



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:30 PM UTC

PDB ID : 4U3C / pdb_00004u3c
Title : Docking Site of Maltotetraose in the Mtb GlgE
Authors : Ronning, D.R.; Lindenberger, J.J.
Deposited on : 2014-07-19
Resolution : 3.98 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

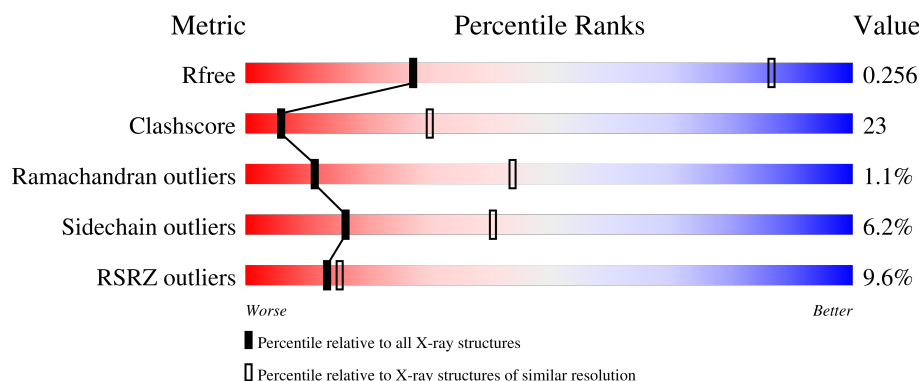
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.98 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.



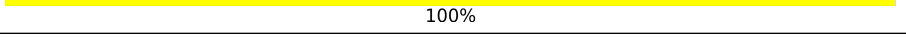
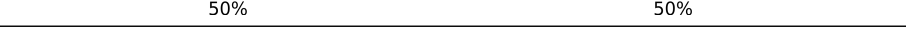
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1016 (4.18-3.78)
Clashscore	190562	1007 (4.16-3.80)
Ramachandran outliers	187476	1000 (4.18-3.78)
Sidechain outliers	187428	1131 (4.20-3.76)
RSRZ outliers	180081	1016 (4.18-3.78)

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	723	7% 51% 36% • 9%
1	B	723	8% 54% 32% 5% • 9%
1	C	723	9% 51% 35% 5% • 9%
1	D	723	9% 46% 39% 5% • 9%
1	E	723	10% 49% 35% 5% • 9%

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Mol	Chain	Length	Quality of chain
1	F	723	
2	G	2	
2	I	2	
2	K	2	
2	M	2	
2	O	2	
2	Q	2	
3	H	6	
3	J	6	
3	L	6	
3	N	6	
3	P	6	
3	R	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31938 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 Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	B	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	C	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	D	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	E	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			
1	F	660	Total	C	N	O	S	0	0	0
			5233	3359	910	950	14			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P9WQ16
A	-20	GLY	-	expression tag	UNP P9WQ16
A	-19	SER	-	expression tag	UNP P9WQ16
A	-18	SER	-	expression tag	UNP P9WQ16
A	-17	HIS	-	expression tag	UNP P9WQ16
A	-16	HIS	-	expression tag	UNP P9WQ16
A	-15	HIS	-	expression tag	UNP P9WQ16
A	-14	HIS	-	expression tag	UNP P9WQ16
A	-13	HIS	-	expression tag	UNP P9WQ16
A	-12	HIS	-	expression tag	UNP P9WQ16
A	-11	SER	-	expression tag	UNP P9WQ16
A	-10	SER	-	expression tag	UNP P9WQ16
A	-9	GLY	-	expression tag	UNP P9WQ16
A	-8	LEU	-	expression tag	UNP P9WQ16
A	-7	GLU	-	expression tag	UNP P9WQ16
A	-6	VAL	-	expression tag	UNP P9WQ16
A	-5	LEU	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PHE	-	expression tag	UNP P9WQ16
A	-3	GLN	-	expression tag	UNP P9WQ16
A	-2	GLY	-	expression tag	UNP P9WQ16
A	-1	PRO	-	expression tag	UNP P9WQ16
A	0	HIS	-	expression tag	UNP P9WQ16
B	-21	MET	-	expression tag	UNP P9WQ16
B	-20	GLY	-	expression tag	UNP P9WQ16
B	-19	SER	-	expression tag	UNP P9WQ16
B	-18	SER	-	expression tag	UNP P9WQ16
B	-17	HIS	-	expression tag	UNP P9WQ16
B	-16	HIS	-	expression tag	UNP P9WQ16
B	-15	HIS	-	expression tag	UNP P9WQ16
B	-14	HIS	-	expression tag	UNP P9WQ16
B	-13	HIS	-	expression tag	UNP P9WQ16
B	-12	HIS	-	expression tag	UNP P9WQ16
B	-11	SER	-	expression tag	UNP P9WQ16
B	-10	SER	-	expression tag	UNP P9WQ16
B	-9	GLY	-	expression tag	UNP P9WQ16
B	-8	LEU	-	expression tag	UNP P9WQ16
B	-7	GLU	-	expression tag	UNP P9WQ16
B	-6	VAL	-	expression tag	UNP P9WQ16
B	-5	LEU	-	expression tag	UNP P9WQ16
B	-4	PHE	-	expression tag	UNP P9WQ16
B	-3	GLN	-	expression tag	UNP P9WQ16
B	-2	GLY	-	expression tag	UNP P9WQ16
B	-1	PRO	-	expression tag	UNP P9WQ16
B	0	HIS	-	expression tag	UNP P9WQ16
C	-21	MET	-	expression tag	UNP P9WQ16
C	-20	GLY	-	expression tag	UNP P9WQ16
C	-19	SER	-	expression tag	UNP P9WQ16
C	-18	SER	-	expression tag	UNP P9WQ16
C	-17	HIS	-	expression tag	UNP P9WQ16
C	-16	HIS	-	expression tag	UNP P9WQ16
C	-15	HIS	-	expression tag	UNP P9WQ16
C	-14	HIS	-	expression tag	UNP P9WQ16
C	-13	HIS	-	expression tag	UNP P9WQ16
C	-12	HIS	-	expression tag	UNP P9WQ16
C	-11	SER	-	expression tag	UNP P9WQ16
C	-10	SER	-	expression tag	UNP P9WQ16
C	-9	GLY	-	expression tag	UNP P9WQ16
C	-8	LEU	-	expression tag	UNP P9WQ16
C	-7	GLU	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	VAL	-	expression tag	UNP P9WQ16
C	-5	LEU	-	expression tag	UNP P9WQ16
C	-4	PHE	-	expression tag	UNP P9WQ16
C	-3	GLN	-	expression tag	UNP P9WQ16
C	-2	GLY	-	expression tag	UNP P9WQ16
C	-1	PRO	-	expression tag	UNP P9WQ16
C	0	HIS	-	expression tag	UNP P9WQ16
D	-21	MET	-	expression tag	UNP P9WQ16
D	-20	GLY	-	expression tag	UNP P9WQ16
D	-19	SER	-	expression tag	UNP P9WQ16
D	-18	SER	-	expression tag	UNP P9WQ16
D	-17	HIS	-	expression tag	UNP P9WQ16
D	-16	HIS	-	expression tag	UNP P9WQ16
D	-15	HIS	-	expression tag	UNP P9WQ16
D	-14	HIS	-	expression tag	UNP P9WQ16
D	-13	HIS	-	expression tag	UNP P9WQ16
D	-12	HIS	-	expression tag	UNP P9WQ16
D	-11	SER	-	expression tag	UNP P9WQ16
D	-10	SER	-	expression tag	UNP P9WQ16
D	-9	GLY	-	expression tag	UNP P9WQ16
D	-8	LEU	-	expression tag	UNP P9WQ16
D	-7	GLU	-	expression tag	UNP P9WQ16
D	-6	VAL	-	expression tag	UNP P9WQ16
D	-5	LEU	-	expression tag	UNP P9WQ16
D	-4	PHE	-	expression tag	UNP P9WQ16
D	-3	GLN	-	expression tag	UNP P9WQ16
D	-2	GLY	-	expression tag	UNP P9WQ16
D	-1	PRO	-	expression tag	UNP P9WQ16
D	0	HIS	-	expression tag	UNP P9WQ16
E	-21	MET	-	expression tag	UNP P9WQ16
E	-20	GLY	-	expression tag	UNP P9WQ16
E	-19	SER	-	expression tag	UNP P9WQ16
E	-18	SER	-	expression tag	UNP P9WQ16
E	-17	HIS	-	expression tag	UNP P9WQ16
E	-16	HIS	-	expression tag	UNP P9WQ16
E	-15	HIS	-	expression tag	UNP P9WQ16
E	-14	HIS	-	expression tag	UNP P9WQ16
E	-13	HIS	-	expression tag	UNP P9WQ16
E	-12	HIS	-	expression tag	UNP P9WQ16
E	-11	SER	-	expression tag	UNP P9WQ16
E	-10	SER	-	expression tag	UNP P9WQ16
E	-9	GLY	-	expression tag	UNP P9WQ16

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	LEU	-	expression tag	UNP P9WQ16
E	-7	GLU	-	expression tag	UNP P9WQ16
E	-6	VAL	-	expression tag	UNP P9WQ16
E	-5	LEU	-	expression tag	UNP P9WQ16
E	-4	PHE	-	expression tag	UNP P9WQ16
E	-3	GLN	-	expression tag	UNP P9WQ16
E	-2	GLY	-	expression tag	UNP P9WQ16
E	-1	PRO	-	expression tag	UNP P9WQ16
E	0	HIS	-	expression tag	UNP P9WQ16
F	-21	MET	-	expression tag	UNP P9WQ16
F	-20	GLY	-	expression tag	UNP P9WQ16
F	-19	SER	-	expression tag	UNP P9WQ16
F	-18	SER	-	expression tag	UNP P9WQ16
F	-17	HIS	-	expression tag	UNP P9WQ16
F	-16	HIS	-	expression tag	UNP P9WQ16
F	-15	HIS	-	expression tag	UNP P9WQ16
F	-14	HIS	-	expression tag	UNP P9WQ16
F	-13	HIS	-	expression tag	UNP P9WQ16
F	-12	HIS	-	expression tag	UNP P9WQ16
F	-11	SER	-	expression tag	UNP P9WQ16
F	-10	SER	-	expression tag	UNP P9WQ16
F	-9	GLY	-	expression tag	UNP P9WQ16
F	-8	LEU	-	expression tag	UNP P9WQ16
F	-7	GLU	-	expression tag	UNP P9WQ16
F	-6	VAL	-	expression tag	UNP P9WQ16
F	-5	LEU	-	expression tag	UNP P9WQ16
F	-4	PHE	-	expression tag	UNP P9WQ16
F	-3	GLN	-	expression tag	UNP P9WQ16
F	-2	GLY	-	expression tag	UNP P9WQ16
F	-1	PRO	-	expression tag	UNP P9WQ16
F	0	HIS	-	expression tag	UNP P9WQ16

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			23	12	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	O	2	Total	C	O	0	0	0
			23	12	11			
2	Q	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

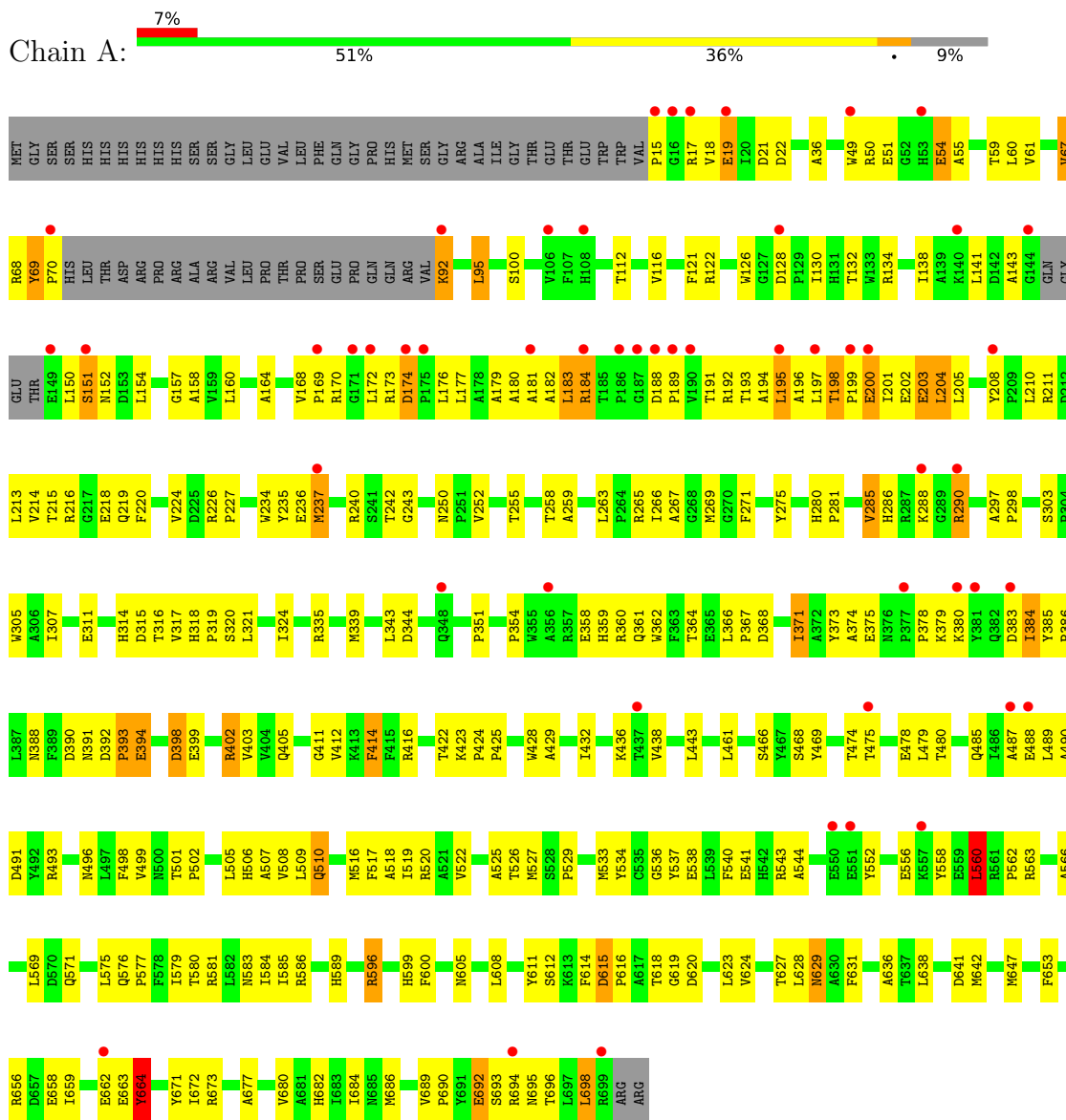


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	H	6	Total	C	O	0	0	0
			67	36	31			
3	J	6	Total	C	O	0	0	0
			67	36	31			
3	L	6	Total	C	O	0	0	0
			67	36	31			
3	N	6	Total	C	O	0	0	0
			67	36	31			
3	P	6	Total	C	O	0	0	0
			67	36	31			
3	R	6	Total	C	O	0	0	0
			67	36	31			

3 Residue-property plots

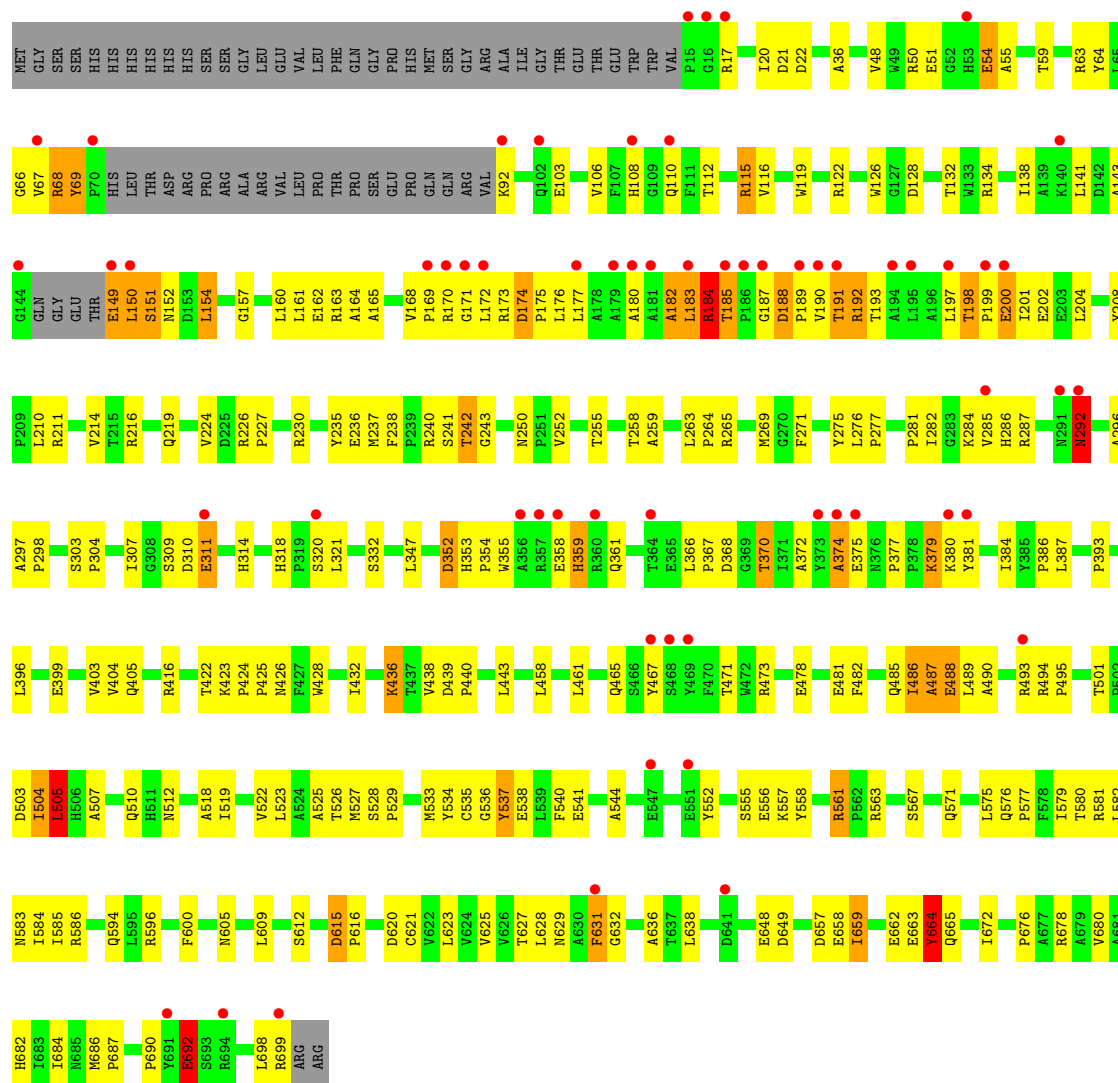
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

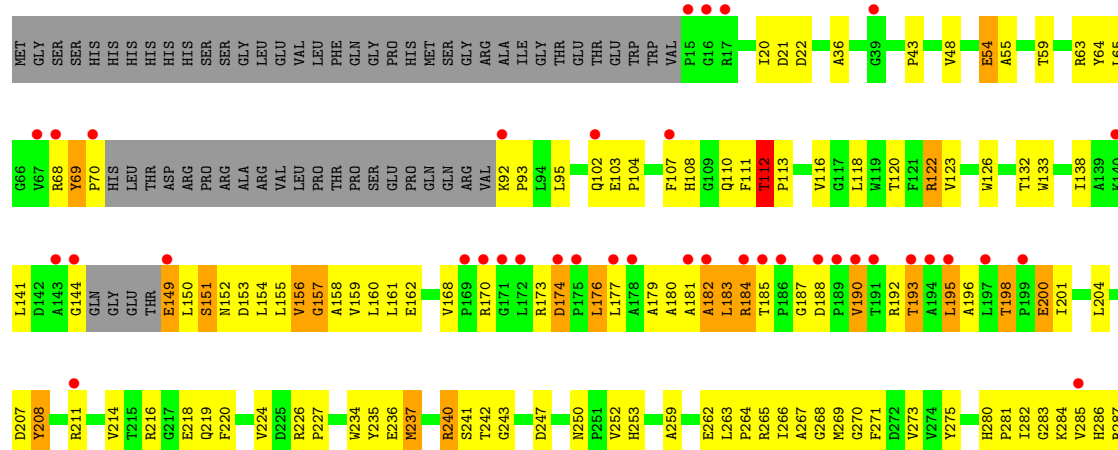


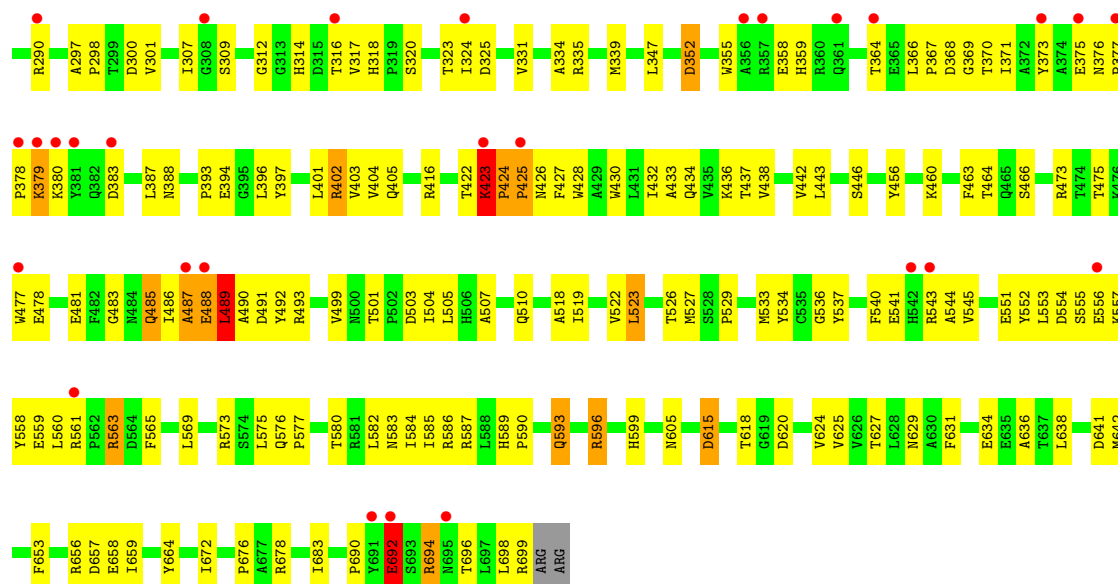
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase



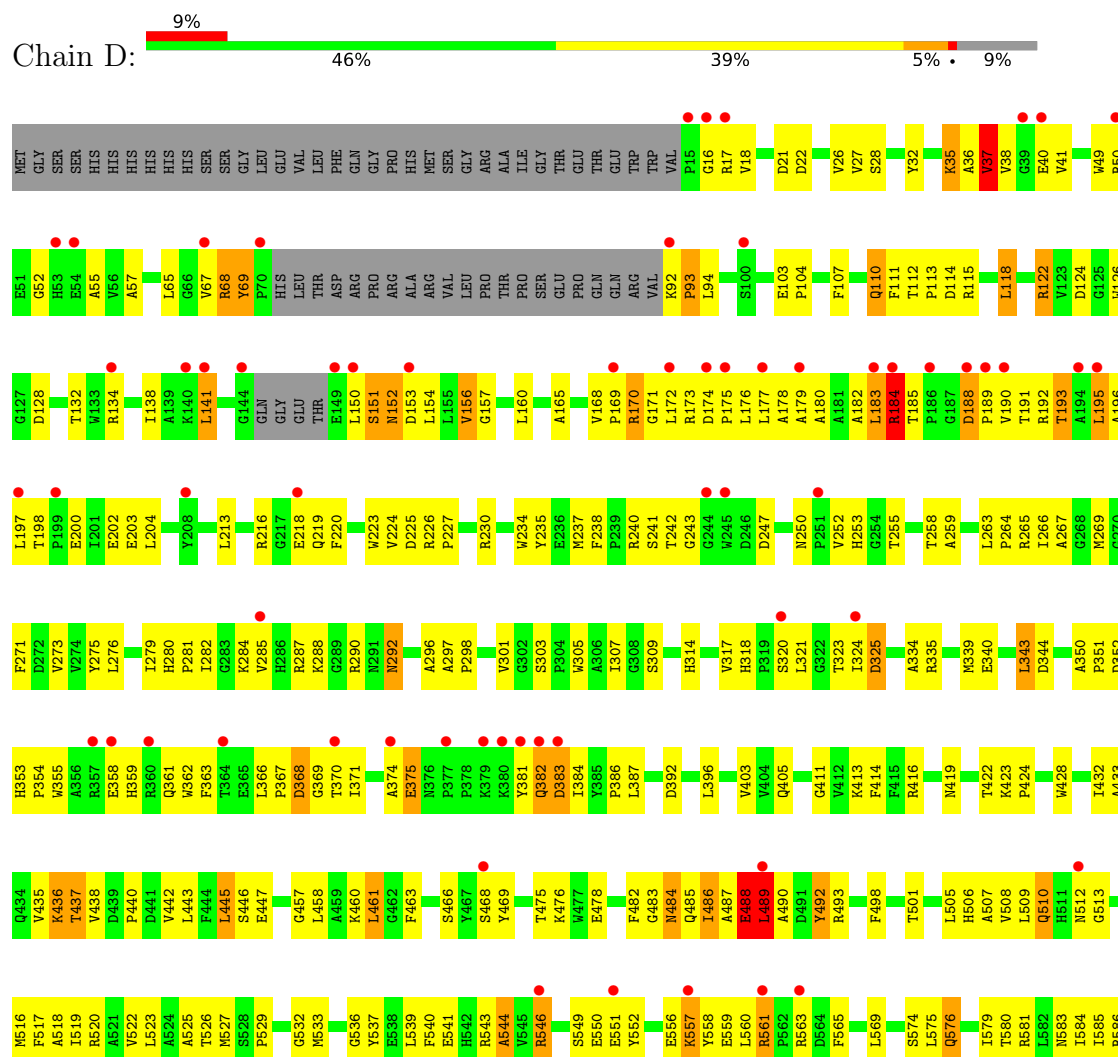


- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

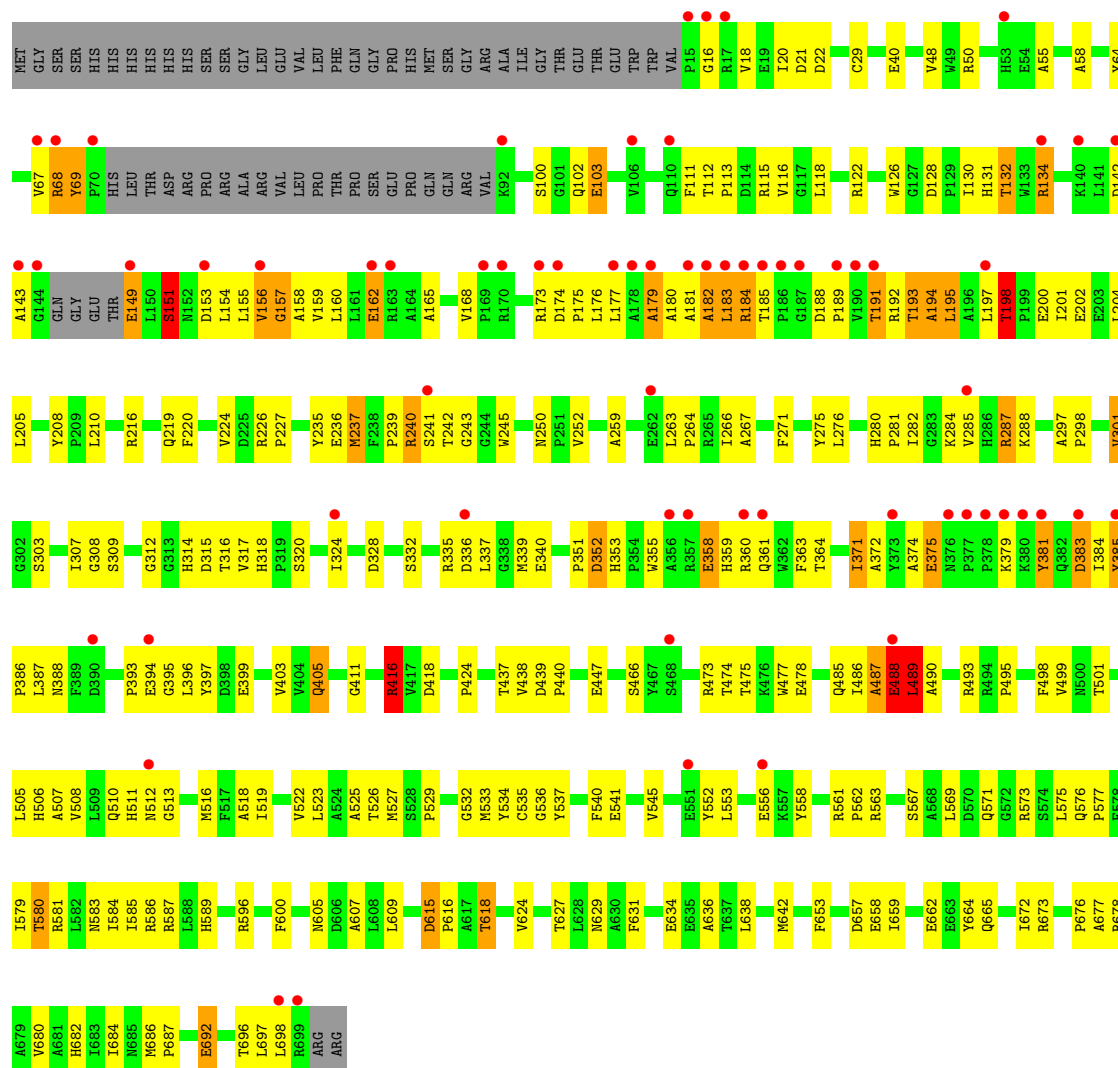




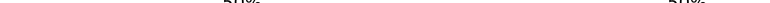
• Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase





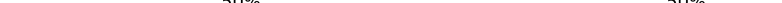


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:  50% 50%

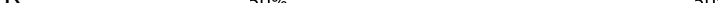


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  50% 50%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:  50% 50%



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  50% 50%

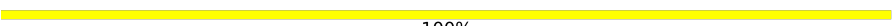
GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:  50% 50%

GLC1
GLC2

- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain Q:  100%

GLC1
GLC2

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  50% 50%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:  33% 67%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:  67% 33%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:  50% 50%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:  50% 50%



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain R:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	338.42Å 239.42Å 239.45Å 90.00° 134.90° 90.00°	Depositor
Resolution (Å)	43.73 – 3.98 43.73 – 3.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.73-3.98) 87.9 (43.73-3.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.224 , 0.256 (Not available) , 0.256	Depositor DCC
R_{free} test set	5681 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	105.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h+2*k,-h-l 0.015 for k+l,h+l,-l 0.014 for -k+l,-h-l,-l 0.015 for -h+k-l,-l,-k 0.013 for -h-k-l,l,k 0.410 for h-k+l,l,-h-l 0.409 for -k-l,-h-l,k 0.418 for h+k+l,-l,-h-l 0.418 for k-l,h+l,-k 0.015 for h,-k,-h-l 0.418 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	31938	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GLC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/5396	1.16	39/7380 (0.5%)
1	B	0.51	0/5396	1.21	58/7380 (0.8%)
1	C	0.52	0/5396	1.20	41/7380 (0.6%)
1	D	0.53	0/5396	1.25	51/7380 (0.7%)
1	E	0.53	0/5396	1.22	56/7380 (0.8%)
1	F	0.50	0/5396	1.20	44/7380 (0.6%)
All	All	0.52	0/32376	1.21	289/44280 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	3
1	E	0	2
All	All	0	7

There are no bond length outliers.

