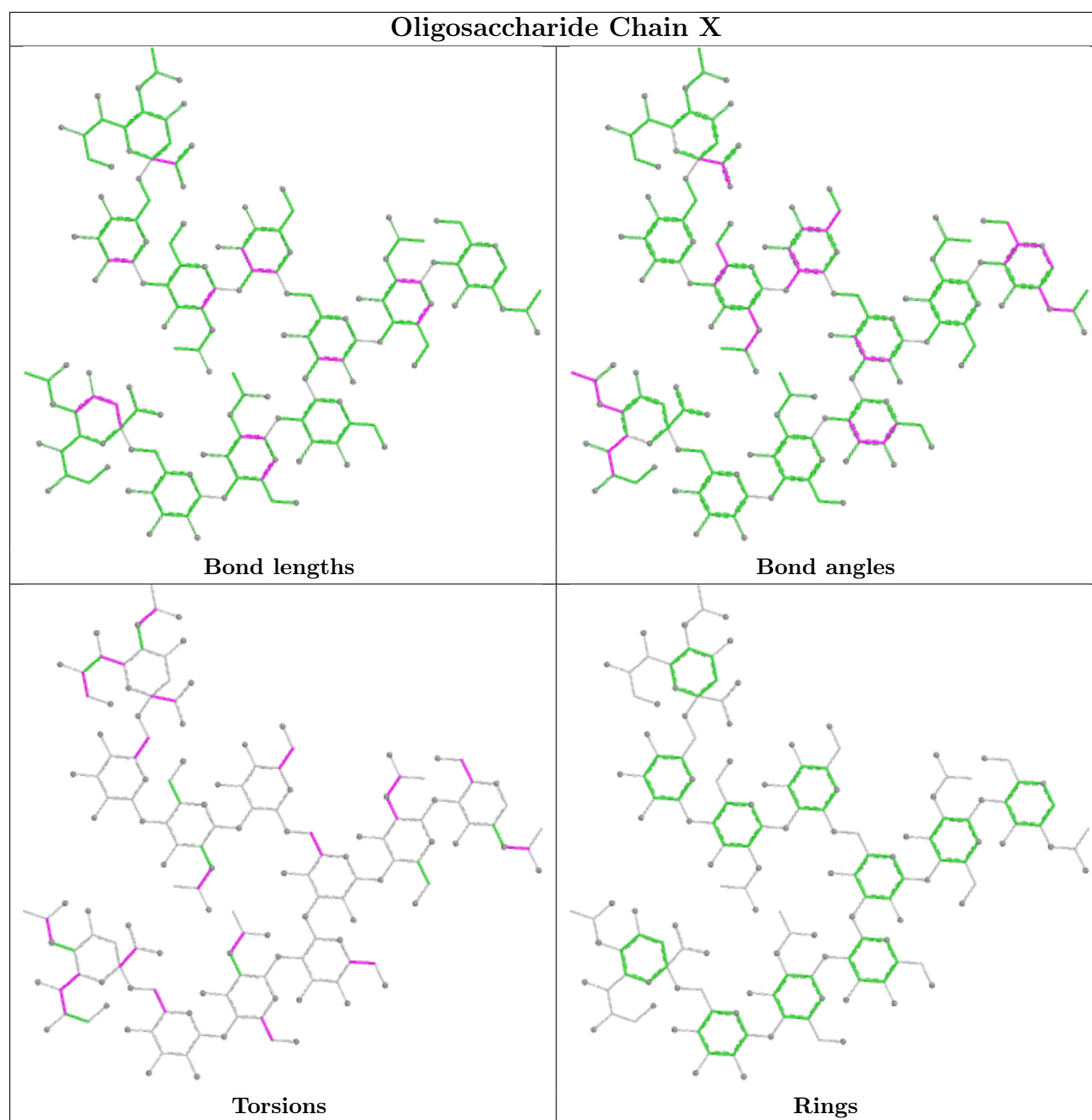
Bond angles

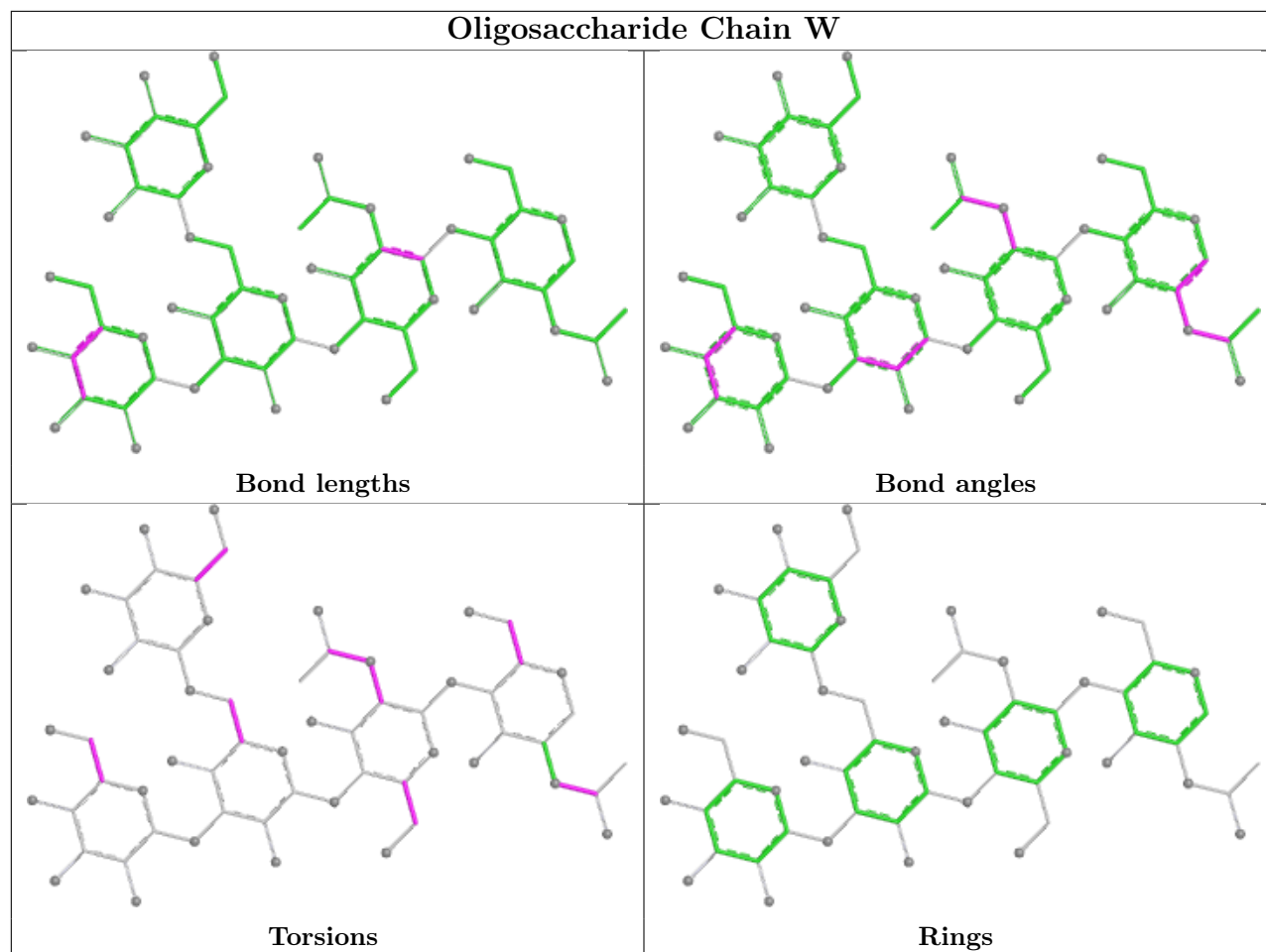


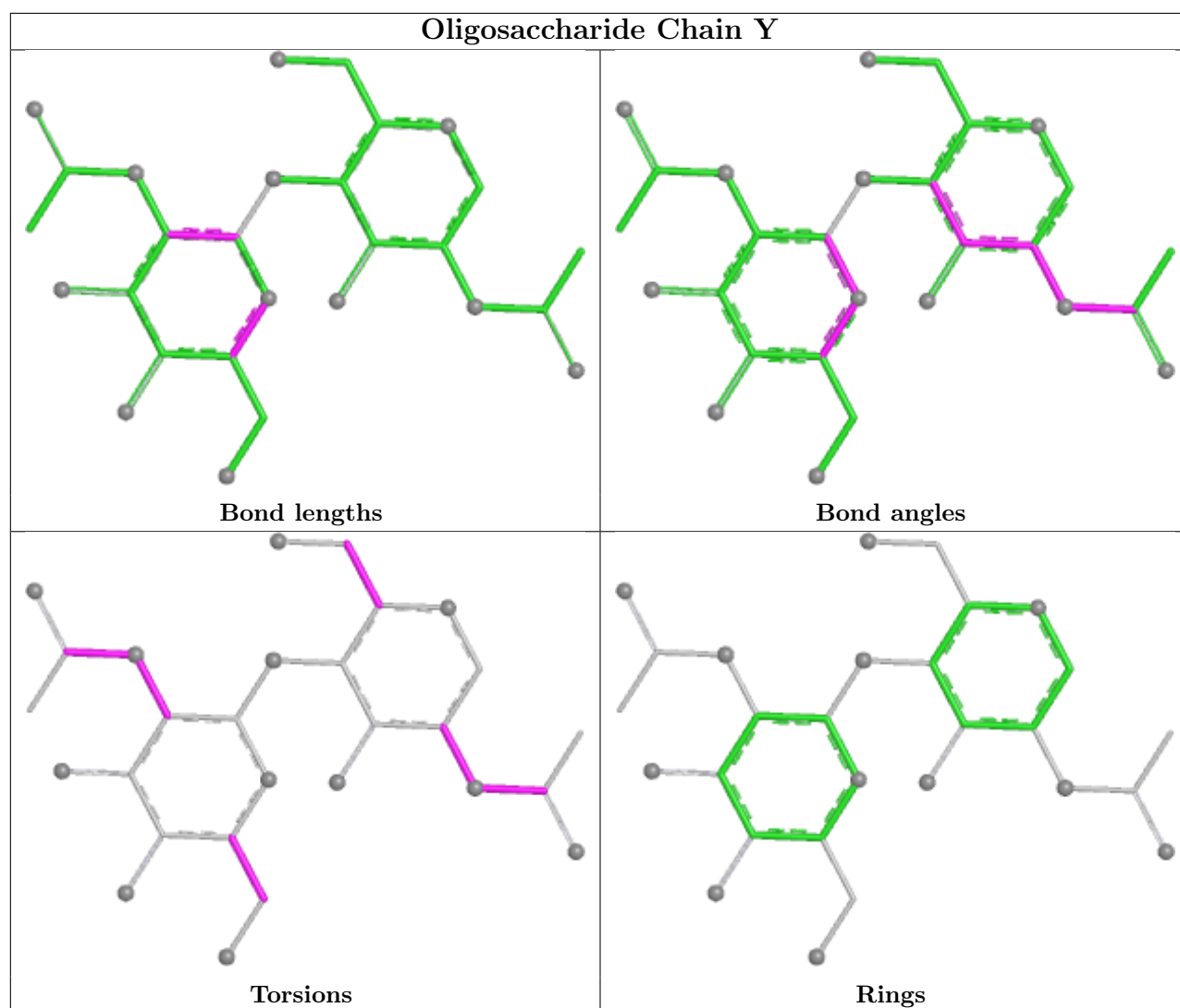
Torsions



Rings







5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	174/562 (30%)	0.49	14 (8%) 18 15	21, 106, 173, 187	0
1	D	174/562 (30%)	1.22	43 (24%) 2 1	62, 137, 231, 238	0
1	G	174/562 (30%)	0.46	9 (5%) 33 26	51, 120, 163, 173	0
1	J	186/562 (33%)	0.90	22 (11%) 9 7	64, 135, 224, 246	0
2	B	401/461 (86%)	0.32	30 (7%) 20 16	21, 53, 151, 184	0
2	E	401/461 (86%)	0.45	34 (8%) 16 14	40, 64, 211, 226	0
2	H	401/461 (86%)	0.17	14 (3%) 47 38	30, 62, 168, 195	0
2	K	401/461 (86%)	0.32	17 (4%) 40 32	40, 64, 156, 164	0
3	C	381/411 (92%)	-0.05	12 (3%) 51 42	8, 39, 189, 232	0
3	F	382/411 (92%)	0.58	33 (8%) 16 13	52, 89, 208, 221	0
3	I	394/411 (95%)	0.43	18 (4%) 37 29	29, 69, 179, 207	0
3	L	391/411 (95%)	0.30	23 (5%) 28 22	35, 70, 177, 203	0
4	M	4/4 (100%)	0.63	0 100 100	63, 64, 103, 108	0
4	N	4/4 (100%)	0.75	0 100 100	119, 131, 149, 154	0
4	Q	4/4 (100%)	0.21	0 100 100	78, 89, 90, 115	0
4	R	4/4 (100%)	0.90	0 100 100	92, 105, 106, 118	0
5	O	4/4 (100%)	0.23	0 100 100	66, 68, 73, 93	0
