



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 PM UTC

PDB ID : 3RT1 / pdb_00003rt1
Title : Maltodextran bound activated state form of yeast glycogen synthase isoform 2
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2011-05-02
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

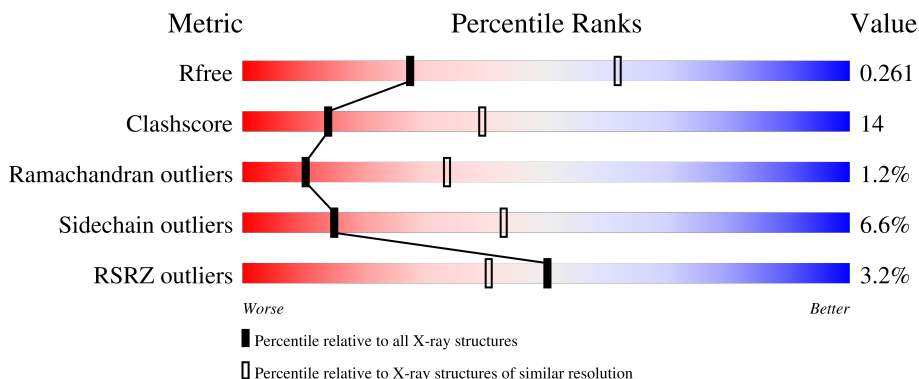
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.




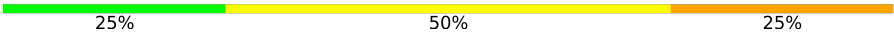

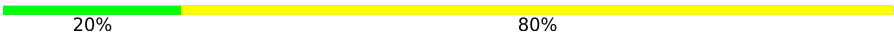
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	725	 3% 63% 22% 12%
1	B	725	 2% 58% 27% 12%
1	C	725	 2% 64% 22% 11%
1	D	725	 4% 56% 28% 12%
2	E	8	 25% 62% 12%

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Mol	Chain	Length	Quality of chain
3	F	3	 33% 67%
4	G	4	 25% 50% 25%
5	H	5	 40% 40% 20%
5	I	5	 20% 80%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 20951 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 PROTEIN (Glycogen [starch] synthase isoform 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	638	5145	3286	896	944	19	0	0	0
1	B	638	5145	3286	896	944	19	0	0	0
1	C	646	5200	3322	907	952	19	0	0	0
1	D	636	5128	3274	894	941	19	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P27472
A	-18	GLY	-	expression tag	UNP P27472
A	-17	SER	-	expression tag	UNP P27472
A	-16	SER	-	expression tag	UNP P27472
A	-15	HIS	-	expression tag	UNP P27472
A	-14	HIS	-	expression tag	UNP P27472
A	-13	HIS	-	expression tag	UNP P27472
A	-12	HIS	-	expression tag	UNP P27472
A	-11	HIS	-	expression tag	UNP P27472
A	-10	HIS	-	expression tag	UNP P27472
A	-9	SER	-	expression tag	UNP P27472
A	-8	SER	-	expression tag	UNP P27472
A	-7	GLY	-	expression tag	UNP P27472
A	-6	LEU	-	expression tag	UNP P27472
A	-5	VAL	-	expression tag	UNP P27472
A	-4	PRO	-	expression tag	UNP P27472
A	-3	ARG	-	expression tag	UNP P27472
A	-2	GLY	-	expression tag	UNP P27472
A	-1	SER	-	expression tag	UNP P27472
A	0	HIS	-	expression tag	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	engineered mutation	UNP P27472
A	592	ALA	ARG	engineered mutation	UNP P27472
B	-19	MET	-	expression tag	UNP P27472
B	-18	GLY	-	expression tag	UNP P27472
B	-17	SER	-	expression tag	UNP P27472
B	-16	SER	-	expression tag	UNP P27472
B	-15	HIS	-	expression tag	UNP P27472
B	-14	HIS	-	expression tag	UNP P27472
B	-13	HIS	-	expression tag	UNP P27472
B	-12	HIS	-	expression tag	UNP P27472
B	-11	HIS	-	expression tag	UNP P27472
B	-10	HIS	-	expression tag	UNP P27472
B	-9	SER	-	expression tag	UNP P27472
B	-8	SER	-	expression tag	UNP P27472
B	-7	GLY	-	expression tag	UNP P27472
B	-6	LEU	-	expression tag	UNP P27472
B	-5	VAL	-	expression tag	UNP P27472
B	-4	PRO	-	expression tag	UNP P27472
B	-3	ARG	-	expression tag	UNP P27472
B	-2	GLY	-	expression tag	UNP P27472
B	-1	SER	-	expression tag	UNP P27472
B	0	HIS	-	expression tag	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	589	ALA	ARG	engineered mutation	UNP P27472
B	592	ALA	ARG	engineered mutation	UNP P27472
C	-19	MET	-	expression tag	UNP P27472
C	-18	GLY	-	expression tag	UNP P27472
C	-17	SER	-	expression tag	UNP P27472
C	-16	SER	-	expression tag	UNP P27472
C	-15	HIS	-	expression tag	UNP P27472
C	-14	HIS	-	expression tag	UNP P27472
C	-13	HIS	-	expression tag	UNP P27472
C	-12	HIS	-	expression tag	UNP P27472
C	-11	HIS	-	expression tag	UNP P27472
C	-10	HIS	-	expression tag	UNP P27472
C	-9	SER	-	expression tag	UNP P27472
C	-8	SER	-	expression tag	UNP P27472
C	-7	GLY	-	expression tag	UNP P27472
C	-6	LEU	-	expression tag	UNP P27472
C	-5	VAL	-	expression tag	UNP P27472
C	-4	PRO	-	expression tag	UNP P27472
C	-3	ARG	-	expression tag	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P27472
C	-1	SER	-	expression tag	UNP P27472
C	0	HIS	-	expression tag	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	589	ALA	ARG	engineered mutation	UNP P27472
C	592	ALA	ARG	engineered mutation	UNP P27472
D	-19	MET	-	expression tag	UNP P27472
D	-18	GLY	-	expression tag	UNP P27472
D	-17	SER	-	expression tag	UNP P27472
D	-16	SER	-	expression tag	UNP P27472
D	-15	HIS	-	expression tag	UNP P27472
D	-14	HIS	-	expression tag	UNP P27472
D	-13	HIS	-	expression tag	UNP P27472
D	-12	HIS	-	expression tag	UNP P27472
D	-11	HIS	-	expression tag	UNP P27472
D	-10	HIS	-	expression tag	UNP P27472
D	-9	SER	-	expression tag	UNP P27472
D	-8	SER	-	expression tag	UNP P27472
D	-7	GLY	-	expression tag	UNP P27472
D	-6	LEU	-	expression tag	UNP P27472
D	-5	VAL	-	expression tag	UNP P27472
D	-4	PRO	-	expression tag	UNP P27472
D	-3	ARG	-	expression tag	UNP P27472
D	-2	GLY	-	expression tag	UNP P27472
D	-1	SER	-	expression tag	UNP P27472
D	0	HIS	-	expression tag	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	589	ALA	ARG	engineered mutation	UNP P27472
D	592	ALA	ARG	engineered mutation	UNP P27472

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	E	8	Total	C	O	0	0	1
			78	42	36			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	F	3	23	12	11	0	0	1

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



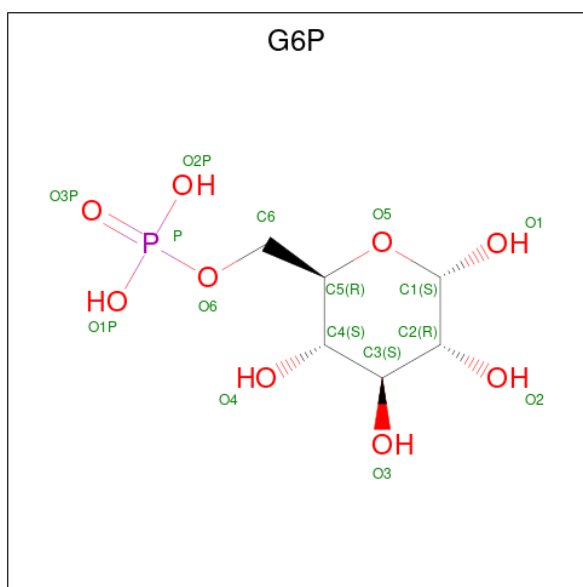
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	G	4	34	18	16	0	0	1

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



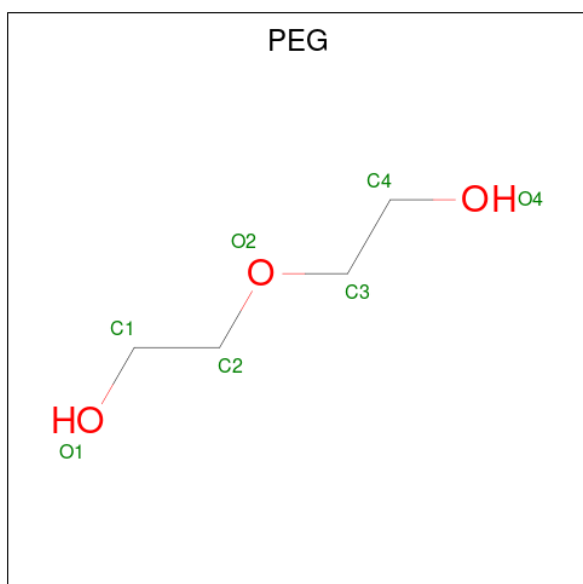
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
5	H	5	45	24	21	0	0	1
5	I	5	45	24	21	0	0	1

- Molecule 6 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: C₆H₁₃O₉P).

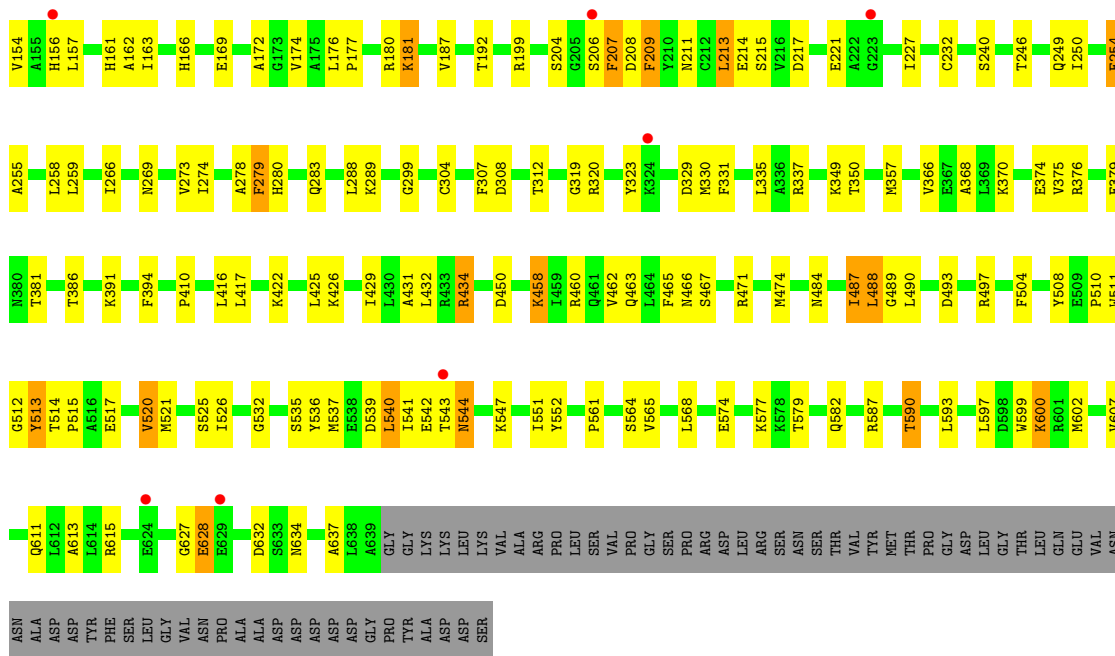


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
6	A	1	16	6	9	1	0	0
6	B	1	16	6	9	1	0	0
6	B	1	16	6	9	1	0	0
6	C	1	16	6	9	1	0	0
6	D	1	16	6	9	1	0	0

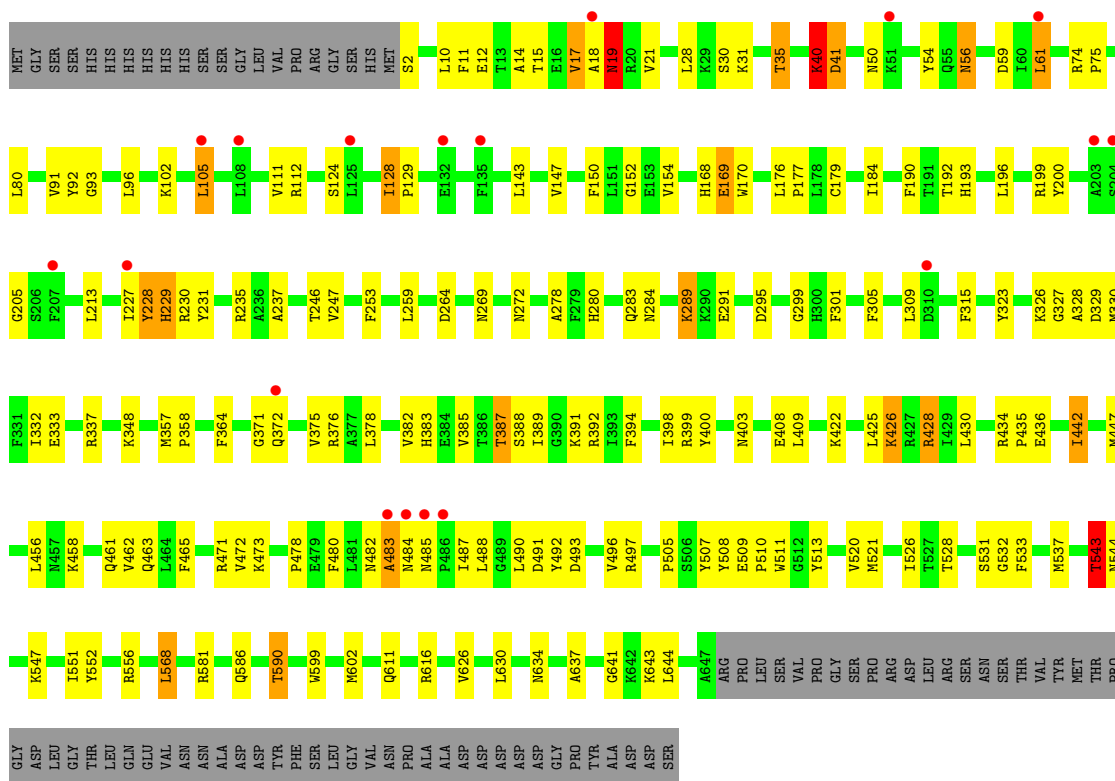
- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 7	C 4	O 3	0	0
7	B	1	Total 7	C 4	O 3	0	0
7	B	1	Total 7	C 4	O 3	0	0
7	C	1	Total 7	C 4	O 3	0	0



• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)

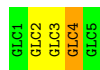


• Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)

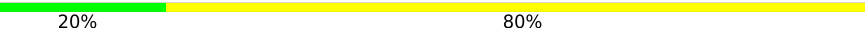


- Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  40% 40% 20%



- Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  20% 80%



4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.44Å 205.33Å 206.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.80 48.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.58-2.80) 99.7 (48.58-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.211 , 0.261 0.213 , 0.261	Depositor DCC
R_{free} test set	5059 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtrriage
Anisotropy	0.403	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20951	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, G6P, 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	0.48	0/5270	0.84	8/7141 (0.1%)
1	B	0.43	0/5270	0.79	4/7141 (0.1%)
1	C	0.43	2/5325 (0.0%)	0.82	9/7212 (0.1%)
1	D	0.48	0/5251	0.83	7/7114 (0.1%)
All	All	0.45	2/21116 (0.0%)	0.82	28/28608 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	434	ARG	C-N	-6.98	1.24	1.33
1	C	435	PRO	C-N	-5.55	1.25	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	434	ARG	CA-C-N	9.94	130.02	119.89
1	C	434	ARG	C-N-CA	9.94	130.02	119.89
1	D	39	TYR	N-CA-C	8.40	124.01	113.43
1	A	612	LEU	N-CA-C	-7.89	103.80	113.50
1	C	434	ARG	CB-CA-C	6.64	119.12	109.09
1	D	128	ILE	CB-CA-C	6.64	116.57	110.13
1	D	39	TYR	CB-CA-C	-6.55	98.64	109.65
1	C	435	PRO	O-C-N	6.32	131.02	122.99
1	A	635	MET	N-CA-C	-6.00	105.45	112.89
1	C	40	LYS	CB-CA-C	-5.87	109.82	116.63
1	D	523	VAL	CA-C-N	5.87	125.83	119.78
1	D	523	VAL	C-N-CA	5.87	125.83	119.78
1	D	434	ARG	CA-C-N	5.50	126.72	119.84
1	D	434	ARG	C-N-CA	5.50	126.72	119.84
1	A	93	GLY	N-CA-C	5.26	117.95	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	VAL	N-CA-C	5.17	115.90	110.62
1	B	467	SER	CA-C-N	5.15	125.19	119.32
1	B	467	SER	C-N-CA	5.15	125.19	119.32
1	C	435	PRO	CA-C-N	-5.14	113.42	121.02
1	C	435	PRO	C-N-CA	-5.14	113.42	121.02
1	A	65	LYS	CA-C-N	5.10	126.21	119.84
1	A	65	LYS	C-N-CA	5.10	126.21	119.84
1	A	513	TYR	N-CA-C	-5.08	105.93	111.82
1	C	128	ILE	N-CA-C	5.05	113.49	107.73
1	A	90	PHE	N-CA-C	5.04	116.24	107.93
1	B	434	ARG	CA-C-N	5.01	126.11	119.84
1	B	434	ARG	C-N-CA	5.01	126.11	119.84
1	C	442	ILE	N-CA-C	-5.01	107.56	113.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5145	0	5054	133	0
1	B	5145	0	5054	141	0
1	C	5200	0	5124	151	0
1	D	5128	0	5039	185	0
2	E	78	0	64	2	0
3	F	23	0	19	2	0
4	G	34	0	28	2	0
5	H	45	0	37	2	0
5	I	45	0	37	0	0
6	A	16	0	11	1	0
6	B	32	0	22	1	0
6	C	16	0	11	1	0
6	D	16	0	11	2	0
7	A	7	0	10	0	0
7	B	14	0	20	2	0
7	C	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20951	0	20551	594	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (594) 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:C:399:ARG:HD3	1:C:403:ASN:HD22	1.20	1.07
1:D:579:THR:H	1:D:582:GLN:HE21	1.17	0.93
1:B:48:PRO:HG3	1:B:143:LEU:HD22	1.53	0.90
1:A:110:SER:O	1:A:111:VAL:HG13	1.78	0.84
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.79	0.83
1:A:108:LEU:O	1:A:111:VAL:HG22	1.80	0.81
1:B:312:THR:HG22	1:B:350:THR:HB	1.62	0.81
1:D:586:GLN:O	1:D:590:THR:HG22	1.82	0.80
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.64	0.80
1:A:542:GLU:OE2	1:A:544:ASN:HB2	1.82	0.79
1:B:192:THR:HG22	1:B:246:THR:HG22	1.65	0.78
1:B:368:ALA:HB1	1:B:487:ILE:HD11	1.65	0.77
1:D:213:LEU:HD21	1:D:253:PHE:HE1	1.49	0.77
1:C:61:LEU:HB2	1:C:93:GLY:HA2	1.69	0.75
1:B:17:VAL:HG21	1:B:46:ILE:O	1.87	0.75
1:D:66:PRO:HA	1:D:74:ARG:HH12	1.51	0.75
1:D:507:TYR:HB2	1:D:556:ARG:NH2	2.01	0.75
1:A:283:GLN:HG2	1:B:280:HIS:CE1	2.22	0.75
1:C:168:HIS:HD2	1:C:193:HIS:NE2	1.85	0.74
1:A:61:LEU:HB2	1:A:93:GLY:HA2	1.69	0.74
1:D:292:LYS:HD3	1:D:490:LEU:HD21	1.69	0.74
1:A:49:LEU:CD1	1:A:105:LEU:HB3	2.17	0.73
1:C:482:ASN:C	1:C:484:ASN:H	1.96	0.73
1:C:284:ASN:HD21	1:D:284:ASN:HD21	1.34	0.73
1:D:264:ASP:O	1:D:635:MET:HG3	1.88	0.73
1:C:200:TYR:CE1	1:C:227:ILE:HD11	2.23	0.73
1:D:482:ASN:HD22	1:D:484:ASN:H	1.37	0.72
1:A:578:LYS:HA	1:A:582:GLN:NE2	2.05	0.71
1:D:579:THR:H	1:D:582:GLN:NE2	1.89	0.71
1:D:456:LEU:O	1:D:460:ARG:HG3	1.90	0.71
1:A:17:VAL:HG21	1:A:47:GLY:HA3	1.73	0.70
1:D:399:ARG:HD3	1:D:403:ASN:HD22	1.56	0.70
1:B:513:TYR:O	1:B:517:GLU:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG21	1:B:46:ILE:C	2.16	0.70
1:B:431:ALA:HB2	1:C:484:ASN:HD21	1.57	0.70
1:D:213:LEU:HD21	1:D:253:PHE:CE1	2.26	0.70
1:C:399:ARG:HD3	1:C:403:ASN:ND2	2.03	0.69
1:D:121:ASP:O	1:D:125:LEU:HB2	1.92	0.69
1:B:579:THR:H	1:B:582:GLN:HE21	1.36	0.69
1:C:283:GLN:HG3	6:C:901:G6P:O1	1.93	0.69
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.74	0.69
1:C:378:LEU:O	1:C:382:VAL:HG23	1.93	0.69
1:A:49:LEU:HD11	1:A:105:LEU:HB3	1.74	0.68
1:C:283:GLN:HG2	1:D:280:HIS:CE1	2.28	0.68
1:A:49:LEU:HD13	1:A:106:PHE:C	2.18	0.68
1:C:493:ASP:HB2	1:C:521:MET:HE1	1.75	0.68
1:D:63:TRP:H	1:D:63:TRP:CD1	2.11	0.68
1:A:49:LEU:HD11	1:A:105:LEU:C	2.18	0.68
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.76	0.68
1:B:542:GLU:OE1	1:B:544:ASN:HB3	1.93	0.68
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.59	0.67
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.30	0.67
1:C:200:TYR:CD1	1:C:227:ILE:HD11	2.30	0.67
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.59	0.67
1:B:579:THR:H	1:B:582:GLN:NE2	1.93	0.67
1:A:192:THR:HG22	1:A:246:THR:HG22	1.76	0.67
1:B:192:THR:CG2	1:B:246:THR:HG22	2.24	0.67
1:D:14:ALA:HB2	1:D:168:HIS:HB2	1.76	0.66
1:C:176:LEU:HD12	1:C:237:ALA:HB1	1.78	0.66
1:A:8:HIS:HB2	1:A:162:ALA:O	1.96	0.66
1:A:110:SER:O	1:A:111:VAL:CG1	2.43	0.66
1:B:254:GLU:HG3	1:B:258:LEU:HD12	1.78	0.65
1:B:431:ALA:HB2	1:C:484:ASN:ND2	2.11	0.65
1:A:339:ASN:O	1:A:343:LYS:HG3	1.96	0.65
1:C:586:GLN:O	1:C:590:THR:HG22	1.96	0.65
1:B:14:ALA:O	1:B:17:VAL:HG23	1.97	0.65
1:C:192:THR:HG22	1:C:246:THR:HG22	1.79	0.64
1:C:634:ASN:HB2	1:C:637:ALA:CB	2.28	0.64
1:D:140:ALA:O	1:D:174:VAL:HG21	1.96	0.64
1:C:482:ASN:O	1:C:484:ASN:N	2.31	0.64
1:A:392:ARG:NH2	1:A:418:LYS:HG2	2.12	0.64
1:B:497:ARG:CZ	1:B:521:MET:HG2	2.26	0.64
1:A:76:VAL:O	1:A:80:LEU:HG	1.98	0.64
1:A:586:GLN:O	1:A:590:THR:HG22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG12	1:B:18:ALA:N	2.12	0.64
1:B:50:ASN:O	1:B:54:TYR:HB3	1.98	0.64
1:B:307:PHE:CD1	1:B:312:THR:HG21	2.32	0.64
1:A:490:LEU:HD22	1:A:494:GLU:HB3	1.79	0.63
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.34	0.63
1:B:379:GLU:HG3	1:D:394:PHE:CE1	2.34	0.63
1:C:50:ASN:O	1:C:54:TYR:HB3	1.99	0.63
1:C:626:VAL:HG11	1:C:630:LEU:HD11	1.81	0.63
1:A:62:ASP:HB3	1:A:65:LYS:HE3	1.80	0.63
1:B:174:VAL:O	1:B:177:PRO:HD2	1.99	0.63
1:A:309:LEU:HA	1:A:312:THR:HG23	1.81	0.63
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.32	0.63
1:D:19:ASN:HD22	1:D:19:ASN:H	1.46	0.63
1:A:213:LEU:HA	1:A:216:VAL:HG23	1.82	0.62
1:C:399:ARG:HH11	1:C:403:ASN:ND2	1.97	0.62
1:D:12:GLU:HG3	1:D:166:HIS:HB3	1.82	0.62
1:D:153:GLU:O	1:D:157:LEU:HG	2.00	0.62
1:D:210:TYR:CZ	1:D:530:VAL:HG13	2.34	0.62
1:A:17:VAL:CG2	1:A:47:GLY:HA3	2.29	0.62
1:B:512:GLY:O	1:B:515:PRO:HD2	1.99	0.62
1:B:51:LYS:HE3	1:B:107:ASP:OD1	1.99	0.62
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.33	0.62
1:B:493:ASP:HB2	1:B:521:MET:HE1	1.80	0.62
1:C:150:PHE:O	1:C:154:VAL:HG23	2.00	0.61
1:A:19:ASN:N	1:A:19:ASN:HD22	1.98	0.61
1:D:74:ARG:N	1:D:75:PRO:HD2	2.16	0.61
1:A:137:THR:O	1:A:141:ILE:HG13	2.00	0.61
1:C:31:LYS:O	1:C:35:THR:HG22	2.01	0.61
1:C:111:VAL:HG12	1:C:111:VAL:O	2.00	0.61
1:B:269:ASN:HB2	1:B:511:TRP:CD1	2.36	0.61
1:B:176:LEU:HB2	1:B:177:PRO:HD3	1.83	0.61
1:A:302:HIS:HB2	1:A:432:LEU:HD22	1.83	0.60
1:A:330:MET:CG	2:E:2:GLC:H61	2.31	0.60
1:D:72:GLU:O	1:D:161:HIS:HE1	1.83	0.60
1:B:227:ILE:O	1:B:227:ILE:HG22	2.01	0.60
1:A:549:TYR:O	1:A:590:THR:HB	2.02	0.60
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.83	0.59
1:D:110:SER:O	1:D:111:VAL:HG23	2.03	0.59
1:B:308:ASP:O	1:B:312:THR:HG23	2.02	0.59
1:C:169:GLU:O	1:C:190:PHE:HE1	1.85	0.59
1:D:125:LEU:HD21	1:D:181:LYS:HZ2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ASN:HB2	1:A:637:ALA:H	1.68	0.59
1:D:19:ASN:HD22	1:D:19:ASN:N	2.00	0.59
1:B:89:HIS:CD2	1:B:110:SER:HB3	2.37	0.58
1:B:597:LEU:HA	1:B:602:MET:HE2	1.84	0.58
1:B:153:GLU:O	1:B:157:LEU:HG	2.03	0.58
1:C:447:MET:HG3	1:C:456:LEU:HD11	1.85	0.58
1:D:217:ASP:O	1:D:221:GLU:HG2	2.03	0.58
1:A:7:ASN:O	1:A:161:HIS:HD2	1.85	0.58
1:A:299:GLY:HA2	1:A:375:VAL:HG21	1.86	0.58
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.84	0.58
1:D:170:TRP:NE1	1:D:196:LEU:HD21	2.19	0.58
1:A:72:GLU:HB2	1:A:161:HIS:HE1	1.68	0.58
1:A:86:ARG:HH11	1:A:86:ARG:HB3	1.68	0.58
1:B:144:GLY:HA3	1:B:174:VAL:HB	1.85	0.58
1:C:399:ARG:CD	1:C:403:ASN:HD22	2.06	0.58
1:B:278:ALA:HB1	1:B:280:HIS:CE1	2.39	0.58
1:C:169:GLU:OE2	1:C:169:GLU:HA	2.03	0.58
1:D:177:PRO:HA	1:D:240:SER:CB	2.33	0.58
4:G:2:GLC:H62	4:G:3:GLC:H5	1.86	0.58
1:B:504:PHE:CE1	1:B:514:THR:HG22	2.39	0.57
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.39	0.57
1:C:399:ARG:HH11	1:C:403:ASN:HD21	1.52	0.57
1:B:206:SER:O	1:B:207:PHE:HB3	2.04	0.57
1:B:537:MET:HG2	1:B:551:ILE:HD13	1.87	0.57
1:C:199:ARG:HG2	1:C:508:TYR:CE2	2.40	0.57
1:C:482:ASN:C	1:C:484:ASN:N	2.63	0.57
1:A:49:LEU:HD11	1:A:105:LEU:CB	2.33	0.57
1:B:368:ALA:HB1	1:B:487:ILE:CD1	2.34	0.57
1:A:83:MET:HE3	1:A:88:VAL:HG21	1.86	0.57
1:D:183:ARG:O	1:D:183:ARG:HG3	2.05	0.57
1:B:249:GLN:OE1	1:B:266:ILE:HD11	2.04	0.57
1:D:447:MET:HB2	1:D:450:ASP:HB2	1.86	0.57
1:B:162:ALA:C	1:B:163:ILE:HG13	2.29	0.56
1:C:634:ASN:HB2	1:C:637:ALA:H	1.70	0.56
1:A:13:THR:HG23	1:A:46:ILE:HB	1.86	0.56
1:A:587:ARG:HA	1:A:590:THR:HG23	1.86	0.56
1:C:19:ASN:N	1:C:19:ASN:HD22	2.02	0.56