All (289) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	184	ARG	N-CA-C	-14.67	93.64	111.69
1	C	184	ARG	N-CA-C	-13.73	94.65	111.40
1	E	185	THR	CA-C-N	13.08	133.26	119.78
1	E	185	THR	C-N-CA	13.08	133.26	119.78
1	B	185	THR	CA-C-N	12.00	132.13	119.89
1	B	185	THR	C-N-CA	12.00	132.13	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	ARG	N-CA-C	-11.76	98.54	111.36
1	D	174	ASP	CA-C-N	-11.53	107.91	119.56
1	D	174	ASP	C-N-CA	-11.53	107.91	119.56
1	C	486	ILE	N-CA-C	-11.09	98.72	110.36
1	A	198	THR	CA-C-N	10.85	133.40	119.84
1	A	198	THR	C-N-CA	10.85	133.40	119.84
1	A	203	GLU	CA-C-N	10.81	135.65	120.29
1	A	203	GLU	C-N-CA	10.81	135.65	120.29
1	B	202	GLU	N-CA-C	-10.65	98.40	111.40
1	F	360	ARG	N-CA-C	-10.34	100.66	113.38
1	F	183	LEU	N-CA-C	10.12	125.19	108.49
1	D	196	ALA	N-CA-C	-9.92	99.49	112.68
1	C	424	PRO	CA-C-N	9.74	129.10	118.97
1	C	424	PRO	C-N-CA	9.74	129.10	118.97
1	C	404	VAL	N-CA-C	9.52	120.33	110.62
1	A	184	ARG	N-CA-C	-9.46	100.97	111.28
1	B	182	ALA	CA-C-N	-9.41	110.42	123.03
1	B	182	ALA	C-N-CA	-9.41	110.42	123.03
1	E	183	LEU	N-CA-C	9.39	128.00	114.39
1	C	174	ASP	CA-C-N	-9.22	109.88	120.12
1	C	174	ASP	C-N-CA	-9.22	109.88	120.12
1	E	184	ARG	N-CA-C	-9.16	101.25	111.14
1	F	194	ALA	N-CA-C	-9.02	102.05	113.23
1	B	380	LYS	N-CA-C	8.94	123.47	108.90
1	B	250	ASN	N-CA-C	8.94	120.56	109.57
1	D	693	SER	N-CA-C	-8.92	101.56	111.28
1	B	185	THR	N-CA-C	8.85	120.88	109.64
1	C	182	ALA	N-CA-C	8.71	123.64	112.92
1	C	112	THR	CA-C-N	8.48	128.49	119.76
1	C	112	THR	C-N-CA	8.48	128.49	119.76
1	F	250	ASN	N-CA-C	8.29	119.77	109.57
1	D	185	THR	CA-C-N	8.22	128.25	119.78
1	D	185	THR	C-N-CA	8.22	128.25	119.78
1	E	188	ASP	CA-C-N	-8.21	109.57	119.84
1	E	188	ASP	C-N-CA	-8.21	109.57	119.84
1	F	185	THR	CA-C-N	8.21	128.24	119.78
1	F	185	THR	C-N-CA	8.21	128.24	119.78
1	E	187	GLY	N-CA-C	8.05	120.92	110.45
1	A	203	GLU	N-CA-C	7.91	127.65	110.80
1	D	92	LYS	CA-C-N	-7.90	109.96	119.84
1	D	92	LYS	C-N-CA	-7.90	109.96	119.84
1	A	250	ASN	N-CA-C	7.88	119.26	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	THR	CA-C-N	7.86	128.16	119.90
1	B	112	THR	C-N-CA	7.86	128.16	119.90
1	E	250	ASN	N-CA-C	7.72	119.06	109.57
1	B	200	GLU	N-CA-C	-7.66	104.54	114.04
1	F	381	TYR	N-CA-C	-7.64	98.26	109.11
1	C	250	ASN	N-CA-C	7.60	118.92	109.57
1	C	208	TYR	CA-C-N	7.57	129.31	119.84
1	C	208	TYR	C-N-CA	7.57	129.31	119.84
1	C	193	THR	N-CA-C	-7.57	102.97	111.14
1	C	176	LEU	N-CA-C	-7.55	102.98	111.14
1	E	376	ASN	CA-C-N	7.52	128.12	120.38
1	E	376	ASN	C-N-CA	7.52	128.12	120.38
1	D	375	GLU	N-CA-C	7.50	121.80	109.06
1	D	292	ASN	CB-CA-C	-7.48	98.76	111.26
1	B	487	ALA	CA-C-N	7.38	134.99	121.70
1	B	487	ALA	C-N-CA	7.38	134.99	121.70
1	D	513	GLY	CA-C-N	7.37	127.08	119.56
1	D	513	GLY	C-N-CA	7.37	127.08	119.56
1	B	374	ALA	N-CA-C	-7.33	99.60	110.23
1	D	250	ASN	N-CA-C	7.33	118.58	109.57
1	B	377	PRO	N-CA-C	7.29	119.59	110.70
1	F	202	GLU	N-CA-C	-7.26	102.54	111.40
1	B	193	THR	N-CA-C	-7.18	103.78	112.54
1	B	191	THR	N-CA-C	7.14	119.06	111.28
1	B	143	ALA	N-CA-C	-7.13	102.55	112.45
1	C	270	GLY	N-CA-C	7.12	125.46	115.43
1	B	292	ASN	N-CA-CB	-7.11	101.18	112.63
1	D	384	ILE	N-CA-C	7.10	120.68	108.90
1	C	485	GLN	N-CA-C	-7.07	103.58	111.71
1	B	174	ASP	CA-C-N	-7.00	112.42	119.56
1	B	174	ASP	C-N-CA	-7.00	112.42	119.56
1	B	375	GLU	N-CA-C	7.00	120.95	109.06
1	C	483	GLY	N-CA-C	-6.94	104.45	112.50
1	A	195	LEU	N-CA-C	-6.93	104.85	113.38
1	A	375	GLU	N-CA-C	6.91	120.81	109.06
1	C	487	ALA	CA-C-N	6.91	134.14	121.70
1	C	487	ALA	C-N-CA	6.91	134.14	121.70
1	F	375	GLU	N-CA-C	6.84	120.70	109.06
1	A	112	THR	CA-C-N	6.82	127.06	119.90
1	A	112	THR	C-N-CA	6.82	127.06	119.90
1	D	615	ASP	CA-C-N	6.78	126.74	119.28
1	D	615	ASP	C-N-CA	6.78	126.74	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	487	ALA	CA-C-N	6.75	133.84	121.70
1	F	487	ALA	C-N-CA	6.75	133.84	121.70
1	D	484	ASN	N-CA-C	-6.72	103.95	111.28
1	F	489	LEU	N-CA-C	6.67	121.09	113.15
1	F	513	GLY	CA-C-N	6.65	126.34	119.56
1	F	513	GLY	C-N-CA	6.65	126.34	119.56
1	B	17	ARG	CA-C-N	-6.65	114.94	123.19
1	B	17	ARG	C-N-CA	-6.65	114.94	123.19
1	C	692	GLU	N-CA-C	-6.62	103.29	112.30
1	D	188	ASP	CA-C-N	-6.61	111.57	119.84
1	D	188	ASP	C-N-CA	-6.61	111.57	119.84
1	E	112	THR	CA-C-N	6.59	126.35	119.76
1	E	112	THR	C-N-CA	6.59	126.35	119.76
1	D	183	LEU	N-CA-C	6.55	120.67	111.30
1	B	197	LEU	N-CA-C	6.55	120.49	112.23
1	B	504	ILE	N-CA-C	6.55	118.25	107.24
1	B	649	ASP	N-CA-C	6.53	118.40	111.28
1	B	537	TYR	N-CA-C	-6.47	104.23	111.28
1	C	425	PRO	CB-CA-C	-6.47	102.78	113.06
1	D	37	VAL	N-CA-C	6.44	118.20	108.80
1	D	220	PHE	CA-C-N	-6.44	117.74	122.18
1	D	220	PHE	C-N-CA	-6.44	117.74	122.18
1	D	561	ARG	CA-C-N	-6.42	113.34	119.76
1	D	561	ARG	C-N-CA	-6.42	113.34	119.76
1	E	487	ALA	CA-C-N	6.42	133.26	121.70
1	E	487	ALA	C-N-CA	6.42	133.26	121.70
1	F	615	ASP	CA-C-N	6.40	126.32	119.28
1	F	615	ASP	C-N-CA	6.40	126.32	119.28
1	B	276	LEU	CA-C-N	6.38	126.95	120.38
1	B	276	LEU	C-N-CA	6.38	126.95	120.38
1	D	544	ALA	N-CA-C	-6.33	100.60	110.42
1	E	384	ILE	N-CA-C	6.33	119.42	108.90
1	D	68	ARG	CB-CA-C	-6.32	109.27	116.54
1	E	185	THR	N-CA-C	6.31	117.84	109.83
1	B	187	GLY	N-CA-C	6.27	118.60	110.45
1	D	424	PRO	CA-C-N	6.26	125.48	118.97
1	D	424	PRO	C-N-CA	6.26	125.48	118.97
1	E	169	PRO	N-CA-C	6.25	120.31	110.50
1	E	198	THR	CA-C-N	6.23	126.35	119.87
1	E	198	THR	C-N-CA	6.23	126.35	119.87
1	D	381	TYR	N-CA-C	-6.22	100.27	109.11
1	E	424	PRO	CA-C-N	6.19	125.41	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	424	PRO	C-N-CA	6.19	125.41	118.97
1	C	615	ASP	CA-C-N	6.16	126.05	119.28
1	C	615	ASP	C-N-CA	6.16	126.05	119.28
1	A	615	ASP	CA-C-N	6.14	126.60	119.47
1	A	615	ASP	C-N-CA	6.14	126.60	119.47
1	B	188	ASP	CA-C-N	-6.14	112.16	119.84
1	B	188	ASP	C-N-CA	-6.14	112.16	119.84
1	F	157	GLY	N-CA-C	-6.14	105.38	112.50
1	B	184	ARG	CA-C-N	6.13	128.91	120.39
1	B	184	ARG	C-N-CA	6.13	128.91	120.39
1	B	198	THR	N-CA-C	6.13	118.30	109.48
1	B	615	ASP	CA-C-N	6.12	126.02	119.28
1	B	615	ASP	C-N-CA	6.12	126.02	119.28
1	B	664	TYR	CA-CB-CG	6.11	124.89	113.90
1	D	489	LEU	CA-C-N	6.10	129.06	120.28
1	D	489	LEU	C-N-CA	6.10	129.06	120.28
1	D	383	ASP	N-CA-C	6.09	120.72	113.16
1	E	93	PRO	N-CA-C	6.08	121.93	111.77
1	E	379	LYS	CA-C-N	-6.05	114.46	122.99
1	E	379	LYS	C-N-CA	-6.05	114.46	122.99
1	C	190	VAL	N-CA-C	6.04	118.60	111.05
1	A	198	THR	N-CA-C	6.04	118.17	109.48
1	A	92	LYS	CA-C-N	-5.99	112.35	119.84
1	A	92	LYS	C-N-CA	-5.99	112.35	119.84
1	A	200	GLU	N-CA-C	-5.99	104.69	112.23
1	F	182	ALA	CA-C-N	-5.98	115.02	123.03
1	F	182	ALA	C-N-CA	-5.98	115.02	123.03
1	F	692	GLU	N-CA-C	-5.98	103.31	111.56
1	B	370	THR	N-CA-C	-5.96	103.08	110.41
1	F	580	THR	N-CA-C	-5.95	104.70	111.07
1	E	425	PRO	CB-CA-C	-5.94	103.62	113.06
1	C	95	LEU	N-CA-C	5.93	118.62	109.07
1	E	50	ARG	N-CA-C	5.92	115.91	108.45
1	A	196	ALA	N-CA-C	-5.91	104.82	112.68
1	F	511	HIS	N-CA-CB	-5.91	102.72	110.88
1	E	61	VAL	N-CA-C	5.91	116.12	107.37
1	E	174	ASP	CA-C-N	-5.91	113.53	119.56
1	E	174	ASP	C-N-CA	-5.91	113.53	119.56
1	B	381	TYR	N-CA-C	-5.89	100.75	109.11
1	D	576	GLN	CA-C-N	-5.88	112.85	118.97
1	D	576	GLN	C-N-CA	-5.88	112.85	118.97
1	F	358	GLU	N-CA-C	5.88	117.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	486	ILE	CA-C-N	-5.88	114.48	122.77
1	D	486	ILE	C-N-CA	-5.88	114.48	122.77
1	E	649	ASP	N-CA-C	5.88	117.69	111.28
1	B	370	THR	CA-C-N	-5.87	115.45	123.14
1	B	370	THR	C-N-CA	-5.87	115.45	123.14
1	E	202	GLU	N-CA-C	-5.84	104.27	111.40
1	C	157	GLY	N-CA-C	-5.82	105.74	112.50
1	F	191	THR	N-CA-C	-5.81	104.95	111.28
1	D	664	TYR	CA-CB-CG	5.80	124.35	113.90
1	E	289	GLY	N-CA-C	-5.79	103.74	112.60
1	C	181	ALA	N-CA-C	5.78	120.03	112.92
1	E	698	LEU	N-CA-C	5.77	117.75	110.24
1	F	112	THR	CA-C-N	5.77	125.96	119.90
1	F	112	THR	C-N-CA	5.77	125.96	119.90
1	A	425	PRO	CB-CA-C	-5.75	103.48	113.20
1	F	395	GLY	N-CA-C	-5.70	105.59	112.49
1	A	571	GLN	CB-CG-CD	-5.67	102.97	112.60
1	A	596	ARG	N-CA-C	5.66	117.53	111.36
1	E	242	THR	N-CA-C	-5.64	106.99	112.97
1	D	510	GLN	N-CA-C	5.63	117.42	111.28
1	E	692	GLU	N-CA-C	-5.62	104.65	112.30
1	B	631	PHE	N-CA-C	5.62	120.14	113.12
1	C	188	ASP	CA-C-N	5.62	126.86	119.84
1	C	188	ASP	C-N-CA	5.62	126.86	119.84
1	D	193	THR	N-CA-C	-5.61	105.69	112.54
1	D	202	GLU	N-CA-C	-5.58	104.59	111.40
1	C	423	LYS	CB-CA-C	5.58	117.70	109.22
1	D	492	TYR	CA-C-N	-5.58	115.12	122.99
1	D	492	TYR	C-N-CA	-5.58	115.12	122.99
1	D	693	SER	CA-C-N	5.54	127.71	120.28
1	D	693	SER	C-N-CA	5.54	127.71	120.28
1	F	184	ARG	N-CA-CB	5.54	118.46	110.20
1	E	238	PHE	CA-C-N	5.54	125.20	119.05
1	E	238	PHE	C-N-CA	5.54	125.20	119.05
1	A	193	THR	N-CA-C	-5.51	105.81	112.54
1	E	664	TYR	CA-CB-CG	5.50	123.81	113.90
1	E	367	PRO	N-CA-C	5.50	121.17	113.53
1	E	280	HIS	CA-C-N	5.50	125.42	119.76
1	E	280	HIS	C-N-CA	5.50	125.42	119.76
1	A	424	PRO	CA-C-N	5.49	124.95	119.24
1	A	424	PRO	C-N-CA	5.49	124.95	119.24
1	E	366	LEU	CA-CB-CG	5.48	135.49	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	635	GLU	N-CA-C	5.48	118.01	109.52
1	A	662	GLU	CA-C-N	5.47	128.64	120.87
1	A	662	GLU	C-N-CA	5.47	128.64	120.87
1	B	628	LEU	N-CA-C	-5.47	106.28	113.17
1	C	373	TYR	N-CA-C	-5.46	102.81	110.50
1	F	511	HIS	N-CA-C	5.45	121.70	114.12
1	F	179	ALA	N-CA-C	-5.45	105.42	111.36
1	A	220	PHE	CA-C-N	-5.45	118.42	122.18
1	A	220	PHE	C-N-CA	-5.45	118.42	122.18
1	E	191	THR	N-CA-C	-5.43	105.36	111.28
1	C	181	ALA	CA-C-N	-5.43	113.97	122.65
1	C	181	ALA	C-N-CA	-5.43	113.97	122.65
1	E	698	LEU	CA-CB-CG	5.42	135.29	116.30
1	A	664	TYR	CA-CB-CG	5.42	123.65	113.90
1	F	151	SER	N-CA-C	5.41	119.38	112.34
1	E	234	TRP	N-CA-C	5.39	118.28	109.59
1	A	95	LEU	N-CA-C	5.38	117.72	109.07
1	B	384	ILE	N-CA-C	5.38	117.82	108.90
1	A	151	SER	N-CA-C	5.37	122.24	110.80
1	D	692	GLU	N-CA-C	-5.34	105.04	112.30
1	D	292	ASN	N-CA-C	-5.33	106.73	113.23
1	B	310	ASP	CA-C-N	5.32	127.84	120.29
1	B	310	ASP	C-N-CA	5.32	127.84	120.29
1	A	100	SER	CA-C-N	-5.31	118.07	122.16
1	A	100	SER	C-N-CA	-5.31	118.07	122.16
1	F	198	THR	CA-C-N	-5.30	114.36	119.87
1	F	198	THR	C-N-CA	-5.30	114.36	119.87
1	F	424	PRO	CA-C-N	5.29	124.47	118.97
1	F	424	PRO	C-N-CA	5.29	124.47	118.97
1	F	132	THR	N-CA-C	-5.29	105.41	111.07
1	A	263	LEU	CA-C-N	-5.28	113.48	118.97
1	A	263	LEU	C-N-CA	-5.28	113.48	118.97
1	C	369	GLY	N-CA-C	-5.26	108.46	115.40
1	E	615	ASP	CA-C-N	5.25	125.56	119.47
1	E	615	ASP	C-N-CA	5.25	125.56	119.47
1	F	134	ARG	CB-CA-C	-5.25	102.88	110.96
1	B	505	LEU	CA-CB-CG	5.24	134.65	116.30
1	F	100	SER	CA-C-N	-5.24	118.13	122.16
1	F	100	SER	C-N-CA	-5.24	118.13	122.16
1	D	369	GLY	N-CA-C	-5.24	108.40	115.21
1	E	282	ILE	CA-C-N	5.23	125.07	120.10
1	E	282	ILE	C-N-CA	5.23	125.07	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	220	PHE	CA-C-N	-5.22	118.58	122.18
1	C	220	PHE	C-N-CA	-5.22	118.58	122.18
1	E	596	ARG	N-CA-C	5.20	117.85	111.82
1	A	560	LEU	CA-CB-CG	5.16	134.37	116.30
1	B	242	THR	N-CA-C	-5.15	107.51	112.97
1	A	698	LEU	N-CA-C	5.14	116.93	110.24
1	B	359	HIS	N-CA-C	5.13	117.16	108.02
1	B	380	LYS	CA-C-N	5.13	129.66	122.79
1	B	380	LYS	C-N-CA	5.13	129.66	122.79
1	A	143	ALA	N-CA-C	-5.12	105.78	111.36
1	E	63	ARG	CA-C-N	5.12	129.58	122.77
1	E	63	ARG	C-N-CA	5.12	129.58	122.77
1	F	384	ILE	N-CA-C	5.12	117.39	108.90
1	A	19	GLU	N-CA-C	5.11	117.89	109.76
1	C	489	LEU	N-CA-C	-5.10	107.08	113.15
1	B	66	GLY	CA-C-N	-5.10	117.93	123.08
1	B	66	GLY	C-N-CA	-5.10	117.93	123.08
1	C	489	LEU	CA-C-N	5.09	127.60	120.28
1	C	489	LEU	C-N-CA	5.09	127.60	120.28
1	B	424	PRO	CA-C-N	5.08	124.25	118.97
1	B	424	PRO	C-N-CA	5.08	124.25	118.97
1	C	187	GLY	N-CA-C	5.07	117.04	110.45
1	E	284	LYS	CA-C-N	-5.06	116.55	122.93
1	E	284	LYS	C-N-CA	-5.06	116.55	122.93
1	D	550	GLU	N-CA-C	5.04	118.74	112.59
1	B	692	GLU	N-CA-C	-5.04	104.61	111.56
1	D	370	THR	N-CA-C	-5.03	104.22	110.41
1	F	220	PHE	CA-C-N	-5.02	118.72	122.18
1	F	220	PHE	C-N-CA	-5.02	118.72	122.18
1	E	382	GLN	N-CA-C	5.02	118.50	112.38
1	F	416	ARG	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLU	Peptide
1	B	292	ASN	Sidechain
1	D	292	ASN	Sidechain
1	D	484	ASN	Sidechain
1	D	488	GLU	Peptide
1	E	379	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	E	62	VAL	Peptide

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	5233	0	5044	246	0
1	B	5233	0	5044	228	0
1	C	5233	0	5044	245	0
1	D	5233	0	5044	282	0
1	E	5233	0	5045	243	1
1	F	5233	0	5045	217	1
2	G	23	0	21	0	0
2	I	23	0	21	0	0
2	K	23	0	21	2	0
2	M	23	0	21	4	0
2	O	23	0	21	1	0
2	Q	23	0	21	2	0
3	H	67	0	57	3	0
3	J	67	0	57	3	0
3	L	67	0	57	3	0
3	N	67	0	57	3	0
3	P	67	0	57	4	0
3	R	67	0	57	5	0
All	All	31938	0	30734	1442	2

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 23.