5	P	4/4 (100%)	0.75	0 100 100	90, 99, 106, 113	0
5	S	4/4 (100%)	0.28	0 100 100	58, 69, 75, 95	0
5	T	4/4 (100%)	0.73	0 100 100	75, 91, 98, 108	0
All	All	3892/5768 (67%)	0.40	269 (6%) 23 18	8, 75, 189, 246	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	76	TYR	8.4
1	D	44	LYS	5.9
2	K	125	TRP	5.7
2	E	218	GLY	5.3
3	F	79	ILE	5.3
1	D	115	LEU	5.3
2	E	153	ILE	5.2
3	F	107	ILE	5.1
1	D	76	TYR	4.9
3	L	5	ARG	4.9
2	B	143	SER	4.8
2	K	150	GLN	4.7
3	I	19	CYS	4.7
2	H	73	GLY	4.6
2	E	150	GLN	4.5
2	B	75	LEU	4.4
1	D	83	SER	4.4
1	J	41	TRP	4.2
2	H	108	SER	4.2
2	H	74	VAL	4.1
3	I	9	CYS	4.1
2	B	74	VAL	4.1
1	D	119	ILE	4.1
1	D	96	GLY	4.0
2	E	219	GLY	4.0
1	J	29	LYS	4.0
1	J	206	LYS	4.0
2	B	219	GLY	4.0
1	D	35	PHE	4.0
1	J	105	ASP	3.9
3	C	68	TYR	3.9
2	E	143	SER	3.9
2	B	115	PHE	3.9
1	J	205	ILE	3.9
3	L	330	ASP	3.8
2	E	417	TYR	3.8
2	H	363	GLU	3.7
3	F	57	VAL	3.7
1	D	94	LEU	3.7
2	E	146	LEU	3.7
2	K	147	GLU	3.7
1	A	87	THR	3.6
2	E	151	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	K	395	SER	3.6
3	L	24	GLY	3.5
1	A	93	ILE	3.5
2	E	157	VAL	3.5
3	F	161	ALA	3.5
2	B	76	CYS	3.4
2	E	74	VAL	3.4
2	H	107	VAL	3.4
1	J	27	ALA	3.4