1:C:91:VAL:HG12	1:C:92:TYR:N	2.19	0.56
1:C:509:GLU:HB3	1:C:531:SER:HB2	1.87	0.56
1:D:402:HIS:O	1:D:404:GLY:N	2.38	0.56
1:D:593:LEU:O	1:D:596:LEU:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:ALA:HB1	1:D:101:PRO:HG3	1.88	0.56
1:B:274:ILE:HG13	1:B:274:ILE:O	2.04	0.56
1:D:180:ARG:HD2	1:D:240:SER:HA	1.86	0.56
1:D:400:TYR:CD2	1:D:401:PRO:HA	2.41	0.56
1:D:170:TRP:HE1	1:D:196:LEU:HD21	1.70	0.56
1:A:264:ASP:O	1:A:635:MET:HG3	2.06	0.56
1:C:196:LEU:O	1:C:200:TYR:HD2	1.88	0.56
1:C:528:THR:HG21	1:C:556:ARG:HG3	1.87	0.56
1:C:634:ASN:CB	1:C:637:ALA:H	2.19	0.56
1:B:9:LEU:HD21	1:B:161:HIS:ND1	2.20	0.56
1:B:79:ALA:O	1:B:83:MET:HG2	2.06	0.56
1:D:594:SER:C	1:D:596:LEU:H	2.13	0.56
1:D:48:PRO:HG3	1:D:143:LEU:HD22	1.88	0.56
1:D:80:LEU:HD22	1:D:90:PHE:CE1	2.40	0.56
1:D:227:ILE:O	1:D:227:ILE:HG22	2.05	0.56
1:D:14:ALA:O	1:D:17:VAL:HG23	2.06	0.55
1:C:383:HIS:O	1:C:387:THR:HG23	2.06	0.55
1:D:75:PRO:HB3	1:D:158:ASP:HB2	1.89	0.55
1:A:85:SER:HB2	1:A:86:ARG:HD3	1.89	0.55
1:B:54:TYR:HE1	1:B:60:ILE:HD11	1.70	0.55
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.42	0.55
1:A:578:LYS:HA	1:A:582:GLN:HE21	1.70	0.55
1:D:292:LYS:CD	1:D:490:LEU:HD21	2.37	0.55
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.89	0.55
1:D:434:ARG:HB2	1:D:435:PRO:HD2	1.88	0.55
1:D:150:PHE:O	1:D:154:VAL:HG23	2.07	0.55
1:D:541:ILE:HG22	1:D:545:GLN:HB3	1.89	0.55
1:D:113:GLY:C	1:D:115:SER:H	2.15	0.55
1:A:74:ARG:N	1:A:75:PRO:CD	2.70	0.54
1:D:144:GLY:O	1:D:175:ALA:HB2	2.06	0.54
1:C:193:HIS:HD1	1:C:247:VAL:HG11	1.72	0.54
1:D:275:LYS:NZ	1:D:279:PHE:HD1	2.05	0.54
1:B:634:ASN:HB2	1:B:637:ALA:CB	2.38	0.54
1:A:266:ILE:HG22	1:A:268:PRO:HD3	1.89	0.54
1:C:507:TYR:HB2	1:C:556:ARG:NH2	2.23	0.54
1:A:153:GLU:O	1:A:157:LEU:HG	2.08	0.54
1:B:536:TYR:O	1:B:540:LEU:HD23	2.08	0.54
1:D:168:HIS:HD2	1:D:193:HIS:NE2	2.06	0.54
1:D:192:THR:HG22	1:D:246:THR:HG22	1.90	0.54
1:C:581:ARG:NH2	1:D:275:LYS:HD3	2.23	0.54
1:D:187:VAL:HG11	1:D:613:ALA:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.90	0.54
1:A:110:SER:C	1:A:111:VAL:HG13	2.32	0.54
1:C:299:GLY:HA2	1:C:375:VAL:HG21	1.90	0.54
1:B:330:MET:HG3	1:B:565:VAL:HG22	1.90	0.53
1:C:269:ASN:O	1:C:602:MET:HE3	2.08	0.53
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.44	0.53
1:D:19:ASN:H	1:D:19:ASN:ND2	2.05	0.53
1:D:59:ASP:O	1:D:61:LEU:HG	2.08	0.53
1:A:192:THR:CG2	1:A:246:THR:HG22	2.39	0.53
1:A:84:GLU:OE2	1:A:84:GLU:HA	2.08	0.53
1:D:176:LEU:N	1:D:177:PRO:HD2	2.24	0.53
1:B:458:LYS:O	1:B:462:VAL:HG22	2.07	0.53
1:A:19:ASN:N	1:A:19:ASN:ND2	2.56	0.53
1:C:170:TRP:CH2	1:C:230:ARG:HG2	2.44	0.53
1:A:368:ALA:HB1	1:A:487:ILE:CD1	2.38	0.53
1:D:17:VAL:HG21	1:D:46:ILE:O	2.08	0.52
1:D:86:ARG:HH11	1:D:86:ARG:HB3	1.74	0.52
1:A:434:ARG:HB2	1:A:435:PRO:HD2	1.91	0.52
1:B:488:LEU:O	1:B:490:LEU:N	2.41	0.52
1:D:21:VAL:HG12	1:D:21:VAL:O	2.09	0.52
1:D:292:LYS:HD3	1:D:490:LEU:CD2	2.38	0.52
1:C:284:ASN:ND2	1:D:284:ASN:HD21	2.06	0.52
1:D:514:THR:HB	1:D:515:PRO:HD3	1.91	0.52
1:A:624:GLU:C	1:A:626:VAL:H	2.17	0.52
1:B:279:PHE:N	1:B:279:PHE:CD1	2.77	0.52
1:C:447:MET:HG3	1:C:456:LEU:CD1	2.40	0.52
1:C:634:ASN:HB2	1:C:637:ALA:HB3	1.91	0.52
1:D:164:VAL:HA	1:D:187:VAL:HG23	1.92	0.52
1:D:537:MET:HG2	1:D:551:ILE:HD13	1.91	0.52
1:C:492:TYR:O	1:C:496:VAL:HG23	2.10	0.52
1:A:80:LEU:HD22	1:A:90:PHE:HE1	1.75	0.52
1:B:335:LEU:HD13	1:B:474:MET:HE1	1.91	0.52
1:C:227:ILE:O	1:C:230:ARG:HB2	2.10	0.52
1:C:269:ASN:HB2	1:C:511:TRP:NE1	2.25	0.51
1:C:278:ALA:HB1	1:C:280:HIS:CE1	2.44	0.51
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.45	0.51
1:D:344:VAL:C	1:D:346:GLY:H	2.18	0.51
1:D:368:ALA:HB1	1:D:487:ILE:CD1	2.40	0.51
1:A:137:THR:HG21	1:A:229:HIS:HD2	1.75	0.51
1:D:31:LYS:NZ	1:D:35:THR:HG21	2.25	0.51
1:A:256:GLU:OE2	1:A:262:LYS:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:OE2	1:C:168:HIS:HE1	1.93	0.51
1:D:167:PHE:HB2	1:D:176:LEU:HD11	1.92	0.51
1:C:30:SER:O	1:C:272:ASN:ND2	2.44	0.51
1:B:42:HIS:CE1	1:B:72:GLU:OE2	2.64	0.51
1:B:249:GLN:HG2	1:B:266:ILE:CD1	2.40	0.51
1:C:482:ASN:C	1:C:490:LEU:O	2.53	0.51
1:D:620:ASP:HA	1:D:623:ARG:NH1	2.26	0.51
1:A:33:PRO:HG3	1:A:98:GLU:HG2	1.92	0.51
1:A:283:GLN:HG3	6:A:901:G6P:O1	2.11	0.51
1:A:31:LYS:O	1:A:34:ILE:HG22	2.11	0.50
1:D:540:LEU:C	1:D:541:ILE:HG13	2.36	0.50
1:B:374:GLU:HB3	1:B:432:LEU:CD2	2.40	0.50
1:B:607:VAL:O	1:B:611:GLN:HG2	2.12	0.50
1:A:187:VAL:HG11	1:A:613:ALA:O	2.12	0.50
1:B:133:ASN:H	1:B:133:ASN:ND2	2.07	0.50
1:D:86:ARG:HB3	1:D:86:ARG:NH1	2.26	0.50
1:B:95:TRP:HB3	1:B:101:PRO:HD2	1.94	0.50
1:C:17:VAL:HG12	1:C:18:ALA:N	2.27	0.50
1:C:269:ASN:HD22	1:C:511:TRP:CD1	2.28	0.50
1:D:612:LEU:HG	1:D:612:LEU:O	2.11	0.50
1:A:542:GLU:OE1	1:A:545:GLN:HB2	2.12	0.50
1:D:543:THR:O	1:D:543:THR:CG2	2.60	0.50
1:A:537:MET:HG2	1:A:551:ILE:HD12	1.94	0.50
1:B:323:TYR:CE1	1:B:329:ASP:HB3	2.47	0.50
1:B:111:VAL:CG1	1:B:118:TRP:CH2	2.95	0.49
1:B:368:ALA:CB	1:B:487:ILE:HD11	2.39	0.49
1:C:510:PRO:O	1:C:532:GLY:HA3	2.12	0.49
1:A:427:ARG:HH21	1:D:482:ASN:HD21	1.60	0.49
1:B:199:ARG:HB3	1:B:508:TYR:CE2	2.48	0.49
1:C:200:TYR:CE2	1:C:227:ILE:HD13	2.48	0.49
1:D:122:LEU:CD2	1:D:128:ILE:HD12	2.41	0.49
1:D:150:PHE:CE2	1:D:154:VAL:HG21	2.47	0.49
1:A:330:MET:HG2	2:E:2:GLC:H61	1.94	0.49
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.94	0.49
1:B:391:LYS:HD3	7:B:1001:PEG:H41	1.94	0.49
1:D:74:ARG:N	1:D:75:PRO:CD	2.75	0.49
1:A:113:GLY:C	1:A:115:SER:H	2.20	0.49
1:B:150:PHE:O	1:B:154:VAL:HG23	2.12	0.49
1:C:18:ALA:HB2	1:C:105:LEU:HD11	1.95	0.49
1:D:6:GLN:NE2	1:D:625:LEU:HD23	2.27	0.49
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:LEU:C	1:D:541:ILE:CG1	2.86	0.49
1:B:13:THR:HG22	1:B:172:ALA:HB1	1.95	0.49
1:B:279:PHE:HD1	1:B:279:PHE:H	1.60	0.49
1:C:533:PHE:O	1:C:537:MET:HB2	2.13	0.49
1:D:368:ALA:HB1	1:D:487:ILE:HD13	1.95	0.49
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.13	0.49
1:A:493:ASP:O	1:A:497:ARG:HG3	2.13	0.49
1:D:19:ASN:N	1:D:19:ASN:ND2	2.61	0.49
1:D:176:LEU:HD13	1:D:190:PHE:HB2	1.95	0.48
1:D:208:ASP:OD1	1:D:209:PHE:N	2.46	0.48
1:B:304:CYS:SG	1:B:434:ARG:HD3	2.53	0.48
1:B:34:ILE:HD13	1:B:599:TRP:HB3	1.95	0.48
1:C:537:MET:HG2	1:C:551:ILE:HG21	1.96	0.48
1:A:218:VAL:HG23	1:A:219:ASP:N	2.29	0.48
1:B:227:ILE:O	1:B:227:ILE:CG2	2.61	0.48
1:C:179:CYS:HA	1:C:184:ILE:HD12	1.95	0.48
1:C:14:ALA:HB3	1:C:28:LEU:HD11	1.96	0.48
1:C:196:LEU:HD13	1:C:227:ILE:CG2	2.43	0.48
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.96	0.48
1:D:289:LYS:HE3	1:D:494:GLU:HG2	1.95	0.48
1:D:617:GLY:C	1:D:619:PRO:HD3	2.38	0.48
1:A:108:LEU:O	1:A:111:VAL:CG2	2.56	0.48
1:A:302:HIS:O	1:A:434:ARG:HD2	2.13	0.48
1:B:319:GLY:O	1:B:357:MET:HG2	2.13	0.48
1:C:442:ILE:HD11	1:C:465:PHE:HA	1.95	0.48
1:A:626:VAL:HG12	1:A:627:GLY:N	2.28	0.48
1:B:15:THR:O	1:B:15:THR:CG2	2.62	0.48
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.48	0.48
1:C:328:ALA:O	1:C:332:ILE:HG13	2.13	0.48
1:D:580:ARG:HE	6:D:901:G6P:H62	1.79	0.48
1:B:600:LYS:O	1:B:600:LYS:HE3	2.14	0.48
1:C:227:ILE:O	1:C:230:ARG:N	2.45	0.48
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.95	0.48
1:D:510:PRO:O	1:D:532:GLY:HA3	2.13	0.48
1:A:3:ARG:H	1:A:621:GLN:HE22	1.62	0.47
1:B:312:THR:CG2	1:B:350:THR:HB	2.40	0.47
1:B:89:HIS:HD2	1:B:110:SER:HB3	1.78	0.47
1:C:200:TYR:CZ	1:C:227:ILE:HD11	2.49	0.47
1:D:238:ALA:O	1:D:261:ARG:HD3	2.15	0.47
3:F:2:GLC:H62	3:F:3:GLC:O5	2.14	0.47
1:A:537:MET:HG2	1:A:551:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:ASN:HB2	1:B:637:ALA:HB3	1.96	0.47
1:D:275:LYS:HZ1	1:D:279:PHE:HD1	1.60	0.47
1:D:606:TYR:O	1:D:610:ARG:HG3	2.14	0.47
1:A:19:ASN:ND2	1:A:19:ASN:H	2.13	0.47
1:B:513:TYR:HD1	1:B:514:THR:N	2.12	0.47
1:D:19:ASN:O	1:D:21:VAL:HG23	2.15	0.47
1:D:620:ASP:HA	1:D:623:ARG:HH12	1.80	0.47
1:A:95:TRP:O	1:A:97:ILE:N	2.47	0.47
1:C:31:LYS:HB2	1:C:599:TRP:CZ2	2.50	0.47
1:C:228:TYR:O	1:C:230:ARG:N	2.48	0.47
1:D:130:SER:O	1:D:132:GLU:N	2.48	0.47
1:A:83:MET:CE	1:A:88:VAL:HG11	2.45	0.47
1:A:392:ARG:CZ	1:A:418:LYS:HG2	2.43	0.47
1:C:235:ARG:HA	1:C:259:LEU:HD22	1.96	0.47
1:C:357:MET:O	1:C:478:PRO:HA	2.14	0.47
1:A:19:ASN:HD22	1:A:19:ASN:H	1.62	0.47
1:B:109:ASP:C	1:B:111:VAL:H	2.23	0.47
1:A:378:LEU:HD13	1:C:394:PHE:CD1	2.50	0.47
1:C:19:ASN:O	1:C:21:VAL:HG23	2.14	0.47
1:A:378:LEU:HD13	1:C:394:PHE:CE1	2.50	0.47
1:D:222:ALA:HB1	1:D:228:TYR:HA	1.97	0.47
1:C:213:LEU:HD21	1:C:253:PHE:HE1	1.81	0.46
1:C:611:GLN:HE21	1:C:611:GLN:HA	1.80	0.46
1:C:644:LEU:HD13	1:C:644:LEU:C	2.40	0.46
1:D:500:HIS:O	1:D:524:PRO:HD2	2.15	0.46
1:A:579:THR:H	1:A:582:GLN:NE2	2.13	0.46
1:A:103:VAL:O	1:A:103:VAL:HG13	2.16	0.46
1:C:176:LEU:HB2	1:C:177:PRO:HD2	1.98	0.46
1:C:385:VAL:O	1:C:389:ILE:HG13	2.15	0.46
1:D:176:LEU:CD2	1:D:188:THR:HB	2.45	0.46
1:C:269:ASN:HB2	1:C:511:TRP:CE2	2.49	0.46
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.96	0.46
1:B:134:ASP:OD2	1:B:137:THR:HG23	2.16	0.46
1:C:10:LEU:HD12	1:C:11:PHE:N	2.31	0.46
1:C:227:ILE:O	1:C:228:TYR:C	2.57	0.46
1:C:371:GLY:O	1:C:375:VAL:HG23	2.15	0.46
1:C:482:ASN:OD1	1:C:483:ALA:N	2.48	0.46
1:D:114:TYR:HD1	1:D:114:TYR:H	1.62	0.46
1:D:279:PHE:CE1	1:D:591:GLU:OE1	2.69	0.46
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.51	0.46
1:C:200:TYR:CD2	1:C:227:ILE:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:N	1:A:75:PRO:HD2	2.31	0.46
1:B:139:ASP:HA	1:B:142:LEU:HD12	1.97	0.46
1:B:627:GLY:C	1:B:628:GLU:HG2	2.40	0.46
1:C:74:ARG:HB2	1:C:75:PRO:HD3	1.98	0.46
1:C:228:TYR:C	1:C:230:ARG:N	2.72	0.46
1:C:388:SER:HB3	1:C:392:ARG:NH2	2.30	0.46
1:D:47:GLY:O	1:D:105:LEU:HA	2.16	0.46
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.97	0.46
1:D:378:LEU:HD22	1:D:382:VAL:HG23	1.97	0.46
1:D:549:TYR:O	1:D:590:THR:HB	2.16	0.46
1:A:63:TRP:H	1:A:63:TRP:CD1	2.34	0.46
1:B:32:ALA:O	1:B:36:VAL:HG23	2.15	0.46
1:C:497:ARG:NH1	1:C:521:MET:HE2	2.31	0.46
1:D:114:TYR:CD1	1:D:114:TYR:N	2.84	0.46