All (1442) 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)
1:D:487:ALA:HA	1:D:488:GLU:HB2	1.13	1.11
1:C:487:ALA:HB1	1:C:488:GLU:HB3	1.30	1.08
1:D:154:LEU:HD22	1:D:183:LEU:HD22	1.38	1.03
1:D:487:ALA:HA	1:D:488:GLU:CB	1.90	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ALA:HB1	1:B:173:ARG:HD2	1.43	0.97
1:A:55:ALA:H	1:A:132:THR:HG22	1.32	0.94
1:C:55:ALA:H	1:C:132:THR:HG22	1.33	0.93
1:F:266:ILE:HG22	1:F:339:MET:HE1	1.51	0.93
1:F:173:ARG:O	1:F:173:ARG:NH1	2.01	0.93
1:E:275:TYR:OH	1:E:416:ARG:NH1	2.00	0.92
1:A:266:ILE:HG22	1:A:339:MET:HE1	1.51	0.92
1:E:266:ILE:HG22	1:E:339:MET:HE1	1.52	0.91
1:E:63:ARG:HG3	1:E:64:TYR:N	1.84	0.91
1:C:149:GLU:N	1:C:151:SER:HG	1.70	0.89
1:D:179:ALA:HA	1:D:195:LEU:HD21	1.55	0.89
1:B:512:ASN:HA	1:B:631:PHE:CZ	2.07	0.89
1:B:512:ASN:HA	1:B:631:PHE:HZ	1.37	0.89
1:D:288:LYS:HZ3	1:D:383:ASP:HB3	1.36	0.88
1:C:266:ILE:HG22	1:C:339:MET:HE1	1.54	0.87
1:D:275:TYR:OH	1:D:416:ARG:NH1	2.07	0.86
1:C:275:TYR:OH	1:C:416:ARG:NH1	2.07	0.86
1:A:629:ASN:C	1:A:629:ASN:HD22	1.84	0.86
1:A:203:GLU:HG3	1:A:205:LEU:H	1.42	0.85
1:C:347:LEU:O	1:C:423:LYS:NZ	2.09	0.85
1:A:560:LEU:HD23	1:A:562:PRO:HD3	1.58	0.85
1:E:284:LYS:HD3	1:E:352:ASP:HB3	1.59	0.85
1:C:265:ARG:HB2	1:E:673:ARG:HH21	1.41	0.84
1:E:698:LEU:HD12	1:E:699:ARG:HG3	1.58	0.84
1:A:491:ASP:OD1	1:A:596:ARG:NH2	2.11	0.84
1:E:533:MET:HE1	1:E:579:ILE:HD13	1.60	0.84
1:D:55:ALA:H	1:D:132:THR:HG22	1.42	0.84
1:E:55:ALA:H	1:E:132:THR:HG22	1.39	0.84
1:F:179:ALA:HB1	1:F:195:LEU:HG	1.58	0.84
1:B:55:ALA:H	1:B:132:THR:HG22	1.44	0.83
1:D:18:VAL:HG22	1:D:50:ARG:HD3	1.59	0.83
1:F:173:ARG:HH12	1:F:177:LEU:H	1.23	0.83
1:D:37:VAL:N	1:D:40:GLU:OE2	2.12	0.82
1:D:151:SER:OG	1:D:152:ASN:N	2.11	0.82
1:D:266:ILE:HG22	1:D:339:MET:HE1	1.62	0.82
1:C:323:THR:HG22	1:C:325:ASP:H	1.44	0.82
1:D:475:THR:HG22	1:D:478:GLU:HG3	1.58	0.82
1:F:241:SER:OG	1:F:561:ARG:O	1.99	0.81
1:C:170:ARG:HA	1:C:173:ARG:HG2	1.62	0.81
1:A:154:LEU:HD13	1:A:183:LEU:HD13	1.61	0.80
1:F:165:ALA:HB1	1:F:173:ARG:HE	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:ALA:HA	1:E:339:MET:HE3	1.64	0.80
1:C:487:ALA:CB	1:C:489:LEU:H	1.94	0.80
1:B:556:GLU:HG3	1:B:561:ARG:HG2	1.63	0.80
1:D:476:LYS:HD3	1:D:628:LEU:HD12	1.63	0.80
1:C:177:LEU:HA	1:C:180:ALA:HB3	1.63	0.80
1:F:201:ILE:HA	1:F:204:LEU:HG	1.62	0.80
1:E:63:ARG:HG3	1:E:64:TYR:H	1.44	0.79
1:B:182:ALA:HB1	1:B:192:ARG:HB3	1.62	0.79
1:D:288:LYS:HE3	1:D:382:GLN:HB3	1.62	0.79
1:F:183:LEU:HD11	1:F:191:THR:HG22	1.64	0.79
1:A:164:ALA:HB2	1:A:210:LEU:HD23	1.66	0.78
1:A:405:GLN:HE22	1:A:438:VAL:HG21	1.49	0.78
1:A:130:ILE:HD11	1:A:210:LEU:HD21	1.67	0.77
1:E:374:ALA:O	1:E:375:GLU:HB2	1.82	0.77
1:B:533:MET:HE3	1:B:537:TYR:HB3	1.65	0.77
1:C:487:ALA:HB1	1:C:488:GLU:CB	2.13	0.77
1:D:169:PRO:O	1:D:171:GLY:N	2.15	0.77
1:B:191:THR:HB	1:B:192:ARG:HD2	1.67	0.76
1:C:284:LYS:N	1:C:352:ASP:OD2	2.18	0.76
1:E:28:SER:OG	1:E:460:LYS:HE3	1.86	0.76
1:C:269:MET:HA	1:C:580:THR:HG23	1.68	0.76
1:D:35:LYS:NZ	1:D:463:PHE:O	2.19	0.76
1:B:629:ASN:HD21	1:B:632:GLY:H	1.32	0.76
1:C:265:ARG:HB2	1:E:673:ARG:NH2	2.00	0.75
1:F:55:ALA:H	1:F:132:THR:HG22	1.51	0.75
1:B:482:PHE:O	1:B:486:ILE:HG22	1.85	0.75
1:D:557:LYS:HE2	2:M:2:GLC:H2	1.68	0.75
1:D:170:ARG:HA	1:D:173:ARG:HG3	1.69	0.75
1:D:241:SER:OG	1:D:561:ARG:O	2.02	0.75
1:E:57:ALA:HA	1:E:107:PHE:HE2	1.51	0.75
1:A:474:THR:HG21	1:A:508:VAL:HG21	1.66	0.75
1:E:149:GLU:N	1:E:149:GLU:OE2	2.20	0.75
1:D:433:ALA:O	1:D:437:THR:OG1	2.04	0.75
1:C:179:ALA:O	1:C:192:ARG:NH1	2.20	0.74
1:F:474:THR:HG21	1:F:508:VAL:HG21	1.69	0.74
1:C:433:ALA:O	1:C:437:THR:OG1	2.05	0.74
1:A:18:VAL:HG21	1:A:213:LEU:HD13	1.70	0.74
1:F:165:ALA:CB	1:F:173:ARG:HE	2.00	0.74
1:E:201:ILE:HA	1:E:204:LEU:HG	1.70	0.74
1:A:265:ARG:NH1	1:A:576:GLN:OE1	2.21	0.74
1:B:318:HIS:CE1	1:B:320:SER:HB3	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:SER:OG	1:C:561:ARG:O	2.05	0.74
1:D:539:LEU:HD12	1:D:563:ARG:HD3	1.69	0.74
1:A:150:LEU:O	1:A:152:ASN:N	2.21	0.74
1:A:275:TYR:OH	1:A:416:ARG:NH1	2.21	0.73
1:E:32:TYR:CD2	1:E:460:LYS:HE2	2.23	0.73
1:F:358:GLU:HG3	1:F:359:HIS:ND1	2.04	0.73
1:A:267:ALA:HA	1:A:339:MET:HE3	1.70	0.73
1:E:375:GLU:HG3	1:E:380:LYS:HD2	1.70	0.73
1:A:130:ILE:HG12	1:A:210:LEU:HD11	1.70	0.73
1:D:517:PHE:HD2	1:D:540:PHE:HD1	1.35	0.73
1:E:605:ASN:HB2	1:E:636:ALA:HB2	1.69	0.73
1:B:629:ASN:ND2	1:B:632:GLY:H	1.85	0.73
1:F:173:ARG:NH1	1:F:177:LEU:H	1.87	0.73
1:B:416:ARG:NH1	1:B:467:TYR:OH	2.22	0.73
1:D:165:ALA:HB2	1:D:176:LEU:HD11	1.71	0.73
1:C:284:LYS:NZ	1:C:309:SER:OG	2.20	0.73
1:E:269:MET:HA	1:E:580:THR:HG23	1.71	0.73
1:E:635:GLU:HB2	1:E:673:ARG:HH11	1.52	0.73
1:F:162:GLU:OE1	1:F:162:GLU:N	2.21	0.73
1:D:267:ALA:HA	1:D:339:MET:HE3	1.71	0.72
1:A:179:ALA:O	1:A:192:ARG:HD2	1.90	0.72
1:F:558:TYR:HH	2:Q:2:GLC:HO3	1.34	0.72
1:D:405:GLN:HE22	1:D:438:VAL:HG21	1.54	0.72
1:A:271:PHE:O	1:A:339:MET:HE2	1.90	0.72
1:A:54:GLU:OE1	1:A:54:GLU:N	2.21	0.71
1:C:183:LEU:HB2	1:C:192:ARG:NE	2.05	0.71
1:D:226:ARG:NH1	1:D:340:GLU:OE2	2.22	0.71
1:D:405:GLN:NE2	1:D:438:VAL:HG21	2.05	0.71
1:F:162:GLU:OE2	1:F:184:ARG:NH2	2.22	0.71
1:B:54:GLU:OE1	1:B:54:GLU:N	2.20	0.71
1:A:335:ARG:NH2	1:A:411:GLY:O	2.22	0.71
1:D:539:LEU:HB2	1:D:563:ARG:NH1	2.05	0.71
1:F:335:ARG:NH2	1:F:411:GLY:O	2.24	0.71
1:F:535:CYS:SG	1:F:563:ARG:NH1	2.63	0.71
1:D:318:HIS:CE1	1:D:320:SER:HB3	2.26	0.71
1:D:223:TRP:NE1	1:D:225:ASP:OD1	2.24	0.71
1:F:183:LEU:O	1:F:192:ARG:NH1	2.23	0.70
1:E:281:PRO:HB2	1:E:309:SER:HB3	1.73	0.70
1:E:536:GLY:HA3	1:E:563:ARG:NH1	2.06	0.70
1:B:493:ARG:HD3	1:B:494:ARG:N	2.06	0.70
1:A:629:ASN:C	1:A:629:ASN:ND2	2.48	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:PRO:O	1:C:380:LYS:NZ	2.24	0.70
1:E:108:HIS:CE1	1:E:698:LEU:HD13	2.27	0.70
1:A:183:LEU:N	1:A:192:ARG:HD3	2.07	0.70
1:C:59:THR:HG23	1:C:126:TRP:HE1	1.57	0.70
1:D:488:GLU:OE2	1:D:493:ARG:NH1	2.24	0.70
1:E:183:LEU:HD11	1:E:192:ARG:HB3	1.74	0.70
1:A:618:THR:HG23	1:A:620:ASP:H	1.55	0.70
1:C:267:ALA:HA	1:C:339:MET:HE3	1.74	0.70
1:C:487:ALA:HB3	1:C:489:LEU:H	1.56	0.70
1:A:368:ASP:OD2	1:B:152:ASN:ND2	2.24	0.70
1:C:240:ARG:HG3	1:C:240:ARG:HH11	1.57	0.70
1:B:529:PRO:O	1:B:586:ARG:NH2	2.24	0.70
1:B:284:LYS:N	1:B:352:ASP:OD2	2.22	0.69
1:E:486:ILE:HG21	1:E:493:ARG:HH21	1.58	0.69
1:E:647:MET:HE1	1:E:687:PRO:HG2	1.74	0.69
1:B:493:ARG:NH1	1:B:494:ARG:H	1.89	0.69
1:A:182:ALA:HB3	1:A:192:ARG:HG3	1.73	0.69
1:A:629:ASN:ND2	1:A:629:ASN:O	2.21	0.69
1:D:122:ARG:HH22	1:D:216:ARG:HD3	1.57	0.69
1:C:318:HIS:CE1	1:C:320:SER:HB3	2.26	0.69
1:E:168:VAL:HG13	1:E:173:ARG:HG2	1.73	0.69
1:B:536:GLY:O	1:B:541:GLU:HG3	1.92	0.69
1:F:158:ALA:HB1	1:F:184:ARG:NH1	2.07	0.69
1:D:110:GLN:NE2	1:D:112:THR:OG1	2.25	0.69
1:D:269:MET:HA	1:D:580:THR:HG23	1.72	0.69
1:A:480:THR:HA	1:A:600:PHE:CE1	2.27	0.69
1:F:267:ALA:HA	1:F:339:MET:HE3	1.73	0.69
1:C:599:HIS:NE2	1:C:641:ASP:OD2	2.25	0.69
1:F:183:LEU:HB2	1:F:192:ARG:HG3	1.73	0.69
1:D:493:ARG:HG2	1:D:493:ARG:HH11	1.57	0.68
1:A:200:GLU:O	1:A:203:GLU:HB3	1.92	0.68
1:A:517:PHE:HD1	1:A:540:PHE:HD1	1.38	0.68
1:D:487:ALA:CA	1:D:488:GLU:HB2	2.08	0.68
1:F:131:HIS:HA	1:F:134:ARG:HG3	1.74	0.68
1:D:305:TRP:NE1	1:D:344:ASP:OD1	2.26	0.68
1:D:368:ASP:N	1:D:368:ASP:OD1	2.26	0.68
1:E:318:HIS:CE1	1:E:320:SER:HB2	2.28	0.68
1:B:505:LEU:HD12	1:B:505:LEU:O	1.94	0.68
1:D:574:SER:OG	1:D:576:GLN:HG2	1.94	0.68
1:C:268:GLY:HA3	1:E:671:TYR:CD2	2.29	0.67
1:D:151:SER:O	1:D:153:ASP:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:O	1:B:180:ALA:N	2.27	0.67
1:B:241:SER:OG	1:B:561:ARG:O	2.13	0.67
1:E:307:ILE:HG21	1:E:314:HIS:CD2	2.29	0.67
1:F:473:ARG:HD2	1:F:478:GLU:HB3	1.77	0.67
1:B:149:GLU:O	1:B:151:SER:N	2.25	0.67
1:E:195:LEU:O	1:E:201:ILE:HD11	1.94	0.67
1:E:509:LEU:HB3	1:E:517:PHE:HE1	1.59	0.67
1:C:358:GLU:HG3	1:C:359:HIS:CD2	2.29	0.67
1:F:176:LEU:O	1:F:180:ALA:N	2.26	0.67
1:F:309:SER:HA	1:F:352:ASP:HB2	1.77	0.67
1:B:505:LEU:HD23	1:B:552:TYR:CD1	2.29	0.67
1:C:394:GLU:N	1:C:394:GLU:OE1	2.25	0.67
1:F:487:ALA:HB2	1:F:490:ALA:HB2	1.76	0.67
1:B:108:HIS:ND1	1:B:698:LEU:HD11	2.10	0.67
1:C:692:GLU:OE1	1:C:692:GLU:HA	1.95	0.67
1:B:150:LEU:O	1:B:152:ASN:N	2.28	0.66
1:D:569:LEU:HD11	1:D:576:GLN:HG3	1.77	0.66
1:C:487:ALA:CB	1:C:488:GLU:HB3	2.15	0.66
1:C:63:ARG:HG3	1:C:93:PRO:HB3	1.76	0.66
1:F:583:ASN:HA	1:F:586:ARG:HD3	1.77	0.66
1:C:618:THR:HG23	1:C:620:ASP:H	1.61	0.66
1:D:122:ARG:HH21	1:D:124:ASP:CG	2.03	0.66
1:D:509:LEU:HB3	1:D:517:PHE:HE1	1.60	0.66
1:D:558:TYR:OH	2:M:2:GLC:O3	2.14	0.66
1:A:509:LEU:HD22	1:A:517:PHE:CD2	2.31	0.66
1:C:192:ARG:HB3	1:C:195:LEU:HD22	1.78	0.66
1:B:165:ALA:HB1	1:B:173:ARG:CD	2.23	0.65
1:F:318:HIS:CE1	1:F:320:SER:HB2	2.31	0.65
1:A:138:ILE:HA	1:A:141:LEU:HD23	1.78	0.65
1:D:36:ALA:HB1	1:D:40:GLU:OE2	1.97	0.65
1:D:57:ALA:HA	1:D:107:PHE:HE2	1.62	0.65
1:E:416:ARG:HH21	1:E:447:GLU:CD	2.03	0.65
1:F:149:GLU:N	1:F:149:GLU:OE1	2.29	0.65
1:C:198:THR:OG1	1:C:200:GLU:HG2	1.96	0.65
1:D:476:LYS:HZ2	1:D:628:LEU:HB2	1.61	0.65
1:F:177:LEU:HA	1:F:180:ALA:HB3	1.78	0.65
1:A:510:GLN:NE2	1:A:544:ALA:HB2	2.12	0.65
1:B:493:ARG:HH11	1:B:494:ARG:H	1.45	0.65
1:D:416:ARG:HH21	1:D:447:GLU:CD	2.04	0.65
1:F:151:SER:HA	1:F:154:LEU:HD13	1.79	0.65
1:F:242:THR:HG21	1:F:259:ALA:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ASN:HD21	1:B:632:GLY:N	1.95	0.65
1:B:347:LEU:HD13	1:B:428:TRP:HH2	1.62	0.65
1:B:541:GLU:OE1	1:B:563:ARG:NH2	2.30	0.65
1:D:605:ASN:HB2	1:D:636:ALA:HB2	1.79	0.64
1:B:432:ILE:HG22	1:B:436:LYS:HZ1	1.62	0.64
1:F:355:TRP:HA	1:F:358:GLU:HG2	1.80	0.64
1:B:465:GLN:HA	1:B:493:ARG:NH1	2.13	0.64
1:A:269:MET:HA	1:A:580:THR:HG23	1.78	0.64
1:B:149:GLU:OE1	1:B:149:GLU:N	2.31	0.64
1:E:50:ARG:HH22	1:E:126:TRP:N	1.95	0.64
1:F:122:ARG:HB3	1:F:219:GLN:HG2	1.79	0.64
1:B:487:ALA:HB1	1:B:489:LEU:N	2.12	0.64
1:C:168:VAL:O	1:C:173:ARG:HD2	1.98	0.64
1:C:54:GLU:OE1	1:C:54:GLU:N	2.20	0.64
1:E:509:LEU:HD21	1:E:520:ARG:HG3	1.80	0.64
1:F:243:GLY:HA3	1:F:252:VAL:O	1.97	0.64
1:F:506:HIS:CE1	1:F:508:VAL:HG23	2.33	0.64
1:A:59:THR:HG23	1:A:126:TRP:HE1	1.63	0.63
1:B:629:ASN:OD1	3:J:2:GLC:O6	2.15	0.63
1:B:149:GLU:C	1:B:151:SER:H	2.06	0.63
1:C:192:ARG:O	1:C:196:ALA:N	2.32	0.63
1:A:203:GLU:HB2	1:A:204:LEU:HD13	1.80	0.63
1:A:237:MET:SD	1:A:266:ILE:HD11	2.39	0.63
1:A:240:ARG:NH2	1:A:556:GLU:O	2.32	0.63
1:B:269:MET:HA	1:B:580:THR:HG23	1.80	0.63
1:E:486:ILE:HD13	1:E:495:PRO:HG3	1.78	0.63
1:C:43:PRO:HD2	1:C:596:ARG:HH11	1.63	0.63
1:E:405:GLN:NE2	1:E:438:VAL:HG21	2.14	0.63
1:F:589:HIS:NE2	1:F:658:GLU:OE2	2.28	0.62
1:A:55:ALA:N	1:A:132:THR:HG22	2.09	0.62
1:B:55:ALA:N	1:B:132:THR:HG22	2.14	0.62
1:B:292:ASN:OD1	1:B:558:TYR:CE2	2.52	0.62
1:D:110:GLN:HG2	1:D:694:ARG:HH22	1.63	0.62
1:E:454:ARG:O	1:E:458:LEU:HD12	1.99	0.62
1:C:522:VAL:O	1:C:526:THR:OG1	2.14	0.62
1:D:419:ASN:HD21	2:M:1:GLC:H61	1.63	0.62
1:E:541:GLU:OE1	1:E:563:ARG:NH1	2.32	0.62
1:E:405:GLN:HE22	1:E:438:VAL:HG21	1.64	0.62
1:F:475:THR:HG22	1:F:478:GLU:CD	2.25	0.62
1:A:529:PRO:O	1:A:586:ARG:NH2	2.32	0.62
1:C:192:ARG:HA	1:C:195:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:ARG:O	1:D:585:ILE:HG12	2.00	0.62
1:A:243:GLY:HA3	1:A:252:VAL:O	1.99	0.62
1:C:487:ALA:HB1	1:C:489:LEU:H	1.63	0.62
1:D:37:VAL:HG11	1:D:227:PRO:HA	1.81	0.62
1:A:318:HIS:CD2	1:A:320:SER:HB3	2.35	0.62
1:C:519:ILE:O	1:C:523:LEU:HD12	2.00	0.62
1:C:563:ARG:HG2	1:C:563:ARG:HH11	1.65	0.62
1:D:325:ASP:OD1	1:D:325:ASP:N	2.28	0.62
1:E:243:GLY:HA3	1:E:252:VAL:O	2.00	0.62
1:E:560:LEU:HD12	1:E:562:PRO:HD3	1.82	0.62
1:F:50:ARG:NH1	1:F:55:ALA:O	2.33	0.62
1:A:475:THR:HG22	1:A:478:GLU:HG3	1.82	0.61
1:A:581:ARG:O	1:A:585:ILE:HG13	2.00	0.61
1:D:576:GLN:O	1:D:580:THR:OG1	2.13	0.61
1:F:126:TRP:HZ3	1:F:128:ASP:HB3	1.65	0.61
1:F:508:VAL:O	1:F:512:ASN:ND2	2.33	0.61
1:E:150:LEU:O	1:E:152:ASN:N	2.33	0.61
1:E:487:ALA:HA	1:E:489:LEU:H	1.65	0.61
1:A:682:HIS:HB3	1:A:684:ILE:HD11	1.82	0.61
1:B:63:ARG:HD3	1:B:64:TYR:N	2.16	0.61
1:D:282:ILE:HD12	1:D:318:HIS:HD2	1.64	0.61
1:F:682:HIS:HB3	1:F:684:ILE:HD11	1.82	0.61
1:B:486:ILE:HG13	1:B:495:PRO:HG3	1.83	0.61
1:D:28:SER:OG	1:D:460:LYS:NZ	2.25	0.61
1:E:110:GLN:N	1:E:110:GLN:OE1	2.34	0.61
1:A:180:ALA:O	1:A:184:ARG:NE	2.29	0.61
1:C:158:ALA:HB1	1:C:184:ARG:CZ	2.31	0.61
1:C:405:GLN:N	1:C:405:GLN:OE1	2.33	0.61
1:D:37:VAL:O	1:D:40:GLU:HG2	2.01	0.61
1:E:536:GLY:O	1:E:541:GLU:HG3	2.01	0.61
1:B:493:ARG:NH1	1:B:494:ARG:O	2.33	0.60
1:C:475:THR:HG22	1:C:478:GLU:HG3	1.82	0.60
1:C:43:PRO:HD2	1:C:596:ARG:NH1	2.15	0.60
1:D:184:ARG:N	1:D:184:ARG:HD2	2.15	0.60
1:E:197:LEU:HD12	1:E:197:LEU:H	1.66	0.60
1:E:583:ASN:HA	1:E:586:ARG:HD3	1.82	0.60
1:D:648:GLU:HG3	1:D:650:TYR:CZ	2.36	0.60
1:B:188:ASP:O	1:B:191:THR:HG23	2.01	0.60
1:C:150:LEU:O	1:C:152:ASN:N	2.34	0.60
1:C:180:ALA:O	1:C:184:ARG:NH2	2.35	0.60
1:C:243:GLY:HA3	1:C:252:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:GLU:HG3	1:D:489:LEU:C	2.26	0.60
1:E:525:ALA:O	1:E:586:ARG:NH1	2.34	0.60
1:D:525:ALA:HB1	1:D:586:ARG:HD2	1.82	0.60
1:F:155:LEU:O	1:F:159:VAL:HG23	2.01	0.60
1:A:371:ILE:HD11	1:A:385:TYR:CG	2.37	0.60
1:A:533:MET:HE1	1:A:538:GLU:HB3	1.83	0.60
1:C:198:THR:HG23	1:C:201:ILE:HG13	1.84	0.60
1:C:656:ARG:NH1	1:C:658:GLU:OE1	2.35	0.60
1:F:282:ILE:HD12	1:F:318:HIS:HD2	1.67	0.60
1:F:416:ARG:HD2	1:F:416:ARG:C	2.26	0.60
1:A:432:ILE:HG23	1:A:436:LYS:NZ	2.17	0.60
1:E:419:ASN:HD21	2:O:1:GLC:H61	1.66	0.60
1:F:536:GLY:O	1:F:541:GLU:HG3	2.01	0.60
1:A:318:HIS:NE2	1:A:320:SER:HB3	2.16	0.59
1:C:387:LEU:HD13	1:C:396:LEU:HD21	1.84	0.59
1:A:583:ASN:HA	1:A:586:ARG:HD3	1.85	0.59
1:B:138:ILE:HA	1:B:141:LEU:HD23	1.84	0.59
1:B:507:ALA:HA	1:B:510:GLN:OE1	2.02	0.59
1:C:446:SER:HB3	1:C:463:PHE:CD1	2.37	0.59
1:A:19:GLU:OE2	1:A:21:ASP:HB2	2.02	0.59
1:C:536:GLY:O	1:C:541:GLU:HG3	2.03	0.59
1:B:465:GLN:HA	1:B:493:ARG:HH12	1.67	0.59
1:A:181:ALA:HA	1:A:184:ARG:HG2	1.84	0.59
1:E:509:LEU:HD22	1:E:517:PHE:CD1	2.38	0.59
1:A:394:GLU:H	1:A:394:GLU:CD	2.11	0.59
1:B:20:ILE:HG12	1:B:48:VAL:HG12	1.84	0.59
1:C:263:LEU:HD21	1:C:334:ALA:HB2	1.84	0.59
1:C:242:THR:HG21	1:C:259:ALA:HA	1.83	0.59
1:C:529:PRO:O	1:C:586:ARG:NH2	2.33	0.59
1:D:234:TRP:CH2	1:D:445:LEU:HD11	2.38	0.59
1:E:68:ARG:HG3	1:E:68:ARG:HH11	1.68	0.59
1:F:183:LEU:HD13	1:F:192:ARG:HA	1.85	0.59
1:A:378:PRO:O	1:A:380:LYS:NZ	2.36	0.59
1:A:509:LEU:HD22	1:A:517:PHE:HD2	1.68	0.59
1:C:271:PHE:O	1:C:339:MET:HE2	2.02	0.59
1:C:430:TRP:NE1	1:C:434:GLN:HE22	2.00	0.59
1:D:288:LYS:HZ3	1:D:383:ASP:CB	2.13	0.59
1:A:525:ALA:O	1:A:586:ARG:NH1	2.36	0.59
1:B:163:ARG:NH1	1:B:210:LEU:HD11	2.18	0.59
1:B:662:GLU:HB3	1:B:664:TYR:HE1	1.67	0.59
1:A:126:TRP:CD2	1:A:211:ARG:HG2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:O	1:A:180:ALA:N	2.33	0.58
1:A:152:ASN:ND2	1:B:368:ASP:OD2	2.36	0.58
1:B:201:ILE:HA	1:B:204:LEU:HB3	1.84	0.58
1:D:416:ARG:HA	1:D:445:LEU:HD13	1.84	0.58
1:D:529:PRO:O	1:D:586:ARG:NH2	2.36	0.58
1:A:480:THR:HA	1:A:600:PHE:HE1	1.67	0.58
1:B:154:LEU:HB3	1:B:183:LEU:HD23	1.86	0.58
1:C:207:ASP:OD1	1:C:208:TYR:N	2.36	0.58
1:D:253:HIS:ND1	1:D:320:SER:OG	2.36	0.58
1:D:539:LEU:HB2	1:D:563:ARG:HH12	1.67	0.58
1:F:485:GLN:NE2	1:F:489:LEU:HD11	2.18	0.58
1:D:509:LEU:HD21	1:D:520:ARG:HG3	1.85	0.58
1:D:533:MET:HG3	1:D:537:TYR:HD2	1.68	0.58
1:A:629:ASN:HB2	3:H:2:GLC:O5	2.03	0.58
1:B:64:TYR:HD2	1:B:115:ARG:HH11	1.50	0.58
1:C:503:ASP:OD2	2:K:1:GLC:O1	2.22	0.58
1:D:498:PHE:CE1	1:D:532:GLY:HA3	2.39	0.58
1:E:285:VAL:HB	1:E:351:PRO:HG3	1.86	0.58
1:A:615:ASP:OD2	1:A:618:THR:HG22	2.02	0.58
1:C:158:ALA:HB1	1:C:184:ARG:NH2	2.19	0.58
1:E:581:ARG:O	1:E:585:ILE:HG13	2.04	0.58
1:A:203:GLU:HG3	1:A:204:LEU:N	2.18	0.58
1:A:692:GLU:HB3	1:A:695:ASN:HD21	1.67	0.58
1:D:695:ASN:O	1:D:698:LEU:HD13	2.04	0.58
1:F:183:LEU:HD22	1:F:192:ARG:HB2	1.85	0.58
1:B:198:THR:OG1	1:B:200:GLU:OE2	2.20	0.58
1:B:243:GLY:HA3	1:B:252:VAL:O	2.04	0.58
1:B:486:ILE:HD11	1:B:528:SER:HB2	1.85	0.58
1:C:154:LEU:H	1:C:154:LEU:HD12	1.68	0.58
1:A:183:LEU:HB2	1:A:192:ARG:HB2	1.86	0.57
1:A:285:VAL:HG12	1:A:286:HIS:ND1	2.19	0.57
1:A:205:LEU:HA	1:A:208:TYR:O	2.04	0.57
1:B:116:VAL:HA	1:B:224:VAL:HG23	1.86	0.57
1:B:493:ARG:HH11	1:B:494:ARG:N	2.02	0.57
1:F:499:VAL:HG11	1:F:537:TYR:CZ	2.39	0.57
1:E:154:LEU:HD12	1:E:154:LEU:H	1.69	0.57
1:C:153:ASP:O	1:C:156:VAL:HG22	2.04	0.57
1:D:65:LEU:HD12	1:D:118:LEU:HD12	1.86	0.57
1:E:150:LEU:HD12	1:E:154:LEU:HD11	1.86	0.57
1:C:587:ARG:HD3	1:E:665:GLN:OE1	2.03	0.57
1:D:309:SER:HA	1:D:352:ASP:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:663:GLU:C	1:E:664:TYR:HD1	2.13	0.57
1:F:363:PHE:HB3	1:F:371:ILE:CD1	2.35	0.57
1:A:692:GLU:OE1	1:A:692:GLU:HA	2.04	0.57
1:B:282:ILE:HD12	1:B:318:HIS:HD2	1.70	0.57
1:D:374:ALA:HA	1:D:386:PRO:HD3	1.86	0.57
1:F:275:TYR:CE1	1:F:416:ARG:HG3	2.39	0.57
1:B:50:ARG:NH1	1:B:51:GLU:OE1	2.37	0.57
1:B:230:ARG:NH1	1:B:594:GLN:OE1	2.38	0.57
1:F:631:PHE:CE1	3:R:5:GLC:H3	2.39	0.57
1:D:169:PRO:C	1:D:171:GLY:H	2.12	0.57
1:E:487:ALA:HB1	1:E:490:ALA:N	2.20	0.57
1:A:19:GLU:OE1	1:A:49:TRP:NE1	2.38	0.57
1:D:182:ALA:O	1:D:183:LEU:HD12	2.05	0.57
1:F:529:PRO:O	1:F:586:ARG:NH2	2.37	0.57
1:A:255:THR:OG1	1:A:321:LEU:O	2.19	0.57
1:B:168:VAL:HG21	1:B:176:LEU:HD12	1.86	0.57
1:C:436:LYS:NZ	1:C:442:VAL:O	2.30	0.57
1:A:318:HIS:HE2	1:A:320:SER:HB3	1.70	0.56
1:B:154:LEU:H	1:B:154:LEU:HD22	1.69	0.56
1:B:374:ALA:CA	1:B:386:PRO:HD3	2.35	0.56
1:D:247:ASP:OD1	1:D:247:ASP:N	2.38	0.56
1:D:363:PHE:HB3	1:D:371:ILE:HD11	1.87	0.56
1:A:506:HIS:CE1	1:A:508:VAL:HG23	2.40	0.56
1:B:182:ALA:O	1:B:192:ARG:HD3	2.05	0.56
1:B:374:ALA:HA	1:B:386:PRO:HD3	1.86	0.56
1:D:362:TRP:HD1	1:D:392:ASP:HB3	1.69	0.56
1:D:556:GLU:HG3	1:D:561:ARG:HB2	1.87	0.56
1:E:271:PHE:HZ	1:E:533:MET:HE3	1.70	0.56
1:E:287:ARG:O	1:E:296:ALA:HB2	2.05	0.56
1:A:122:ARG:HB3	1:A:219:GLN:HG2	1.86	0.56
1:A:154:LEU:O	1:A:192:ARG:NH2	2.36	0.56
1:C:554:ASP:HB3	1:C:559:GLU:OE2	2.05	0.56
1:E:157:GLY:O	1:E:161:LEU:HD12	2.05	0.56
1:F:168:VAL:CG2	1:F:173:ARG:HD3	2.34	0.56
1:F:605:ASN:HB2	1:F:636:ALA:HB2	1.88	0.56
1:B:177:LEU:HA	1:B:180:ALA:HB3	1.86	0.56
1:E:182:ALA:O	1:E:183:LEU:HD13	2.05	0.56
1:F:498:PHE:CE1	1:F:532:GLY:HA3	2.41	0.56
1:A:388:ASN:ND2	1:A:391:ASN:H	2.02	0.56
1:B:292:ASN:OD1	1:B:558:TYR:CZ	2.58	0.56
1:C:149:GLU:N	1:C:151:SER:OG	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:LEU:HD13	1:E:396:LEU:HD21	1.87	0.56
1:F:317:VAL:HG23	1:F:324:ILE:HG12	1.87	0.56
1:A:536:GLY:O	1:A:541:GLU:HG3	2.05	0.56
1:B:533:MET:HE2	1:B:538:GLU:HG3	1.88	0.56
1:C:488:GLU:C	1:C:490:ALA:H	2.13	0.56
1:F:519:ILE:HD13	1:F:627:THR:O	2.05	0.56
1:F:525:ALA:O	1:F:586:ARG:NH1	2.39	0.56
1:C:198:THR:HG23	1:C:201:ILE:CG1	2.36	0.56
1:C:615:ASP:OD2	1:C:618:THR:HG22	2.05	0.56
1:D:282:ILE:HD12	1:D:318:HIS:CD2	2.41	0.56
1:D:366:LEU:HB3	1:D:367:PRO:HD2	1.87	0.56
1:E:476:LYS:HD3	1:E:628:LEU:HD12	1.88	0.56
1:D:122:ARG:HB3	1:D:219:GLN:HG2	1.87	0.56
1:D:154:LEU:HD12	1:D:154:LEU:H	1.70	0.56
1:D:509:LEU:HD22	1:D:517:PHE:CD1	2.41	0.56
1:E:134:ARG:O	1:E:138:ILE:HG12	2.05	0.56
1:E:575:LEU:HD23	1:E:579:ILE:HD11	1.86	0.56
1:F:192:ARG:C	1:F:194:ALA:H	2.14	0.56
1:B:432:ILE:HG22	1:B:436:LYS:NZ	2.20	0.56
1:F:173:ARG:HH12	1:F:177:LEU:N	1.99	0.56
1:C:247:ASP:N	1:C:247:ASP:OD1	2.39	0.56
1:C:543:ARG:HB3	1:C:553:LEU:HD12	1.88	0.56
1:F:571:GLN:OE1	1:F:573:ARG:NH1	2.38	0.56
1:A:179:ALA:HA	1:A:195:LEU:HD13	1.88	0.55
1:E:486:ILE:HG21	1:E:493:ARG:NH2	2.21	0.55
1:A:92:LYS:HD2	1:A:92:LYS:O	2.06	0.55
1:C:183:LEU:HD22	1:C:192:ARG:HG3	1.87	0.55
1:B:238:PHE:CE1	1:B:277:PRO:HG2	2.41	0.55
1:C:183:LEU:HB2	1:C:192:ARG:CD	2.37	0.55
1:D:17:ARG:HG2	1:D:213:LEU:HD11	1.88	0.55
1:D:173:ARG:O	1:D:176:LEU:HG	2.05	0.55
1:D:179:ALA:CA	1:D:195:LEU:HD21	2.33	0.55
1:F:287:ARG:NH2	1:F:301:VAL:O	2.34	0.55
1:F:692:GLU:OE1	1:F:692:GLU:HA	2.06	0.55
1:B:581:ARG:O	1:B:585:ILE:HG13	2.06	0.55
1:E:607:ALA:HB3	1:E:634:GLU:HG2	1.88	0.55
1:F:394:GLU:HA	1:F:397:TYR:HB2	1.88	0.55
1:C:120:THR:HG21	1:C:219:GLN:OE1	2.07	0.55
1:D:519:ILE:HD13	1:D:627:THR:O	2.06	0.55
1:E:191:THR:HG23	1:E:192:ARG:HG3	1.87	0.55
1:E:652:ARG:HD3	1:E:665:GLN:NE2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:682:HIS:HB3	1:E:684:ILE:HD11	1.88	0.55
1:C:59:THR:OG1	1:C:211:ARG:NH2	2.36	0.55
1:C:183:LEU:HB2	1:C:192:ARG:HE	1.70	0.55
1:A:195:LEU:O	1:A:201:ILE:HG13	2.06	0.55
1:B:122:ARG:HB3	1:B:219:GLN:HG2	1.88	0.55
1:B:485:GLN:HA	1:B:488:GLU:OE1	2.07	0.55
1:D:536:GLY:O	1:D:541:GLU:HG3	2.06	0.55
1:E:55:ALA:N	1:E:132:THR:HG22	2.15	0.55
1:F:581:ARG:O	1:F:585:ILE:HG13	2.06	0.55
1:D:170:ARG:HA	1:D:173:ARG:CG	2.36	0.55
1:E:519:ILE:HD13	1:E:627:THR:O	2.06	0.55
1:F:198:THR:HG21	1:F:201:ILE:HD13	1.88	0.55
1:B:522:VAL:O	1:B:526:THR:OG1	2.17	0.55
1:C:481:GLU:O	1:C:485:GLN:N	2.40	0.55
1:D:682:HIS:HB3	1:D:684:ILE:HD11	1.89	0.55
1:E:265:ARG:NH1	1:E:576:GLN:OE1	2.40	0.55
1:E:285:VAL:HG12	1:E:286:HIS:CE1	2.41	0.55
1:A:519:ILE:HD13	1:A:627:THR:O	2.08	0.54
1:B:292:ASN:OD1	1:B:558:TYR:OH	2.14	0.54
1:E:375:GLU:CD	1:E:379:LYS:O	2.50	0.54
1:E:671:TYR:HE1	1:E:673:ARG:CZ	2.20	0.54
1:F:180:ALA:O	1:F:184:ARG:CZ	2.55	0.54
1:C:285:VAL:HG12	1:C:286:HIS:ND1	2.22	0.54
1:C:505:LEU:HB2	1:C:552:TYR:CE2	2.43	0.54
1:C:505:LEU:HD13	1:C:552:TYR:HE2	1.72	0.54
1:A:188:ASP:HB3	1:A:191:THR:OG1	2.07	0.54
1:B:67:VAL:HG11	1:B:440:PRO:HG3	1.89	0.54
1:B:505:LEU:HB3	1:B:552:TYR:HE1	1.72	0.54
1:E:280:HIS:HB3	1:E:281:PRO:HD2	1.89	0.54
1:E:476:LYS:NZ	1:E:606:ASP:O	2.27	0.54
1:E:631:PHE:CE1	3:P:5:GLC:H3	2.43	0.54
1:F:275:TYR:CZ	1:F:416:ARG:HG3	2.42	0.54
1:B:238:PHE:CD1	1:B:277:PRO:HG2	2.41	0.54
1:E:589:HIS:NE2	1:E:658:GLU:OE2	2.35	0.54
1:D:362:TRP:CD1	1:D:392:ASP:HB3	2.41	0.54
1:A:236:GLU:HB3	1:A:534:TYR:HA	1.89	0.54
1:E:64:TYR:HE2	1:E:117:GLY:HA3	1.71	0.54
1:E:540:PHE:CZ	1:E:575:LEU:HB2	2.43	0.54
1:D:153:ASP:O	1:D:156:VAL:HG22	2.08	0.54
1:B:575:LEU:HD23	1:B:579:ILE:HD11	1.90	0.54
1:D:242:THR:HG21	1:D:259:ALA:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:LYS:HZ1	3:N:1:GLC:H4	1.73	0.54
1:E:183:LEU:CD1	1:E:192:ARG:HB3	2.37	0.54
1:C:182:ALA:C	1:C:192:ARG:HD3	2.33	0.54
1:C:582:LEU:O	1:C:586:ARG:HG2	2.07	0.54
1:D:335:ARG:NH2	1:D:411:GLY:O	2.41	0.54
1:E:509:LEU:HD22	1:E:517:PHE:HD1	1.72	0.54
1:B:59:THR:HG23	1:B:126:TRP:HE1	1.73	0.54
1:C:176:LEU:O	1:C:180:ALA:N	2.39	0.54
1:C:657:ASP:OD1	1:C:659:ILE:HG12	2.08	0.54
1:E:251:PRO:HB2	1:E:560:LEU:HD11	1.90	0.54
1:C:240:ARG:NH1	1:C:560:LEU:HD23	2.23	0.53
1:C:317:VAL:HG23	1:C:324:ILE:HG12	1.90	0.53
1:D:35:LYS:HD2	1:D:492:TYR:O	2.08	0.53
1:F:111:PHE:CE1	1:F:113:PRO:HG3	2.43	0.53
1:A:158:ALA:HB1	1:A:184:ARG:NE	2.23	0.53
1:B:168:VAL:HG12	1:B:208:TYR:HB2	1.90	0.53
1:C:179:ALA:HA	1:C:195:LEU:HD11	1.91	0.53
1:C:499:VAL:HG11	1:C:537:TYR:CZ	2.42	0.53
1:C:605:ASN:HB2	1:C:636:ALA:HB2	1.89	0.53
1:D:188:ASP:OD1	1:D:189:PRO:HD2	2.08	0.53
1:B:126:TRP:CZ3	1:B:128:ASP:HB3	2.44	0.53
1:C:92:LYS:HG3	1:C:93:PRO:HD2	1.90	0.53
1:D:134:ARG:O	1:D:138:ILE:HG13	2.08	0.53
1:D:184:ARG:HD2	1:D:184:ARG:H	1.73	0.53
1:A:242:THR:HG21	1:A:259:ALA:HA	1.88	0.53
1:F:485:GLN:O	1:F:489:LEU:HD12	2.08	0.53
1:A:362:TRP:HH2	1:A:399:GLU:HG3	1.74	0.53
1:C:156:VAL:O	1:C:160:LEU:HD23	2.08	0.53
1:E:212:ASP:CG	1:E:213:LEU:HD12	2.34	0.53
1:E:374:ALA:HB2	1:E:386:PRO:N	2.23	0.53
1:B:387:LEU:HD13	1:B:396:LEU:HD21	1.91	0.53
1:D:190:VAL:HA	1:D:193:THR:OG1	2.08	0.53
1:D:226:ARG:HH12	1:D:340:GLU:CD	2.17	0.53
1:B:151:SER:HA	1:B:154:LEU:HD23	1.91	0.53
1:D:275:TYR:CZ	1:D:416:ARG:HD3	2.43	0.53
1:F:55:ALA:N	1:F:132:THR:HG22	2.21	0.53
1:F:405:GLN:NE2	1:F:438:VAL:HG21	2.24	0.53
1:E:485:GLN:O	1:E:489:LEU:HG	2.09	0.53
1:A:280:HIS:ND1	1:A:314:HIS:HA	2.24	0.53
1:D:488:GLU:HB3	1:D:490:ALA:HB2	1.91	0.53
1:F:505:LEU:HB2	1:F:552:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:677:ALA:HB2	3:R:6:GLC:H61	1.91	0.53
1:A:305:TRP:NE1	1:A:344:ASP:OD1	2.39	0.53
1:B:682:HIS:HB3	1:B:684:ILE:HD11	1.90	0.53
1:F:569:LEU:HD11	1:F:576:GLN:NE2	2.24	0.53
1:B:103:GLU:OE1	1:B:106:VAL:HG23	2.09	0.52
1:C:207:ASP:OD1	1:C:208:TYR:HD2	1.90	0.52
1:E:398:ASP:OD1	1:E:402:ARG:NH1	2.42	0.52
1:F:282:ILE:HD12	1:F:318:HIS:CD2	2.43	0.52
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.90	0.52
1:B:184:ARG:HG3	1:B:185:THR:H	1.73	0.52
1:C:519:ILE:HD13	1:C:627:THR:O	2.09	0.52
1:E:284:LYS:CD	1:E:352:ASP:HB3	2.36	0.52
1:E:621:CYS:HB2	1:E:689:VAL:HG23	1.91	0.52
1:A:134:ARG:O	1:A:138:ILE:HG13	2.09	0.52
1:B:567:SER:O	1:B:571:GLN:HG2	2.08	0.52
1:C:473:ARG:HD2	1:C:478:GLU:HB3	1.91	0.52
1:C:589:HIS:NE2	1:C:658:GLU:OE2	2.39	0.52
1:E:556:GLU:CD	1:E:563:ARG:HH21	2.16	0.52
1:F:126:TRP:CZ3	1:F:128:ASP:HB3	2.45	0.52
1:C:69:TYR:HB3	1:C:70:PRO:HD3	1.92	0.52
1:D:276:LEU:HD11	1:D:343:LEU:HD12	1.92	0.52
1:E:242:THR:HG21	1:E:259:ALA:HA	1.91	0.52
1:F:284:LYS:N	1:F:352:ASP:OD2	2.30	0.52
1:C:265:ARG:HA	1:E:671:TYR:CE1	2.44	0.52
1:D:282:ILE:O	1:D:287:ARG:NH2	2.42	0.52
1:E:580:THR:O	1:E:584:ILE:HG13	2.10	0.52
1:F:130:ILE:HD13	1:F:160:LEU:HD13	1.91	0.52
1:A:15:PRO:N	1:B:426:ASN:HD22	2.07	0.52
1:B:503:ASP:OD1	1:B:557:LYS:HE3	2.10	0.52
1:E:170:ARG:O	1:E:173:ARG:HG3	2.09	0.52
1:E:218:GLU:HG3	1:E:220:PHE:CZ	2.45	0.52
1:A:692:GLU:O	1:A:696:THR:HG23	2.10	0.52
1:F:157:GLY:O	1:F:160:LEU:HB2	2.10	0.52
1:C:176:LEU:HD21	1:C:204:LEU:HD11	1.92	0.52
1:D:457:GLY:O	1:D:460:LYS:HB3	2.09	0.52
1:E:149:GLU:HG2	1:E:150:LEU:H	1.75	0.52
1:E:269:MET:SD	1:E:576:GLN:HG3	2.50	0.52
1:A:364:THR:HG22	1:A:388:ASN:HB2	1.91	0.52
1:A:374:ALA:HA	1:A:386:PRO:HD3	1.90	0.52
1:A:695:ASN:HA	1:A:698:LEU:CD1	2.40	0.52
1:B:662:GLU:HB3	1:B:664:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TRP:CE2	1:C:157:GLY:HA3	2.44	0.52
1:D:27:VAL:HG12	1:D:460:LYS:HE3	1.92	0.52
1:E:21:ASP:OD2	1:E:22:ASP:N	2.43	0.52
1:E:32:TYR:HD2	1:E:460:LYS:HE2	1.74	0.52
1:A:361:GLN:H	1:A:361:GLN:CD	2.17	0.51
1:B:540:PHE:CZ	1:B:575:LEU:HB2	2.44	0.51
1:B:665:GLN:OE1	1:F:587:ARG:NH1	2.43	0.51
1:C:422:THR:HA	1:D:52:GLY:HA2	1.93	0.51
1:C:541:GLU:CD	1:C:563:ARG:HH12	2.18	0.51
1:D:482:PHE:O	1:D:486:ILE:HG12	2.09	0.51
1:D:698:LEU:O	1:D:699:ARG:HB2	2.10	0.51
1:E:671:TYR:CZ	1:E:673:ARG:HG3	2.44	0.51
1:F:374:ALA:HA	1:F:386:PRO:HD3	1.91	0.51
1:F:657:ASP:OD1	1:F:659:ILE:HG12	2.10	0.51
1:A:656:ARG:NH1	1:A:658:GLU:OE1	2.44	0.51
1:C:156:VAL:O	1:C:159:VAL:HG12	2.09	0.51
1:D:36:ALA:O	1:D:224:VAL:HA	2.10	0.51
1:D:200:GLU:O	1:D:204:LEU:HG	2.10	0.51
1:E:428:TRP:O	1:E:432:ILE:HG13	2.10	0.51
1:E:476:LYS:CD	1:E:628:LEU:HD12	2.40	0.51
1:C:355:TRP:HA	1:C:358:GLU:HG2	1.91	0.51
1:D:103:GLU:HG3	1:D:104:PRO:HD2	1.92	0.51
1:D:200:GLU:O	1:D:203:GLU:HG2	2.10	0.51
1:D:317:VAL:HG23	1:D:324:ILE:HG12	1.91	0.51
1:D:505:LEU:HD12	1:D:552:TYR:CE1	2.46	0.51
1:F:153:ASP:O	1:F:156:VAL:HG22	2.10	0.51
1:F:235:TYR:HB2	1:F:271:PHE:CD1	2.45	0.51
1:F:405:GLN:HE22	1:F:438:VAL:HG21	1.76	0.51
1:A:509:LEU:HB3	1:A:517:PHE:HE2	1.75	0.51
1:D:414:PHE:CE1	1:D:443:LEU:HD12	2.46	0.51
1:E:288:LYS:HZ3	1:E:383:ASP:CG	2.18	0.51
1:F:168:VAL:HG12	1:F:208:TYR:HB2	1.91	0.51
1:F:375:GLU:N	1:F:375:GLU:OE1	2.43	0.51
1:C:583:ASN:HA	1:C:586:ARG:HD3	1.92	0.51
1:B:519:ILE:HD13	1:B:627:THR:O	2.10	0.51
1:C:126:TRP:CD2	1:C:211:ARG:HG2	2.46	0.51
1:C:397:TYR:HB3	1:C:430:TRP:CH2	2.45	0.51
1:D:111:PHE:CE1	1:D:113:PRO:HG3	2.46	0.51
1:D:642:MET:HE1	1:D:653:PHE:HE2	1.75	0.51
1:D:657:ASP:OD2	1:D:659:ILE:HG12	2.11	0.51
1:E:693:SER:OG	1:E:694:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:O	1:A:403:VAL:HG23	2.11	0.51
1:A:509:LEU:HD21	1:A:520:ARG:HG3	1.93	0.51
1:A:527:MET:HE1	1:A:600:PHE:CZ	2.46	0.51
1:C:149:GLU:N	1:C:149:GLU:OE1	2.43	0.51
1:E:505:LEU:HD12	1:E:552:TYR:CE1	2.46	0.51
1:E:647:MET:HE1	1:E:687:PRO:CG	2.39	0.51
1:B:698:LEU:O	1:B:699:ARG:HB2	2.11	0.51
1:C:240:ARG:NH2	1:C:556:GLU:O	2.43	0.51
1:D:157:GLY:O	1:D:160:LEU:HB2	2.11	0.51
1:E:657:ASP:OD1	1:E:659:ILE:HG12	2.11	0.51
1:F:416:ARG:NH1	1:F:447:GLU:HB2	2.25	0.51
1:F:556:GLU:CD	1:F:556:GLU:H	2.19	0.51
1:B:173:ARG:O	1:B:173:ARG:HG2	2.10	0.51
1:D:68:ARG:O	1:D:69:TYR:HB2	2.10	0.51
1:D:541:GLU:OE2	1:D:563:ARG:NH2	2.44	0.51
1:A:275:TYR:CZ	1:A:416:ARG:HD3	2.45	0.51
1:D:280:HIS:HB2	1:D:307:ILE:HG23	1.91	0.51
1:B:366:LEU:HG	1:B:372:ALA:HB2	1.93	0.50
1:E:126:TRP:HZ3	1:E:128:ASP:HB2	1.75	0.50
1:A:362:TRP:CD1	1:A:392:ASP:HB3	2.46	0.50
1:A:605:ASN:HB2	1:A:636:ALA:HB2	1.93	0.50
1:E:314:HIS:HB3	1:E:403:VAL:HG11	1.93	0.50
1:A:21:ASP:OD1	1:A:22:ASP:N	2.42	0.50
1:A:358:GLU:C	1:A:359:HIS:HD2	2.19	0.50
1:B:236:GLU:HB3	1:B:534:TYR:HA	1.93	0.50
1:B:307:ILE:HG21	1:B:314:HIS:CD2	2.47	0.50
1:C:64:TYR:OH	1:C:116:VAL:O	2.22	0.50
1:C:240:ARG:HG3	1:C:240:ARG:NH1	2.25	0.50
1:D:35:LYS:CG	1:D:492:TYR:HA	2.41	0.50
1:E:275:TYR:CZ	1:E:416:ARG:HD3	2.46	0.50
1:E:371:ILE:HD11	1:E:385:TYR:CE2	2.46	0.50
1:F:173:ARG:HD2	1:F:176:LEU:HD13	1.92	0.50
1:A:428:TRP:O	1:A:432:ILE:HG13	2.11	0.50
1:A:485:GLN:NE2	1:A:489:LEU:HD12	2.25	0.50
1:B:191:THR:CB	1:B:192:ARG:HD2	2.40	0.50
1:C:122:ARG:HG2	1:C:123:VAL:N	2.25	0.50
1:C:375:GLU:N	1:C:375:GLU:OE1	2.45	0.50
1:E:68:ARG:O	1:E:69:TYR:HB2	2.11	0.50
1:E:126:TRP:CD2	1:E:211:ARG:HG2	2.47	0.50
1:E:126:TRP:CZ3	1:E:128:ASP:HB2	2.47	0.50
1:F:179:ALA:O	1:F:195:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:573:ARG:O	1:F:573:ARG:HG2	2.11	0.50
1:A:307:ILE:HG21	1:A:314:HIS:CD2	2.45	0.50
1:B:242:THR:HG21	1:B:259:ALA:HA	1.93	0.50
1:B:512:ASN:CA	1:B:631:PHE:CZ	2.88	0.50
1:C:161:LEU:HD12	1:C:161:LEU:H	1.77	0.50
1:D:630:ALA:O	3:N:6:GLC:O4	2.28	0.50
1:A:690:PRO:C	1:A:692:GLU:H	2.20	0.50
1:B:126:TRP:HZ3	1:B:128:ASP:HB3	1.77	0.50
1:D:195:LEU:HA	1:D:198:THR:OG1	2.12	0.50
1:A:499:VAL:HG11	1:A:537:TYR:CZ	2.47	0.50
1:C:366:LEU:HB3	1:C:367:PRO:HD2	1.94	0.50
1:E:507:ALA:O	1:E:510:GLN:HB2	2.11	0.50
1:E:536:GLY:HA3	1:E:563:ARG:HH11	1.75	0.50
1:A:631:PHE:CE1	3:H:5:GLC:H3	2.47	0.50
1:B:505:LEU:HD23	1:B:552:TYR:CE1	2.47	0.50
1:B:505:LEU:HD11	1:B:544:ALA:HB2	1.94	0.50
1:C:590:PRO:O	1:C:593:GLN:HG3	2.12	0.50
1:C:631:PHE:CE1	3:L:5:GLC:H3	2.47	0.50
1:E:382:GLN:OE1	1:E:382:GLN:N	2.33	0.50
1:A:414:PHE:CE1	1:A:443:LEU:HB2	2.46	0.50
1:C:314:HIS:HB3	1:C:403:VAL:HG11	1.93	0.50
1:D:176:LEU:O	1:D:180:ALA:N	2.44	0.50
1:D:583:ASN:O	1:D:587:ARG:HG3	2.11	0.50
1:E:517:PHE:CE2	1:E:540:PHE:HA	2.47	0.50
1:E:18:VAL:HG11	1:E:50:ARG:CZ	2.42	0.49
1:E:366:LEU:HD23	1:E:368:ASP:H	1.77	0.49
1:A:234:TRP:HZ2	1:A:414:PHE:CE2	2.31	0.49
1:A:235:TYR:OH	1:A:538:GLU:OE1	2.18	0.49
1:A:517:PHE:HD1	1:A:540:PHE:CD1	2.25	0.49
1:D:263:LEU:HD21	1:D:334:ALA:HB2	1.94	0.49
1:D:265:ARG:HH21	1:D:565:PHE:HB3	1.77	0.49
1:F:151:SER:HA	1:F:154:LEU:CD1	2.41	0.49
1:F:505:LEU:HB2	1:F:552:TYR:CE2	2.46	0.49
1:A:317:VAL:HG23	1:A:324:ILE:HG12	1.94	0.49
1:B:134:ARG:O	1:B:138:ILE:HG23	2.12	0.49
1:D:631:PHE:CE1	3:N:5:GLC:H3	2.48	0.49
1:E:672:ILE:HD11	1:E:682:HIS:CD2	2.47	0.49
1:A:116:VAL:HA	1:A:224:VAL:HG23	1.93	0.49
1:A:174:ASP:HA	1:A:177:LEU:HD13	1.94	0.49
1:B:157:GLY:O	1:B:161:LEU:HD22	2.13	0.49
1:D:177:LEU:HA	1:D:180:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:GLU:O	1:E:203:GLU:HG2	2.12	0.49
1:B:505:LEU:HB3	1:B:552:TYR:CE1	2.46	0.49
1:D:21:ASP:OD1	1:D:22:ASP:N	2.43	0.49
1:D:436:LYS:HG3	1:D:440:PRO:HA	1.93	0.49
1:D:489:LEU:HD23	1:D:492:TYR:OH	2.13	0.49
1:C:183:LEU:N	1:C:192:ARG:HD3	2.27	0.49
1:A:371:ILE:HD11	1:A:385:TYR:CD1	2.48	0.49
1:B:108:HIS:CG	1:B:698:LEU:HD11	2.47	0.49
1:B:534:TYR:OH	1:B:556:GLU:OE1	2.14	0.49
1:C:151:SER:HA	1:C:154:LEU:HD13	1.95	0.49
1:E:188:ASP:O	1:E:192:ARG:HG3	2.12	0.49
1:F:180:ALA:O	1:F:184:ARG:NH2	2.46	0.49
1:A:479:LEU:HD12	1:A:628:LEU:HD21	1.94	0.49
1:B:189:PRO:C	1:B:191:THR:H	2.21	0.49
1:C:491:ASP:OD2	1:C:596:ARG:NH2	2.35	0.49
1:C:631:PHE:CD1	3:L:5:GLC:H3	2.48	0.49
1:D:165:ALA:HA	1:D:176:LEU:HD21	1.95	0.49