2	E	118	MET	3.4
1	D	114	ASP	3.4
3	L	87	ARG	3.3
1	A	28	CYS	3.3
2	B	218	GLY	3.3
3	C	60	LEU	3.3
1	D	62	PHE	3.3
2	E	115	PHE	3.3
2	H	355	ASP	3.2
1	D	194	LEU	3.2
1	A	111	VAL	3.2
1	D	118	ARG	3.2
1	J	69	LEU	3.2
2	E	73	GLY	3.2
2	H	219	GLY	3.2
3	L	16	GLY	3.2
2	E	139	VAL	3.1
3	F	364	ASP	3.1
1	D	126	VAL	3.1
3	F	46	ILE	3.1
3	F	110	LEU	3.1
2	B	205	VAL	3.1
3	I	381	LYS	3.1
1	J	158	ILE	3.1
2	K	121	LEU	3.1
3	I	21	THR	3.1
2	B	68	ALA	3.0
2	E	125	TRP	3.0
1	J	37	SER	3.0
3	F	53	LYS	3.0
2	B	229	PRO	3.0
3	F	68	TYR	2.9
3	F	50	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	90	ILE	2.9
1	J	181	GLN	2.9
2	B	142	TYR	2.9
3	L	83	THR	2.9
1	J	90	ILE	2.9
2	B	73	GLY	2.9
3	C	50	VAL	2.8
2	H	115	PHE	2.8
2	B	150	GLN	2.8
1	A	108	TYR	2.8
2	E	128	ARG	2.8
2	H	121	LEU	2.8
2	K	168	LEU	2.8
3	C	43	LEU	2.8
3	I	85	LYS	2.8
3	L	20	PRO	2.8
1	G	108	TYR	2.8
1	J	80	ASN	2.8
3	C	57	VAL	2.8
3	I	25	ILE	2.8
3	F	63	ALA	2.7
2	B	121	LEU	2.7
2	E	124	LEU	2.7
2	K	417	TYR	2.7
1	J	83	SER	2.7
2	K	107	VAL	2.7
1	D	93	ILE	2.7
1	D	122	LEU	2.7
2	H	218	GLY	2.7
2	K	433	ASP	2.7
2	B	204	PRO	2.7
2	E	93	ILE	2.7
3	F	64	ILE	2.7
1	D	127	ILE	2.7
1	D	168	ALA	2.7
1	A	76	TYR	2.7