1:A:17:VAL:HG23	1:A:18:ALA:N	2.30	0.46
1:D:13:THR:HB	1:D:167:PHE:CD1	2.51	0.46
1:D:122:LEU:HD21	1:D:128:ILE:HD12	1.96	0.46
1:A:50:ASN:O	1:A:54:TYR:HB3	2.16	0.45
1:A:134:ASP:OD1	1:A:137:THR:HG23	2.16	0.45
1:A:587:ARG:HA	1:A:590:THR:CG2	2.44	0.45
1:D:123:TRP:O	1:D:123:TRP:CE3	2.69	0.45
1:D:167:PHE:CD2	1:D:176:LEU:HD21	2.51	0.45
1:A:330:MET:HE2	1:A:568:LEU:HD22	1.97	0.45
1:C:333:GLU:HG3	1:C:337:ARG:HD2	1.98	0.45
1:D:487:ILE:HG22	1:D:488:LEU:N	2.32	0.45
1:C:227:ILE:O	1:C:227:ILE:HG22	2.16	0.45
1:D:81:GLN:HA	1:D:84:GLU:HB3	1.99	0.45
1:A:71:ASP:O	1:A:74:ARG:HG2	2.17	0.45
1:C:485:ASN:HB2	1:C:488:LEU:O	2.17	0.45
1:C:487:ILE:HG23	1:C:488:LEU:N	2.31	0.45
1:C:168:HIS:CD2	1:C:193:HIS:NE2	2.75	0.45
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.86	0.45
1:C:509:GLU:O	1:C:531:SER:HA	2.17	0.45
1:C:547:LYS:HG2	1:C:552:TYR:CE1	2.52	0.45
1:D:16:GLU:OE2	1:D:24:ILE:HD12	2.17	0.45
1:A:114:TYR:N	1:A:114:TYR:CD1	2.84	0.45
1:B:510:PRO:O	1:B:532:GLY:HA3	2.16	0.45
1:D:92:TYR:OH	1:D:102:LYS:HD3	2.16	0.45
1:D:164:VAL:HG13	1:D:187:VAL:HG23	1.98	0.45
1:D:200:TYR:CE2	1:D:227:ILE:HD13	2.52	0.45
1:A:4:ASP:HB2	1:A:160:GLN:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:MET:O	1:A:88:VAL:HB	2.17	0.45
1:D:140:ALA:C	1:D:174:VAL:HG21	2.42	0.45
1:D:279:PHE:HE1	1:D:591:GLU:OE1	2.00	0.45
1:D:615:ARG:HD3	1:D:622:PHE:CD1	2.52	0.45
1:C:387:THR:O	1:C:391:LYS:HG3	2.17	0.45
1:C:463:GLN:HG2	1:C:465:PHE:HE2	1.82	0.45
1:A:268:PRO:HB2	1:A:602:MET:CE	2.46	0.45
1:A:550:GLY:HA2	1:A:586:GLN:NE2	2.32	0.45
1:B:180:ARG:HD2	1:B:240:SER:O	2.17	0.45
1:B:283:GLN:O	6:B:901:G6P:H1	2.17	0.45
1:B:561:PRO:O	1:B:565:VAL:HG23	2.17	0.45
1:D:150:PHE:CD2	1:D:150:PHE:C	2.95	0.45
1:B:32:ALA:HB1	1:B:101:PRO:HG3	1.99	0.44
1:D:512:GLY:O	1:D:515:PRO:HD2	2.17	0.44
1:A:54:TYR:CE1	1:A:91:VAL:HG21	2.52	0.44
1:A:418:LYS:HD3	1:A:418:LYS:HA	1.47	0.44
1:D:543:THR:O	1:D:543:THR:HG22	2.17	0.44
1:A:39:TYR:CB	1:A:43:TYR:HB2	2.47	0.44
1:C:112:ARG:O	1:C:112:ARG:HG2	2.16	0.44
1:D:54:TYR:O	1:D:58:VAL:HG23	2.18	0.44
1:D:441:PRO:HA	5:H:3:GLC:H62	1.98	0.44
1:D:557:ARG:HD3	1:D:558:PHE:CZ	2.52	0.44
1:D:618:TYR:N	1:D:618:TYR:CD1	2.86	0.44
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.98	0.44
1:B:577:LYS:HA	1:B:577:LYS:HD3	1.80	0.44
1:C:91:VAL:CG1	1:C:92:TYR:N	2.79	0.44
1:D:66:PRO:O	1:D:74:ARG:NH2	2.50	0.44
1:D:144:GLY:HA3	1:D:174:VAL:CB	2.42	0.44
1:B:49:LEU:HA	1:B:105:LEU:HB3	1.98	0.44
1:B:63:TRP:CD1	1:B:63:TRP:H	2.35	0.44
1:B:273:VAL:HG13	1:B:520:VAL:HG13	1.99	0.44
1:A:114:TYR:N	1:A:114:TYR:HD1	2.16	0.44
1:A:134:ASP:CG	1:A:137:THR:HG23	2.43	0.44
1:B:330:MET:HE1	1:B:564:SER:HB3	1.99	0.44
1:C:152:GLY:CA	4:G:4:GLC:H61	2.48	0.44
1:C:581:ARG:HH22	1:D:275:LYS:HD3	1.83	0.44
1:B:181:LYS:O	1:B:181:LYS:HD3	2.18	0.44
1:C:315:PHE:CD1	1:C:315:PHE:N	2.84	0.44
1:C:547:LYS:HB2	1:C:547:LYS:HE3	1.73	0.44
1:D:200:TYR:CE1	1:D:227:ILE:HD11	2.53	0.44
1:D:283:GLN:HG3	6:D:901:G6P:O1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:LYS:O	1:D:426:LYS:HG3	2.17	0.44
1:D:507:TYR:HB2	1:D:556:ARG:HH21	1.78	0.44
1:B:422:LYS:O	1:B:426:LYS:HG3	2.18	0.43
1:C:428:ARG:HA	1:C:428:ARG:HD2	1.42	0.43
1:D:174:VAL:O	1:D:177:PRO:HD2	2.18	0.43
1:C:31:LYS:O	1:C:35:THR:CG2	2.66	0.43
1:B:249:GLN:HG2	1:B:266:ILE:HD11	1.98	0.43
1:B:133:ASN:ND2	1:B:133:ASN:N	2.66	0.43
1:B:374:GLU:HB3	1:B:432:LEU:HD23	2.00	0.43
1:C:169:GLU:OE2	1:C:169:GLU:CA	2.65	0.43
1:C:422:LYS:O	1:C:426:LYS:HD3	2.18	0.43
1:D:266:ILE:O	1:D:267:LEU:HD23	2.19	0.43
1:A:432:LEU:HD13	1:C:398:ILE:HD12	2.00	0.43
1:B:587:ARG:HA	1:B:590:THR:HG23	2.00	0.43
1:C:364:PHE:CE1	1:C:487:ILE:HG21	2.53	0.43
1:B:391:LYS:CD	7:B:1001:PEG:H41	2.48	0.43
1:B:394:PHE:CE1	1:D:378:LEU:HD13	2.53	0.43
1:B:18:ALA:HB3	1:B:105:LEU:HD11	2.01	0.43
1:C:169:GLU:O	1:C:190:PHE:CE1	2.68	0.43
1:D:321:TYR:OH	1:D:455:ILE:HG12	2.19	0.43
1:A:213:LEU:HA	1:A:216:VAL:CG2	2.48	0.43
1:B:425:LEU:O	1:B:429:ILE:HG13	2.19	0.43
1:D:209:PHE:O	1:D:213:LEU:HB3	2.18	0.43
1:A:114:TYR:HD1	1:A:114:TYR:H	1.66	0.42
1:B:526:ILE:HG12	1:B:552:TYR:HB2	2.01	0.42
1:C:92:TYR:OH	1:C:102:LYS:HD3	2.19	0.42
1:D:67:GLU:C	1:D:69:PHE:H	2.27	0.42
1:D:163:ILE:O	1:D:187:VAL:HG22	2.19	0.42
1:D:523:VAL:HA	1:D:524:PRO:HD3	1.84	0.42
1:A:308:ASP:O	1:A:312:THR:HG23	2.19	0.42
1:B:370:LYS:HB3	1:B:370:LYS:HE2	1.82	0.42
1:C:326:LYS:HA	1:C:326:LYS:HD3	1.74	0.42
1:C:458:LYS:O	1:C:462:VAL:HG22	2.19	0.42
1:D:108:LEU:HD22	1:D:142:LEU:HB3	2.01	0.42
1:B:458:LYS:O	1:B:458:LYS:HD3	2.19	0.42
1:B:217:ASP:O	1:B:221:GLU:HB2	2.19	0.42
1:D:594:SER:C	1:D:596:LEU:N	2.76	0.42
1:A:338:LEU:HD22	1:A:572:MET:HB3	2.01	0.42
1:B:63:TRP:HZ3	1:B:81:GLN:HG3	1.84	0.42
1:C:14:ALA:CB	1:C:28:LEU:HD11	2.50	0.42
1:D:218:VAL:HG11	1:D:260:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:LEU:HD12	5:H:4:GLC:H61	2.01	0.42
1:B:34:ILE:HG13	1:B:35:THR:N	2.35	0.42
1:B:465:PHE:O	1:B:466:ASN:HB2	2.19	0.42
1:C:289:LYS:HD2	1:C:289:LYS:HA	1.72	0.42
1:D:587:ARG:HA	1:D:590:THR:CG2	2.50	0.42
1:B:208:ASP:OD2	1:B:211:ASN:HB2	2.20	0.42
1:D:82:THR:O	1:D:82:THR:HG22	2.20	0.42
1:D:107:ASP:OD1	1:D:109:ASP:HB2	2.20	0.42
1:D:192:THR:HG23	1:D:192:THR:O	2.19	0.42
1:D:520:VAL:HA	1:D:594:SER:HB2	2.02	0.42
1:A:65:LYS:HA	1:A:66:PRO:HD3	1.79	0.42
1:B:250:ILE:HD12	1:B:535:SER:HB3	2.02	0.42
1:B:615:ARG:HD2	1:B:615:ARG:O	2.20	0.42
1:C:228:TYR:O	1:C:229:HIS:C	2.63	0.42
1:D:30:SER:O	1:D:33:PRO:HD2	2.20	0.42
1:D:176:LEU:H	1:D:177:PRO:HD2	1.84	0.42
1:D:257:HIS:O	1:D:258:LEU:HD23	2.19	0.42
1:A:32:ALA:O	1:A:33:PRO:C	2.62	0.42
1:A:268:PRO:HB2	1:A:602:MET:HE1	2.02	0.42
1:C:56:ASN:OD1	1:C:56:ASN:N	2.52	0.42
1:D:482:ASN:ND2	1:D:484:ASN:H	2.12	0.42
1:A:10:LEU:HD21	1:A:610:ARG:HE	1.85	0.42
1:B:149:TRP:C	1:B:149:TRP:CD1	2.98	0.42
1:B:187:VAL:HG11	1:B:613:ALA:O	2.20	0.42
1:A:86:ARG:HG3	1:A:149:TRP:CH2	2.55	0.41
1:D:70:SER:O	1:D:74:ARG:HG2	2.20	0.41
1:A:265:GLY:HA3	1:A:635:MET:HE2	2.01	0.41
1:B:17:VAL:CG2	1:B:46:ILE:O	2.62	0.41
1:B:83:MET:HE2	1:B:106:PHE:CE1	2.55	0.41
1:C:408:GLU:O	1:C:409:LEU:HD23	2.20	0.41
1:D:3:ARG:NH2	1:D:155:ALA:O	2.52	0.41
1:D:383:HIS:O	1:D:387:THR:HG23	2.20	0.41
1:B:10:LEU:HD12	1:B:11:PHE:N	2.35	0.41
1:B:255:ALA:O	1:B:259:LEU:HB2	2.21	0.41
1:B:536:TYR:CD2	1:B:536:TYR:C	2.99	0.41
1:C:18:ALA:CB	1:C:105:LEU:HD11	2.50	0.41
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.93	0.41
1:C:483:ALA:N	1:C:491:ASP:OD1	2.29	0.41
1:C:611:GLN:HA	1:C:611:GLN:NE2	2.35	0.41
1:D:3:ARG:NH2	1:D:158:ASP:O	2.53	0.41
1:D:283:GLN:HE22	1:D:587:ARG:HE	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:O	1:A:161:HIS:CD2	2.71	0.41
1:A:56:ASN:OD1	1:A:56:ASN:N	2.53	0.41
1:B:39:TYR:O	1:B:40:LYS:HB2	2.21	0.41
1:C:372:GLN:HG3	1:C:487:ILE:HD12	2.02	0.41
1:C:400:TYR:CD1	1:C:408:GLU:HA	2.55	0.41
1:D:74:ARG:O	1:D:77:GLN:N	2.53	0.41
1:D:191:THR:HA	1:D:245:THR:O	2.20	0.41
1:A:54:TYR:CE2	1:A:55:GLN:HG3	2.55	0.41
1:A:128:ILE:HG12	1:A:232:CYS:HB3	2.02	0.41
1:B:59:ASP:HB2	1:B:96:LEU:HD21	2.02	0.41
1:B:74:ARG:N	1:B:75:PRO:CD	2.83	0.41
1:B:122:LEU:HG	1:B:128:ILE:HB	2.01	0.41
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.84	0.41
1:A:484:ASN:HB3	1:D:428:ARG:NH1	2.35	0.41
1:A:550:GLY:HA2	1:A:586:GLN:HE21	1.85	0.41
1:C:327:GLY:HA3	1:C:505:PRO:O	2.21	0.41
1:D:149:TRP:CD1	1:D:149:TRP:C	2.98	0.41
1:D:435:PRO:HD2	1:D:438:GLN:NE2	2.35	0.41
1:B:134:ASP:OD1	1:B:136:GLU:HB2	2.21	0.41
1:C:128:ILE:HA	1:C:129:PRO:HD3	1.77	0.41
1:C:358:PRO:HG2	1:C:480:PHE:CE2	2.55	0.41
1:C:31:LYS:HG2	1:C:35:THR:HG22	2.03	0.41
1:C:143:LEU:O	1:C:147:VAL:HG23	2.21	0.41
1:C:513:TYR:CD2	1:C:513:TYR:N	2.85	0.41
1:D:125:LEU:HD11	1:D:181:LYS:NZ	2.36	0.41
1:A:86:ARG:HB3	1:A:86:ARG:NH1	2.36	0.41
1:A:133:ASN:OD1	1:A:133:ASN:N	2.42	0.41
1:A:144:GLY:HA3	1:A:174:VAL:HB	2.03	0.41
1:A:458:LYS:O	1:A:458:LYS:HD3	2.21	0.41
1:A:620:ASP:O	1:A:624:GLU:HG2	2.21	0.41
1:C:176:LEU:HB2	1:C:177:PRO:CD	2.51	0.41
1:C:200:TYR:CE2	1:C:227:ILE:CD1	3.04	0.41
1:D:31:LYS:HZ3	1:D:35:THR:HG21	1.85	0.41
1:D:337:ARG:HE	1:D:565:VAL:HG11	1.85	0.41
1:A:123:TRP:O	1:A:127:GLY:HA2	2.21	0.41
1:C:228:TYR:O	1:C:231:TYR:N	2.53	0.41
1:D:409:LEU:HD12	1:D:409:LEU:HA	1.78	0.41
1:A:36:VAL:HG21	1:A:99:GLY:O	2.21	0.40
1:A:500:HIS:O	1:A:524:PRO:HD2	2.20	0.40
1:B:394:PHE:CD1	1:D:378:LEU:HD13	2.55	0.40
1:C:264:ASP:OD2	1:C:616:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:HD11	1:D:54:TYR:CG	2.55	0.40
1:D:330:MET:HE3	1:D:330:MET:HB3	1.89	0.40
1:D:417:LEU:HD23	1:D:417:LEU:HA	1.52	0.40
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.84	0.40
1:A:78:HIS:O	1:A:81:GLN:HB2	2.21	0.40
1:A:573:GLU:O	1:A:577:LYS:HG3	2.20	0.40
1:C:54:TYR:CD1	1:C:54:TYR:O	2.74	0.40
1:C:301:PHE:HE1	1:C:473:LYS:HD2	1.86	0.40
1:D:344:VAL:C	1:D:346:GLY:N	2.79	0.40
1:D:513:TYR:CD2	1:D:513:TYR:N	2.90	0.40
1:D:635:MET:HB3	1:D:635:MET:HE3	1.86	0.40
1:A:337:ARG:HG3	3:F:3:GLC:O2	2.22	0.40
1:B:49:LEU:HD22	1:B:91:VAL:HG23	2.04	0.40
1:B:119:LYS:NZ	1:B:130:SER:HB2	2.36	0.40
1:C:40:LYS:HB3	1:C:41:ASP:H	1.44	0.40
1:C:330:MET:HE2	1:C:568:LEU:HD12	2.03	0.40
1:A:109:ASP:C	1:A:111:VAL:H	2.29	0.40
1:A:262:LYS:HA	1:A:263:PRO:HD3	1.83	0.40
1:B:493:ASP:O	1:B:497:ARG:HG3	2.22	0.40
1:B:513:TYR:CD1	1:B:514:THR:N	2.89	0.40
1:C:200:TYR:CZ	1:C:227:ILE:CD1	3.05	0.40
1:A:227:ILE:HA	1:A:227:ILE:HD13	1.67	0.40
1:B:209:PHE:O	1:B:213:LEU:HB3	2.22	0.40
1:B:386:THR:HG21	1:D:390:GLY:CA	2.51	0.40
1:B:410:PRO:HG2	1:B:416:LEU:HD21	2.02	0.40
1:B:547:LYS:HE3	1:B:574:GLU:OE1	2.21	0.40
1:C:372:GLN:CG	1:C:487:ILE:HD12	2.51	0.40
1:C:543:THR:HB	1:C:544:ASN:H	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	636/725 (88%)	586 (92%)	44 (7%)	6 (1%)	14	41
1	B	636/725 (88%)	581 (91%)	48 (8%)	7 (1%)	11	36
1	C	644/725 (89%)	598 (93%)	38 (6%)	8 (1%)	10	34
1	D	632/725 (87%)	556 (88%)	67 (11%)	9 (1%)	9	30
All	All	2548/2900 (88%)	2321 (91%)	197 (8%)	30 (1%)	10	34