1:D:489:LEU:HD12	1:D:489:LEU:H	1.77	0.49
1:F:605:ASN:HD21	1:F:634:GLU:HG3	1.78	0.49
1:A:533:MET:HG3	1:A:537:TYR:HD1	1.77	0.49
1:B:493:ARG:HD3	1:B:494:ARG:C	2.38	0.49
1:C:583:ASN:O	1:C:587:ARG:HG3	2.12	0.49
1:D:276:LEU:HD13	1:D:279:ILE:HG23	1.94	0.49
1:D:600:PHE:CD1	1:D:611:TYR:HB3	2.47	0.49
1:E:523:LEU:O	1:E:527:MET:HG3	2.13	0.49
1:E:630:ALA:O	3:P:6:GLC:O4	2.28	0.49
1:F:240:ARG:CZ	1:F:301:VAL:HG11	2.43	0.49
1:F:358:GLU:HG3	1:F:359:HIS:N	2.26	0.49
1:A:468:SER:OG	1:A:469:TYR:N	2.44	0.49
1:A:505:LEU:HB2	1:A:552:TYR:CE2	2.48	0.49
1:F:173:ARG:CZ	1:F:176:LEU:HB2	2.42	0.49
1:B:226:ARG:NE	1:B:443:LEU:HD11	2.28	0.48
1:B:282:ILE:HD12	1:B:318:HIS:CD2	2.47	0.48
1:B:533:MET:HE3	1:B:537:TYR:CD1	2.47	0.48
1:D:476:LYS:CD	1:D:628:LEU:HD12	2.40	0.48
1:D:489:LEU:HD12	1:D:489:LEU:N	2.27	0.48
1:D:589:HIS:NE2	1:D:658:GLU:OE2	2.36	0.48
1:E:468:SER:OG	1:E:469:TYR:N	2.46	0.48
1:E:508:VAL:O	1:E:512:ASN:ND2	2.32	0.48
1:A:575:LEU:HD23	1:A:579:ILE:HD11	1.95	0.48
1:B:275:TYR:CZ	1:B:416:ARG:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ALA:CA	1:C:339:MET:HE3	2.42	0.48
1:D:518:ALA:O	1:D:522:VAL:HG23	2.13	0.48
1:F:122:ARG:HH11	1:F:219:GLN:HE21	1.60	0.48
1:F:153:ASP:OD1	1:F:154:LEU:HD12	2.13	0.48
1:F:155:LEU:HA	1:F:158:ALA:HB3	1.94	0.48
1:A:311:GLU:OE1	1:A:319:PRO:HG3	2.14	0.48
1:A:475:THR:HG22	1:A:478:GLU:CG	2.44	0.48
1:A:533:MET:HE2	1:A:537:TYR:HB3	1.95	0.48
1:B:405:GLN:NE2	1:B:438:VAL:HG21	2.28	0.48
1:C:195:LEU:C	1:C:198:THR:HG22	2.37	0.48
1:D:265:ARG:NH2	1:D:565:PHE:HB3	2.28	0.48
1:D:271:PHE:O	1:D:339:MET:HE2	2.13	0.48
1:E:180:ALA:O	1:E:184:ARG:HG2	2.13	0.48
1:E:193:THR:O	1:E:195:LEU:N	2.47	0.48
1:E:374:ALA:N	1:E:386:PRO:HD3	2.28	0.48
1:C:275:TYR:CZ	1:C:416:ARG:HD3	2.48	0.48
1:D:533:MET:HG3	1:D:537:TYR:CD2	2.48	0.48
1:E:179:ALA:HB1	1:E:195:LEU:HD22	1.96	0.48
1:F:21:ASP:OD1	1:F:22:ASP:N	2.46	0.48
1:F:374:ALA:HB3	1:F:381:TYR:HB2	1.96	0.48
1:A:642:MET:HE1	1:A:653:PHE:HE2	1.78	0.48
1:E:57:ALA:HA	1:E:107:PHE:CE2	2.40	0.48
1:E:241:SER:OG	1:E:561:ARG:O	2.21	0.48
1:E:475:THR:OG1	1:E:478:GLU:HG3	2.12	0.48
1:F:336:ASP:OD1	1:F:337:LEU:N	2.47	0.48
1:B:501:THR:OG1	1:B:504:ILE:HG12	2.12	0.48
1:C:157:GLY:O	1:C:160:LEU:HB2	2.13	0.48
1:C:280:HIS:HB3	1:C:281:PRO:HD2	1.94	0.48
1:E:283:GLY:O	1:E:287:ARG:NH2	2.46	0.48
1:A:280:HIS:HB3	1:A:281:PRO:HD2	1.94	0.48
1:A:366:LEU:HB3	1:A:367:PRO:HD2	1.96	0.48
1:A:371:ILE:HD11	1:A:385:TYR:CD2	2.49	0.48
1:C:201:ILE:HA	1:C:204:LEU:HD21	1.95	0.48
1:B:240:ARG:NH2	1:B:304:PRO:HG3	2.29	0.48
1:B:269:MET:SD	1:B:576:GLN:HG3	2.53	0.48
1:B:663:GLU:O	1:B:664:TYR:HD1	1.97	0.48
1:C:312:GLY:HA3	1:C:316:THR:OG1	2.14	0.48
1:D:498:PHE:HD2	1:D:501:THR:HG22	1.79	0.48
1:A:508:VAL:HG11	1:A:516:MET:HE2	1.96	0.48
1:C:170:ARG:HG3	1:C:170:ARG:O	2.13	0.48
1:C:253:HIS:CE1	1:C:320:SER:HG	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ARG:HE	1:D:559:GLU:CD	2.20	0.48
1:D:314:HIS:HB3	1:D:403:VAL:HG11	1.95	0.48
1:D:607:ALA:HB3	1:D:634:GLU:HG2	1.95	0.48
1:D:663:GLU:C	1:D:664:TYR:HD1	2.22	0.48
1:E:366:LEU:HD23	1:E:367:PRO:N	2.29	0.48
1:F:314:HIS:HB3	1:F:403:VAL:HG11	1.95	0.48
1:C:20:ILE:HG12	1:C:48:VAL:HG12	1.95	0.48
1:C:569:LEU:HD11	1:C:576:GLN:NE2	2.29	0.48
1:D:662:GLU:HG3	1:D:664:TYR:HE1	1.79	0.48
1:E:141:LEU:HD13	1:E:142:ASP:N	2.29	0.48
1:E:235:TYR:HE1	1:E:538:GLU:OE2	1.95	0.48
1:E:573:ARG:O	1:E:573:ARG:HG2	2.14	0.48
1:F:165:ALA:HB1	1:F:173:ARG:NE	2.20	0.48
1:F:173:ARG:HH12	1:F:177:LEU:HB2	1.79	0.48
1:F:204:LEU:HD12	1:F:205:LEU:HG	1.95	0.48
1:C:475:THR:HG23	1:C:478:GLU:H	1.79	0.47
1:C:573:ARG:O	1:C:573:ARG:HG3	2.14	0.47
1:D:263:LEU:N	1:D:264:PRO:HD2	2.29	0.47
1:E:235:TYR:HB2	1:E:271:PHE:CD1	2.49	0.47
1:E:283:GLY:HA2	1:E:352:ASP:OD1	2.14	0.47
1:F:188:ASP:OD1	1:F:189:PRO:HD2	2.14	0.47
1:F:297:ALA:HB1	1:F:298:PRO:HD2	1.96	0.47
1:F:508:VAL:HG12	1:F:512:ASN:ND2	2.28	0.47
1:A:663:GLU:O	1:A:664:TYR:HD1	1.98	0.47
1:C:92:LYS:HG3	1:C:93:PRO:N	2.29	0.47
1:C:265:ARG:CZ	1:C:565:PHE:CD2	2.96	0.47
1:D:176:LEU:HD12	1:D:177:LEU:N	2.30	0.47
1:E:32:TYR:CE2	1:E:460:LYS:HE2	2.48	0.47
1:E:271:PHE:CZ	1:E:533:MET:HE3	2.49	0.47
1:F:102:GLN:HG2	1:F:103:GLU:H	1.79	0.47
1:A:358:GLU:C	1:A:359:HIS:CD2	2.93	0.47
1:A:580:THR:O	1:A:584:ILE:HG13	2.13	0.47
1:B:36:ALA:O	1:B:224:VAL:HA	2.14	0.47
1:B:405:GLN:HE22	1:B:438:VAL:HG21	1.80	0.47
1:B:473:ARG:HD2	1:B:478:GLU:HB3	1.97	0.47
1:B:600:PHE:HE1	1:B:609:LEU:HD11	1.79	0.47
1:E:138:ILE:O	1:E:141:LEU:HD12	2.14	0.47
1:E:297:ALA:HB1	1:E:298:PRO:HD2	1.96	0.47
1:F:615:ASP:OD2	1:F:618:THR:OG1	2.32	0.47
1:A:269:MET:SD	1:A:576:GLN:HG3	2.55	0.47
1:B:226:ARG:HB2	1:B:227:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ARG:HH11	1:B:494:ARG:C	2.21	0.47
1:C:201:ILE:HA	1:C:204:LEU:CD2	2.44	0.47
1:C:563:ARG:HG2	1:C:563:ARG:NH1	2.28	0.47
1:D:255:THR:OG1	1:D:321:LEU:O	2.28	0.47
1:D:359:HIS:HD2	1:D:362:TRP:CH2	2.32	0.47
1:D:507:ALA:O	1:D:510:GLN:HB2	2.15	0.47
1:E:18:VAL:HG21	1:E:50:ARG:NH1	2.30	0.47
1:E:161:LEU:O	1:E:165:ALA:N	2.44	0.47
1:F:642:MET:HE1	1:F:653:PHE:HE2	1.79	0.47
1:A:188:ASP:OD1	1:A:189:PRO:HD2	2.13	0.47
1:A:235:TYR:HB2	1:A:271:PHE:CD1	2.48	0.47
1:C:269:MET:HG3	1:C:271:PHE:CE2	2.50	0.47
1:C:422:THR:HA	1:D:52:GLY:CA	2.45	0.47
1:D:287:ARG:O	1:D:296:ALA:HB2	2.14	0.47
1:A:556:GLU:CD	1:A:563:ARG:HH12	2.22	0.47
1:B:600:PHE:CE1	1:B:609:LEU:HD11	2.49	0.47
1:C:698:LEU:O	1:C:699:ARG:HB3	2.14	0.47
1:E:375:GLU:HG3	1:E:380:LYS:HA	1.96	0.47
1:A:210:LEU:O	1:A:210:LEU:HD12	2.14	0.47
1:A:499:VAL:HG11	1:A:537:TYR:CE1	2.49	0.47
1:B:21:ASP:OD1	1:B:22:ASP:N	2.46	0.47
1:B:235:TYR:HB2	1:B:271:PHE:CD1	2.49	0.47
1:B:582:LEU:O	1:B:586:ARG:HG2	2.15	0.47
1:B:663:GLU:C	1:B:664:TYR:HD1	2.22	0.47
1:C:92:LYS:HG3	1:C:93:PRO:CD	2.45	0.47
1:C:110:GLN:HE22	1:C:694:ARG:NH1	2.12	0.47
1:C:290:ARG:NH2	1:C:300:ASP:OD1	2.48	0.47
1:C:428:TRP:O	1:C:432:ILE:HG13	2.14	0.47
1:D:165:ALA:HB2	1:D:176:LEU:CD1	2.42	0.47
1:D:436:LYS:HD2	1:D:442:VAL:O	2.14	0.47
1:E:271:PHE:O	1:E:339:MET:HE2	2.14	0.47
1:E:505:LEU:HD23	1:E:505:LEU:O	2.14	0.47
1:E:663:GLU:O	1:E:664:TYR:HD1	1.98	0.47
1:F:142:ASP:OD1	1:F:143:ALA:N	2.48	0.47
1:F:416:ARG:NH1	1:F:418:ASP:HA	2.30	0.47
1:A:589:HIS:NE2	1:A:658:GLU:OE2	2.40	0.47
1:C:263:LEU:N	1:C:264:PRO:HD2	2.30	0.47
1:D:485:GLN:NE2	1:D:488:GLU:OE1	2.48	0.47
1:E:686:MET:HE3	1:E:686:MET:HB3	1.85	0.47
1:B:161:LEU:HA	1:B:164:ALA:HB3	1.97	0.47
1:B:309:SER:HA	1:B:352:ASP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:HIS:HD2	1:D:560:LEU:HD21	1.80	0.47
1:D:662:GLU:HG3	1:D:664:TYR:CE1	2.49	0.47
1:E:173:ARG:O	1:E:177:LEU:HD12	2.14	0.47
1:E:280:HIS:C	1:E:318:HIS:HB2	2.39	0.47
1:B:108:HIS:HD1	1:B:698:LEU:HD11	1.79	0.47
1:B:354:PRO:O	1:B:358:GLU:HG2	2.15	0.47
1:B:534:TYR:HE2	1:B:552:TYR:CE2	2.32	0.47
1:C:283:GLY:O	1:C:287:ARG:NE	2.43	0.47
1:C:367:PRO:HG2	1:D:152:ASN:OD1	2.15	0.47
1:F:192:ARG:O	1:F:195:LEU:HB3	2.15	0.47
1:F:615:ASP:HA	1:F:616:PRO:HD2	1.79	0.47
1:A:69:TYR:HB3	1:A:70:PRO:HD3	1.97	0.46
1:A:198:THR:C	1:A:200:GLU:H	2.22	0.46
1:A:354:PRO:O	1:A:358:GLU:HG3	2.14	0.46
1:A:695:ASN:O	1:A:698:LEU:HD13	2.15	0.46
1:B:122:ARG:HH11	1:B:219:GLN:HE21	1.63	0.46
1:B:172:LEU:C	1:B:174:ASP:H	2.23	0.46
1:B:533:MET:CE	1:B:538:GLU:HG3	2.44	0.46
1:B:581:ARG:NH2	1:B:658:GLU:O	2.38	0.46
1:D:512:ASN:ND2	1:D:516:MET:HB2	2.30	0.46
1:D:695:ASN:HA	1:D:698:LEU:CD1	2.46	0.46
1:E:255:THR:OG1	1:E:321:LEU:O	2.28	0.46
1:E:605:ASN:ND2	1:E:635:GLU:O	2.44	0.46
1:B:583:ASN:HA	1:B:586:ARG:HD3	1.96	0.46
1:C:507:ALA:O	1:C:510:GLN:HB2	2.16	0.46
1:D:67:VAL:HG23	1:D:68:ARG:H	1.81	0.46
1:D:234:TRP:HH2	1:D:445:LEU:HD11	1.80	0.46
1:D:419:ASN:ND2	2:M:1:GLC:H61	2.29	0.46
1:A:414:PHE:CD1	1:A:443:LEU:HB2	2.51	0.46
1:B:157:GLY:O	1:B:160:LEU:HB2	2.15	0.46
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.97	0.46
1:B:556:GLU:HG3	1:B:561:ARG:CG	2.41	0.46
1:E:676:PRO:C	1:E:678:ARG:H	2.23	0.46
1:C:526:THR:HG21	1:C:624:VAL:HG21	1.97	0.46
1:C:583:ASN:O	1:C:586:ARG:HG3	2.16	0.46
1:D:517:PHE:HD2	1:D:540:PHE:CD1	2.24	0.46
1:E:36:ALA:O	1:E:224:VAL:HA	2.14	0.46
1:E:522:VAL:O	1:E:526:THR:OG1	2.20	0.46
1:F:475:THR:HG23	1:F:477:TRP:H	1.81	0.46
1:B:255:THR:HG23	1:B:258:THR:H	1.81	0.46
1:B:281:PRO:HB3	1:B:311:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:TRP:O	1:B:432:ILE:HG13	2.16	0.46
1:C:216:ARG:HG3	1:C:216:ARG:HH11	1.80	0.46
1:C:309:SER:HA	1:C:352:ASP:HB2	1.97	0.46
1:C:456:TYR:O	1:C:460:LYS:HG3	2.16	0.46
1:D:41:VAL:HG21	1:D:616:PRO:HB2	1.97	0.46
1:D:475:THR:HG22	1:D:478:GLU:CG	2.37	0.46
1:E:280:HIS:ND1	1:E:314:HIS:HA	2.31	0.46
1:A:488:GLU:C	1:A:490:ALA:H	2.22	0.46
1:B:64:TYR:HD2	1:B:115:ARG:NH1	2.12	0.46
1:C:110:GLN:N	1:C:110:GLN:OE1	2.48	0.46
1:C:235:TYR:HB2	1:C:271:PHE:CD1	2.50	0.46
1:D:297:ALA:HB1	1:D:298:PRO:HD2	1.96	0.46
1:D:575:LEU:HD23	1:D:579:ILE:HD11	1.98	0.46
1:F:522:VAL:O	1:F:526:THR:OG1	2.23	0.46
1:A:183:LEU:HD12	1:A:192:ARG:HB2	1.98	0.46
1:A:677:ALA:HB2	3:H:6:GLC:H62	1.98	0.46
1:B:59:THR:OG1	1:B:211:ARG:NH2	2.42	0.46
1:E:698:LEU:CD1	1:E:699:ARG:HG3	2.40	0.46
1:F:130:ILE:HD11	1:F:210:LEU:HD23	1.98	0.46
1:F:371:ILE:HG13	1:F:372:ALA:N	2.30	0.46
1:A:203:GLU:HG3	1:A:204:LEU:H	1.79	0.46
1:B:68:ARG:O	1:B:69:TYR:HB2	2.15	0.46
1:D:175:PRO:O	1:D:178:ALA:HB3	2.15	0.46
1:E:318:HIS:HE1	1:E:320:SER:HB2	1.80	0.46
1:E:499:VAL:HG11	1:E:537:TYR:CZ	2.50	0.46
1:A:517:PHE:O	1:A:537:TYR:OH	2.23	0.46
1:B:265:ARG:NH2	1:B:538:GLU:OE1	2.48	0.46
1:B:657:ASP:OD1	1:B:659:ILE:HG13	2.15	0.46
1:C:383:ASP:OD1	1:C:383:ASP:N	2.39	0.46
1:D:37:VAL:HG12	1:D:38:VAL:H	1.81	0.46
1:B:487:ALA:HB1	1:B:490:ALA:N	2.31	0.46
1:C:307:ILE:HG21	1:C:314:HIS:CD2	2.51	0.46
1:C:364:THR:OG1	1:C:388:ASN:HB2	2.16	0.46
1:D:234:TRP:CE2	1:D:273:VAL:HG11	2.51	0.46
1:D:458:LEU:HA	1:D:461:LEU:CD1	2.46	0.46
1:E:361:GLN:CD	1:E:361:GLN:H	2.23	0.46
1:F:68:ARG:NH2	1:F:118:LEU:HD23	2.30	0.46
1:F:263:LEU:N	1:F:264:PRO:HD2	2.31	0.46
1:A:36:ALA:O	1:A:224:VAL:HA	2.15	0.45
1:A:475:THR:CG2	1:A:478:GLU:HG3	2.44	0.45
1:B:150:LEU:HD12	1:B:154:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:VAL:O	1:C:335:ARG:HG3	2.16	0.45
1:D:240:ARG:HD3	1:D:560:LEU:HD23	1.98	0.45
1:D:271:PHE:CZ	1:D:533:MET:HE2	2.51	0.45
1:D:662:GLU:OE1	1:D:662:GLU:HA	2.17	0.45
1:E:631:PHE:CD1	3:P:5:GLC:H3	2.51	0.45
1:F:182:ALA:C	1:F:183:LEU:HD12	2.41	0.45
1:F:387:LEU:HD13	1:F:396:LEU:HD21	1.98	0.45
1:A:61:VAL:HG22	1:A:95:LEU:HD22	1.98	0.45
1:A:290:ARG:H	1:A:290:ARG:HD2	1.80	0.45
1:A:522:VAL:O	1:A:526:THR:OG1	2.20	0.45
1:A:686:MET:HE3	1:A:686:MET:HB3	1.87	0.45
1:B:309:SER:O	1:B:354:PRO:HD3	2.16	0.45
1:B:698:LEU:HD12	1:B:699:ARG:H	1.80	0.45
1:F:174:ASP:N	1:F:175:PRO:CD	2.79	0.45
1:A:183:LEU:HB2	1:A:192:ARG:HD3	1.99	0.45
1:B:493:ARG:HD3	1:B:493:ARG:C	2.42	0.45
1:C:487:ALA:HB1	1:C:489:LEU:N	2.30	0.45
1:D:442:VAL:C	1:D:443:LEU:HD23	2.41	0.45
1:E:371:ILE:HD11	1:E:385:TYR:CZ	2.51	0.45
1:A:195:LEU:HA	1:A:195:LEU:HD23	1.66	0.45
1:A:432:ILE:HG23	1:A:436:LYS:HZ3	1.81	0.45
1:C:180:ALA:O	1:C:184:ARG:CZ	2.64	0.45
1:D:122:ARG:NH2	1:D:216:ARG:HD3	2.28	0.45
1:D:475:THR:CG2	1:D:478:GLU:HG3	2.38	0.45
1:D:539:LEU:HD11	1:D:565:PHE:HD1	1.82	0.45
1:E:64:TYR:CE2	1:E:117:GLY:HA3	2.51	0.45
1:E:525:ALA:HB1	1:E:586:ARG:HD2	1.98	0.45
1:F:288:LYS:NZ	1:F:383:ASP:OD1	2.50	0.45
1:A:235:TYR:HE2	1:A:237:MET:HG3	1.82	0.45
1:A:255:THR:HG23	1:A:258:THR:H	1.81	0.45
1:A:280:HIS:N	1:A:280:HIS:CD2	2.82	0.45
1:A:673:ARG:NH2	1:E:570:ASP:OD1	2.49	0.45
1:B:439:ASP:HA	1:B:440:PRO:HD3	1.81	0.45
1:B:692:GLU:OE1	1:B:692:GLU:HA	2.15	0.45
1:C:112:THR:HA	1:C:113:PRO:HD3	1.71	0.45
1:C:425:PRO:HG3	1:D:49:TRP:CZ3	2.51	0.45
1:E:312:GLY:HA3	1:E:316:THR:OG1	2.16	0.45
1:F:162:GLU:OE2	1:F:180:ALA:HB1	2.15	0.45
1:B:358:GLU:C	1:B:359:HIS:CD2	2.95	0.45
1:B:436:LYS:HA	1:B:439:ASP:O	2.17	0.45
1:C:493:ARG:NH1	1:C:493:ARG:HG2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:625:VAL:HG11	1:D:672:ILE:HD13	1.97	0.45
1:F:177:LEU:HD12	1:F:180:ALA:HB3	1.99	0.45
1:F:487:ALA:HA	1:F:489:LEU:N	2.31	0.45
1:A:49:TRP:CZ3	1:B:425:PRO:HG3	2.51	0.45
1:B:161:LEU:O	1:B:165:ALA:N	2.49	0.45
1:B:615:ASP:HA	1:B:616:PRO:HD2	1.81	0.45
1:C:642:MET:HE1	1:C:653:PHE:HE2	1.82	0.45
1:D:237:MET:HG3	1:D:238:PHE:N	2.31	0.45
1:D:323:THR:OG1	1:D:325:ASP:OD1	2.26	0.45
1:E:41:VAL:HG21	1:E:616:PRO:HB2	1.98	0.45
1:E:188:ASP:O	1:E:191:THR:HG22	2.16	0.45
1:E:529:PRO:O	1:E:586:ARG:NH2	2.45	0.45
1:F:48:VAL:HG21	1:F:58:ALA:HB2	1.97	0.45
1:B:169:PRO:O	1:B:171:GLY:N	2.50	0.45
1:B:629:ASN:HD21	1:B:632:GLY:CA	2.29	0.45
1:C:555:SER:OG	1:C:557:LYS:HG3	2.17	0.45
1:D:165:ALA:CB	1:D:176:LEU:HD11	2.46	0.45
1:D:276:LEU:HD11	1:D:343:LEU:CD1	2.47	0.45
1:E:18:VAL:HB	1:E:215:THR:OG1	2.16	0.45
1:E:211:ARG:HH21	1:E:214:VAL:HG11	1.81	0.45
1:E:458:LEU:HA	1:E:461:LEU:HD13	1.98	0.45
1:F:64:TYR:CD1	1:F:115:ARG:HD2	2.51	0.45
1:F:168:VAL:HG23	1:F:173:ARG:HD3	1.99	0.45
1:F:200:GLU:HG2	1:F:201:ILE:HD12	1.98	0.45
1:F:226:ARG:HH12	1:F:340:GLU:CD	2.25	0.45
1:A:362:TRP:HD1	1:A:392:ASP:HB3	1.82	0.45
1:A:518:ALA:O	1:A:522:VAL:HG23	2.17	0.45
1:E:122:ARG:NH2	1:E:124:ASP:OD2	2.50	0.45
1:F:280:HIS:HB2	1:F:307:ILE:HG23	1.99	0.45
1:A:130:ILE:CG1	1:A:210:LEU:HD11	2.45	0.45
1:A:318:HIS:CD2	1:A:320:SER:H	2.35	0.45
1:B:162:GLU:CG	1:B:180:ALA:HB1	2.47	0.45
1:B:242:THR:O	1:B:258:THR:HB	2.17	0.45
1:B:698:LEU:HD12	1:B:698:LEU:HA	1.59	0.45
1:C:265:ARG:NE	1:C:576:GLN:OE1	2.50	0.45
1:D:114:ASP:OD1	1:D:115:ARG:HG2	2.17	0.45
1:E:229:ALA:HB2	1:E:443:LEU:HD13	1.99	0.45
1:E:612:SER:HB3	1:E:623:LEU:HD12	1.99	0.45
1:F:583:ASN:O	1:F:587:ARG:HG3	2.16	0.45
1:A:67:VAL:O	1:A:68:ARG:HG2	2.17	0.44
1:C:200:GLU:O	1:C:204:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:MET:HE3	1:C:642:MET:HB3	1.92	0.44
1:D:37:VAL:HG21	1:D:230:ARG:HB2	1.98	0.44
1:E:255:THR:HG23	1:E:258:THR:H	1.82	0.44
1:E:526:THR:HG21	1:E:624:VAL:HG21	1.98	0.44
1:F:493:ARG:HG2	1:F:493:ARG:HH11	1.82	0.44
1:A:18:VAL:HB	1:A:215:THR:OG1	2.18	0.44
1:B:525:ALA:O	1:B:586:ARG:NH1	2.51	0.44
1:C:236:GLU:HB3	1:C:534:TYR:HA	1.99	0.44
1:C:424:PRO:O	1:C:427:PHE:HB3	2.18	0.44
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.98	0.44
1:F:487:ALA:HA	1:F:488:GLU:C	2.43	0.44
1:B:535:CYS:SG	1:B:563:ARG:NH1	2.91	0.44
1:C:426:ASN:HD21	1:D:17:ARG:NH1	2.15	0.44
1:C:523:LEU:O	1:C:527:MET:HG3	2.17	0.44
1:E:106:VAL:C	1:E:107:PHE:HD1	2.25	0.44
1:E:635:GLU:HB2	1:E:673:ARG:HG2	1.98	0.44
1:A:183:LEU:H	1:A:192:ARG:HD3	1.80	0.44
1:A:496:ASN:HD22	1:A:498:PHE:HE1	1.64	0.44
1:C:103:GLU:CD	1:C:104:PRO:HD2	2.42	0.44
1:C:368:ASP:C	1:C:370:THR:H	2.25	0.44
1:C:544:ALA:C	1:C:553:LEU:HG	2.43	0.44
1:C:558:TYR:OH	2:K:2:GLC:O3	2.22	0.44
1:D:122:ARG:NH2	1:D:124:ASP:OD2	2.41	0.44
1:D:243:GLY:HA3	1:D:252:VAL:O	2.17	0.44
1:E:50:ARG:HH12	1:E:126:TRP:HA	1.82	0.44
1:F:307:ILE:HG21	1:F:314:HIS:CE1	2.52	0.44
1:F:498:PHE:HD2	1:F:501:THR:HG22	1.82	0.44
1:A:17:ARG:NH1	1:B:426:ASN:HD21	2.16	0.44
1:A:393:PRO:HG2	1:A:394:GLU:OE1	2.16	0.44
1:B:263:LEU:N	1:B:264:PRO:HD2	2.33	0.44
1:C:297:ALA:HB1	1:C:298:PRO:HD2	1.99	0.44
1:D:265:ARG:NH2	1:D:576:GLN:OE1	2.51	0.44
1:D:361:GLN:CD	1:D:361:GLN:H	2.25	0.44
1:F:282:ILE:HB	1:F:287:ARG:NH2	2.33	0.44
1:A:128:ASP:O	1:A:132:THR:HG23	2.17	0.44
1:A:509:LEU:HD22	1:A:517:PHE:CE2	2.52	0.44
1:A:527:MET:HE1	1:A:600:PHE:HZ	1.82	0.44
1:B:138:ILE:O	1:B:141:LEU:HG	2.18	0.44
1:F:281:PRO:HA	1:F:318:HIS:CD2	2.53	0.44
1:F:576:GLN:N	1:F:577:PRO:HD2	2.33	0.44
1:F:607:ALA:HB3	1:F:634:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:HE1	1:A:693:SER:HB2	1.82	0.44
1:C:582:LEU:O	1:C:585:ILE:HG12	2.17	0.44
1:D:280:HIS:HB3	1:D:281:PRO:HD2	2.00	0.44
1:F:193:THR:O	1:F:197:LEU:HG	2.16	0.44
1:A:360:ARG:O	1:A:360:ARG:HG3	2.18	0.44
1:A:373:TYR:CE1	1:A:385:TYR:HE1	2.36	0.44
1:A:526:THR:OG1	1:A:611:TYR:OH	2.31	0.44
1:A:543:ARG:H	1:A:543:ARG:HG2	1.65	0.44
1:B:165:ALA:CB	1:B:173:ARG:HD2	2.32	0.44
1:B:512:ASN:HA	1:B:631:PHE:CE1	2.52	0.44
1:B:555:SER:OG	1:B:557:LYS:NZ	2.50	0.44
1:B:612:SER:HB3	1:B:623:LEU:HD12	1.99	0.44
1:B:690:PRO:C	1:B:692:GLU:H	2.25	0.44
1:D:522:VAL:O	1:D:526:THR:OG1	2.18	0.44
1:D:580:THR:O	1:D:584:ILE:HG13	2.16	0.44
1:E:114:ASP:OD2	1:E:115:ARG:HG3	2.17	0.44
1:F:352:ASP:OD1	1:F:352:ASP:N	2.50	0.44
1:B:185:THR:OG1	1:B:192:ARG:NH2	2.47	0.44
1:B:358:GLU:C	1:B:359:HIS:HD2	2.25	0.44
1:C:237:MET:HE1	1:C:262:GLU:HB2	1.99	0.44
1:D:288:LYS:N	1:D:288:LYS:CD	2.81	0.44
1:D:523:LEU:O	1:D:527:MET:HG3	2.17	0.44
1:B:576:GLN:N	1:B:577:PRO:HD2	2.32	0.43
1:B:627:THR:HG22	1:B:680:VAL:O	2.18	0.43
1:C:545:VAL:HA	1:C:553:LEU:CD2	2.48	0.43
1:D:505:LEU:HD23	1:D:505:LEU:O	2.17	0.43
1:F:580:THR:O	1:F:584:ILE:HG13	2.18	0.43
1:A:493:ARG:HG2	1:A:493:ARG:HH11	1.83	0.43
1:A:505:LEU:HB2	1:A:552:TYR:CD2	2.54	0.43
1:C:489:LEU:HD13	1:C:492:TYR:CZ	2.53	0.43
1:D:67:VAL:HG23	1:D:68:ARG:N	2.33	0.43
1:D:493:ARG:NH1	1:D:493:ARG:HG2	2.26	0.43
1:E:413:LYS:NZ	1:E:439:ASP:OD2	2.46	0.43
1:E:663:GLU:C	1:E:664:TYR:CD1	2.95	0.43
1:F:162:GLU:O	1:F:165:ALA:HB3	2.19	0.43
1:F:237:MET:HE3	1:F:237:MET:HB2	1.80	0.43
1:F:558:TYR:OH	2:Q:2:GLC:O3	2.15	0.43
1:A:50:ARG:HG2	1:A:51:GLU:H	1.83	0.43
1:A:612:SER:HB3	1:A:623:LEU:HD12	2.00	0.43
1:A:663:GLU:C	1:A:664:TYR:HD1	2.26	0.43
1:B:110:GLN:N	1:B:110:GLN:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ARG:O	1:B:296:ALA:HB2	2.18	0.43
1:B:523:LEU:O	1:B:527:MET:HG3	2.18	0.43
1:C:529:PRO:HB3	1:C:593:GLN:HA	2.01	0.43
1:D:35:LYS:HG3	1:D:492:TYR:HA	2.01	0.43
1:D:255:THR:HG23	1:D:258:THR:H	1.84	0.43
1:D:488:GLU:HB3	1:D:490:ALA:N	2.33	0.43
1:E:61:VAL:HG22	1:E:95:LEU:CD1	2.49	0.43
1:F:540:PHE:CZ	1:F:575:LEU:HB2	2.53	0.43
1:F:677:ALA:HB2	3:R:6:GLC:C6	2.48	0.43
1:F:692:GLU:O	1:F:696:THR:HG23	2.19	0.43
1:A:429:ALA:HB2	1:A:461:LEU:HD23	2.00	0.43
1:D:354:PRO:O	1:D:358:GLU:HG2	2.18	0.43
1:D:488:GLU:C	1:D:490:ALA:H	2.27	0.43
1:D:648:GLU:HG3	1:D:650:TYR:CE1	2.53	0.43
1:E:150:LEU:C	1:E:152:ASN:H	2.26	0.43
1:E:309:SER:HA	1:E:352:ASP:CG	2.43	0.43
1:E:457:GLY:O	1:E:460:LYS:HB3	2.19	0.43
1:E:642:MET:HE3	1:E:642:MET:HB3	1.94	0.43
1:A:388:ASN:HD22	1:A:391:ASN:H	1.67	0.43
1:A:501:THR:HB	1:A:502:PRO:HD2	1.99	0.43
1:B:108:HIS:CD2	1:B:698:LEU:HD21	2.54	0.43
1:B:150:LEU:C	1:B:152:ASN:H	2.25	0.43
1:B:605:ASN:HB2	1:B:636:ALA:HB2	2.00	0.43
1:C:540:PHE:CZ	1:C:575:LEU:HB2	2.54	0.43
1:C:580:THR:O	1:C:584:ILE:HG13	2.19	0.43
1:C:625:VAL:HG11	1:C:672:ILE:HD13	2.01	0.43
1:D:138:ILE:HA	1:D:141:LEU:HD23	2.00	0.43
1:D:445:LEU:HD12	1:D:445:LEU:N	2.34	0.43
1:E:629:ASN:ND2	1:E:632:GLY:H	2.15	0.43
1:F:523:LEU:O	1:F:527:MET:HG3	2.19	0.43
1:A:59:THR:HG23	1:A:126:TRP:NE1	2.31	0.43
1:A:398:ASP:O	1:A:402:ARG:NH1	2.51	0.43
1:B:255:THR:OG1	1:B:321:LEU:O	2.25	0.43
1:C:234:TRP:CE2	1:C:273:VAL:HG11	2.54	0.43
1:C:493:ARG:HG2	1:C:493:ARG:HH11	1.82	0.43
1:C:543:ARG:HA	1:C:543:ARG:HD2	1.67	0.43
1:D:539:LEU:HD23	1:D:539:LEU:HA	1.76	0.43
1:F:493:ARG:HG2	1:F:493:ARG:NH1	2.33	0.43
1:F:507:ALA:O	1:F:510:GLN:HB2	2.19	0.43
1:F:627:THR:HG22	1:F:680:VAL:O	2.19	0.43
1:F:629:ASN:HB2	3:R:2:GLC:H2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:HB1	1:A:184:ARG:HH21	1.84	0.43
1:C:21:ASP:OD1	1:C:22:ASP:N	2.47	0.43
1:C:144:GLY:C	1:C:150:LEU:HD23	2.44	0.43
1:C:422:THR:HA	1:D:52:GLY:N	2.33	0.43
1:D:184:ARG:H	1:D:184:ARG:CD	2.32	0.43
1:D:226:ARG:NH2	1:D:413:LYS:O	2.52	0.43
1:D:387:LEU:HD13	1:D:396:LEU:HD21	2.00	0.43
1:D:487:ALA:HB3	1:D:595:LEU:O	2.19	0.43
1:D:509:LEU:HD22	1:D:517:PHE:HD1	1.80	0.43
1:F:383:ASP:OD1	1:F:383:ASP:N	2.51	0.43
1:A:126:TRP:CZ3	1:A:128:ASP:HB2	2.54	0.43
1:A:642:MET:HE1	1:A:653:PHE:CE2	2.53	0.43
1:B:108:HIS:HB3	1:B:698:LEU:HD11	2.01	0.43
1:B:485:GLN:O	1:B:487:ALA:HA	2.19	0.43
1:D:605:ASN:ND2	1:D:635:GLU:O	2.46	0.43
1:F:177:LEU:O	1:F:181:ALA:N	2.51	0.43
1:A:599:HIS:HE1	1:A:641:ASP:OD2	2.02	0.43
1:C:446:SER:HB3	1:C:463:PHE:HD1	1.82	0.43
1:D:40:GLU:O	1:D:112:THR:HG23	2.19	0.43
1:D:517:PHE:CD1	1:D:537:TYR:HE1	2.37	0.43
1:E:398:ASP:O	1:E:402:ARG:HG3	2.19	0.43
1:E:660:THR:HG22	1:E:662:GLU:HG2	2.01	0.43
1:F:631:PHE:CD1	3:R:5:GLC:H3	2.54	0.43
1:B:399:GLU:O	1:B:403:VAL:HG23	2.19	0.43
1:C:443:LEU:HB3	1:C:464:THR:HG21	2.01	0.43
1:D:168:VAL:HA	1:D:169:PRO:HD3	1.70	0.43
1:D:218:GLU:OE1	1:D:219:GLN:N	2.52	0.43
1:D:461:LEU:HD13	1:D:461:LEU:H	1.84	0.43
1:D:549:SER:OG	1:D:551:GLU:OE1	2.37	0.43
1:E:375:GLU:CD	1:E:376:ASN:N	2.77	0.43
1:E:487:ALA:O	1:E:596:ARG:HA	2.19	0.43
1:E:605:ASN:HD21	1:E:634:GLU:HG3	1.84	0.43
1:F:204:LEU:HD12	1:F:205:LEU:N	2.33	0.43
1:F:351:PRO:HA	1:F:385:TYR:OH	2.19	0.43
1:A:201:ILE:HA	1:A:203:GLU:CD	2.44	0.42
1:A:493:ARG:HG2	1:A:493:ARG:NH1	2.34	0.42
1:A:608:LEU:HD23	1:A:608:LEU:HA	1.82	0.42
1:B:162:GLU:HG2	1:B:180:ALA:HB1	2.01	0.42
1:C:111:PHE:CE1	1:C:113:PRO:HG3	2.55	0.42
1:E:164:ALA:HA	1:E:210:LEU:HD13	2.01	0.42
1:E:170:ARG:HB2	1:E:171:GLY:H	1.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLY:O	1:E:689:VAL:N	2.50	0.42
1:F:16:GLY:C	1:F:18:VAL:H	2.26	0.42
1:F:676:PRO:C	1:F:678:ARG:H	2.27	0.42
1:A:18:VAL:CG2	1:A:213:LEU:HD13	2.44	0.42
1:A:168:VAL:HG23	1:A:169:PRO:HD2	2.01	0.42
1:C:36:ALA:O	1:C:224:VAL:HA	2.19	0.42
1:D:191:THR:C	1:D:192:ARG:HG3	2.45	0.42
1:D:280:HIS:ND1	1:D:314:HIS:HA	2.34	0.42
1:D:374:ALA:CA	1:D:386:PRO:HD3	2.49	0.42
1:D:676:PRO:C	1:D:678:ARG:H	2.26	0.42
1:E:69:TYR:HB3	1:E:70:PRO:HD3	2.01	0.42
1:E:168:VAL:O	1:E:173:ARG:HG2	2.18	0.42
1:E:575:LEU:O	1:E:579:ILE:HG13	2.20	0.42
1:F:285:VAL:HG23	1:F:352:ASP:OD1	2.19	0.42
1:F:567:SER:O	1:F:571:GLN:HG3	2.17	0.42
1:A:285:VAL:O	1:A:286:HIS:HB2	2.19	0.42
1:B:379:LYS:H	1:B:379:LYS:HG3	1.35	0.42
1:C:226:ARG:HB2	1:C:227:PRO:HD2	2.02	0.42
1:C:226:ARG:HE	1:C:443:LEU:HD11	1.82	0.42
1:C:422:THR:HA	1:D:52:GLY:H	1.84	0.42
1:C:605:ASN:HD21	1:C:634:GLU:HG3	1.85	0.42
1:D:40:GLU:O	1:D:40:GLU:HG3	2.19	0.42
1:D:428:TRP:O	1:D:432:ILE:HG13	2.18	0.42
1:D:541:GLU:HG2	1:D:563:ARG:HH22	1.84	0.42
1:D:591:ALA:HA	1:D:615:ASP:HB2	2.01	0.42
1:F:439:ASP:HA	1:F:440:PRO:HD3	1.78	0.42
1:A:60:LEU:HD11	1:A:121:PHE:HB2	2.01	0.42
1:B:518:ALA:O	1:B:522:VAL:HG23	2.19	0.42
1:C:358:GLU:HG3	1:C:359:HIS:CG	2.54	0.42
1:D:265:ARG:NH1	1:D:269:MET:HE2	2.34	0.42
1:E:205:LEU:HA	1:E:208:TYR:O	2.19	0.42
1:E:497:LEU:HD22	1:E:528:SER:HB3	2.02	0.42
1:E:599:HIS:HD2	1:E:644:ALA:CB	2.31	0.42
1:F:486:ILE:HG23	1:F:495:PRO:HG3	2.01	0.42
1:F:697:LEU:O	1:F:697:LEU:HG	2.20	0.42
1:A:179:ALA:HA	1:A:195:LEU:CD1	2.49	0.42
1:A:475:THR:HG23	1:A:478:GLU:H	1.84	0.42
1:A:671:TYR:HD1	1:E:264:PRO:HB2	1.84	0.42
1:B:416:ARG:NH1	1:B:467:TYR:CZ	2.82	0.42
1:C:501:THR:OG1	1:C:504:ILE:HG12	2.19	0.42
1:E:226:ARG:HH12	1:E:340:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:THR:O	1:E:258:THR:HB	2.19	0.42
1:F:364:THR:OG1	1:F:388:ASN:HB2	2.20	0.42
1:F:533:MET:HE2	1:F:533:MET:HB3	1.84	0.42
1:A:569:LEU:HD11	1:A:576:GLN:NE2	2.35	0.42
1:A:615:ASP:HA	1:A:616:PRO:HD2	1.79	0.42
1:B:200:GLU:HG2	1:B:201:ILE:HG23	2.01	0.42
1:B:512:ASN:ND2	3:J:1:GLC:O6	2.51	0.42
1:C:690:PRO:C	1:C:692:GLU:H	2.26	0.42
1:F:184:ARG:HH11	1:F:192:ARG:NH2	2.17	0.42
1:A:351:PRO:HA	1:A:385:TYR:CE2	2.55	0.42
1:A:405:GLN:NE2	1:A:438:VAL:HG21	2.26	0.42
1:B:368:ASP:OD1	1:B:370:THR:HG22	2.19	0.42
1:C:107:PHE:C	1:C:108:HIS:HD2	2.28	0.42
1:D:446:SER:HB3	1:D:463:PHE:CD1	2.54	0.42
1:E:238:PHE:CD2	1:E:556:GLU:OE1	2.73	0.42
1:E:414:PHE:CE1	1:E:443:LEU:HB2	2.55	0.42
1:E:608:LEU:HD23	1:E:608:LEU:HA	1.83	0.42
1:F:245:TRP:CZ2	1:F:562:PRO:HB2	2.55	0.42
3:J:4:GLC:H5	3:J:5:GLC:O5	2.18	0.42
1:A:18:VAL:HG22	1:A:50:ARG:HD3	2.01	0.42
1:B:172:LEU:O	1:B:175:PRO:HD2	2.20	0.42
1:B:580:THR:O	1:B:584:ILE:HG13	2.19	0.42
1:C:138:ILE:O	1:C:141:LEU:HB3	2.20	0.42
1:C:253:HIS:ND1	1:C:320:SER:OG	2.52	0.42
1:C:475:THR:CG2	1:C:478:GLU:HG3	2.49	0.42
1:C:629:ASN:OD1	3:L:2:GLC:H61	2.19	0.42
1:D:126:TRP:CZ3	1:D:128:ASP:HB3	2.55	0.42
1:D:509:LEU:HD22	1:D:517:PHE:CE1	2.54	0.42
1:F:271:PHE:O	1:F:339:MET:HE2	2.19	0.42
1:F:353:HIS:CE1	1:F:355:TRP:CG	3.07	0.42
1:F:506:HIS:ND1	1:F:508:VAL:HG23	2.33	0.42
1:A:198:THR:HA	1:A:199:PRO:HD3	1.66	0.42
1:B:126:TRP:CD2	1:B:211:ARG:HG2	2.55	0.42
1:C:207:ASP:OD1	1:C:208:TYR:CD2	2.73	0.42
1:C:477:TRP:NE1	1:C:481:GLU:OE2	2.53	0.42
1:D:122:ARG:HH22	1:D:216:ARG:CD	2.29	0.42
1:E:600:PHE:CE1	1:E:609:LEU:HD11	2.54	0.42
1:F:312:GLY:HA3	1:F:316:THR:OG1	2.20	0.42
1:A:288:LYS:HZ2	1:A:288:LYS:HG3	1.71	0.42
1:A:526:THR:HG21	1:A:624:VAL:HG21	2.02	0.42
1:A:566:ALA:O	1:A:569:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HB3	1:B:367:PRO:HD2	2.02	0.42
1:C:108:HIS:ND1	1:C:698:LEU:HD22	2.35	0.42
1:C:487:ALA:HB1	1:C:488:GLU:CA	2.49	0.42
1:C:576:GLN:N	1:C:577:PRO:HD2	2.35	0.42
1:D:188:ASP:O	1:D:191:THR:HG22	2.20	0.42
1:D:223:TRP:HZ2	1:D:436:LYS:HZ2	1.64	0.42
1:D:353:HIS:CE1	1:D:355:TRP:CG	3.08	0.42
1:D:695:ASN:HA	1:D:698:LEU:HD13	2.02	0.42
1:E:103:GLU:HG3	1:E:104:PRO:HD2	2.02	0.42
1:E:375:GLU:HG3	1:E:381:TYR:H	1.85	0.42
1:A:422:THR:C	1:A:423:LYS:HD2	2.45	0.41
1:B:138:ILE:HA	1:B:141:LEU:CD2	2.50	0.41
1:D:55:ALA:N	1:D:132:THR:HG22	2.23	0.41
1:E:307:ILE:HG21	1:E:314:HIS:HD2	1.78	0.41
1:F:518:ALA:O	1:F:522:VAL:HG23	2.19	0.41
1:A:19:GLU:HG3	1:A:49:TRP:CZ2	2.55	0.41
1:A:558:TYR:CD1	1:A:558:TYR:N	2.87	0.41
1:A:576:GLN:N	1:A:577:PRO:HD2	2.35	0.41
1:B:458:LEU:HA	1:B:461:LEU:HD23	2.02	0.41
1:C:155:LEU:HA	1:C:158:ALA:HB3	2.02	0.41
1:C:190:VAL:O	1:C:193:THR:OG1	2.29	0.41
1:C:226:ARG:NE	1:C:443:LEU:HD11	2.35	0.41
1:C:266:ILE:O	1:C:269:MET:HG2	2.20	0.41
1:E:201:ILE:HG22	1:E:204:LEU:HD21	2.03	0.41
1:E:305:TRP:NE1	1:E:344:ASP:OD2	2.44	0.41
1:E:576:GLN:N	1:E:577:PRO:HD2	2.35	0.41
1:F:508:VAL:HG12	1:F:512:ASN:HD21	1.85	0.41
1:F:526:THR:HG21	1:F:624:VAL:HG21	2.03	0.41
1:A:203:GLU:HG3	1:A:205:LEU:N	2.22	0.41
1:A:506:HIS:ND1	1:A:507:ALA:N	2.67	0.41
1:A:517:PHE:CE1	1:A:540:PHE:HA	2.55	0.41
1:A:576:GLN:O	1:A:580:THR:OG1	2.35	0.41
1:B:358:GLU:O	1:B:359:HIS:HD2	2.02	0.41
1:B:471:THR:HG21	1:B:504:ILE:HD12	2.02	0.41
1:C:150:LEU:C	1:C:152:ASN:H	2.29	0.41
1:C:505:LEU:HB2	1:C:552:TYR:CD2	2.55	0.41
1:C:533:MET:HE2	1:C:533:MET:HB3	1.83	0.41
1:C:541:GLU:OE1	1:C:563:ARG:NH2	2.35	0.41
1:E:350:ALA:HB1	1:E:351:PRO:HD2	2.02	0.41
1:B:318:HIS:HE1	1:B:320:SER:HB3	1.77	0.41
1:B:366:LEU:HD23	1:B:366:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:ILE:O	1:B:486:ILE:HG12	2.21	0.41
1:C:377:PRO:HA	1:C:378:PRO:HA	1.72	0.41
1:D:37:VAL:HG12	1:D:38:VAL:N	2.35	0.41
1:D:110:GLN:HG2	1:D:694:ARG:NH2	2.33	0.41
1:D:265:ARG:NH2	1:D:576:GLN:CD	2.78	0.41
1:E:157:GLY:O	1:E:160:LEU:HB2	2.20	0.41
1:E:189:PRO:O	1:E:193:THR:N	2.47	0.41
1:F:308:GLY:HA3	1:F:353:HIS:CD2	2.54	0.41
1:A:343:LEU:HD12	1:A:412:VAL:HG11	2.01	0.41
1:B:64:TYR:HB2	1:B:119:TRP:CE3	2.56	0.41
1:B:353:HIS:CE1	1:B:355:TRP:CG	3.09	0.41
1:B:625:VAL:HG11	1:B:672:ILE:HD13	2.01	0.41
1:C:402:ARG:HH11	1:C:402:ARG:CG	2.34	0.41
1:C:518:ALA:O	1:C:522:VAL:HG23	2.20	0.41
1:C:683:ILE:N	1:C:683:ILE:HD12	2.36	0.41
1:D:309:SER:HA	1:D:352:ASP:CB	2.48	0.41
1:D:489:LEU:H	1:D:489:LEU:CD1	2.34	0.41
1:E:204:LEU:HD12	1:E:205:LEU:N	2.35	0.41
1:E:358:GLU:C	1:E:359:HIS:HD2	2.28	0.41
1:F:508:VAL:CG1	1:F:516:MET:HE3	2.51	0.41
1:A:194:ALA:HA	1:A:197:LEU:HD12	2.03	0.41
1:A:383:ASP:OD1	1:A:384:ILE:HG13	2.20	0.41
1:C:183:LEU:HB2	1:C:192:ARG:HD3	2.02	0.41
1:D:458:LEU:O	1:D:461:LEU:HD13	2.20	0.41
1:F:173:ARG:NH1	1:F:177:LEU:HB2	2.35	0.41
1:F:416:ARG:HD2	1:F:416:ARG:O	2.20	0.41
1:F:575:LEU:HD23	1:F:579:ILE:HD11	2.03	0.41
1:A:432:ILE:HG23	1:A:436:LYS:HZ2	1.84	0.41
1:C:676:PRO:C	1:C:678:ARG:H	2.27	0.41
1:D:57:ALA:HA	1:D:107:PHE:CE2	2.49	0.41
1:D:182:ALA:O	1:D:192:ARG:NE	2.52	0.41
1:E:185:THR:H	1:E:185:THR:HG22	1.65	0.41
1:F:399:GLU:O	1:F:403:VAL:HG23	2.21	0.41
1:A:157:GLY:O	1:A:160:LEU:HB2	2.21	0.41
1:A:364:THR:CG2	1:A:388:ASN:HB2	2.51	0.41
1:A:388:ASN:ND2	1:A:390:ASP:H	2.19	0.41
1:B:108:HIS:CG	1:B:698:LEU:HD21	2.56	0.41
1:B:507:ALA:O	1:B:510:GLN:HB2	2.21	0.41
1:F:475:THR:HG23	1:F:477:TRP:N	2.35	0.41
1:F:545:VAL:HA	1:F:553:LEU:HD13	2.02	0.41
1:A:68:ARG:O	1:A:69:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HB2	1:A:227:PRO:HD2	2.03	0.41
1:A:627:THR:HG22	1:A:680:VAL:O	2.21	0.41
1:A:642:MET:HE3	1:A:647:MET:HB2	2.03	0.41
1:B:557:LYS:HB2	1:B:558:TYR:CD1	2.56	0.41
1:B:558:TYR:CD1	1:B:558:TYR:N	2.88	0.41
1:B:676:PRO:C	1:B:678:ARG:H	2.28	0.41
1:C:240:ARG:HH11	1:C:240:ARG:CG	2.31	0.41
1:C:283:GLY:O	1:C:287:ARG:HG3	2.21	0.41
1:D:37:VAL:CG1	1:D:227:PRO:HA	2.49	0.41
1:D:280:HIS:C	1:D:318:HIS:HB2	2.45	0.41
1:D:505:LEU:HD22	1:D:544:ALA:HB2	2.02	0.41
1:D:506:HIS:ND1	1:D:508:VAL:HG12	2.36	0.41
1:D:546:ARG:HA	1:D:546:ARG:HD3	1.20	0.41
1:D:619:GLY:O	1:D:689:VAL:N	2.52	0.41
1:E:236:GLU:HB3	1:E:534:TYR:HA	2.02	0.41
1:E:509:LEU:HB3	1:E:517:PHE:CE1	2.48	0.41
1:F:20:ILE:HG12	1:F:48:VAL:HG12	2.02	0.41
1:F:642:MET:HE3	1:F:642:MET:HB3	1.86	0.41
1:A:315:ASP:OD1	1:A:316:THR:HG23	2.20	0.41
1:A:672:ILE:HD12	1:A:673:ARG:H	1.85	0.41
1:B:686:MET:HB3	1:B:687:PRO:HD2	2.03	0.41
1:D:663:GLU:O	1:D:664:TYR:HD1	2.04	0.41
1:E:629:ASN:OD1	3:P:2:GLC:C6	2.69	0.41
1:F:195:LEU:HD23	1:F:195:LEU:O	2.21	0.41
1:F:236:GLU:HB3	1:F:534:TYR:HA	2.03	0.41
1:F:600:PHE:CE1	1:F:609:LEU:HD11	2.56	0.41
1:F:686:MET:HB3	1:F:687:PRO:HD2	2.03	0.41
1:A:487:ALA:HA	1:A:488:GLU:HA	1.82	0.40
1:C:155:LEU:O	1:C:158:ALA:HB3	2.20	0.40
1:C:280:HIS:C	1:C:318:HIS:HB2	2.46	0.40
1:C:358:GLU:O	1:C:359:HIS:HD2	2.04	0.40
1:C:446:SER:O	1:C:446:SER:OG	2.40	0.40
1:D:435:VAL:O	1:D:438:VAL:HG22	2.20	0.40
1:E:100:SER:HB2	1:E:107:PHE:CE1	2.55	0.40
1:E:374:ALA:CA	1:E:386:PRO:HD3	2.50	0.40
1:E:518:ALA:O	1:E:522:VAL:HG23	2.21	0.40
1:F:40:GLU:OE1	1:F:596:ARG:NH1	2.53	0.40
1:F:116:VAL:HA	1:F:224:VAL:HG23	2.02	0.40
1:F:168:VAL:HG12	1:F:208:TYR:CB	2.49	0.40
1:F:226:ARG:HB2	1:F:227:PRO:HD2	2.02	0.40
1:F:239:PRO:HG3	1:F:276:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:575:LEU:O	1:F:579:ILE:HG13	2.21	0.40
1:B:154:LEU:H	1:B:154:LEU:CD2	2.34	0.40
1:C:65:LEU:HD12	1:C:118:LEU:HD23	2.03	0.40
1:C:271:PHE:N	1:C:271:PHE:CD2	2.90	0.40
1:D:285:VAL:HG23	1:D:352:ASP:CG	2.46	0.40
1:D:362:TRP:C	1:D:363:PHE:HD1	2.29	0.40
1:D:686:MET:HE3	1:D:686:MET:HB3	1.80	0.40
1:E:251:PRO:HB2	1:E:560:LEU:CD1	2.50	0.40
1:F:68:ARG:HG2	1:F:69:TYR:N	2.37	0.40
1:F:158:ALA:HB1	1:F:184:ARG:HH12	1.81	0.40
1:F:198:THR:OG1	1:F:200:GLU:OE1	2.39	0.40
1:A:599:HIS:CE1	1:A:641:ASP:OD2	2.74	0.40
1:B:422:THR:C	1:B:423:LYS:HD2	2.47	0.40
1:B:620:ASP:OD2	1:B:621:CYS:N	2.55	0.40
1:C:218:GLU:H	1:C:218:GLU:HG2	1.66	0.40
1:C:376:ASN:O	1:C:379:LYS:HG3	2.20	0.40
1:D:288:LYS:N	1:D:288:LYS:HD3	2.36	0.40
1:D:468:SER:OG	1:D:469:TYR:N	2.54	0.40
1:D:627:THR:HG22	1:D:680:VAL:O	2.21	0.40
1:E:240:ARG:NH2	1:E:304:PRO:HG3	2.36	0.40
1:E:416:ARG:NH2	1:E:447:GLU:OE1	2.54	0.40
1:E:533:MET:HE1	1:E:579:ILE:HG21	2.03	0.40
1:E:543:ARG:HH11	1:E:543:ARG:HD2	1.76	0.40
1:F:68:ARG:HH22	1:F:118:LEU:HD23	1.85	0.40
1:F:315:ASP:OD1	1:F:316:THR:HG23	2.21	0.40
1:F:317:VAL:HG21	1:F:324:ILE:HA	2.04	0.40
1:A:534:TYR:OH	1:A:556:GLU:OE2	2.37	0.40
1:A:619:GLY:O	1:A:689:VAL:N	2.51	0.40
1:B:285:VAL:HG12	1:B:286:HIS:ND1	2.36	0.40
1:C:545:VAL:HG23	1:C:551:GLU:O	2.21	0.40
1:D:93:PRO:HB2	1:D:94:LEU:H	1.71	0.40
1:D:235:TYR:HB2	1:D:271:PHE:CD1	2.56	0.40
1:D:422:THR:C	1:D:423:LYS:HD3	2.47	0.40
1:D:612:SER:HB3	1:D:623:LEU:HD12	2.03	0.40
1:E:63:ARG:HD2	1:E:92:LYS:O	2.22	0.40
1:F:374:ALA:CA	1:F:386:PRO:HD3	2.51	0.40
1:F:473:ARG:CD	1:F:478:GLU:HB3	2.49	0.40
1:A:67:VAL:HG12	1:A:68:ARG:N	2.36	0.40
1:A:150:LEU:CD2	1:A:154:LEU:HG	2.52	0.40
1:A:344:ASP:OD1	1:A:416:ARG:NH1	2.55	0.40
1:D:190:VAL:HA	1:D:193:THR:HG1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ALA:CA	1:D:339:MET:HE3	2.46	0.40
1:D:483:GLY:HA3	1:D:600:PHE:CZ	2.57	0.40
1:F:672:ILE:HD12	1:F:673:ARG:H	1.85	0.40