2	E	152	TYR	2.7
2	B	208	GLY	2.7
1	J	38	ASP	2.7
2	B	112	SER	2.7
3	F	82	ALA	2.6
1	A	194	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	78	MET	2.6
2	E	164	ASN	2.6
3	I	20	PRO	2.6
1	J	210	VAL	2.6
3	C	394	ILE	2.6
3	L	79	ILE	2.6
1	D	27	ALA	2.6
3	L	161	ALA	2.6
3	F	208	TRP	2.6
1	D	43	TYR	2.6
1	D	163	GLY	2.6
1	G	150	LEU	2.6
2	E	165	LEU	2.6
3	F	47	LEU	2.5
3	C	61	ILE	2.5
3	F	56	GLU	2.5
1	D	101	ALA	2.5
1	J	35	PHE	2.5
1	D	33	TRP	2.5
2	B	64	GLY	2.5
3	I	169	ILE	2.5
3	L	82	ALA	2.5
1	G	56	ASP	2.5
2	E	395	SER	2.5
1	D	169	LEU	2.5
2	H	146	LEU	2.5
3	F	60	LEU	2.5
2	B	153	ILE	2.5
3	F	209	ILE	2.5
2	B	132	VAL	2.5
2	E	122	LYS	2.5
2	E	353	LEU	2.5
3	I	76	PRO	2.5
1	D	158	ILE	2.5
1	G	158	ILE	2.5
2	K	422	TYR	2.5
1	D	116	ARG	2.5
2	B	221	THR	2.5
1	G	105	ASP	2.4
1	G	194	LEU	2.4
2	K	115	PHE	2.4
3	I	13	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	80	ASN	2.4
1	J	86	LEU	2.4
3	I	43	LEU	2.4
2	E	104	VAL	2.4
3	L	57	VAL	2.4
1	D	50	ARG	2.4
2	B	94	ARG	2.4
3	F	58	LYS	2.4
3	F	381	LYS	2.4
3	L	18	TYR	2.4
1	D	73	LEU	2.4
1	J	194	LEU	2.4
3	F	179	LEU	2.4
3	F	394	ILE	2.4
3	I	8	CYS	2.4
1	D	81	LYS	2.4
3	C	18	TYR	2.4
3	F	109	TYR	2.4