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	SER
1	C	483	ALA
1	C	543	THR
1	D	132	GLU
1	D	204	SER
1	D	403	ASN
1	A	38	GLN
1	A	111	VAL
1	B	209	PHE
1	B	489	GLY
1	C	17	VAL
1	D	107	ASP
1	D	111	VAL
1	D	115	SER
1	D	131	PRO
1	A	96	LEU
1	A	625	LEU
1	B	17	VAL
1	C	19	ASN
1	C	229	HIS
1	D	40	LYS
1	B	169	GLU
1	B	215	SER
1	A	631	ASN
1	B	543	THR
1	C	228	TYR
1	C	641	GLY
1	D	402	HIS
1	C	205	GLY
1	A	626	VAL

5.3.2 Protein sidechains [i](#)

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	551/623 (88%)	511 (93%)	40 (7%)	13	38
1	B	551/623 (88%)	509 (92%)	42 (8%)	12	36
1	C	556/623 (89%)	527 (95%)	29 (5%)	21	53
1	D	549/623 (88%)	515 (94%)	34 (6%)	16	45
All	All	2207/2492 (89%)	2062 (93%)	145 (7%)	15	43

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	19	ASN
1	A	56	ASN
1	A	67	GLU
1	A	71	ASP
1	A	81	GLN
1	A	82	THR
1	A	86	ARG
1	A	114	TYR
1	A	124	SER
1	A	136	GLU
1	A	156	HIS
1	A	181	LYS
1	A	192	THR
1	A	227	ILE
1	A	289	LYS
1	A	295	ASP
1	A	312	THR
1	A	337	ARG
1	A	360	LYS
1	A	376	ARG
1	A	378	LEU
1	A	387	THR
1	A	399	ARG

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Mol	Chain	Res	Type
1	A	406	THR
1	A	415	GLU
1	A	458	LYS
1	A	467	SER
1	A	471	ARG
1	A	484	ASN
1	A	487	ILE
1	A	488	LEU
1	A	493	ASP
1	A	521	MET
1	A	531	SER
1	A	543	THR
1	A	551	ILE
1	A	556	ARG
1	A	590	THR
1	A	629	GLU
1	B	2	SER
1	B	15	THR
1	B	19	ASN
1	B	45	LEU
1	B	126	VAL
1	B	133	ASN
1	B	136	GLU
1	B	156	HIS
1	B	181	LYS
1	B	207	PHE
1	B	213	LEU
1	B	214	GLU
1	B	232	CYS
1	B	254	GLU
1	B	279	PHE
1	B	288	LEU
1	B	289	LYS
1	B	320	ARG
1	B	337	ARG
1	B	349	LYS
1	B	366	VAL
1	B	376	ARG
1	B	381	THR
1	B	417	LEU
1	B	458	LYS
1	B	471	ARG

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Mol	Chain	Res	Type
1	B	484	ASN
1	B	487	ILE
1	B	488	LEU
1	B	513	TYR
1	B	520	VAL
1	B	525	SER
1	B	539	ASP
1	B	540	LEU
1	B	541	ILE
1	B	544	ASN
1	B	568	LEU
1	B	590	THR
1	B	593	LEU
1	B	600	LYS
1	B	628	GLU
1	B	632	ASP
1	C	2	SER
1	C	15	THR
1	C	19	ASN
1	C	35	THR
1	C	40	LYS
1	C	41	ASP
1	C	56	ASN
1	C	61	LEU
1	C	105	LEU
1	C	124	SER
1	C	169	GLU
1	C	289	LYS
1	C	291	GLU
1	C	295	ASP
1	C	348	LYS
1	C	376	ARG
1	C	387	THR
1	C	426	LYS
1	C	428	ARG
1	C	430	LEU
1	C	436	GLU
1	C	461	GLN
1	C	471	ARG
1	C	472	VAL
1	C	520	VAL
1	C	543	THR