All (2) 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)
1:E:29:CYS:CB	1:E:29:CYS:SG[2_556]	1.75	0.45
1:F:29:CYS:SG	1:F:29:CYS:SG[2_555]	2.03	0.17

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	654/723 (90%)	629 (96%)	20 (3%)	5 (1%)	16	51
1	B	654/723 (90%)	624 (95%)	21 (3%)	9 (1%)	9	39
1	C	654/723 (90%)	628 (96%)	20 (3%)	6 (1%)	14	48
1	D	654/723 (90%)	621 (95%)	24 (4%)	9 (1%)	9	39
1	E	654/723 (90%)	624 (95%)	22 (3%)	8 (1%)	10	42
1	F	654/723 (90%)	629 (96%)	19 (3%)	6 (1%)	14	48
All	All	3924/4338 (90%)	3755 (96%)	126 (3%)	43 (1%)	11	44

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	TYR
1	A	151	SER
1	B	68	ARG
1	B	69	TYR

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Mol	Chain	Res	Type
1	B	150	LEU
1	B	151	SER
1	B	170	ARG
1	C	68	ARG
1	C	69	TYR
1	C	151	SER
1	C	174	ASP
1	C	488	GLU
1	D	16	GLY
1	D	69	TYR
1	D	151	SER
1	D	152	ASN
1	D	170	ARG
1	D	382	GLN
1	D	488	GLU
1	E	69	TYR
1	E	151	SER
1	E	194	ALA
1	F	488	GLU
1	A	67	VAL
1	B	190	VAL
1	D	93	PRO
1	D	172	LEU
1	E	375	GLU
1	A	170	ARG
1	B	488	GLU
1	F	69	TYR
1	F	193	THR
1	F	68	ARG
1	E	171	GLY
1	E	172	LEU
1	E	197	LEU
1	F	67	VAL
1	F	393	PRO
1	B	393	PRO
1	A	393	PRO
1	E	393	PRO
1	B	199	PRO
1	C	393	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	542/597 (91%)	513 (95%)	29 (5%)	20	44
1	B	542/597 (91%)	513 (95%)	29 (5%)	20	44
1	C	542/597 (91%)	507 (94%)	35 (6%)	15	40
1	D	542/597 (91%)	508 (94%)	34 (6%)	16	40
1	E	542/597 (91%)	502 (93%)	40 (7%)	13	36
1	F	542/597 (91%)	509 (94%)	33 (6%)	17	41
All	All	3252/3582 (91%)	3052 (94%)	200 (6%)	16	41

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	172	LEU
1	A	173	ARG
1	A	174	ASP
1	A	183	LEU
1	A	204	LEU
1	A	214	VAL
1	A	216	ARG
1	A	218	GLU
1	A	237	MET
1	A	285	VAL
1	A	290	ARG
1	A	303	SER
1	A	371	ILE
1	A	379	LYS
1	A	384	ILE
1	A	394	GLU
1	A	398	ASP
1	A	402	ARG
1	A	414	PHE
1	A	466	SER
1	A	510	GLN

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Mol	Chain	Res	Type
1	A	560	LEU
1	A	629	ASN
1	A	638	LEU
1	A	659	ILE
1	A	664	TYR
1	A	692	GLU
1	A	694	ARG
1	B	54	GLU
1	B	92	LYS
1	B	115	ARG
1	B	149	GLU
1	B	154	LEU
1	B	183	LEU
1	B	184	ARG
1	B	192	ARG
1	B	214	VAL
1	B	216	ARG
1	B	237	MET
1	B	303	SER
1	B	311	GLU
1	B	332	SER
1	B	352	ASP
1	B	361	GLN
1	B	379	LYS
1	B	404	VAL
1	B	436	LYS
1	B	481	GLU
1	B	486	ILE
1	B	505	LEU
1	B	561	ARG
1	B	596	ARG
1	B	638	LEU
1	B	648	GLU
1	B	659	ILE
1	B	664	TYR
1	B	692	GLU
1	C	54	GLU
1	C	102	GLN
1	C	112	THR
1	C	122	ARG
1	C	149	GLU
1	C	156	VAL

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Mol	Chain	Res	Type
1	C	162	GLU
1	C	183	LEU
1	C	185	THR
1	C	195	LEU
1	C	198	THR
1	C	200	GLU
1	C	214	VAL
1	C	237	MET
1	C	240	ARG
1	C	282	ILE
1	C	301	VAL
1	C	352	ASP
1	C	371	ILE
1	C	379	LYS
1	C	401	LEU
1	C	402	ARG
1	C	423	LYS
1	C	438	VAL
1	C	466	SER
1	C	489	LEU
1	C	523	LEU
1	C	563	ARG
1	C	593	GLN
1	C	596	ARG
1	C	638	LEU
1	C	664	TYR
1	C	692	GLU
1	C	694	ARG
1	C	696	THR
1	D	26	VAL
1	D	32	TYR
1	D	35	LYS
1	D	37	VAL
1	D	110	GLN
1	D	118	LEU
1	D	122	ARG
1	D	141	LEU
1	D	150	LEU
1	D	156	VAL
1	D	184	ARG
1	D	195	LEU
1	D	197	LEU

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Mol	Chain	Res	Type
1	D	284	LYS
1	D	301	VAL
1	D	303	SER
1	D	325	ASP
1	D	343	LEU
1	D	368	ASP
1	D	375	GLU
1	D	436	LYS
1	D	437	THR
1	D	445	LEU
1	D	461	LEU
1	D	466	SER
1	D	488	GLU
1	D	489	LEU
1	D	543	ARG
1	D	546	ARG
1	D	557	LYS
1	D	638	LEU
1	D	648	GLU
1	D	664	TYR
1	D	692	GLU
1	E	29	CYS
1	E	63	ARG
1	E	112	THR
1	E	122	ARG
1	E	141	LEU
1	E	149	GLU
1	E	170	ARG
1	E	183	LEU
1	E	184	ARG
1	E	185	THR
1	E	188	ASP
1	E	197	LEU
1	E	201	ILE
1	E	211	ARG
1	E	213	LEU
1	E	216	ARG
1	E	286	HIS
1	E	287	ARG
1	E	348	GLN
1	E	357	ARG
1	E	358	GLU

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Mol	Chain	Res	Type
1	E	366	LEU
1	E	371	ILE
1	E	436	LYS
1	E	458	LEU
1	E	466	SER
1	E	476	LYS
1	E	527	MET
1	E	533	MET
1	E	560	LEU
1	E	563	ARG
1	E	581	ARG
1	E	638	LEU
1	E	645	LEU
1	E	648	GLU
1	E	652	ARG
1	E	663	GLU
1	E	664	TYR
1	E	674	ILE
1	E	698	LEU
1	F	103	GLU
1	F	149	GLU
1	F	151	SER
1	F	156	VAL
1	F	162	GLU
1	F	195	LEU
1	F	198	THR
1	F	216	ARG
1	F	237	MET
1	F	240	ARG
1	F	287	ARG
1	F	301	VAL
1	F	303	SER
1	F	328	ASP
1	F	332	SER
1	F	352	ASP
1	F	361	GLN
1	F	371	ILE
1	F	379	LYS
1	F	383	ASP
1	F	385	TYR
1	F	405	GLN
1	F	416	ARG

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Mol	Chain	Res	Type
1	F	437	THR
1	F	466	SER
1	F	488	GLU
1	F	489	LEU
1	F	618	THR
1	F	638	LEU
1	F	662	GLU
1	F	664	TYR
1	F	665	GLN
1	F	698	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	314	HIS
1	A	388	ASN
1	A	405	GLN
1	A	485	GLN
1	A	629	ASN
1	A	695	ASN
1	B	152	ASN
1	B	286	HIS
1	B	314	HIS
1	B	388	ASN
1	B	405	GLN
1	B	406	HIS
1	B	455	GLN
1	B	465	GLN
1	C	286	HIS
1	C	292	ASN
1	C	314	HIS
1	C	434	GLN
1	C	485	GLN
1	D	280	HIS
1	D	314	HIS
1	D	405	GLN
1	D	419	ASN
1	D	484	ASN
1	E	152	ASN
1	E	286	HIS
1	E	314	HIS

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Mol	Chain	Res	Type
1	E	388	ASN
1	E	405	GLN
1	E	406	HIS
1	E	419	ASN
1	E	455	GLN
1	E	465	GLN
1	E	484	ASN
1	F	291	ASN
1	F	485	GLN
1	F	512	ASN
1	F	576	GLN
1	F	665	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