3	F	379	MET	2.4
2	E	77	PRO	2.4
3	L	50	VAL	2.4
1	G	76	TYR	2.4
2	B	238	VAL	2.3
2	B	72	LEU	2.3
2	E	78	THR	2.3
1	D	34	PRO	2.3
3	I	16	GLY	2.3
1	D	74	PHE	2.3
1	J	62	PHE	2.3
1	J	28	CYS	2.3
2	B	226	LEU	2.3
2	K	64	GLY	2.3
2	K	277	ALA	2.3
1	J	200	GLN	2.3
3	L	60	LEU	2.3
1	A	90	ILE	2.3
1	D	123	LYS	2.3
1	D	46	PRO	2.3
2	K	457	PHE	2.3
3	L	90	LEU	2.3
3	L	339	CYS	2.3
2	K	74	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	97	ASP	2.2
2	B	93	ILE	2.2
3	L	10	ILE	2.2
3	L	93	ILE	2.2
1	D	162	ARG	2.2
3	C	153	CYS	2.2
2	B	440	TRP	2.2
3	C	22	THR	2.2
3	I	17	SER	2.2
3	L	81	ALA	2.2
3	F	76	PRO	2.2
1	A	83	SER	2.2
2	E	426	MET	2.2
2	E	161	ILE	2.2
1	G	146	ASP	2.2
2	B	71	ASP	2.2
1	D	41	TRP	2.2
2	H	193	CYS	2.2
1	D	68	LYS	2.2
2	H	72	LEU	2.2
2	H	168	LEU	2.2
3	F	213	GLU	2.2
1	D	167	ARG	2.2
1	D	98	PHE	2.2
2	B	236	TYR	2.2
2	K	86	LEU	2.2
3	L	22	THR	2.1
3	C	23	CYS	2.1
3	I	23	CYS	2.1
3	C	64	ILE	2.1
2	B	284	ASN	2.1
1	A	56	ASP	2.1
3	F	28	PHE	2.1
3	L	15	PHE	2.1
3	F	197	ARG	2.1
3	F	368	ILE	2.1
3	I	61	ILE	2.1
1	A	73	LEU	2.1
1	A	82	ASP	2.1
2	E	378	TYR	2.1
3	F	367	ILE	2.1
3	L	8	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	85	LYS	2.1
1	D	195	PRO	2.1