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Mol	Chain	Res	Type
1	C	568	LEU
1	C	590	THR
1	C	643	LYS
1	D	6	GLN
1	D	19	ASN
1	D	42	HIS
1	D	86	ARG
1	D	114	TYR
1	D	122	LEU
1	D	132	GLU
1	D	136	GLU
1	D	164	VAL
1	D	181	LYS
1	D	213	LEU
1	D	288	LEU
1	D	310	ASP
1	D	324	LYS
1	D	337	ARG
1	D	376	ARG
1	D	378	LEU
1	D	379	GLU
1	D	409	LEU
1	D	412	ASP
1	D	450	ASP
1	D	457	ASN
1	D	461	GLN
1	D	482	ASN
1	D	487	ILE
1	D	488	LEU
1	D	517	GLU
1	D	519	THR
1	D	525	SER
1	D	557	ARG
1	D	590	THR
1	D	591	GLU
1	D	596	LEU
1	D	597	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN

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Mol	Chain	Res	Type
1	A	19	ASN
1	A	44	HIS
1	A	161	HIS
1	A	239	HIS
1	A	396	HIS
1	A	484	ASN
1	A	545	GLN
1	A	582	GLN
1	A	621	GLN
1	B	44	HIS
1	B	78	HIS
1	B	81	GLN
1	B	89	HIS
1	B	133	ASN
1	B	484	ASN
1	B	582	GLN
1	C	8	HIS
1	C	19	ASN
1	C	81	GLN
1	C	133	ASN
1	C	168	HIS
1	C	249	GLN
1	C	277	GLN
1	C	284	ASN
1	C	403	ASN
1	C	477	HIS
1	C	484	ASN
1	C	611	GLN
1	D	6	GLN
1	D	19	ASN
1	D	50	ASN
1	D	55	GLN
1	D	81	GLN
1	D	161	HIS
1	D	168	HIS
1	D	239	HIS
1	D	257	HIS
1	D	283	GLN
1	D	402	HIS
1	D	403	ASN
1	D	482	ASN
1	D	582	GLN

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Mol	Chain	Res	Type
1	D	585	ASN
1	D	621	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](#)

Of 25 monosaccharides modelled in this entry, 20 were used for Mogul analysis.

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	E	2	2	11,11,12	0.80	0	15,15,17	1.23	1 (6%)
2	GLC	E	3	2	11,11,12	0.54	0	15,15,17	1.16	1 (6%)
2	GLC	E	4	2	11,11,12	0.28	0	15,15,17	1.19	2 (13%)
2	GLC	E	5	2	11,11,12	0.36	0	15,15,17	0.85	1 (6%)
2	GLC	E	6	2	11,11,12	0.53	0	15,15,17	0.69	0
2	GLC	E	7	2	11,11,12	0.83	0	15,15,17	1.11	1 (6%)
2	GLC	E	8	2	11,11,12	0.83	0	15,15,17	1.53	2 (13%)
3	GLC	F	2	3	11,11,12	0.61	0	15,15,17	1.94	4 (26%)
3	GLC	F	3	3	11,11,12	0.71	0	15,15,17	0.84	1 (6%)
4	GLC	G	2	4	11,11,12	0.26	0	15,15,17	0.77	0
4	GLC	G	3	4	11,11,12	0.40	0	15,15,17	0.76	0
4	GLC	G	4	4	11,11,12	0.38	0	15,15,17	1.03	2 (13%)
5	GLC	H	2	5	11,11,12	0.84	0	15,15,17	2.00	3 (20%)
5	GLC	H	3	5	11,11,12	0.36	0	15,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLC	H	4	5	11,11,12	0.35	0	15,15,17	1.07	1 (6%)
5	GLC	H	5	5	11,11,12	0.54	0	15,15,17	0.85	0
5	GLC	I	2	5	11,11,12	0.63	0	15,15,17	1.40	1 (6%)
5	GLC	I	3	5	11,11,12	0.36	0	15,15,17	1.48	1 (6%)
5	GLC	I	4	5	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
5	GLC	I	5	5	11,11,12	0.66	0	15,15,17	1.56	2 (13%)

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	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	2/2/19/22	0/1/1/1
2	GLC	E	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	5	2	-	0/2/19/22	0/1/1/1
2	GLC	E	6	2	-	0/2/19/22	0/1/1/1
2	GLC	E	7	2	-	1/2/19/22	0/1/1/1
2	GLC	E	8	2	-	1/2/19/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	3	3	-	2/2/19/22	0/1/1/1
4	GLC	G	2	4	-	0/2/19/22	0/1/1/1
4	GLC	G	3	4	-	2/2/19/22	0/1/1/1
4	GLC	G	4	4	-	2/2/19/22	0/1/1/1
5	GLC	H	2	5	-	2/2/19/22	0/1/1/1
5	GLC	H	3	5	-	0/2/19/22	0/1/1/1
5	GLC	H	4	5	-	0/2/19/22	0/1/1/1
5	GLC	H	5	5	-	1/2/19/22	0/1/1/1
5	GLC	I	2	5	-	0/2/19/22	0/1/1/1
5	GLC	I	3	5	-	2/2/19/22	0/1/1/1
5	GLC	I	4	5	-	2/2/19/22	0/1/1/1
5	GLC	I	5	5	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	GLC	C1-O5-C5	6.29	120.62	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	GLC	C1-O5-C5	5.73	119.86	112.19
5	I	3	GLC	C1-O5-C5	4.56	118.30	112.19
5	I	5	GLC	C1-C2-C3	4.47	116.16	109.64
2	E	8	GLC	C1-O5-C5	4.33	117.99	112.19
5	I	2	GLC	C1-O5-C5	4.04	117.60	112.19
2	E	7	GLC	C1-O5-C5	3.57	116.97	112.19
2	E	3	GLC	C1-O5-C5	3.51	116.89	112.19
5	H	4	GLC	C1-C2-C3	2.80	113.72	109.64
4	G	4	GLC	C1-O5-C5	2.77	115.90	112.19
2	E	4	GLC	C2-C3-C4	-2.55	106.37	110.86
5	I	4	GLC	C1-C2-C3	2.47	113.24	109.64
5	I	5	GLC	C1-O5-C5	2.45	115.47	112.19
3	F	2	GLC	O5-C5-C4	2.39	116.65	110.83
5	H	2	GLC	C2-C3-C4	-2.33	106.77	110.86
5	H	2	GLC	O2-C2-C1	2.31	114.52	109.22
2	E	2	GLC	C1-O5-C5	2.31	115.28	112.19
3	F	2	GLC	O2-C2-C1	2.29	114.47	109.22
2	E	8	GLC	C1-C2-C3	2.29	112.97	109.64
4	G	4	GLC	C1-C2-C3	2.28	112.97	109.64
2	E	4	GLC	C1-O5-C5	2.26	115.22	112.19
3	F	3	GLC	C1-C2-C3	2.20	112.85	109.64
2	E	5	GLC	C1-O5-C5	2.20	115.13	112.19
5	I	4	GLC	C2-C3-C4	2.19	114.71	110.86
3	F	2	GLC	O4-C4-C3	-2.01	105.63	110.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
3	F	3	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6
5	I	4	GLC	O5-C5-C6-O6
2	E	3	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
5	I	3	GLC	C4-C5-C6-O6
4	G	4	GLC	O5-C5-C6-O6
5	I	4	GLC	C4-C5-C6-O6
4	G	4	GLC	C4-C5-C6-O6
3	F	3	GLC	C4-C5-C6-O6
5	I	3	GLC	O5-C5-C6-O6
5	H	2	GLC	C4-C5-C6-O6

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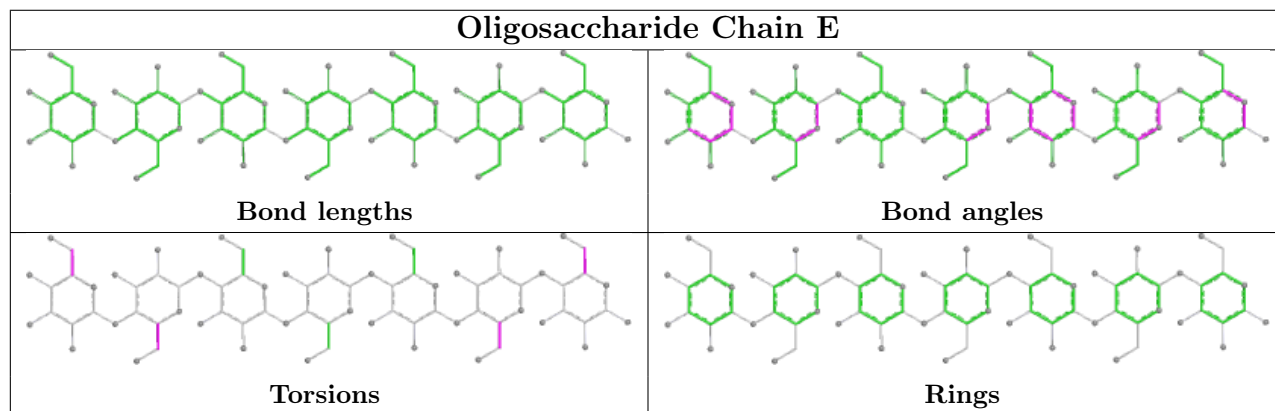
Mol	Chain	Res	Type	Atoms
2	E	8	GLC	O5-C5-C6-O6
5	H	2	GLC	O5-C5-C6-O6
4	G	3	GLC	C4-C5-C6-O6
4	G	3	GLC	O5-C5-C6-O6
2	E	7	GLC	O5-C5-C6-O6
5	H	5	GLC	C4-C5-C6-O6
5	I	5	GLC	C4-C5-C6-O6
5	I	5	GLC	O5-C5-C6-O6

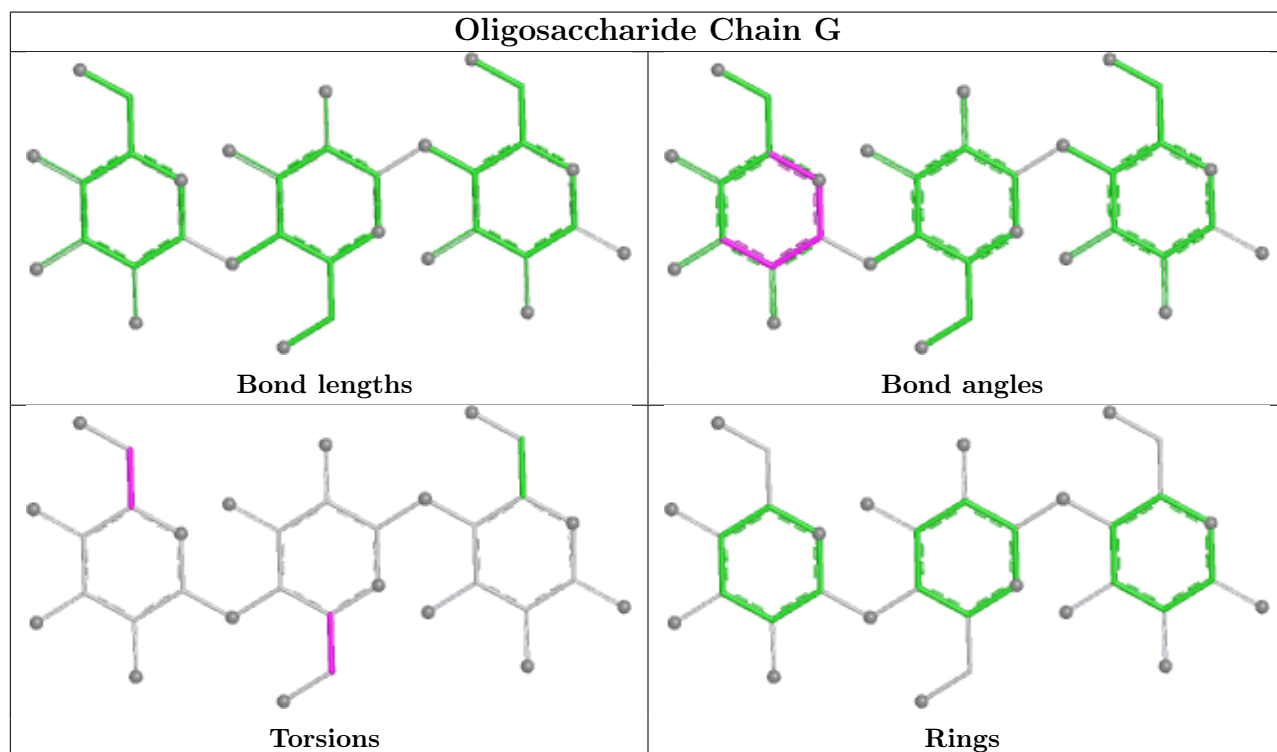
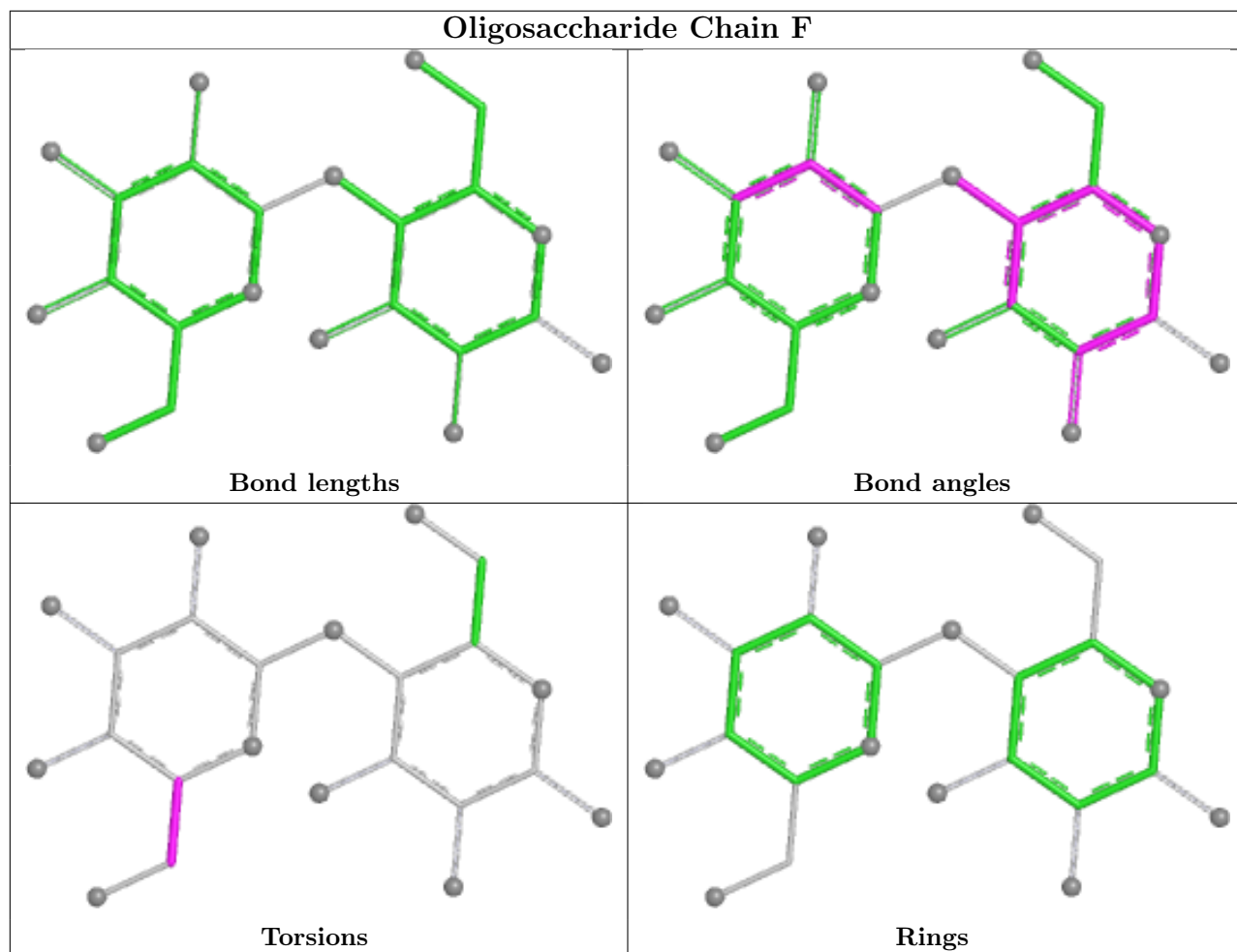
There are no ring outliers.