48 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	G	1	2	12,12,12	0.65	0	17,17,17	1.67	3 (17%)
2	GLC	G	2	2	11,11,12	0.60	0	15,15,17	0.66	0
3	GLC	H	1	3	12,12,12	2.05	5 (41%)	17,17,17	1.34	3 (17%)
3	GLC	H	2	3	11,11,12	2.70	7 (63%)	15,15,17	1.49	4 (26%)
3	GLC	H	3	3	11,11,12	2.84	5 (45%)	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	H	4	3	11,11,12	2.76	6 (54%)	15,15,17	1.44	4 (26%)
3	GLC	H	5	3	11,11,12	2.94	7 (63%)	15,15,17	2.02	3 (20%)
3	GLC	H	6	3	11,11,12	2.65	4 (36%)	15,15,17	0.67	0
2	GLC	I	1	2	12,12,12	0.58	0	17,17,17	0.96	1 (5%)
2	GLC	I	2	2	11,11,12	0.61	0	15,15,17	0.60	0
3	GLC	J	1	3	12,12,12	2.05	5 (41%)	17,17,17	1.04	3 (17%)
3	GLC	J	2	3	11,11,12	2.69	7 (63%)	15,15,17	1.60	3 (20%)
3	GLC	J	3	3	11,11,12	2.84	4 (36%)	15,15,17	1.45	3 (20%)
3	GLC	J	4	3	11,11,12	2.87	6 (54%)	15,15,17	1.34	2 (13%)
3	GLC	J	5	3	11,11,12	2.90	7 (63%)	15,15,17	1.93	3 (20%)
3	GLC	J	6	3	11,11,12	2.62	4 (36%)	15,15,17	1.27	2 (13%)
2	GLC	K	1	2	12,12,12	0.58	0	17,17,17	1.10	1 (5%)
2	GLC	K	2	2	11,11,12	0.64	0	15,15,17	0.64	0
3	GLC	L	1	3	12,12,12	2.07	5 (41%)	17,17,17	1.05	0
3	GLC	L	2	3	11,11,12	2.67	7 (63%)	15,15,17	1.13	2 (13%)
3	GLC	L	3	3	11,11,12	2.86	4 (36%)	15,15,17	1.12	1 (6%)
3	GLC	L	4	3	11,11,12	2.76	6 (54%)	15,15,17	1.12	1 (6%)
3	GLC	L	5	3	11,11,12	2.80	5 (45%)	15,15,17	1.69	3 (20%)
3	GLC	L	6	3	11,11,12	2.64	4 (36%)	15,15,17	1.03	0
2	GLC	M	1	2	12,12,12	0.55	0	17,17,17	1.38	2 (11%)
2	GLC	M	2	2	11,11,12	0.72	0	15,15,17	0.69	0
3	GLC	N	1	3	12,12,12	2.05	5 (41%)	17,17,17	0.96	0
3	GLC	N	2	3	11,11,12	2.69	7 (63%)	15,15,17	1.10	2 (13%)
3	GLC	N	3	3	11,11,12	2.93	5 (45%)	15,15,17	1.98	2 (13%)
3	GLC	N	4	3	11,11,12	2.94	6 (54%)	15,15,17	1.79	2 (13%)
3	GLC	N	5	3	11,11,12	2.89	7 (63%)	15,15,17	1.79	4 (26%)
3	GLC	N	6	3	11,11,12	2.61	4 (36%)	15,15,17	1.03	0
2	GLC	O	1	2	12,12,12	0.55	0	17,17,17	1.33	2 (11%)
2	GLC	O	2	2	11,11,12	0.62	0	15,15,17	0.58	0
3	GLC	P	1	3	12,12,12	2.08	5 (41%)	17,17,17	0.82	0
3	GLC	P	2	3	11,11,12	2.68	7 (63%)	15,15,17	1.03	1 (6%)
3	GLC	P	3	3	11,11,12	2.90	4 (36%)	15,15,17	1.31	1 (6%)
3	GLC	P	4	3	11,11,12	2.74	6 (54%)	15,15,17	1.03	2 (13%)
3	GLC	P	5	3	11,11,12	2.70	5 (45%)	15,15,17	1.80	3 (20%)
3	GLC	P	6	3	11,11,12	2.64	4 (36%)	15,15,17	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	Q	1	2	12,12,12	0.45	0	17,17,17	0.89	1 (5%)
2	GLC	Q	2	2	11,11,12	0.62	0	15,15,17	0.62	0
3	GLC	R	1	3	12,12,12	2.07	5 (41%)	17,17,17	0.99	0
3	GLC	R	2	3	11,11,12	2.67	8 (72%)	15,15,17	1.27	1 (6%)
3	GLC	R	3	3	11,11,12	2.96	5 (45%)	15,15,17	1.74	2 (13%)
3	GLC	R	4	3	11,11,12	2.75	6 (54%)	15,15,17	1.40	4 (26%)
3	GLC	R	5	3	11,11,12	2.97	8 (72%)	15,15,17	2.06	6 (40%)
3	GLC	R	6	3	11,11,12	2.62	4 (36%)	15,15,17	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
3	GLC	H	1	3	-	2/2/22/22	0/1/1/1
3	GLC	H	2	3	-	2/2/19/22	0/1/1/1
3	GLC	H	3	3	-	2/2/19/22	0/1/1/1
3	GLC	H	4	3	-	2/2/19/22	0/1/1/1
3	GLC	H	5	3	-	2/2/19/22	0/1/1/1
3	GLC	H	6	3	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	2/2/22/22	0/1/1/1
3	GLC	J	2	3	-	2/2/19/22	0/1/1/1
3	GLC	J	3	3	-	1/2/19/22	0/1/1/1
3	GLC	J	4	3	-	2/2/19/22	0/1/1/1
3	GLC	J	5	3	-	2/2/19/22	0/1/1/1
3	GLC	J	6	3	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	2/2/22/22	0/1/1/1
3	GLC	L	2	3	-	2/2/19/22	0/1/1/1
3	GLC	L	3	3	-	0/2/19/22	0/1/1/1
3	GLC	L	4	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	L	5	3	-	1/2/19/22	0/1/1/1
3	GLC	L	6	3	-	1/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	1/2/19/22	0/1/1/1
3	GLC	N	1	3	-	2/2/22/22	0/1/1/1
3	GLC	N	2	3	-	2/2/19/22	0/1/1/1
3	GLC	N	3	3	-	2/2/19/22	0/1/1/1
3	GLC	N	4	3	-	2/2/19/22	0/1/1/1
3	GLC	N	5	3	-	2/2/19/22	0/1/1/1
3	GLC	N	6	3	-	2/2/19/22	0/1/1/1
2	GLC	O	1	2	-	0/2/22/22	0/1/1/1
2	GLC	O	2	2	-	1/2/19/22	0/1/1/1
3	GLC	P	1	3	-	2/2/22/22	0/1/1/1
3	GLC	P	2	3	-	2/2/19/22	0/1/1/1
3	GLC	P	3	3	-	0/2/19/22	0/1/1/1
3	GLC	P	4	3	-	2/2/19/22	0/1/1/1
3	GLC	P	5	3	-	2/2/19/22	0/1/1/1
3	GLC	P	6	3	-	2/2/19/22	0/1/1/1
2	GLC	Q	1	2	-	0/2/22/22	0/1/1/1
2	GLC	Q	2	2	-	0/2/19/22	0/1/1/1
3	GLC	R	1	3	-	2/2/22/22	0/1/1/1
3	GLC	R	2	3	-	2/2/19/22	0/1/1/1
3	GLC	R	3	3	-	2/2/19/22	0/1/1/1
3	GLC	R	4	3	-	2/2/19/22	0/1/1/1
3	GLC	R	5	3	-	0/2/19/22	0/1/1/1
3	GLC	R	6	3	-	2/2/19/22	0/1/1/1

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	6	GLC	O5-C5	6.32	1.55	1.43
3	P	3	GLC	O5-C5	6.25	1.55	1.43
3	R	3	GLC	O5-C5	6.25	1.55	1.43
3	H	6	GLC	O5-C5	6.25	1.55	1.43
3	R	6	GLC	O5-C5	6.23	1.55	1.43
3	N	3	GLC	O5-C5	6.23	1.55	1.43
3	J	6	GLC	O5-C5	6.16	1.55	1.43
3	N	6	GLC	O5-C5	6.15	1.55	1.43
3	L	6	GLC	O5-C5	6.10	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	3	GLC	O5-C5	6.06	1.55	1.43
3	L	3	GLC	O5-C5	6.05	1.55	1.43
3	H	3	GLC	O5-C5	5.96	1.55	1.43
3	N	4	GLC	O5-C5	5.83	1.54	1.43
3	J	4	GLC	O5-C5	5.54	1.54	1.43
3	P	4	GLC	O5-C5	5.39	1.53	1.43
3	L	4	GLC	O5-C5	5.35	1.53	1.43
3	R	4	GLC	O5-C5	5.35	1.53	1.43
3	R	5	GLC	C2-C3	-5.33	1.44	1.52
3	H	4	GLC	O5-C5	5.31	1.53	1.43
3	J	4	GLC	C2-C3	-5.30	1.44	1.52
3	N	4	GLC	C2-C3	-5.27	1.44	1.52
3	H	5	GLC	C2-C3	-5.22	1.44	1.52
3	J	2	GLC	O5-C5	5.18	1.53	1.43
3	N	2	GLC	O5-C5	5.15	1.53	1.43
3	P	2	GLC	O5-C5	5.10	1.53	1.43
3	L	5	GLC	C2-C3	-5.06	1.44	1.52
3	R	2	GLC	O5-C5	5.06	1.53	1.43
3	L	2	GLC	O5-C5	5.04	1.53	1.43
3	N	5	GLC	C2-C3	-5.03	1.44	1.52
3	H	2	GLC	O5-C5	4.98	1.53	1.43
3	L	4	GLC	C2-C3	-4.96	1.44	1.52
3	H	4	GLC	C2-C3	-4.86	1.45	1.52
3	R	4	GLC	C2-C3	-4.86	1.45	1.52
3	R	5	GLC	O5-C5	4.84	1.52	1.43
3	J	5	GLC	O5-C5	4.82	1.52	1.43
3	J	5	GLC	C2-C3	-4.71	1.45	1.52
3	H	5	GLC	O5-C5	4.67	1.52	1.43
3	R	3	GLC	C2-C3	-4.63	1.45	1.52
3	P	4	GLC	C2-C3	-4.63	1.45	1.52
3	N	5	GLC	O5-C5	4.62	1.52	1.43
3	P	5	GLC	C2-C3	-4.52	1.45	1.52
3	N	3	GLC	C2-C3	-4.49	1.45	1.52
3	L	3	GLC	C2-C3	-4.39	1.45	1.52
3	P	3	GLC	C2-C3	-4.34	1.45	1.52
3	H	3	GLC	C2-C3	-4.30	1.45	1.52
3	L	5	GLC	O5-C5	4.27	1.51	1.43
3	P	5	GLC	O5-C5	4.14	1.51	1.43
3	J	3	GLC	C2-C3	-4.09	1.46	1.52
3	P	1	GLC	O5-C5	3.90	1.53	1.44
3	L	1	GLC	O5-C5	3.84	1.53	1.44
3	R	1	GLC	O5-C5	3.83	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	GLC	C2-C3	-3.83	1.46	1.52
3	N	1	GLC	O5-C5	3.83	1.53	1.44
3	H	1	GLC	O5-C5	3.77	1.53	1.44
3	J	1	GLC	O5-C5	3.77	1.53	1.44
3	P	2	GLC	C2-C3	-3.75	1.46	1.52
3	R	2	GLC	C2-C3	-3.72	1.46	1.52
3	J	3	GLC	C6-C5	-3.69	1.39	1.51
3	H	3	GLC	C6-C5	-3.67	1.39	1.51
3	R	3	GLC	C6-C5	-3.66	1.39	1.51
3	N	2	GLC	O2-C2	3.62	1.50	1.43
3	L	3	GLC	C6-C5	-3.61	1.39	1.51
3	L	2	GLC	C2-C3	-3.61	1.47	1.52
3	J	2	GLC	C2-C3	-3.61	1.47	1.52
3	P	3	GLC	C6-C5	-3.59	1.39	1.51
3	N	3	GLC	C6-C5	-3.58	1.39	1.51
3	H	2	GLC	O2-C2	3.57	1.50	1.43
3	N	2	GLC	C2-C3	-3.55	1.47	1.52
3	L	2	GLC	O2-C2	3.52	1.50	1.43
3	R	2	GLC	O2-C2	3.49	1.50	1.43
3	L	6	GLC	C6-C5	-3.43	1.40	1.51
3	P	2	GLC	O2-C2	3.42	1.50	1.43
3	P	5	GLC	C6-C5	-3.41	1.40	1.51
3	N	6	GLC	C6-C5	-3.41	1.40	1.51
3	R	6	GLC	C6-C5	-3.34	1.40	1.51
3	J	6	GLC	C6-C5	-3.34	1.40	1.51
3	H	5	GLC	C6-C5	-3.34	1.40	1.51
3	H	6	GLC	C6-C5	-3.33	1.40	1.51
3	L	5	GLC	C6-C5	-3.33	1.40	1.51
3	J	2	GLC	O2-C2	3.31	1.50	1.43
3	P	6	GLC	C6-C5	-3.29	1.40	1.51
3	J	5	GLC	O2-C2	3.29	1.50	1.43
3	L	6	GLC	C2-C3	-3.26	1.47	1.52
3	H	6	GLC	C2-C3	-3.26	1.47	1.52
3	N	5	GLC	C6-C5	-3.24	1.41	1.51
3	H	4	GLC	O2-C2	3.23	1.50	1.43
3	R	4	GLC	O2-C2	3.19	1.50	1.43
3	P	4	GLC	O2-C2	3.17	1.50	1.43
3	N	1	GLC	O3-C3	3.14	1.50	1.43
3	R	5	GLC	C6-C5	-3.14	1.41	1.51
3	L	4	GLC	O2-C2	3.12	1.49	1.43
3	P	5	GLC	O3-C3	3.09	1.50	1.43
3	J	5	GLC	O3-C3	3.09	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	GLC	C3-C2	-3.08	1.44	1.52
3	P	1	GLC	C3-C2	-3.07	1.44	1.52
3	H	5	GLC	O3-C3	3.07	1.50	1.43
3	H	5	GLC	O2-C2	3.07	1.49	1.43
3	L	1	GLC	C3-C2	-3.06	1.44	1.52
3	J	5	GLC	C6-C5	-3.05	1.41	1.51
3	P	5	GLC	O2-C2	3.04	1.49	1.43
3	R	5	GLC	O3-C3	3.03	1.50	1.43
3	N	5	GLC	O2-C2	3.02	1.49	1.43
3	R	5	GLC	O2-C2	3.01	1.49	1.43
3	L	5	GLC	O3-C3	3.01	1.50	1.43
3	L	5	GLC	O2-C2	2.99	1.49	1.43
3	H	1	GLC	O3-C3	2.99	1.50	1.43
3	N	5	GLC	O3-C3	2.98	1.50	1.43
3	P	6	GLC	C2-C3	-2.97	1.47	1.52
3	N	4	GLC	O2-C2	2.96	1.49	1.43
3	R	6	GLC	C2-C3	-2.96	1.48	1.52
3	L	1	GLC	O3-C3	2.95	1.50	1.43
3	H	1	GLC	C3-C2	-2.94	1.44	1.52
3	J	1	GLC	C3-C2	-2.91	1.44	1.52
3	J	4	GLC	O2-C2	2.90	1.49	1.43
3	J	1	GLC	O3-C3	2.89	1.50	1.43
3	R	1	GLC	O3-C3	2.89	1.50	1.43
3	N	6	GLC	C2-C3	-2.87	1.48	1.52
3	P	1	GLC	O3-C3	2.86	1.50	1.43
3	J	6	GLC	C2-C3	-2.83	1.48	1.52
3	N	1	GLC	C3-C2	-2.82	1.45	1.52
3	H	2	GLC	O5-C1	2.71	1.48	1.43
3	L	2	GLC	O5-C1	2.66	1.48	1.43
3	J	2	GLC	O5-C1	2.64	1.48	1.43
3	N	2	GLC	O5-C1	2.63	1.48	1.43
3	J	5	GLC	O5-C1	2.61	1.48	1.43
3	J	6	GLC	O2-C2	2.52	1.48	1.43
3	R	2	GLC	O5-C1	2.52	1.47	1.43
3	P	2	GLC	O5-C1	2.48	1.47	1.43
3	N	4	GLC	O3-C3	2.47	1.49	1.43
3	R	2	GLC	C6-C5	-2.46	1.43	1.51
3	R	4	GLC	O3-C3	2.43	1.49	1.43
3	H	3	GLC	O3-C3	2.43	1.49	1.43
3	H	4	GLC	O3-C3	2.43	1.49	1.43
3	J	3	GLC	O3-C3	2.41	1.48	1.43
3	N	6	GLC	O2-C2	2.40	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	GLC	O3-C3	2.39	1.48	1.43
3	N	2	GLC	C6-C5	-2.38	1.43	1.51
3	L	4	GLC	O3-C3	2.37	1.48	1.43
3	L	6	GLC	O2-C2	2.37	1.48	1.43
3	P	3	GLC	O3-C3	2.36	1.48	1.43
3	P	6	GLC	O2-C2	2.36	1.48	1.43
3	P	4	GLC	O3-C3	2.36	1.48	1.43
3	H	2	GLC	C6-C5	-2.35	1.43	1.51
3	P	2	GLC	C6-C5	-2.35	1.43	1.51
3	J	2	GLC	C6-C5	-2.35	1.43	1.51
3	R	3	GLC	O3-C3	2.35	1.48	1.43
3	R	6	GLC	O2-C2	2.32	1.48	1.43
3	L	2	GLC	C6-C5	-2.31	1.44	1.51
3	N	3	GLC	O3-C3	2.29	1.48	1.43
3	P	1	GLC	C6-C5	-2.29	1.44	1.51
3	J	1	GLC	C6-C5	-2.28	1.44	1.51
3	R	1	GLC	C6-C5	-2.28	1.44	1.51
3	L	3	GLC	O3-C3	2.28	1.48	1.43
3	N	2	GLC	O3-C3	2.27	1.48	1.43
3	H	6	GLC	O2-C2	2.26	1.48	1.43
3	P	2	GLC	O3-C3	2.25	1.48	1.43
3	N	4	GLC	C1-C2	-2.25	1.46	1.52
3	H	1	GLC	C6-C5	-2.24	1.44	1.51
3	P	4	GLC	C1-C2	-2.23	1.46	1.52
3	R	4	GLC	C1-C2	-2.23	1.46	1.52
3	H	2	GLC	O3-C3	2.21	1.48	1.43
3	L	2	GLC	O3-C3	2.21	1.48	1.43
3	P	4	GLC	C6-C5	-2.20	1.44	1.51
3	R	5	GLC	C4-C5	2.19	1.57	1.53
3	J	4	GLC	C1-C2	-2.19	1.47	1.52
3	J	2	GLC	O3-C3	2.18	1.48	1.43
3	L	1	GLC	C6-C5	-2.18	1.44	1.51
3	R	5	GLC	C4-C3	-2.17	1.46	1.52
3	J	1	GLC	O2-C2	2.17	1.48	1.43
3	H	4	GLC	C1-C2	-2.16	1.47	1.52
3	N	3	GLC	O5-C1	2.16	1.47	1.43
3	N	5	GLC	C4-C3	-2.16	1.46	1.52
3	L	4	GLC	C1-C2	-2.16	1.47	1.52
3	N	1	GLC	C6-C5	-2.16	1.44	1.51
3	L	4	GLC	C6-C5	-2.15	1.44	1.51
3	R	5	GLC	O5-C1	2.14	1.47	1.43
3	J	2	GLC	O4-C4	2.14	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	3	GLC	O5-C1	2.13	1.47	1.43
3	P	1	GLC	O2-C2	2.13	1.48	1.43
3	N	5	GLC	C4-C5	2.13	1.57	1.53
3	H	4	GLC	C6-C5	-2.13	1.44	1.51
3	N	1	GLC	O2-C2	2.12	1.48	1.43
3	H	5	GLC	C4-C5	2.11	1.57	1.53
3	R	2	GLC	O3-C3	2.10	1.48	1.43
3	H	1	GLC	O2-C2	2.09	1.48	1.43
3	H	3	GLC	C4-C5	2.09	1.57	1.53
3	R	4	GLC	C6-C5	-2.08	1.44	1.51
3	J	4	GLC	C6-C5	-2.08	1.44	1.51
3	H	5	GLC	C4-C3	-2.07	1.47	1.52
3	L	2	GLC	O4-C4	2.06	1.48	1.43
3	R	1	GLC	O2-C2	2.06	1.48	1.43
3	J	5	GLC	C4-C5	2.05	1.57	1.53
3	P	2	GLC	O4-C4	2.05	1.48	1.43
3	N	4	GLC	C6-C5	-2.04	1.45	1.51
3	L	1	GLC	O2-C2	2.03	1.48	1.43
3	H	2	GLC	O4-C4	2.02	1.48	1.43
3	N	2	GLC	O4-C4	2.02	1.47	1.43
3	R	2	GLC	C1-C2	-2.02	1.47	1.52
3	R	2	GLC	O4-C4	2.00	1.47	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	GLC	C1-O5-C5	6.37	120.73	112.19
3	R	3	GLC	C1-O5-C5	5.74	119.88	112.19
3	H	5	GLC	C1-O5-C5	5.66	119.77	112.19
3	J	5	GLC	C1-O5-C5	5.39	119.41	112.19
3	N	4	GLC	C1-O5-C5	5.05	118.96	112.19
3	R	5	GLC	C1-O5-C5	4.98	118.86	112.19
2	G	1	GLC	O5-C1-C2	4.80	118.75	110.30
3	N	5	GLC	C1-O5-C5	4.19	117.80	112.19
3	P	5	GLC	C1-C2-C3	4.11	115.63	109.64
3	P	3	GLC	C1-O5-C5	3.90	117.41	112.19
3	P	5	GLC	C2-C3-C4	3.79	117.53	110.86
3	J	4	GLC	C1-O5-C5	3.77	117.24	112.19
3	H	5	GLC	C3-C4-C5	3.77	117.06	110.23
3	L	5	GLC	C3-C4-C5	3.70	116.95	110.23
2	M	1	GLC	C1-O5-C5	3.49	120.41	113.65
3	J	5	GLC	C3-C4-C5	3.46	116.51	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	4	GLC	C3-C4-C5	3.45	116.48	110.23
3	R	5	GLC	C3-C4-C5	3.40	116.40	110.23
2	O	1	GLC	C1-O5-C5	3.35	120.14	113.65
3	J	2	GLC	O6-C6-C5	-3.33	100.00	111.33
3	H	3	GLC	C1-O5-C5	3.32	116.64	112.19
3	L	5	GLC	C2-C3-C4	3.31	116.69	110.86
3	N	5	GLC	C3-C4-C5	3.24	116.10	110.23
3	H	2	GLC	C1-C2-C3	3.05	114.08	109.64
3	J	3	GLC	C1-O5-C5	3.04	116.26	112.19
3	L	3	GLC	C1-O5-C5	3.03	116.24	112.19
3	J	2	GLC	C1-C2-C3	2.97	113.96	109.64
3	R	4	GLC	C2-C3-C4	2.86	115.89	110.86
3	H	4	GLC	C2-C3-C4	2.83	115.84	110.86
3	N	3	GLC	O5-C1-C2	2.80	117.47	110.79
3	J	6	GLC	C1-C2-C3	2.78	113.69	109.64
3	H	1	GLC	C4-C3-C2	2.74	115.64	110.83
3	H	1	GLC	O4-C4-C3	-2.71	103.98	110.38
3	R	2	GLC	C1-C2-C3	2.71	113.59	109.64
3	L	5	GLC	C1-C2-C3	2.64	113.49	109.64
3	J	2	GLC	O5-C5-C4	-2.53	104.68	110.83
3	H	4	GLC	C1-C2-C3	2.51	113.29	109.64
2	M	1	GLC	O5-C5-C6	2.47	112.56	106.44
3	R	5	GLC	O5-C1-C2	2.44	116.61	110.79
3	J	5	GLC	O5-C5-C6	2.43	112.40	107.66
3	P	5	GLC	C3-C4-C5	2.42	114.61	110.23
2	K	1	GLC	C4-C3-C2	2.41	115.06	110.83
3	R	4	GLC	C3-C4-C5	2.41	114.60	110.23
3	H	1	GLC	C3-C4-C5	2.37	114.53	110.23
3	H	2	GLC	C2-C3-C4	2.37	115.02	110.86
3	N	2	GLC	O5-C5-C6	2.36	112.26	107.66
3	N	5	GLC	O5-C1-C2	2.35	116.40	110.79
3	H	4	GLC	O4-C4-C3	-2.35	104.85	110.38
3	H	2	GLC	C1-O5-C5	2.32	115.30	112.19
3	P	2	GLC	C1-C2-C3	2.32	113.03	109.64
3	R	4	GLC	O4-C4-C3	-2.31	104.92	110.38
3	H	4	GLC	C3-C4-C5	2.29	114.38	110.23
3	L	2	GLC	C1-C2-C3	2.25	112.91	109.64
2	G	1	GLC	C1-O5-C5	2.23	117.97	113.65
3	J	3	GLC	O4-C4-C3	-2.22	105.14	110.38
2	O	1	GLC	O5-C5-C6	2.22	111.93	106.44
3	P	4	GLC	C2-C3-C4	2.19	114.72	110.86
3	J	6	GLC	O5-C5-C4	-2.19	105.51	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	1	GLC	O5-C5-C6	2.18	111.85	106.44
3	H	2	GLC	O4-C4-C3	-2.18	105.24	110.38
3	R	4	GLC	C1-C2-C3	2.16	112.78	109.64
3	J	4	GLC	O4-C4-C3	-2.15	105.32	110.38
3	J	3	GLC	C1-C2-C3	2.15	112.77	109.64
2	I	1	GLC	C4-C3-C2	2.10	114.52	110.83
3	R	3	GLC	O5-C1-C2	2.10	115.79	110.79
3	R	5	GLC	C1-C2-C3	2.09	112.69	109.64
3	R	5	GLC	O4-C4-C3	-2.08	105.47	110.38
3	J	1	GLC	C3-C4-C5	2.08	114.00	110.23
2	G	1	GLC	C1-C2-C3	2.07	114.58	110.36
3	L	4	GLC	C1-C2-C3	2.07	112.65	109.64
3	R	5	GLC	C2-C3-C4	2.06	114.49	110.86
3	H	3	GLC	C3-C4-C5	2.06	113.96	110.23
3	L	2	GLC	O5-C5-C4	-2.04	105.86	110.83
3	N	5	GLC	O4-C4-C3	-2.02	105.61	110.38
3	N	2	GLC	C1-C2-C3	2.02	112.58	109.64
3	J	1	GLC	O4-C4-C3	-2.01	105.64	110.38
3	J	1	GLC	C4-C3-C2	2.01	114.36	110.83
3	H	5	GLC	O5-C1-C2	2.01	115.58	110.79
3	P	4	GLC	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	GLC	O5-C5-C6-O6
3	R	2	GLC	O5-C5-C6-O6
3	R	6	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
3	L	1	GLC	O5-C5-C6-O6
3	N	2	GLC	O5-C5-C6-O6
3	P	2	GLC	O5-C5-C6-O6
3	N	3	GLC	O5-C5-C6-O6
3	R	3	GLC	O5-C5-C6-O6
3	R	1	GLC	O5-C5-C6-O6
3	R	6	GLC	C4-C5-C6-O6
3	J	6	GLC	O5-C5-C6-O6
3	L	4	GLC	O5-C5-C6-O6
3	P	2	GLC	C4-C5-C6-O6
3	J	1	GLC	O5-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	4	GLC	C4-C5-C6-O6
3	R	2	GLC	C4-C5-C6-O6
3	R	4	GLC	O5-C5-C6-O6
3	H	4	GLC	O5-C5-C6-O6
3	H	5	GLC	O5-C5-C6-O6
3	H	2	GLC	C4-C5-C6-O6
3	H	3	GLC	O5-C5-C6-O6
3	N	4	GLC	O5-C5-C6-O6
3	J	6	GLC	C4-C5-C6-O6
3	N	2	GLC	C4-C5-C6-O6
3	J	1	GLC	C4-C5-C6-O6
3	N	3	GLC	C4-C5-C6-O6
3	N	4	GLC	C4-C5-C6-O6
3	H	5	GLC	C4-C5-C6-O6
3	R	3	GLC	C4-C5-C6-O6
3	H	3	GLC	C4-C5-C6-O6
3	J	5	GLC	C4-C5-C6-O6
3	L	4	GLC	C4-C5-C6-O6
3	J	4	GLC	O5-C5-C6-O6
3	H	1	GLC	C4-C5-C6-O6
3	N	1	GLC	C4-C5-C6-O6
3	P	4	GLC	O5-C5-C6-O6
3	P	1	GLC	O5-C5-C6-O6
3	R	4	GLC	C4-C5-C6-O6
3	H	4	GLC	C4-C5-C6-O6
3	P	6	GLC	O5-C5-C6-O6
3	L	1	GLC	C4-C5-C6-O6
3	N	1	GLC	O5-C5-C6-O6
3	N	6	GLC	O5-C5-C6-O6
3	P	5	GLC	C4-C5-C6-O6
3	H	1	GLC	O5-C5-C6-O6
3	R	1	GLC	C4-C5-C6-O6
3	N	5	GLC	O5-C5-C6-O6
3	J	5	GLC	O5-C5-C6-O6
3	N	5	GLC	C4-C5-C6-O6
3	H	6	GLC	O5-C5-C6-O6
3	J	3	GLC	O5-C5-C6-O6
3	L	2	GLC	C4-C5-C6-O6
2	M	2	GLC	O5-C5-C6-O6
3	P	4	GLC	C4-C5-C6-O6
2	O	2	GLC	O5-C5-C6-O6
3	N	6	GLC	C4-C5-C6-O6

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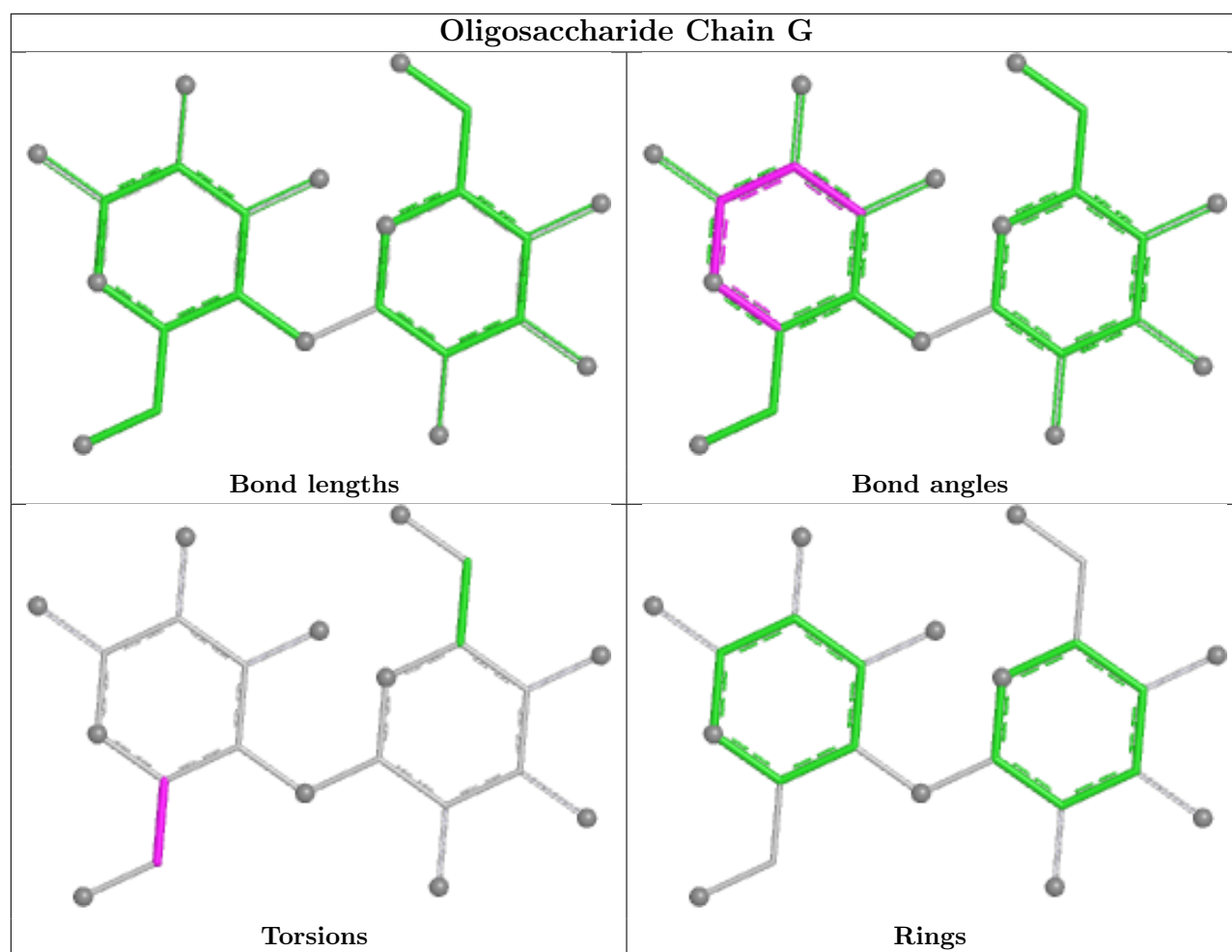
Mol	Chain	Res	Type	Atoms
3	P	6	GLC	C4-C5-C6-O6
3	J	2	GLC	O5-C5-C6-O6
3	L	5	GLC	O5-C5-C6-O6
3	P	5	GLC	O5-C5-C6-O6
3	L	2	GLC	O5-C5-C6-O6
3	J	2	GLC	C4-C5-C6-O6
3	P	1	GLC	C4-C5-C6-O6
3	H	6	GLC	C4-C5-C6-O6
3	L	6	GLC	O5-C5-C6-O6

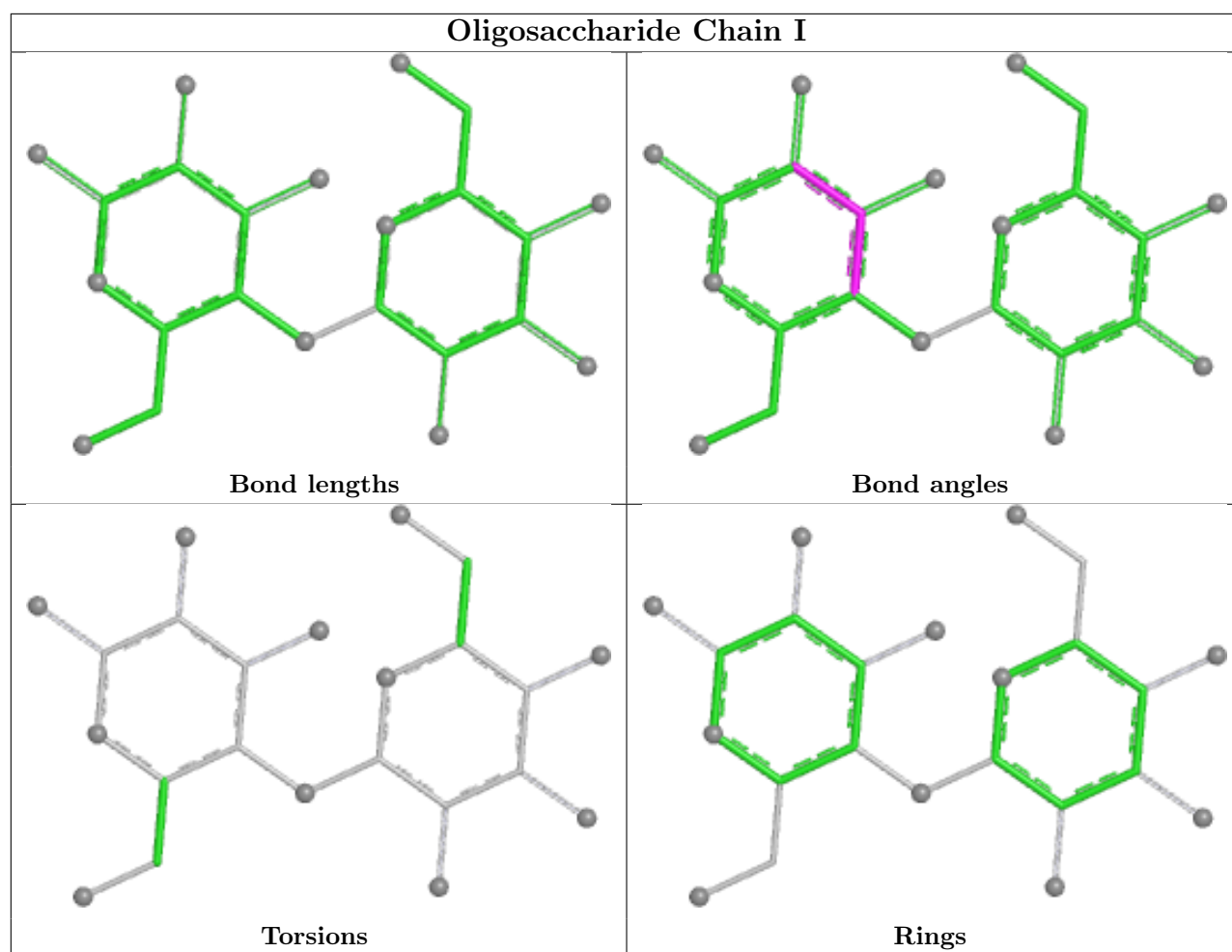
There are no ring outliers.