2	E	64	GLY	2.1
3	F	61	ILE	2.1
2	E	363	GLU	2.1
1	D	112	SER	2.0
2	E	114	SER	2.0
3	F	134	GLN	2.0
2	E	72	LEU	2.0
3	L	63	ALA	2.0
1	G	186	GLU	2.0
1	D	85	SER	2.0
2	K	435	VAL	2.0
1	A	86	LEU	2.0
3	I	386	ILE	2.0
1	A	81	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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
6	NAG	V	9	14/15	-0.10	0.19	105,109,111,115	0
6	NAG	X	9	14/15	0.01	0.18	106,111,112,115	0
6	NAG	U	5	14/15	0.06	0.17	104,111,112,113	0
6	NAG	V	5	14/15	0.08	0.18	103,110,115,117	0
6	SIA	X	11	20/21	0.08	0.19	105,113,116,116	0
6	SIA	U	7	20/21	0.09	0.20	99,104,108,108	0
6	SIA	V	11	20/21	0.10	0.18	109,114,119,125	0
6	BMA	X	3	11/12	0.10	0.16	101,104,107,107	0
6	MAN	V	4	11/12	0.12	0.17	106,108,109,112	0
6	NAG	X	2	14/15	0.14	0.18	97,100,102,104	0
6	MAN	U	4	11/12	0.16	0.15	109,111,112,113	0
6	SIA	U	11	20/21	0.18	0.17	97,103,109,111	0

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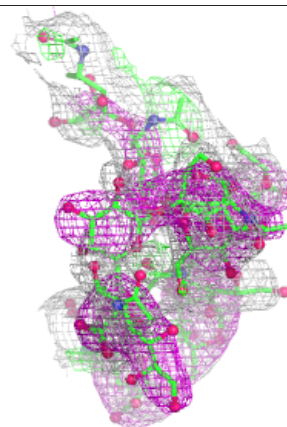
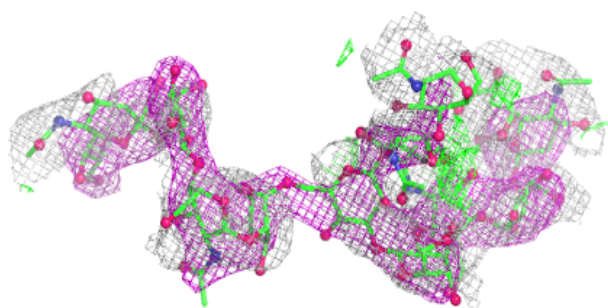
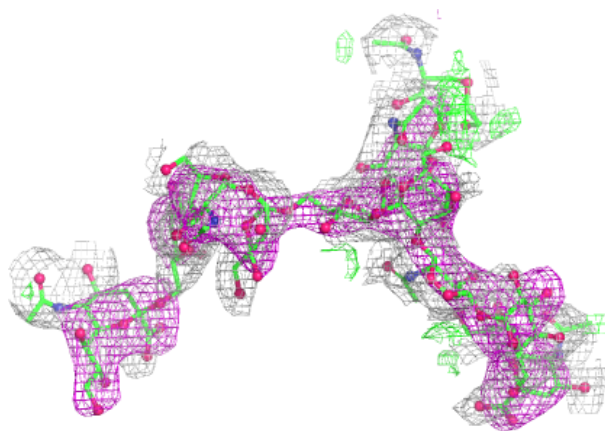
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	U	8	11/12	0.18	0.16	104,108,109,109	0