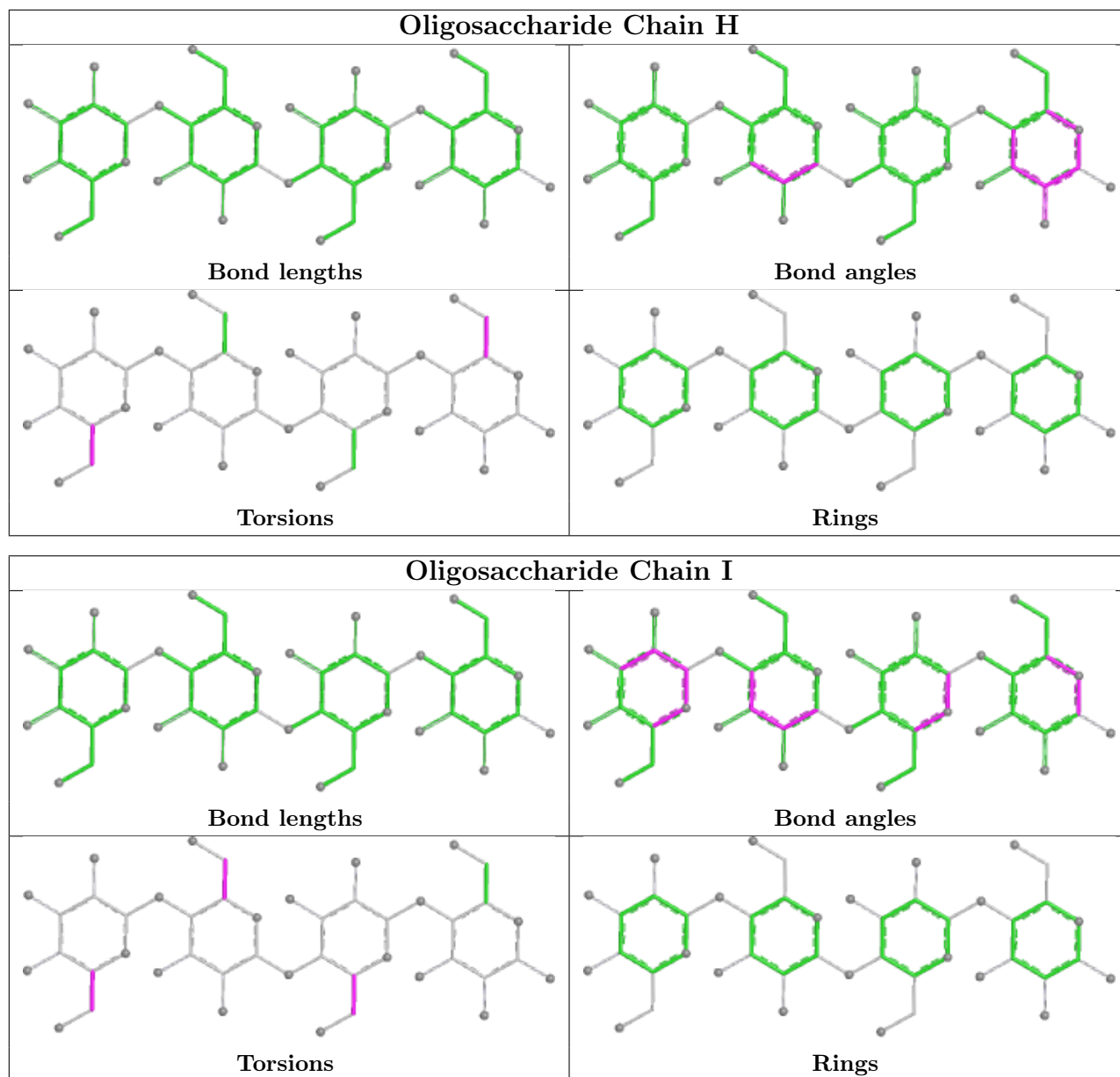
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GLC	2	0
4	G	3	GLC	1	0
3	F	2	GLC	1	0
5	H	4	GLC	1	0
5	H	3	GLC	1	0
4	G	4	GLC	1	0
3	F	3	GLC	2	0
4	G	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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PEG	B	706	-	6,6,6	0.55	0	5,5,5	0.18	0
6	G6P	B	901	-	16,16,16	0.56	0	23,24,24	1.04	1 (4%)
6	G6P	B	902	-	16,16,16	0.70	0	23,24,24	1.53	3 (13%)
6	G6P	A	901	-	16,16,16	0.53	0	23,24,24	0.84	0
7	PEG	B	1001	-	6,6,6	0.54	0	5,5,5	0.19	0
7	PEG	C	1004	-	6,6,6	0.55	0	5,5,5	0.14	0
6	G6P	D	901	-	16,16,16	0.45	0	23,24,24	0.91	0
6	G6P	C	901	-	16,16,16	0.54	0	23,24,24	0.86	0
7	PEG	A	1009	-	6,6,6	0.53	0	5,5,5	0.23	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
7	PEG	B	706	-	-	3/4/4/4	-
6	G6P	B	901	-	-	0/6/26/26	0/1/1/1
6	G6P	B	902	-	-	3/6/26/26	0/1/1/1
6	G6P	A	901	-	-	0/6/26/26	0/1/1/1
7	PEG	B	1001	-	-	3/4/4/4	-
7	PEG	C	1004	-	-	2/4/4/4	-
6	G6P	D	901	-	-	5/6/26/26	0/1/1/1
6	G6P	C	901	-	-	4/6/26/26	0/1/1/1
7	PEG	A	1009	-	-	4/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	902	G6P	O5-C5-C6	3.92	114.46	106.69
6	B	902	G6P	C3-C4-C5	-3.49	103.90	110.23
6	B	902	G6P	C4-C3-C2	-3.14	105.33	110.83
6	B	901	G6P	O5-C5-C6	2.42	111.50	106.69

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	902	G6P	C4-C5-C6-O6
6	B	902	G6P	O5-C5-C6-O6
6	C	901	G6P	O5-C5-C6-O6
6	C	901	G6P	C6-O6-P-O3P
6	D	901	G6P	C4-C5-C6-O6
6	D	901	G6P	O5-C5-C6-O6
6	D	901	G6P	C6-O6-P-O1P
6	D	901	G6P	C6-O6-P-O2P
7	B	1001	PEG	O1-C1-C2-O2
7	C	1004	PEG	O1-C1-C2-O2
7	B	1001	PEG	O2-C3-C4-O4
7	B	706	PEG	O2-C3-C4-O4
7	A	1009	PEG	O2-C3-C4-O4
7	C	1004	PEG	O2-C3-C4-O4
7	A	1009	PEG	O1-C1-C2-O2
7	B	706	PEG	O1-C1-C2-O2
6	D	901	G6P	C6-O6-P-O3P
7	A	1009	PEG	C1-C2-O2-C3
6	C	901	G6P	C6-O6-P-O2P
6	B	902	G6P	C5-C6-O6-P
7	B	706	PEG	C4-C3-O2-C2
6	C	901	G6P	C4-C5-C6-O6
7	A	1009	PEG	C4-C3-O2-C2
7	B	1001	PEG	C4-C3-O2-C2

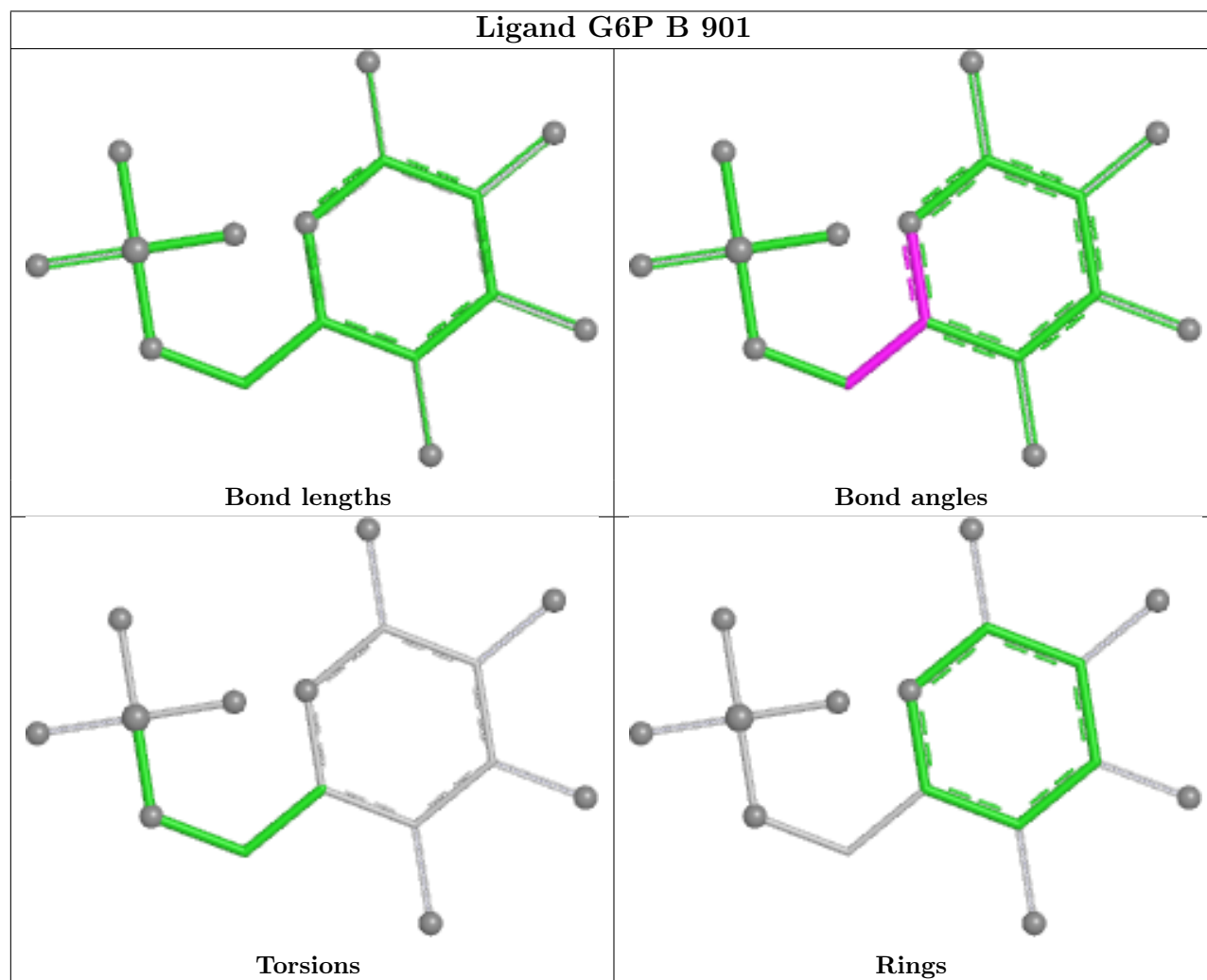
There are no ring outliers.