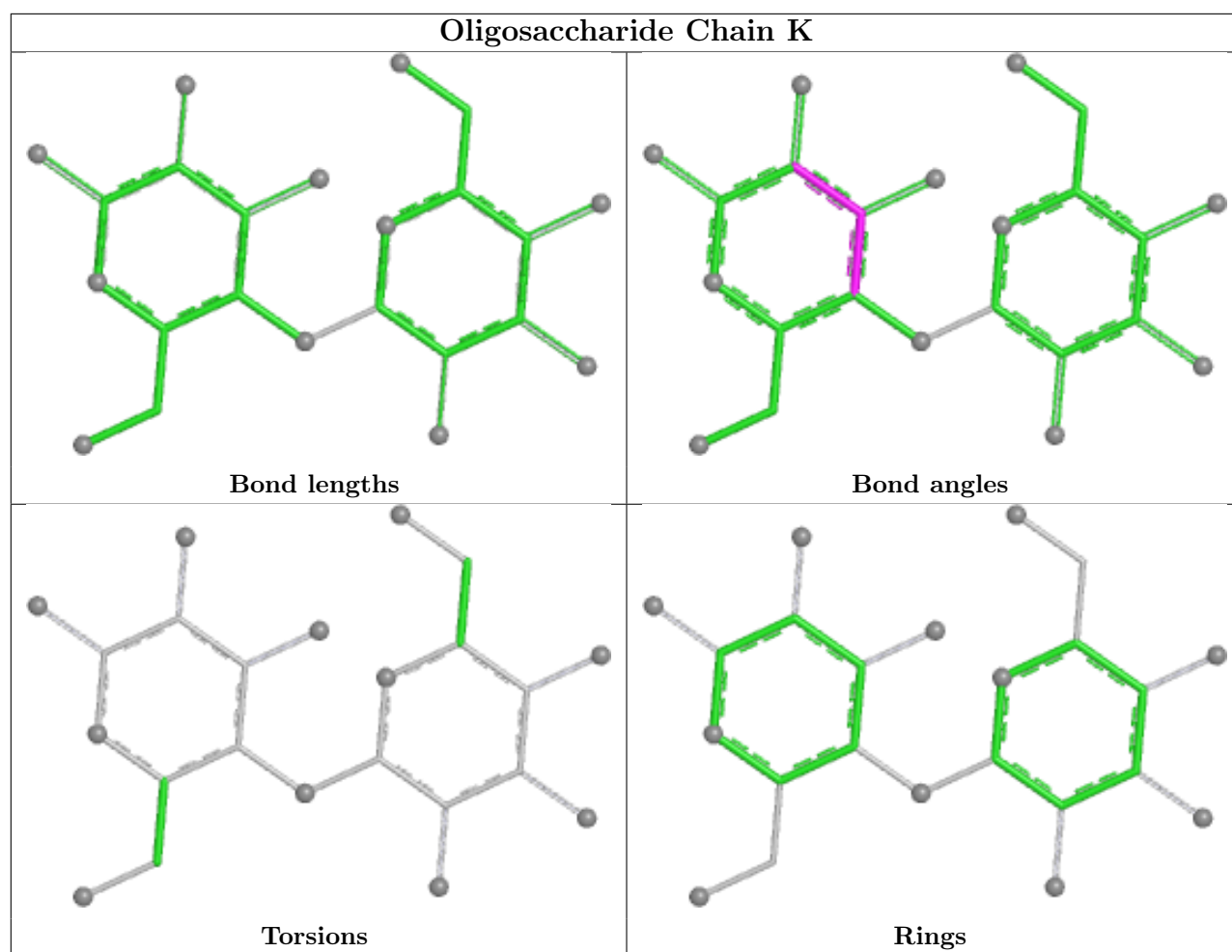
24 monomers are involved in 30 short contacts:

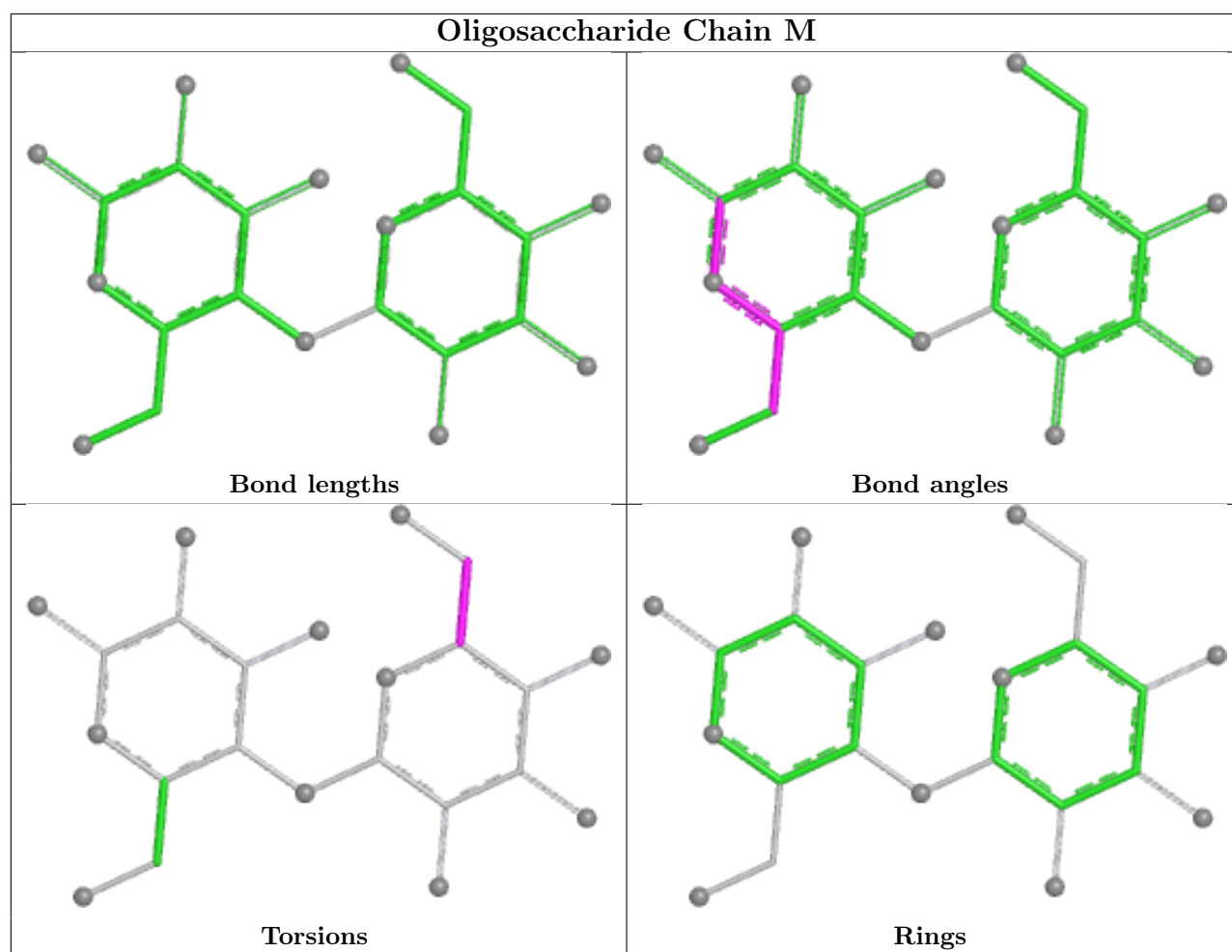
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	2	GLC	1	0
3	R	6	GLC	2	0
2	Q	2	GLC	2	0
3	J	1	GLC	1	0
3	H	5	GLC	1	0
3	J	2	GLC	1	0
3	R	2	GLC	1	0
3	H	2	GLC	1	0
2	O	1	GLC	1	0
3	J	4	GLC	1	0
3	P	6	GLC	1	0
3	N	6	GLC	1	0
3	L	5	GLC	2	0
2	K	1	GLC	1	0
3	P	5	GLC	2	0
2	K	2	GLC	1	0
2	M	1	GLC	2	0
3	J	5	GLC	1	0
3	N	1	GLC	1	0
3	H	6	GLC	1	0
2	M	2	GLC	2	0
3	R	5	GLC	2	0
3	N	5	GLC	1	0
3	L	2	GLC	1	0

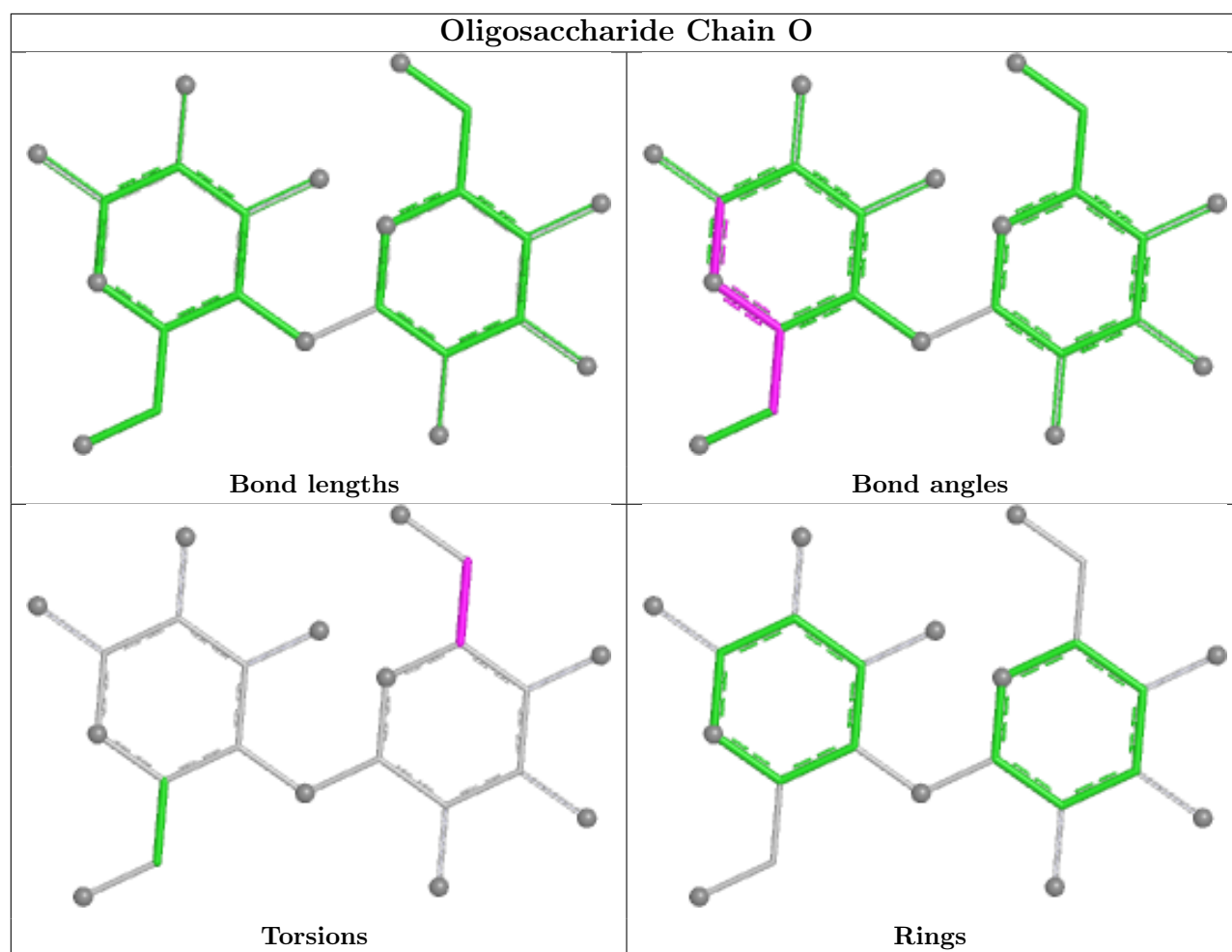
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

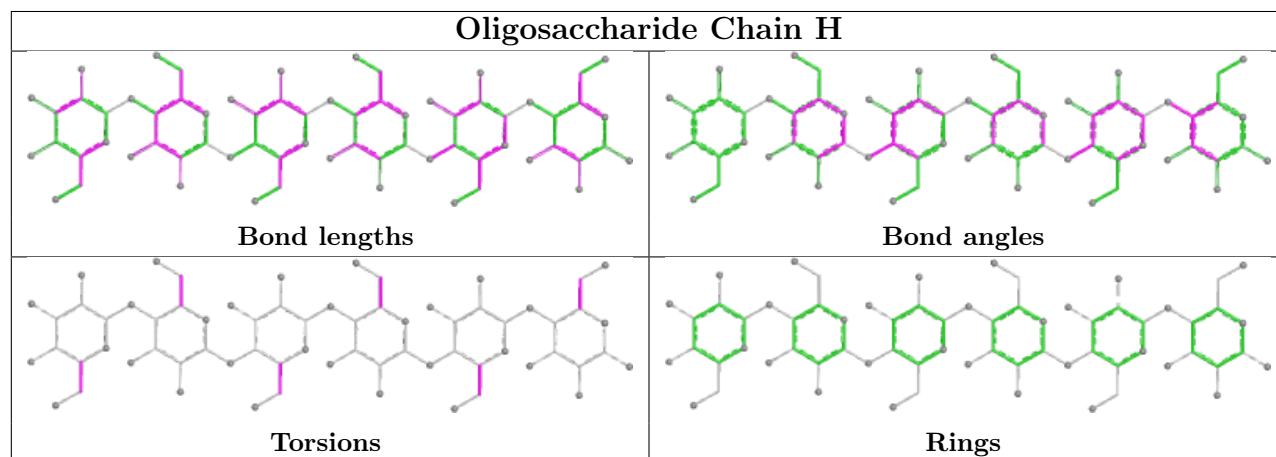
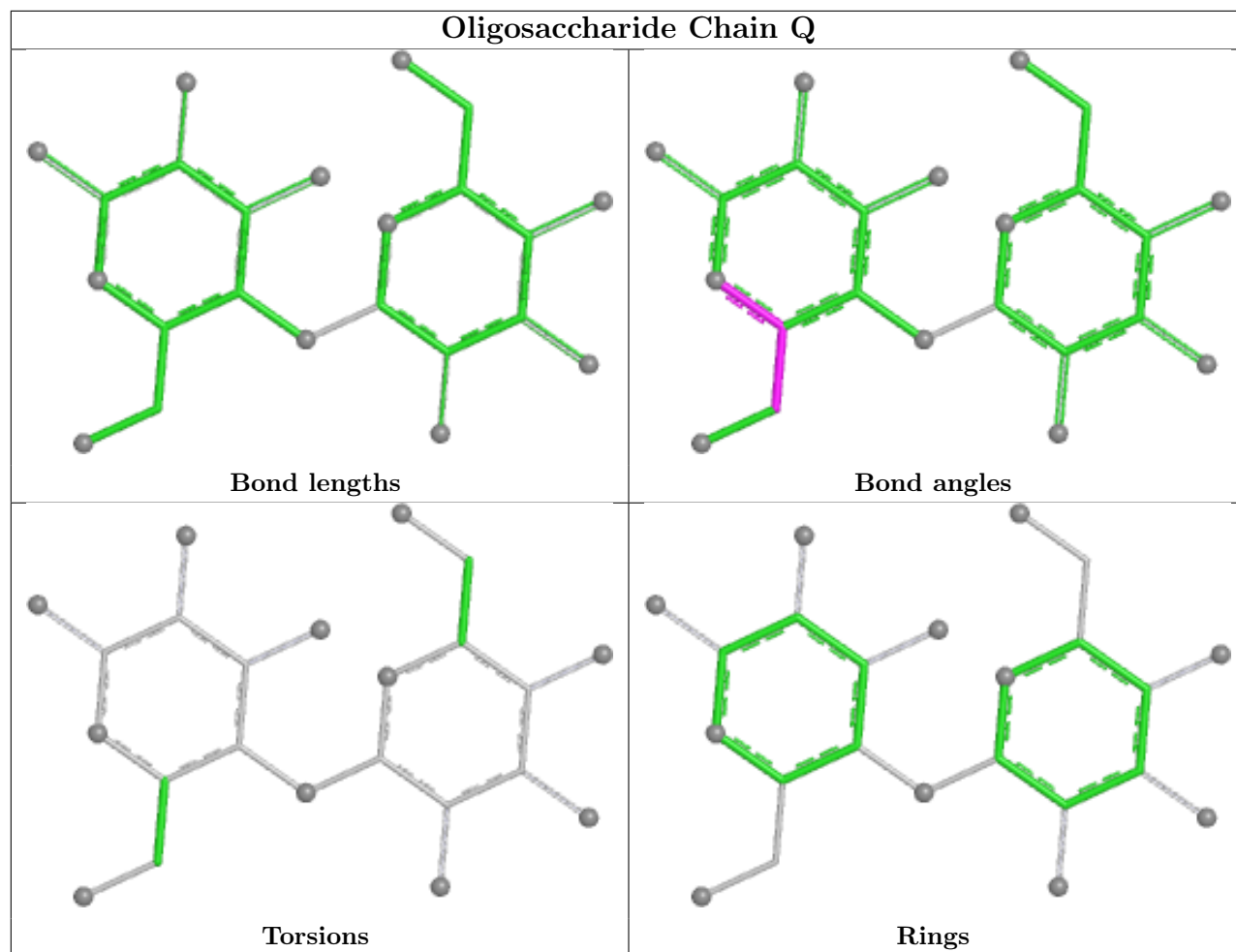


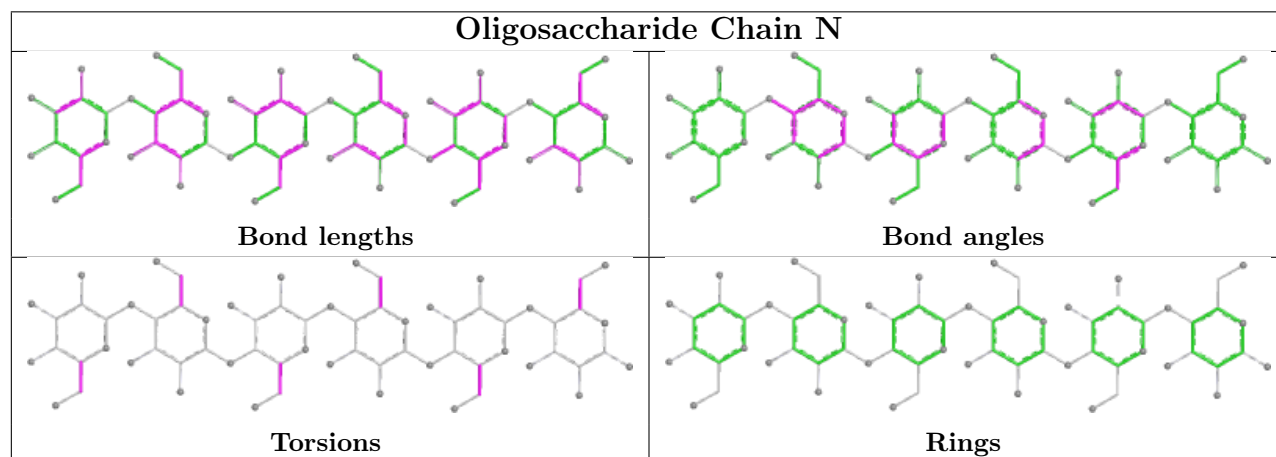
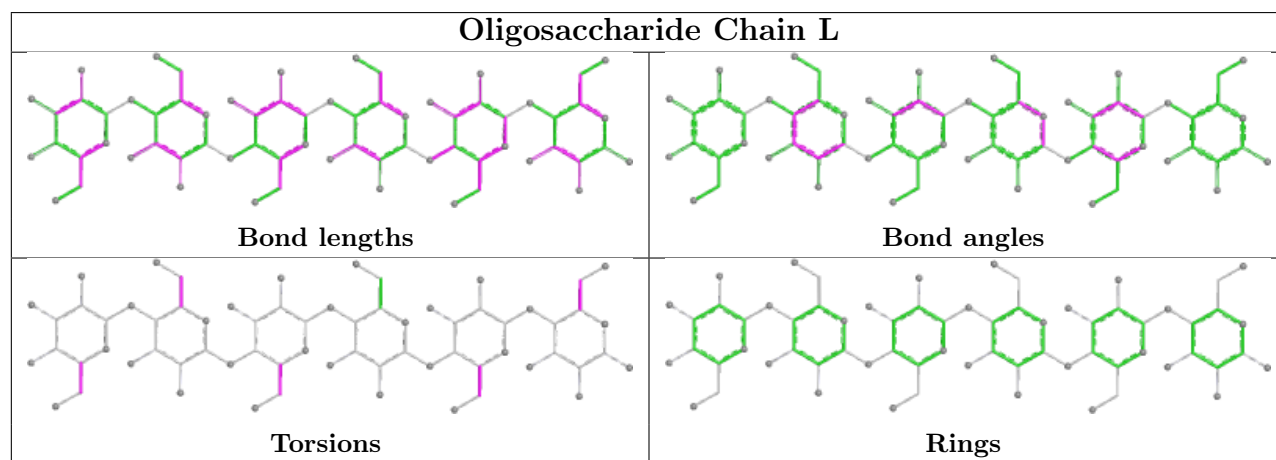
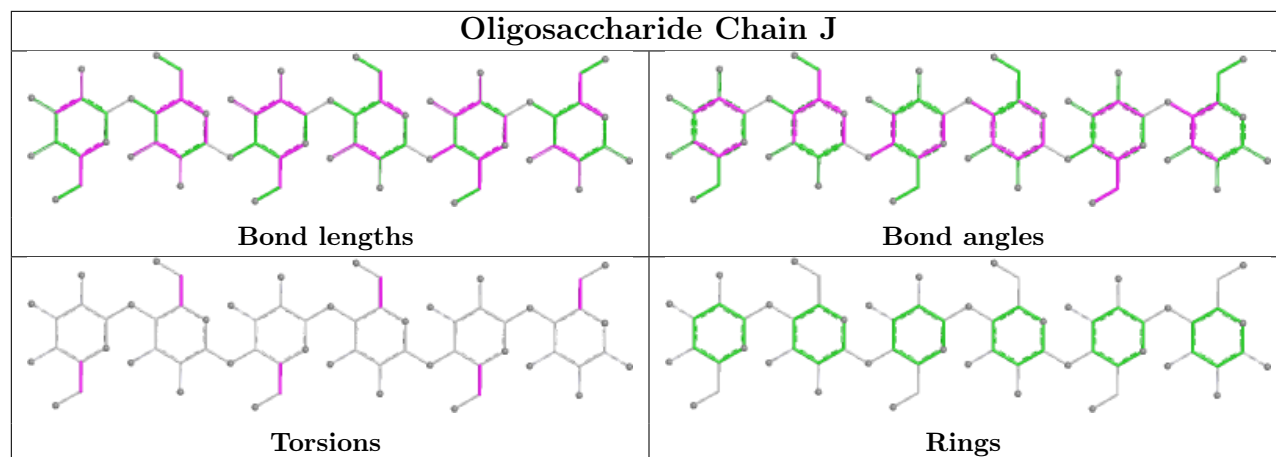


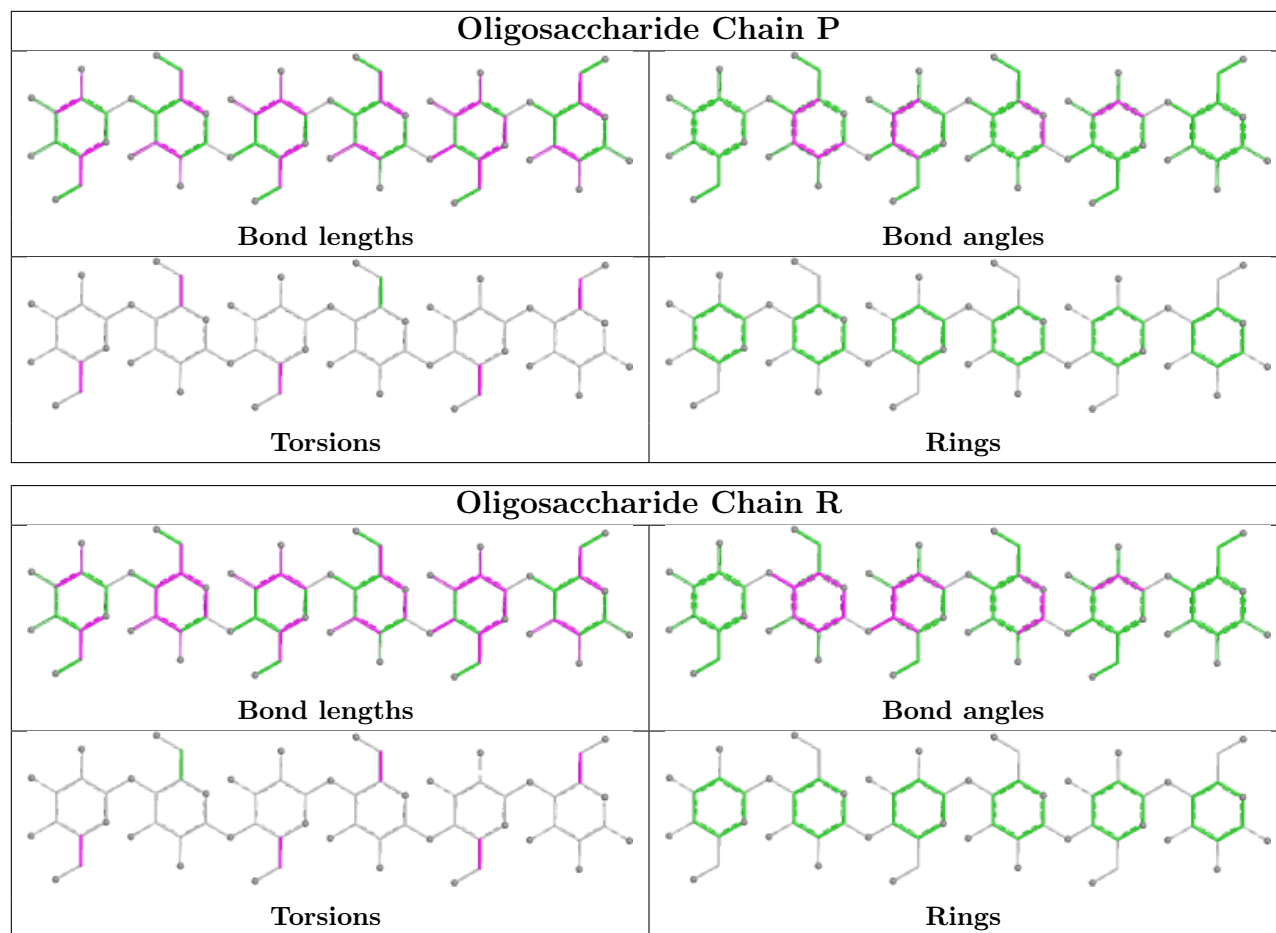












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	660/723 (91%)	0.66	51 (7%) 19 19	86, 118, 165, 185	0
1	B	660/723 (91%)	0.69	60 (9%) 15 16	86, 117, 162, 185	0
1	C	660/723 (91%)	0.77	66 (10%) 12 15	88, 119, 167, 201	0
1	D	660/723 (91%)	0.76	66 (10%) 12 15	87, 117, 162, 192	0
1	E	660/723 (91%)	0.77	72 (10%) 10 13	85, 119, 165, 191	0
1	F	660/723 (91%)	0.70	65 (9%) 13 15	84, 117, 167, 190	0
All	All	3960/4338 (91%)	0.72	380 (9%) 13 15	84, 118, 165, 201	0

All (380) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	PRO	8.9
1	E	15	PRO	8.3
1	C	144	GLY	7.7
1	B	15	PRO	6.9
1	F	70	PRO	6.9
1	D	15	PRO	6.2
1	B	70	PRO	6.2
1	D	70	PRO	6.1
1	B	180	ALA	6.1
1	E	70	PRO	6.0
1	C	70	PRO	5.9
1	F	15	PRO	5.9
1	C	15	PRO	5.8
1	B	144	GLY	5.7
1	F	197	LEU	5.7
1	A	348	GLN	5.7
1	E	190	VAL	5.6
1	A	144	GLY	5.5
1	E	144	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	190	VAL	5.4
1	A	70	PRO	5.4
1	A	197	LEU	5.3
1	F	181	ALA	5.3
1	C	197	LEU	5.1
1	C	186	PRO	5.0
1	F	190	VAL	5.0
1	D	144	GLY	4.9
1	C	191	THR	4.8
1	D	197	LEU	4.7
1	D	377	PRO	4.7
1	B	186	PRO	4.7
1	E	162	GLU	4.6
1	E	181	ALA	4.5
1	B	171	GLY	4.4
1	D	563	ARG	4.4
1	A	189	PRO	4.4
1	F	182	ALA	4.4
1	E	16	GLY	4.3
1	F	92	LYS	4.3
1	C	357	ARG	4.3
1	F	356	ALA	4.3
1	C	194	ALA	4.2
1	E	197	LEU	4.1
1	B	380	LYS	4.1
1	F	178	ALA	4.1
1	F	149	GLU	4.1
1	F	556	GLU	4.1
1	B	16	GLY	4.1
1	E	50	ARG	4.1
1	F	381	TYR	4.1
1	E	17	ARG	4.1
1	D	186	PRO	4.1
1	B	17	ARG	4.0
1	E	185	THR	4.0
1	C	169	PRO	4.0
1	D	190	VAL	3.9
1	C	140	LYS	3.9
1	F	156	VAL	3.9
1	D	380	LYS	3.9
1	A	149	GLU	3.8
1	A	172	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	179	ALA	3.8
1	E	169	PRO	3.8
1	E	149	GLU	3.8
1	F	169	PRO	3.8
1	D	153	ASP	3.7
1	D	195	LEU	3.7
1	C	178	ALA	3.7
1	B	311	GLU	3.7
1	E	379	LYS	3.7
1	D	150	LEU	3.7
1	A	169	PRO	3.7
1	B	177	LEU	3.7
1	B	694	ARG	3.7
1	C	174	ASP	3.7
1	B	172	LEU	3.6
1	C	377	PRO	3.6
1	E	394	GLU	3.6
1	F	377	PRO	3.6
1	C	171	GLY	3.5
1	A	92	LYS	3.5
1	B	360	ARG	3.5
1	C	170	ARG	3.5
1	F	144	GLY	3.5
1	A	237	MET	3.5
1	D	551	GLU	3.5
1	D	382	GLN	3.5
1	F	379	LYS	3.5
1	B	364	THR	3.5
1	C	17	ARG	3.5
1	C	189	PRO	3.5
1	E	189	PRO	3.5
1	F	191	THR	3.4
1	E	182	ALA	3.4
1	F	551	GLU	3.4
1	E	487	ALA	3.4
1	E	551	GLU	3.4
1	B	149	GLU	3.4
1	D	149	GLU	3.4
1	B	197	LEU	3.4
1	A	662	GLU	3.3
1	D	699	ARG	3.3
1	A	190	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	50	ARG	3.3
1	C	172	LEU	3.3
1	B	189	PRO	3.3
1	C	199	PRO	3.3
1	D	169	PRO	3.3
1	D	92	LYS	3.3
1	F	378	PRO	3.3
1	B	195	LEU	3.3
1	A	187	GLY	3.3
1	B	381	TYR	3.3
1	A	186	PRO	3.3
1	F	186	PRO	3.2
1	A	140	LYS	3.2
1	F	184	ARG	3.2
1	A	377	PRO	3.2
1	B	187	GLY	3.2
1	F	383	ASP	3.2
1	A	16	GLY	3.1
1	B	375	GLU	3.1
1	E	191	THR	3.1
1	C	182	ALA	3.1
1	D	381	TYR	3.1
1	D	245	TRP	3.0
1	A	199	PRO	3.0
1	F	153	ASP	3.0
1	C	67	VAL	3.0
1	C	488	GLU	3.0
1	B	631	PHE	3.0
1	D	357	ARG	3.0
1	A	208	TYR	3.0
1	C	375	GLU	3.0
1	E	92	LYS	3.0
1	A	188	ASP	3.0
1	C	175	PRO	3.0
1	F	185	THR	3.0
1	E	29	CYS	2.9
1	A	181	ALA	2.9
1	A	356	ALA	2.9
1	A	19	GLU	2.9
1	F	68	ARG	2.9
1	F	142	ASP	2.9
1	B	140	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	244	GLY	2.9
1	D	557	LYS	2.9
1	D	184	ARG	2.9
1	E	128	ASP	2.8
1	E	153	ASP	2.8
1	E	662	GLU	2.9
1	D	324	ILE	2.8
1	F	170	ARG	2.8
1	E	381	TYR	2.8
1	D	172	LEU	2.8
1	E	172	LEU	2.8
1	A	195	LEU	2.8
1	B	190	VAL	2.8
1	B	150	LEU	2.8
1	B	285	VAL	2.8
1	C	193	THR	2.8
1	D	546	ARG	2.8
1	B	169	PRO	2.8
1	A	380	LYS	2.8
1	D	53	HIS	2.8
1	C	181	ALA	2.8
1	E	699	ARG	2.7
1	D	174	ASP	2.7
1	E	186	PRO	2.7
1	E	357	ARG	2.7
1	F	360	ARG	2.7
1	C	324	ILE	2.7
1	F	53	HIS	2.7
1	A	290	ARG	2.7
1	A	694	ARG	2.7
1	B	468	SER	2.7
1	D	199	PRO	2.7
1	C	149	GLU	2.7
1	F	173	ARG	2.7
1	D	512	ASN	2.7
1	A	171	GLY	2.7
1	E	286	HIS	2.7
1	F	468	SER	2.7
1	E	140	LYS	2.7
1	E	284	LYS	2.7
1	C	691	TYR	2.6
1	F	380	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	370	THR	2.6
1	F	373	TYR	2.6
1	B	358	GLU	2.6
1	C	16	GLY	2.6
1	A	381	TYR	2.6
1	C	543	ARG	2.6
1	C	364	THR	2.6
1	D	17	ARG	2.6
1	C	308	GLY	2.6
1	C	316	THR	2.6
1	E	547	GLU	2.6
1	B	292	ASN	2.6
1	F	177	LEU	2.6
1	F	189	PRO	2.6
1	E	245	TRP	2.5
1	A	699	ARG	2.5
1	E	374	ALA	2.5
1	E	356	ALA	2.5
1	C	184	ARG	2.5
1	E	561	ARG	2.5
1	E	54	GLU	2.5
1	E	324	ILE	2.5
1	D	134	ARG	2.5
1	D	561	ARG	2.5
1	F	357	ARG	2.5
1	B	373	TYR	2.5
1	E	51	GLU	2.5
1	B	356	ALA	2.5
1	E	199	PRO	2.5
1	D	39	GLY	2.5
1	A	17	ARG	2.5
1	C	561	ARG	2.5
1	F	16	GLY	2.5
1	B	469	TYR	2.5
1	C	188	ASP	2.4
1	E	106	VAL	2.4
1	D	140	LYS	2.4
1	C	477	TRP	2.4
1	B	493	ARG	2.4
1	C	361	GLN	2.4
1	C	423	LYS	2.4
1	D	67	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	324	ILE	2.4
1	B	194	ALA	2.4
1	F	163	ARG	2.4
1	C	185	THR	2.4
1	B	200	GLU	2.4
1	D	694	ARG	2.4
1	B	110	GLN	2.4
1	E	372	ALA	2.4
1	D	489	LEU	2.4
1	E	694	ARG	2.4
1	F	488	GLU	2.4
1	F	140	LYS	2.4
1	D	100	SER	2.4
1	A	128	ASP	2.4
1	B	641	ASP	2.4
1	E	364	THR	2.3
1	F	67	VAL	2.3
1	E	596	ARG	2.3
1	D	379	LYS	2.3
1	D	383	ASP	2.3
1	F	390	ASP	2.3
1	D	374	ALA	2.3
1	E	115	ARG	2.3
1	D	208	TYR	2.3
1	B	551	GLU	2.3
1	E	131	HIS	2.3
1	C	211	ARG	2.3
1	A	487	ALA	2.3
1	C	177	LEU	2.3
1	A	551	GLU	2.3
1	F	162	GLU	2.3
1	F	336	ASP	2.3
1	B	320	SER	2.3
1	F	187	GLY	2.3
1	F	285	VAL	2.3
1	B	185	THR	2.3
1	C	695	ASN	2.3
1	B	357	ARG	2.3
1	D	360	ARG	2.3
1	E	335	ARG	2.3
1	F	699	ARG	2.3
1	F	262	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	241	SER	2.3
1	A	175	PRO	2.3
1	F	174	ASP	2.3
1	D	364	THR	2.3
1	E	184	ARG	2.3
1	D	177	LEU	2.3
1	C	381	TYR	2.3
1	A	200	GLU	2.3
1	F	394	GLU	2.3
1	C	195	LEU	2.2
1	D	179	ALA	2.2
1	E	178	ALA	2.2
1	C	380	LYS	2.2
1	B	374	ALA	2.2
1	C	487	ALA	2.2
1	A	106	VAL	2.2
1	A	488	GLU	2.2
1	B	547	GLU	2.2
1	D	54	GLU	2.2
1	D	285	VAL	2.2
1	E	141	LEU	2.2
1	A	437	THR	2.2
1	F	143	ALA	2.2
1	B	183	LEU	2.2
1	E	67	VAL	2.2
1	F	106	VAL	2.2
1	E	383	ASP	2.2
1	C	68	ARG	2.2
1	B	291	ASN	2.2
1	C	143	ALA	2.2
1	F	179	ALA	2.2
1	B	102	GLN	2.2
1	D	141	LEU	2.2
1	F	385	TYR	2.2
1	E	375	GLU	2.2
1	E	376	ASN	2.2
1	C	356	ALA	2.1
1	A	151	SER	2.1
1	B	53	HIS	2.1
1	D	468	SER	2.1
1	E	247	ASP	2.1
1	C	102	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	691	TYR	2.1
1	E	691	TYR	2.1
1	C	379	LYS	2.1
1	E	193	THR	2.1
1	E	316	THR	2.1
1	A	53	HIS	2.1
1	A	288	LYS	2.1
1	C	425	PRO	2.1
1	D	16	GLY	2.1
1	C	556	GLU	2.1
1	D	189	PRO	2.1
1	D	183	LEU	2.1
1	A	184	ARG	2.1
1	B	181	ALA	2.1
1	C	290	ARG	2.1
1	F	17	ARG	2.1
1	F	134	ARG	2.1
1	A	383	ASP	2.1
1	C	383	ASP	2.1
1	D	188	ASP	2.1
1	E	244	GLY	2.1
1	D	358	GLU	2.1
1	E	19	GLU	2.1
1	B	170	ARG	2.1
1	F	512	ASN	2.1
1	B	67	VAL	2.1
1	A	49	TRP	2.1
1	C	373	TYR	2.1
1	A	550	GLU	2.1
1	B	699	ARG	2.1
1	D	320	SER	2.1
1	C	107	PHE	2.1
1	D	695	ASN	2.1
1	F	376	ASN	2.1
1	C	285	VAL	2.1
1	A	108	HIS	2.1
1	B	467	TYR	2.1
1	C	378	PRO	2.1
1	A	475	THR	2.1
1	B	92	LYS	2.1
1	D	194	ALA	2.1
1	F	183	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	199	PRO	2.0
1	E	360	ARG	2.0
1	A	557	LYS	2.0
1	E	164	ALA	2.0
1	E	107	PHE	2.0
1	C	39	GLY	2.0
1	B	108	HIS	2.0
1	C	92	LYS	2.0
1	D	175	PRO	2.0
1	D	40	GLU	2.0
1	E	644	ALA	2.0
1	E	285	VAL	2.0
1	F	110	GLN	2.0
1	F	361	GLN	2.0
1	D	251	PRO	2.0
1	E	134	ARG	2.0
1	B	191	THR	2.0
1	C	542	HIS	2.0
1	E	314	HIS	2.0
1	E	511	HIS	2.0
1	C	692	GLU	2.0
1	D	218	GLU	2.0
1	E	218	GLU	2.0
1	A	174	ASP	2.0
1	F	698	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	J	5	11/12	0.59	0.26	146,159,169,171	0
2	GLC	G	1	12/12	0.60	0.20	111,143,149,153	0
2	GLC	K	1	12/12	0.62	0.24	110,148,156,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	Q	1	12/12	0.65	0.21	122,142,150,156	0
2	GLC	I	1	12/12	0.66	0.20	117,147,154,155	0
2	GLC	O	1	12/12	0.67	0.21	121,147,155,156	0
3	GLC	J	4	11/12	0.71	0.19	133,139,154,160	0
2	GLC	M	1	12/12	0.71	0.20	127,150,159,160	0
3	GLC	H	5	11/12	0.76	0.15	109,125,132,139	0
3	GLC	P	3	11/12	0.79	0.14	123,129,131,136	0
3	GLC	H	1	12/12	0.81	0.17	108,117,120,121	0
3	GLC	R	3	11/12	0.83	0.12	116,123,130,130	0
3	GLC	L	3	11/12	0.84	0.13	119,126,130,131	0
3	GLC	P	2	11/12	0.85	0.13	119,128,134,137	0
3	GLC	H	3	11/12	0.86	0.12	123,127,130,130	0
3	GLC	J	6	11/12	0.86	0.18	106,123,136,147	0
3	GLC	N	1	12/12	0.87	0.12	109,117,121,122	0
3	GLC	H	6	11/12	0.87	0.18	105,118,126,126	0
3	GLC	N	5	11/12	0.88	0.11	120,124,126,133	0
3	GLC	P	1	12/12	0.88	0.12	117,125,130,130	0
3	GLC	L	1	12/12	0.88	0.11	110,118,124,126	0
2	GLC	M	2	11/12	0.88	0.14	140,144,148,155	0
3	GLC	P	5	11/12	0.88	0.10	116,125,129,137	0
3	GLC	H	2	11/12	0.88	0.14	118,123,127,133	0
3	GLC	R	5	11/12	0.88	0.13	118,128,135,148	0
3	GLC	P	4	11/12	0.89	0.12	124,127,133,134	0
3	GLC	N	3	11/12	0.89	0.10	116,126,128,129	0
3	GLC	R	1	12/12	0.89	0.12	108,117,120,125	0
3	GLC	N	4	11/12	0.89	0.13	115,126,133,134	0
3	GLC	H	4	11/12	0.89	0.10	118,126,132,133	0
3	GLC	N	6	11/12	0.90	0.12	111,116,128,129	0
3	GLC	R	2	11/12	0.90	0.11	116,119,126,126	0
2	GLC	G	2	11/12	0.90	0.14	132,139,147,148	0
3	GLC	R	4	11/12	0.90	0.10	116,122,127,130	0
3	GLC	P	6	11/12	0.90	0.13	110,118,129,130	0
3	GLC	J	2	11/12	0.91	0.11	112,120,127,130	0
3	GLC	L	2	11/12	0.91	0.11	120,125,128,132	0
3	GLC	J	1	12/12	0.91	0.14	109,115,117,122	0
3	GLC	L	6	11/12	0.91	0.12	115,121,130,131	0
2	GLC	K	2	11/12	0.92	0.12	132,137,140,141	0
3	GLC	J	3	11/12	0.92	0.10	114,128,130,136	0
3	GLC	L	4	11/12	0.92	0.10	122,128,140,141	0
2	GLC	I	2	11/12	0.92	0.12	132,137,145,146	0
3	GLC	R	6	11/12	0.92	0.12	110,121,132,132	0
2	GLC	O	2	11/12	0.93	0.15	135,144,149,150	0