6	NAG	U	9	14/15	0.18	0.17	104,107,109,110	0
7	MAN	W	5	11/12	0.19	0.16	104,108,110,110	0
6	SIA	X	7	20/21	0.20	0.19	102,107,109,109	0
6	MAN	V	8	11/12	0.20	0.17	99,104,107,107	0
6	NAG	X	5	14/15	0.21	0.17	97,105,107,109	0
8	NAG	Y	2	14/15	0.21	0.16	105,108,109,109	0
6	MAN	X	8	11/12	0.22	0.17	99,101,106,108	0
6	GAL	V	10	11/12	0.23	0.14	115,118,118,119	0
6	GAL	X	10	11/12	0.26	0.17	113,116,117,117	0
6	GAL	U	10	11/12	0.28	0.15	106,107,108,112	0
6	GAL	X	6	11/12	0.29	0.15	105,110,111,111	0
6	GAL	V	6	11/12	0.29	0.15	109,112,115,116	0
6	BMA	V	3	11/12	0.30	0.14	98,103,106,108	0
6	NAG	U	2	14/15	0.32	0.16	96,98,101,102	0
8	NAG	Y	1	14/15	0.33	0.15	106,109,110,111	0
6	NAG	V	2	14/15	0.35	0.17	95,97,101,101	0
7	MAN	W	4	11/12	0.37	0.16	100,103,105,107	0
6	SIA	V	7	20/21	0.40	0.16	103,107,111,112	0
6	MAN	X	4	11/12	0.42	0.15	93,103,105,105	0
6	NAG	V	1	14/15	0.43	0.21	80,85,89,92	0
6	GAL	U	6	11/12	0.47	0.12	98,104,107,108	0
6	NAG	U	1	14/15	0.48	0.19	83,89,92,95	0
6	NAG	X	1	14/15	0.49	0.18	83,87,92,96	0
6	BMA	U	3	11/12	0.51	0.12	99,105,108,109	0
7	NAG	W	2	14/15	0.52	0.13	94,97,102,103	0
7	NAG	W	1	14/15	0.53	0.17	83,87,91,93	0