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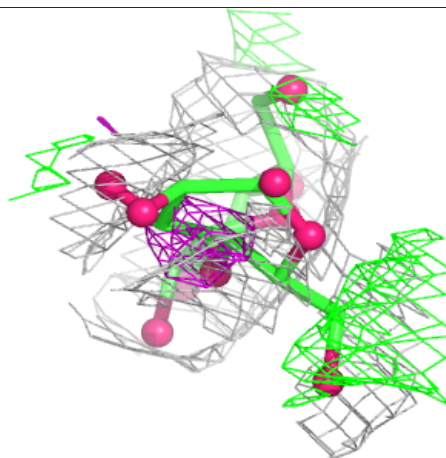
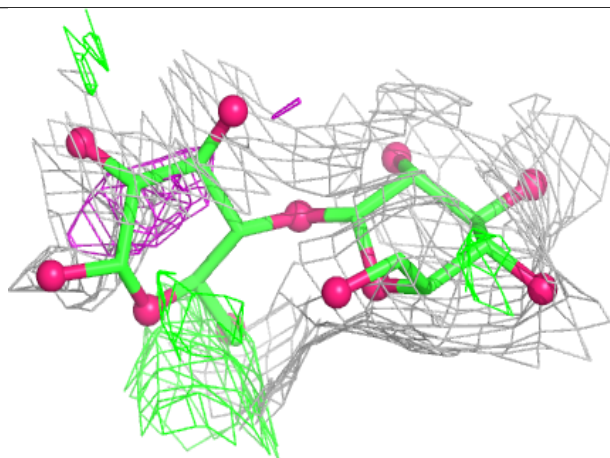
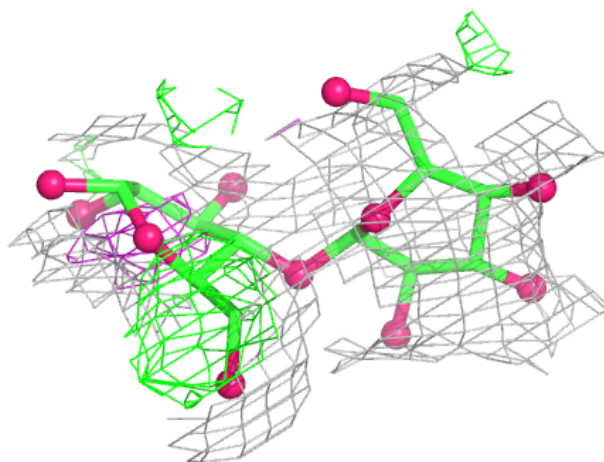
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	Q	2	11/12	0.93	0.14	129,136,144,144	0
3	GLC	L	5	11/12	0.94	0.08	117,128,131,131	0
3	GLC	N	2	11/12	0.94	0.10	118,123,127,127	0

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.

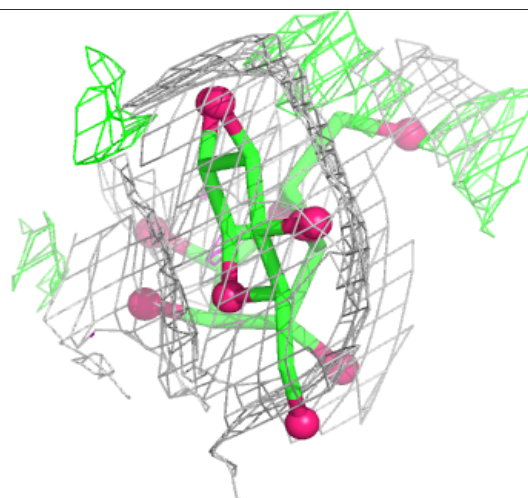
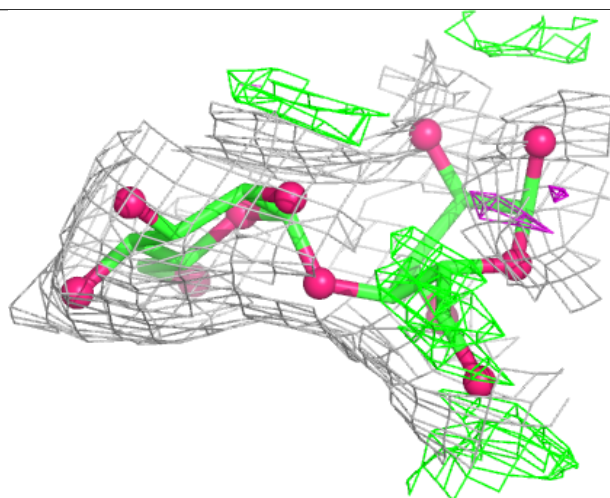
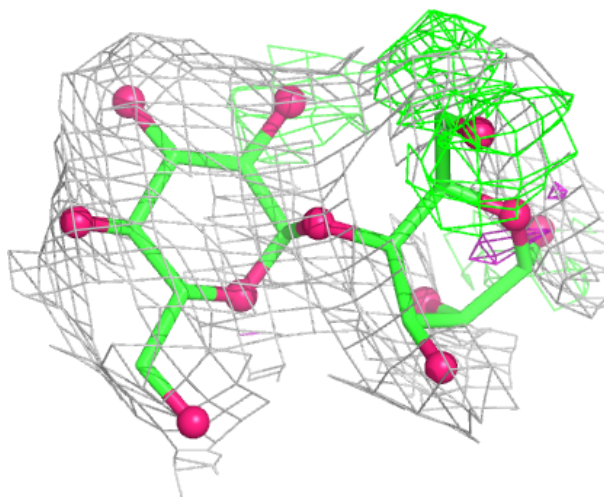
Electron density around Chain G:

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



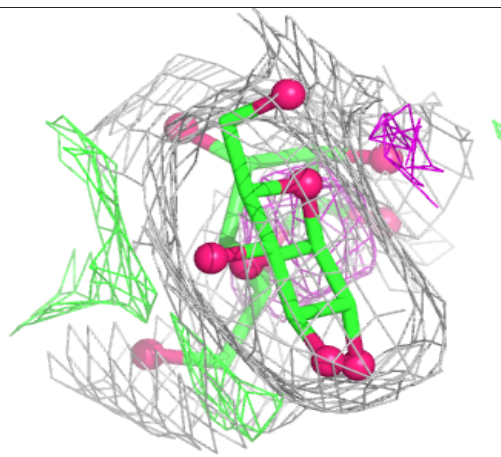
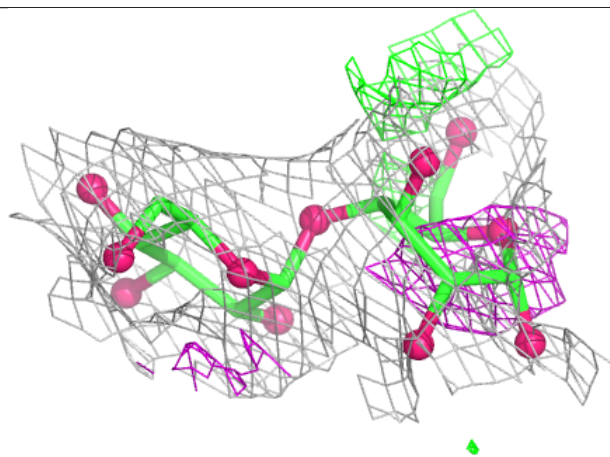
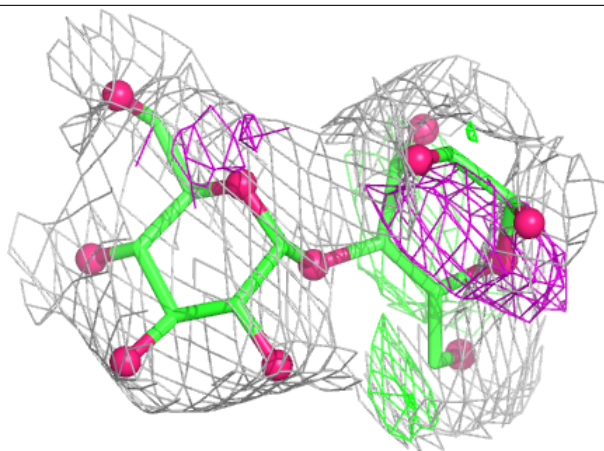
Electron density around Chain I:

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



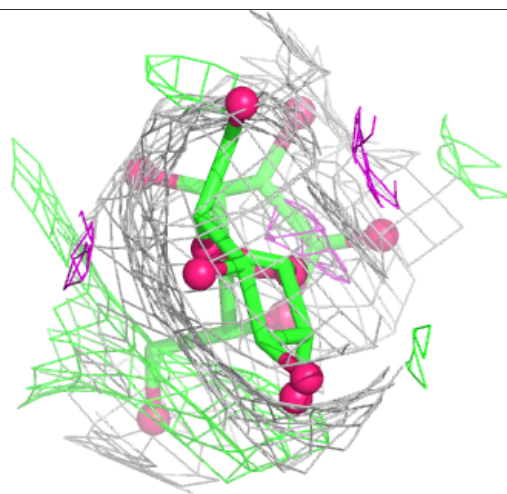
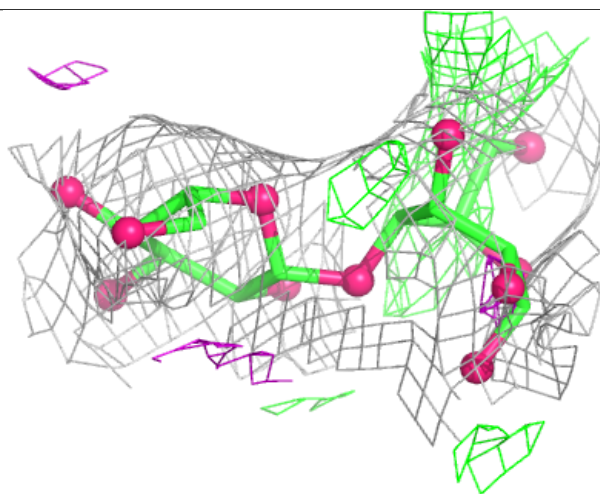
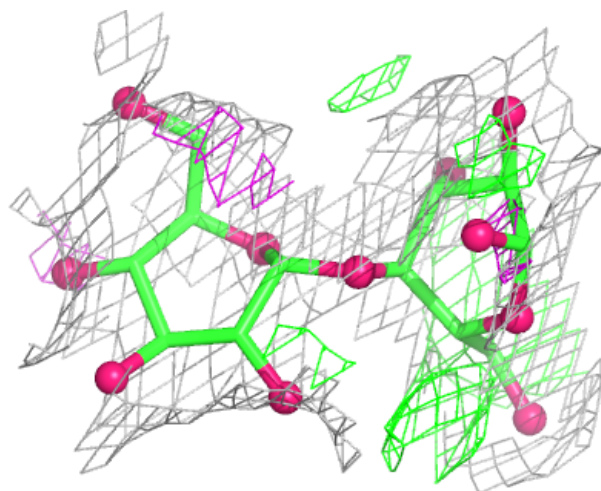
Electron density around Chain K:

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



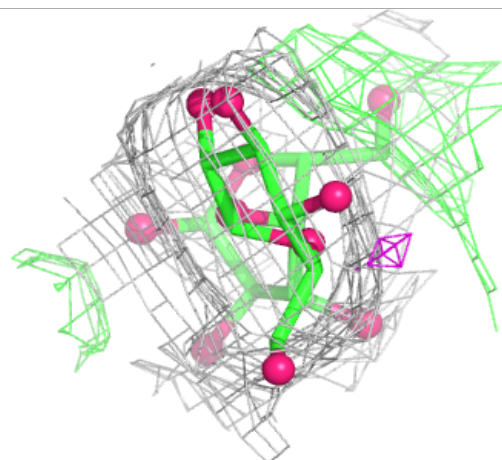
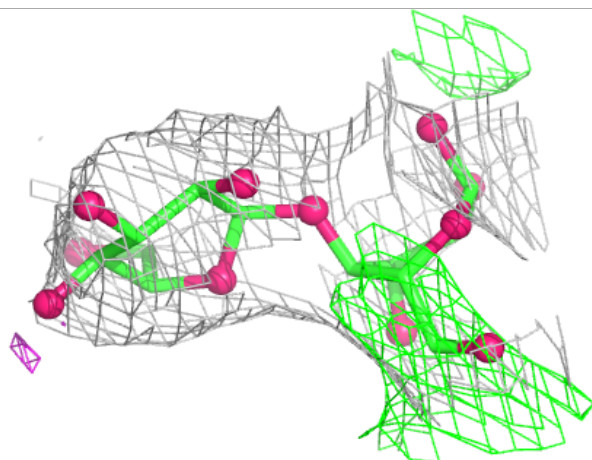
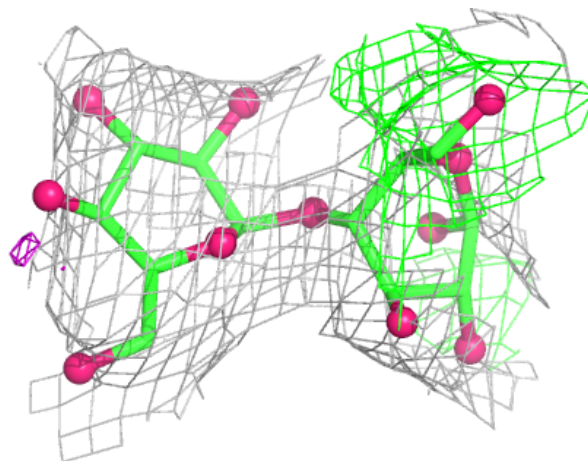
Electron density around Chain M:

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



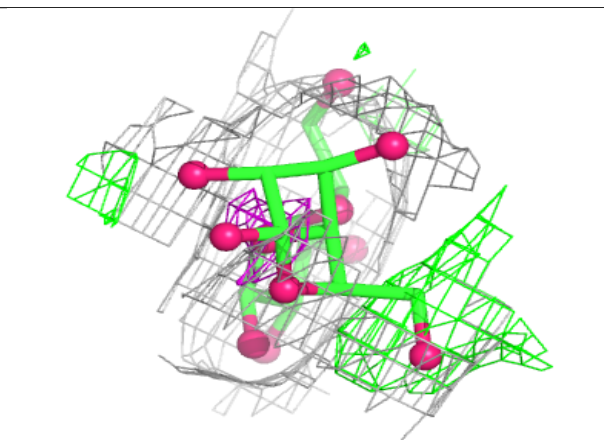
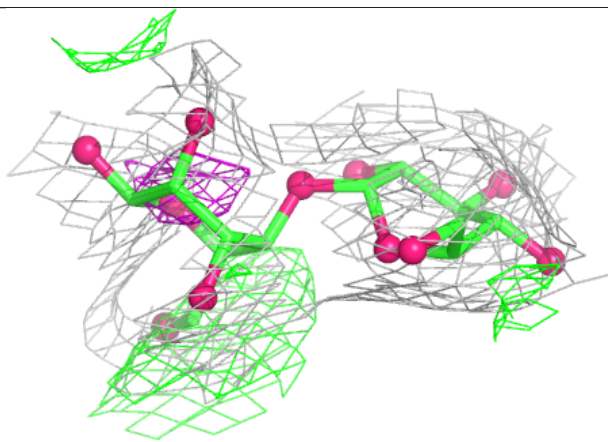
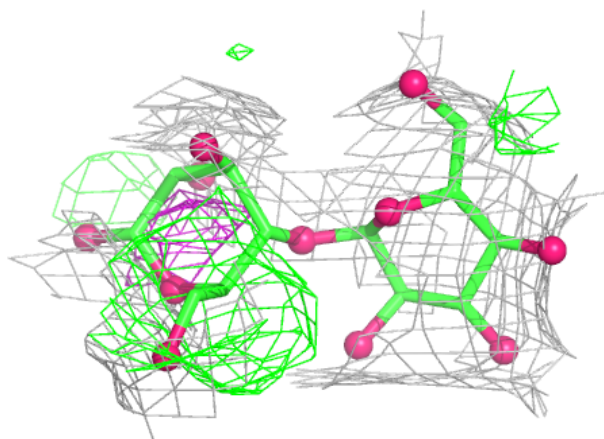
Electron density around Chain O:

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

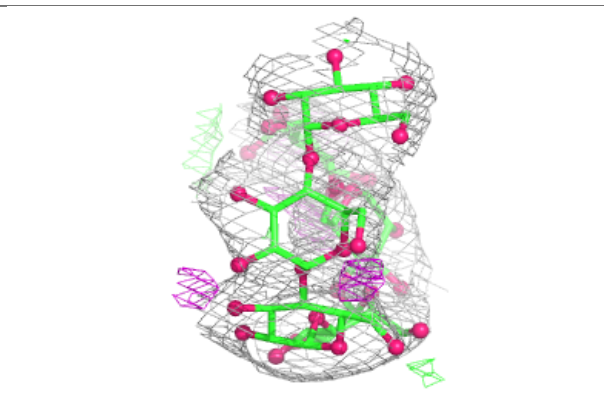
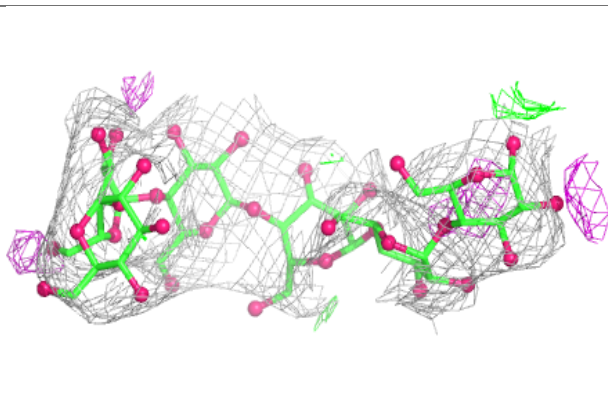
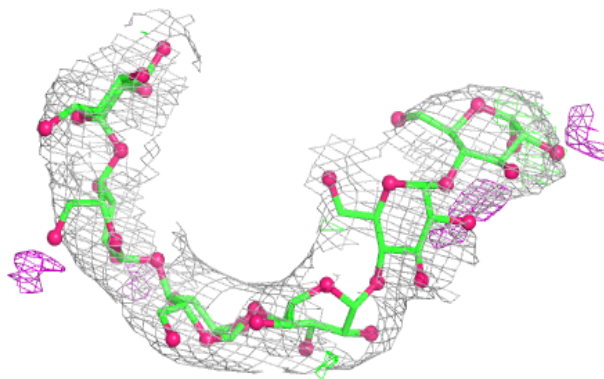


Electron density around Chain Q:

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

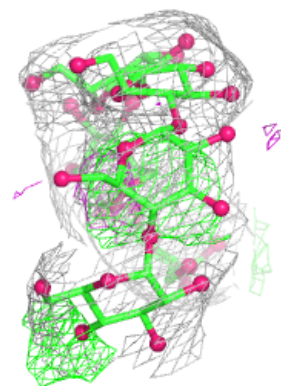
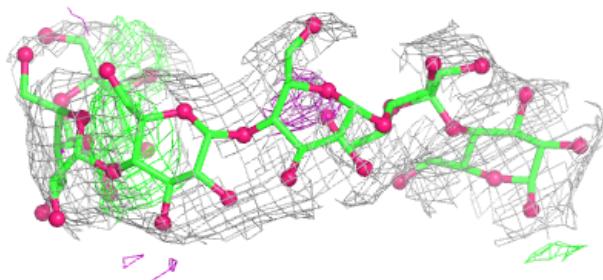
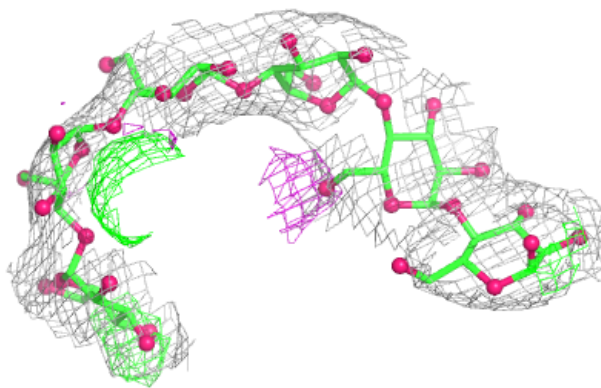
**Electron density around Chain H:**

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

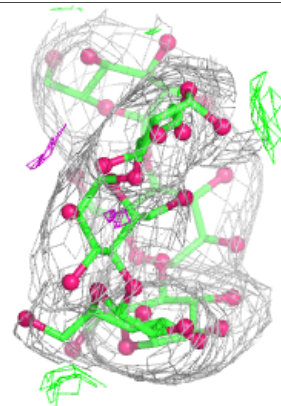
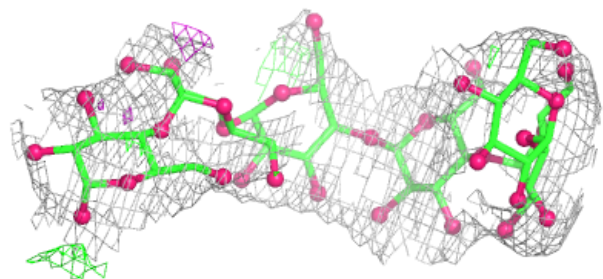
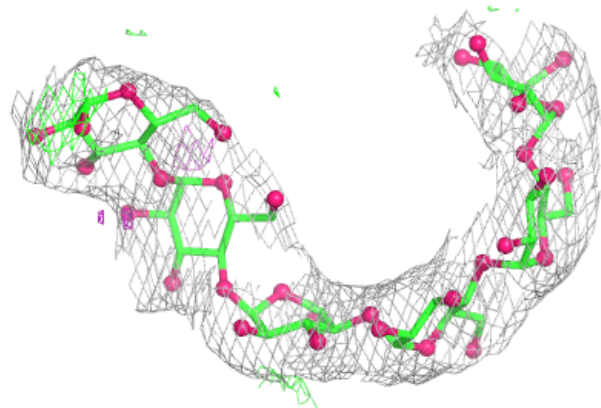


Electron density around Chain J:

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

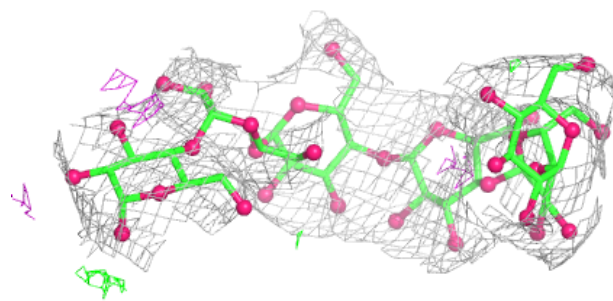
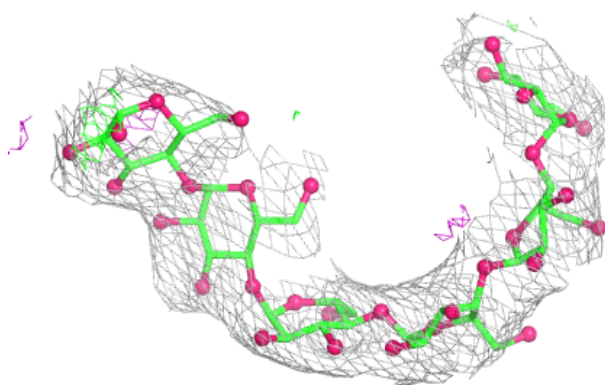
**Electron density around Chain L:**

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

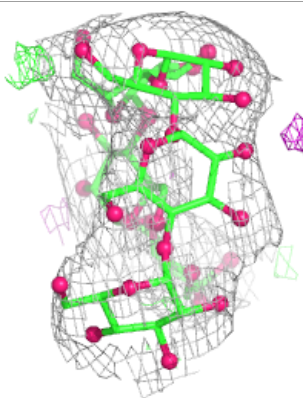
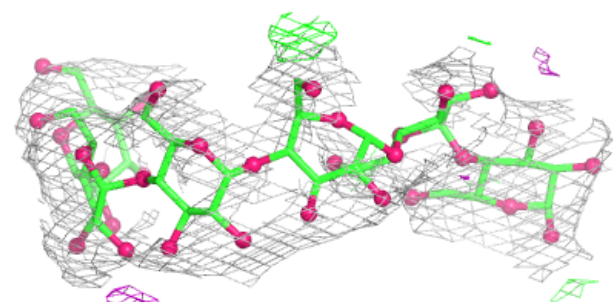
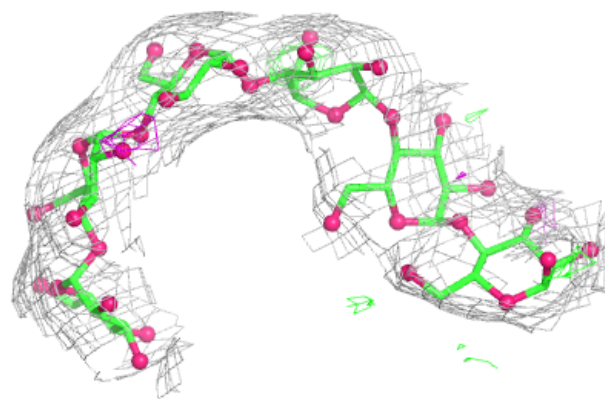


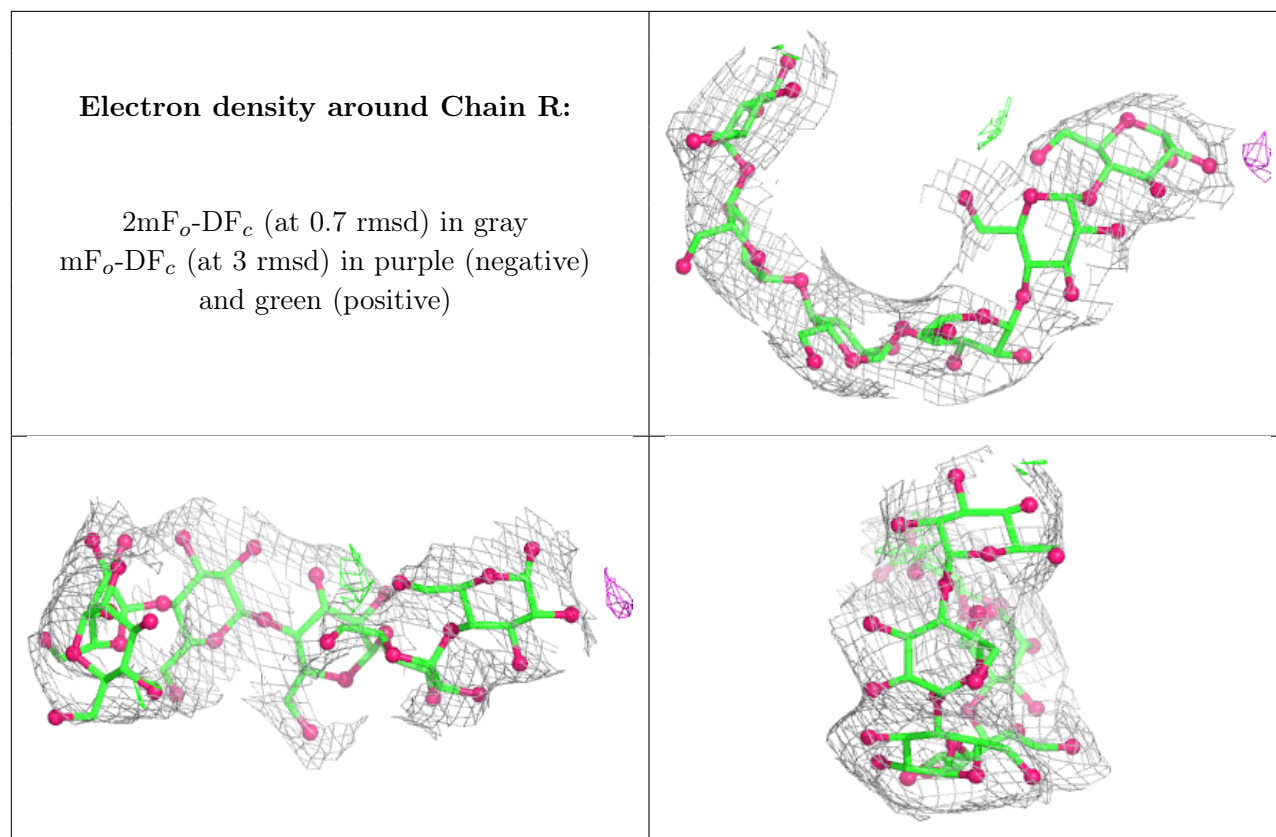
Electron density around Chain N:

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

**Electron density around Chain P:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.