7	BMA	W	3	11/12	0.59	0.11	100,104,108,110	0

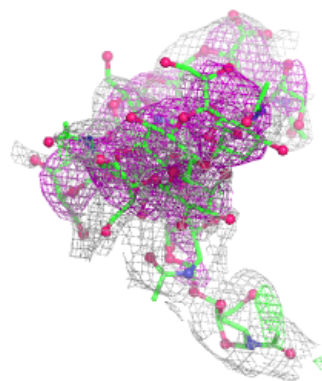
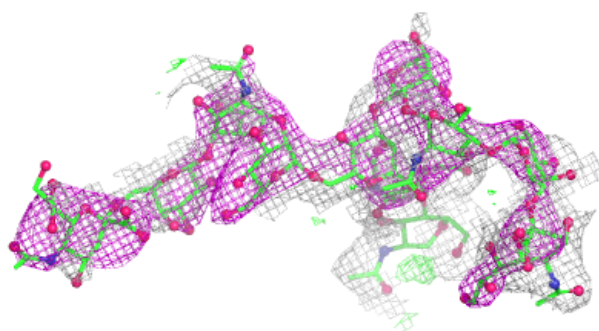
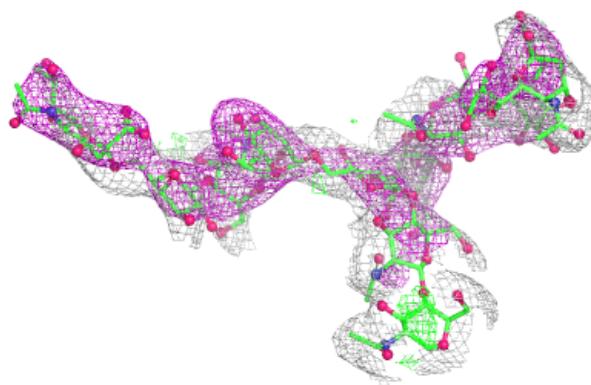
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

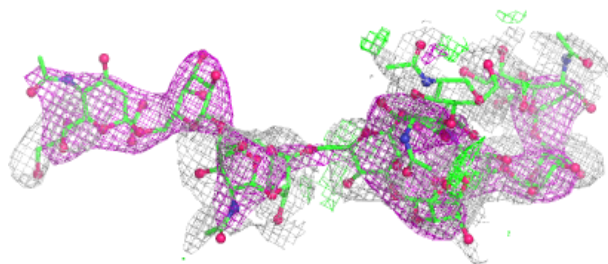
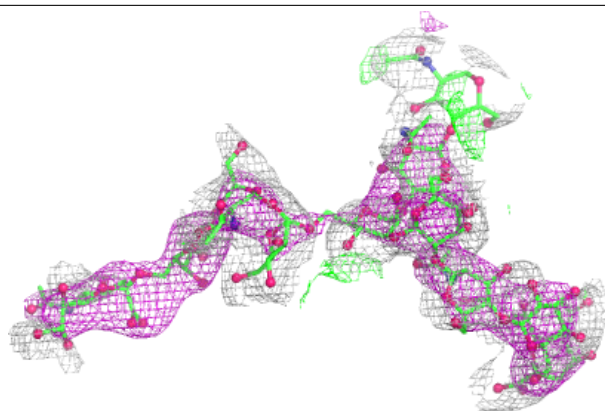
**Electron density around Chain V:**

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



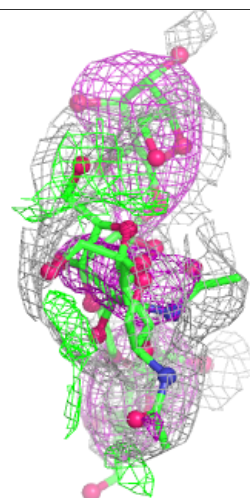
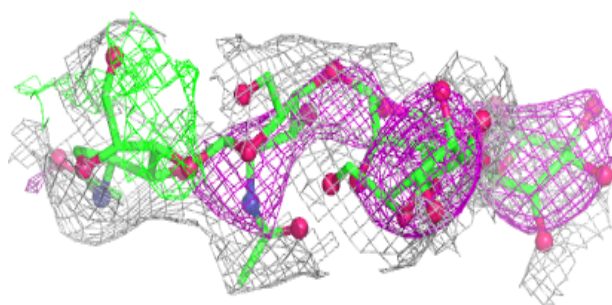
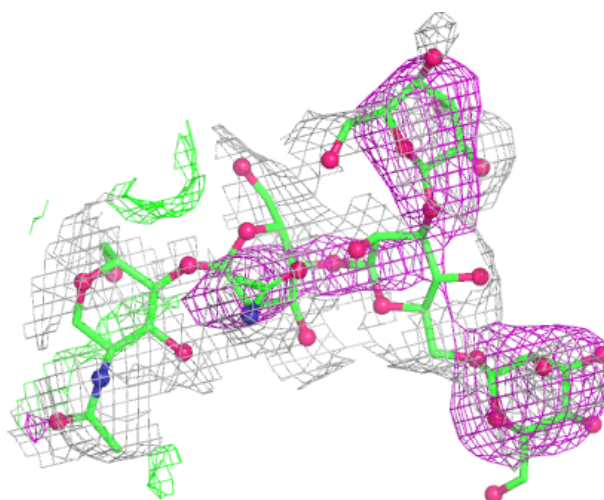
Electron density around Chain X:

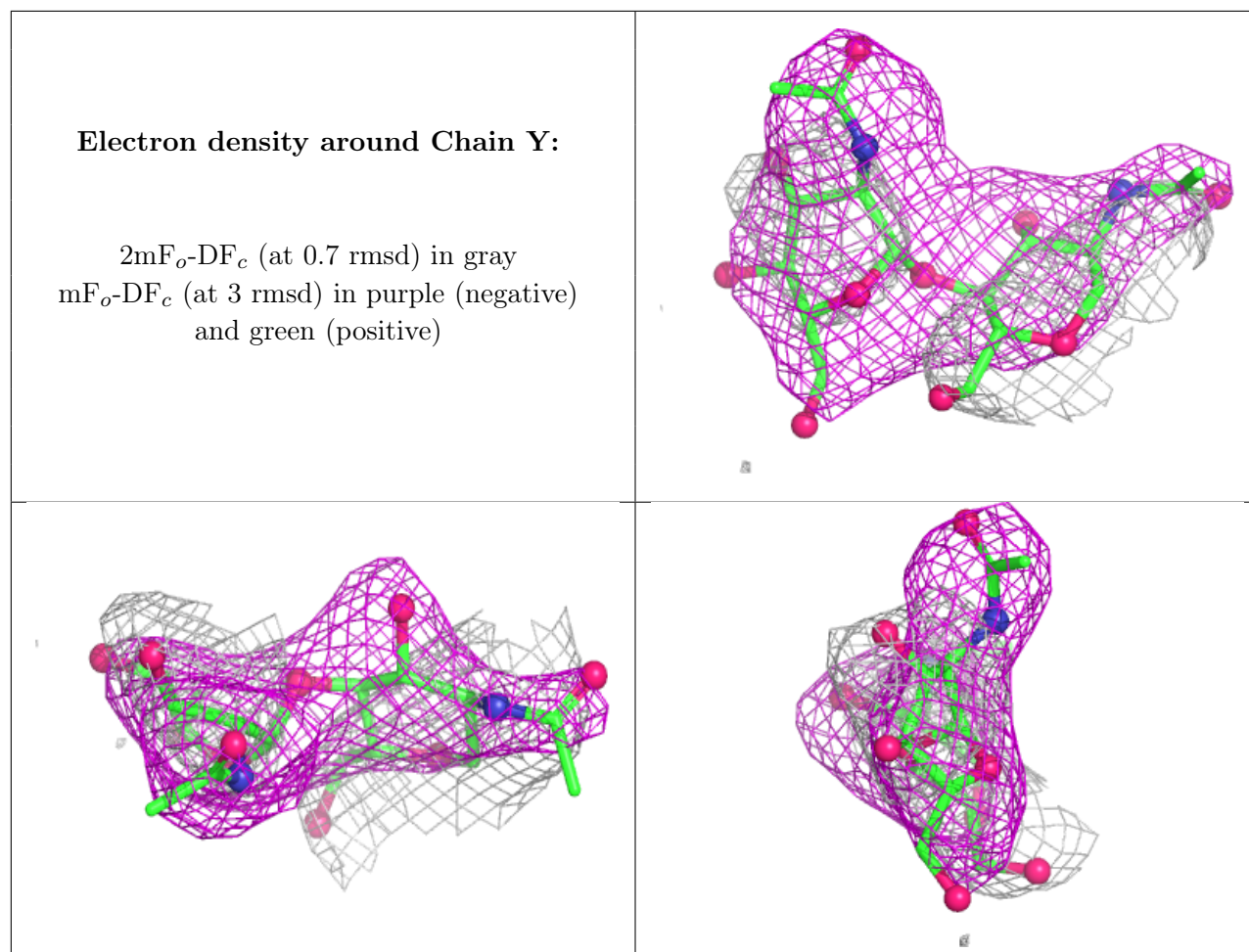
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

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





6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
9	CA	C	601	1/1	0.91	0.09	31,31,31,31	0
9	CA	K	501	1/1	0.92	0.07	68,68,68,68	0
9	CA	E	501	1/1	0.94	0.17	47,47,47,47	0
9	CA	L	601	1/1	0.95	0.11	51,51,51,51	0
9	CA	F	601	1/1	0.96	0.08	49,49,49,49	0
9	CA	I	601	1/1	0.96	0.06	56,56,56,56	0
9	CA	B	501	1/1	0.98	0.04	77,77,77,77	0
9	CA	H	501	1/1	0.99	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.