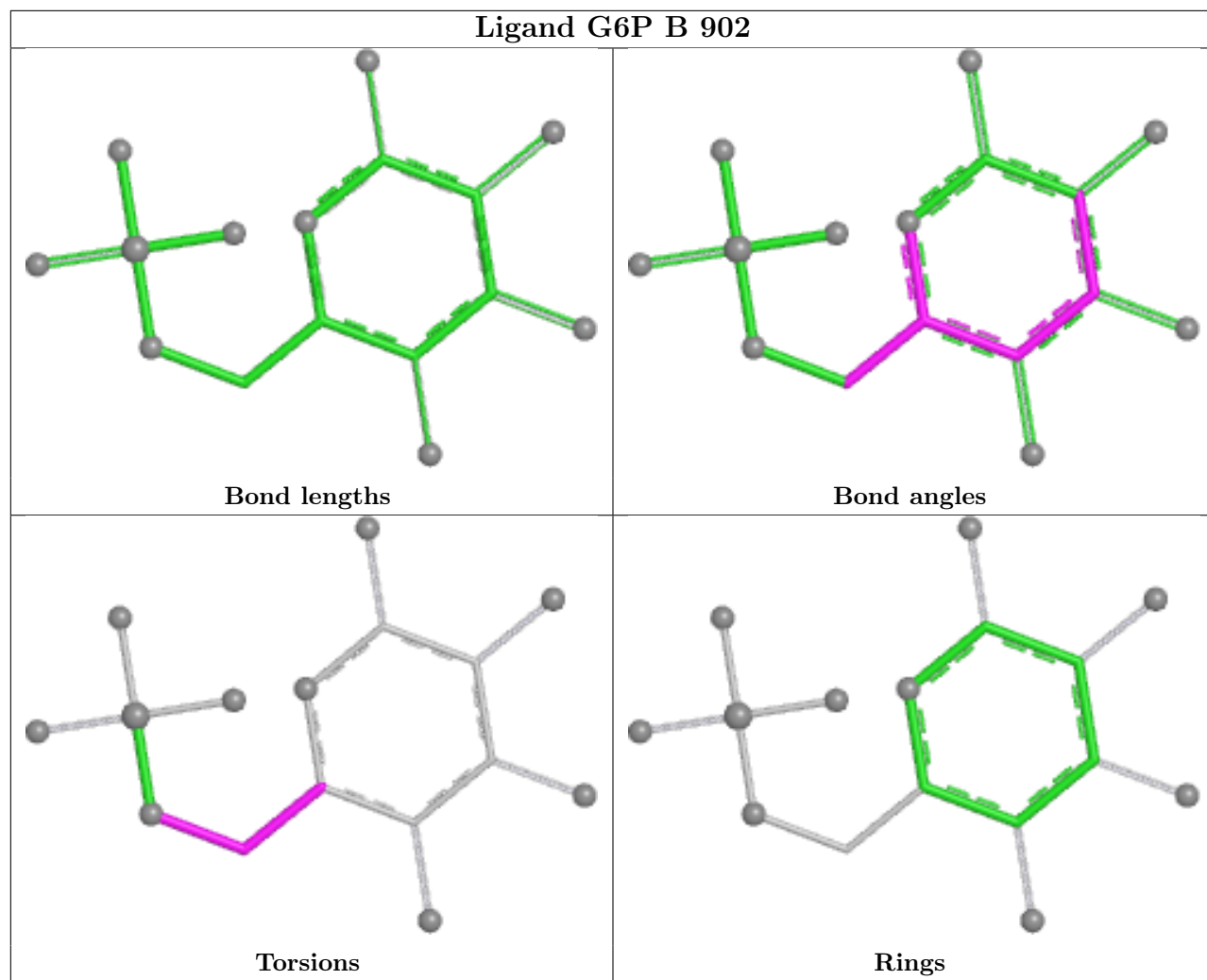
5 monomers are involved in 7 short contacts:

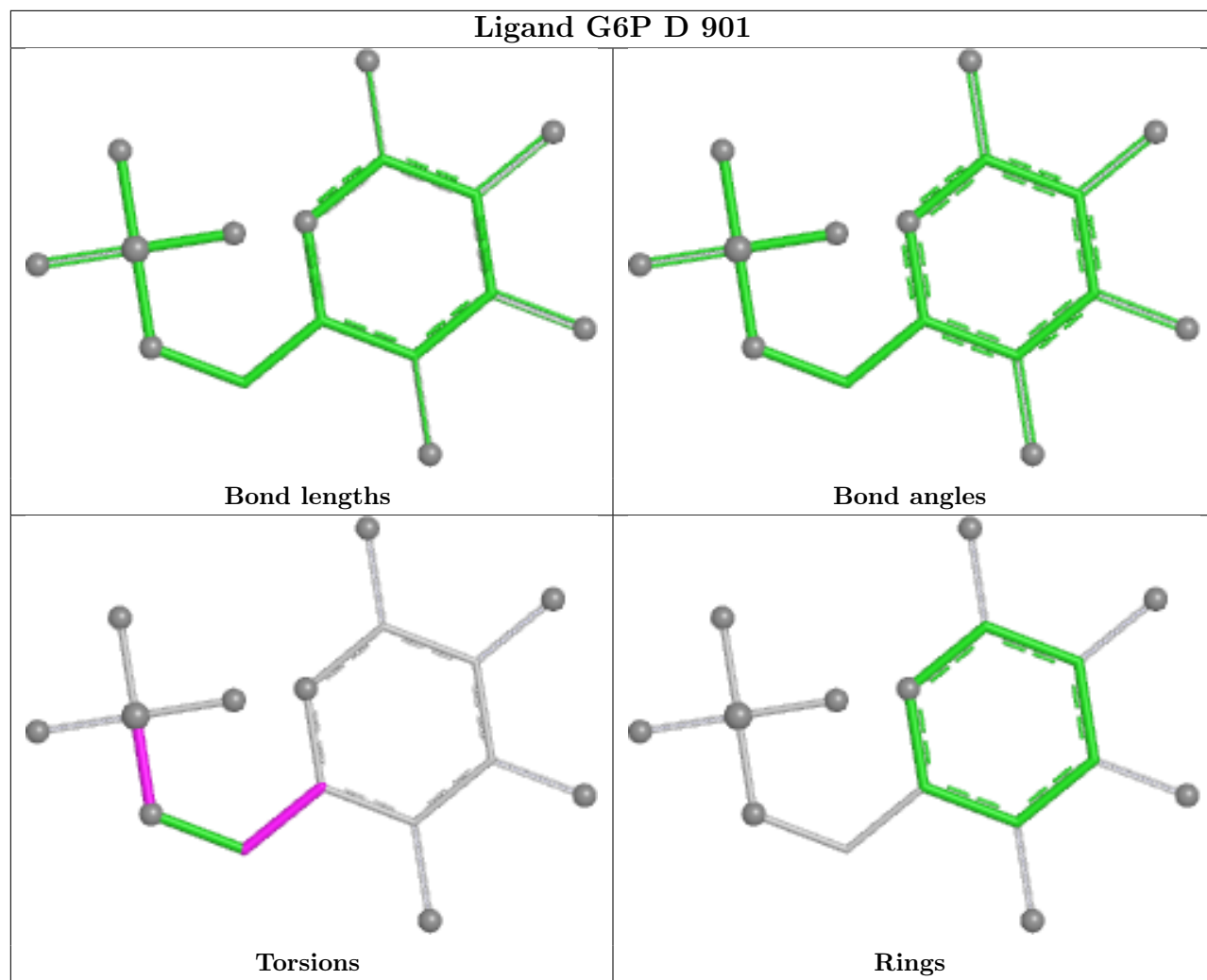
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	901	G6P	1	0
6	A	901	G6P	1	0
7	B	1001	PEG	2	0
6	D	901	G6P	2	0
6	C	901	G6P	1	0

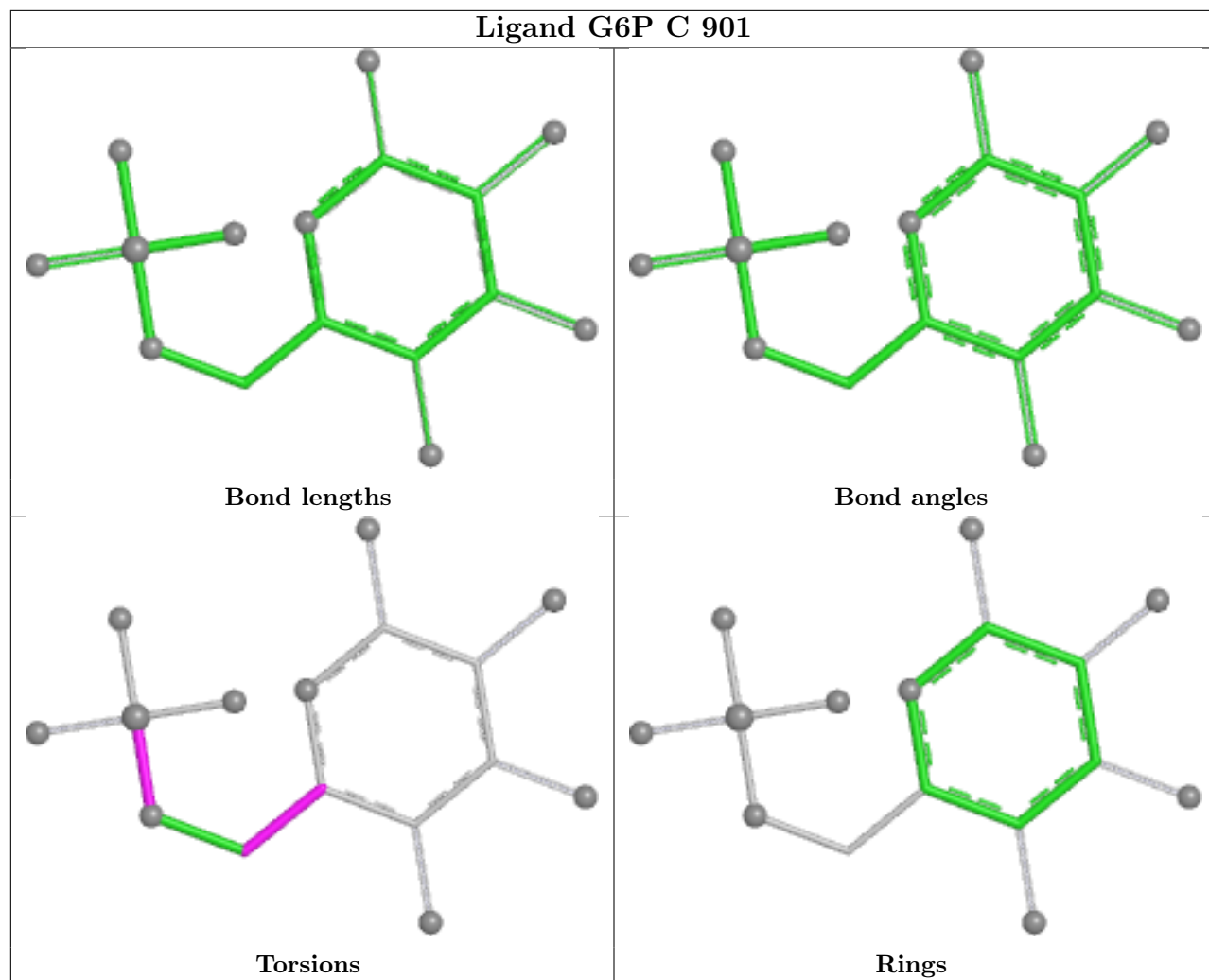
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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









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	638/725 (88%)	0.09	23 (3%) 46 37	27, 58, 110, 124	0
1	B	638/725 (88%)	0.19	13 (2%) 65 56	38, 65, 110, 123	0
1	C	646/725 (89%)	0.30	18 (2%) 55 45	42, 70, 111, 126	0
1	D	636/725 (87%)	0.31	29 (4%) 37 29	32, 76, 127, 136	0
All	All	2558/2900 (88%)	0.23	83 (3%) 50 40	27, 66, 118, 136	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	483	ALA	6.1
1	D	205	GLY	4.7
1	B	128	ILE	3.8
1	D	639	ALA	3.5
1	D	630	LEU	3.4
1	C	485	ASN	3.2
1	A	637	ALA	3.2
1	B	206	SER	3.2
1	D	113	GLY	3.1
1	D	118	TRP	3.1
1	A	632	ASP	3.1
1	A	2	SER	3.0
1	C	310	ASP	2.9
1	A	157	LEU	2.8
1	C	18	ALA	2.7
1	D	114	TYR	2.7
1	D	75	PRO	2.7
1	A	61	LEU	2.7
1	C	125	LEU	2.7
1	D	85	SER	2.7
1	B	108	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	135	PHE	2.7
1	A	162	ALA	2.6
1	C	135	PHE	2.6
1	C	51	LYS	2.6
1	A	68	ALA	2.6
1	B	629	GLU	2.5
1	A	63	TRP	2.5
1	A	78	HIS	2.5
1	A	5	LEU	2.4
1	A	163	ILE	2.4
1	B	103	VAL	2.4
1	A	85	SER	2.4
1	D	125	LEU	2.4
1	B	156	HIS	2.4
1	C	227	ILE	2.4
1	A	18	ALA	2.4
1	A	625	LEU	2.4
1	D	625	LEU	2.4
1	D	78	HIS	2.3
1	B	543	THR	2.3
1	D	60	ILE	2.3
1	D	618	TYR	2.3
1	D	279	PHE	2.3
1	C	132	GLU	2.3
1	D	624	GLU	2.3
1	D	242	ASP	2.3
1	D	620	ASP	2.3
1	D	212	CYS	2.3
1	C	484	ASN	2.3
1	C	204	SER	2.3
1	D	622	PHE	2.2
1	C	372	GLN	2.2
1	A	60	ILE	2.2
1	D	627	GLY	2.2
1	D	82	THR	2.2
1	A	630	LEU	2.2
1	C	61	LEU	2.2
1	A	591	GLU	2.2
1	B	324	LYS	2.2
1	B	624	GLU	2.2
1	D	119	LYS	2.1
1	A	274	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	631	ASN	2.1
1	B	129	PRO	2.1
1	D	158	ASP	2.1
1	B	223	GLY	2.1
1	C	108	LEU	2.1
1	C	486	PRO	2.1
1	D	178	LEU	2.1
1	D	591	GLU	2.1
1	A	160	GLN	2.1
1	A	279	PHE	2.1
1	C	207	PHE	2.1
1	D	135	PHE	2.0
1	A	543	THR	2.0
1	D	16	GLU	2.0
1	D	153	GLU	2.0
1	A	111	VAL	2.0
1	C	105	LEU	2.0
1	C	203	ALA	2.0
1	D	63	TRP	2.0
1	B	21	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

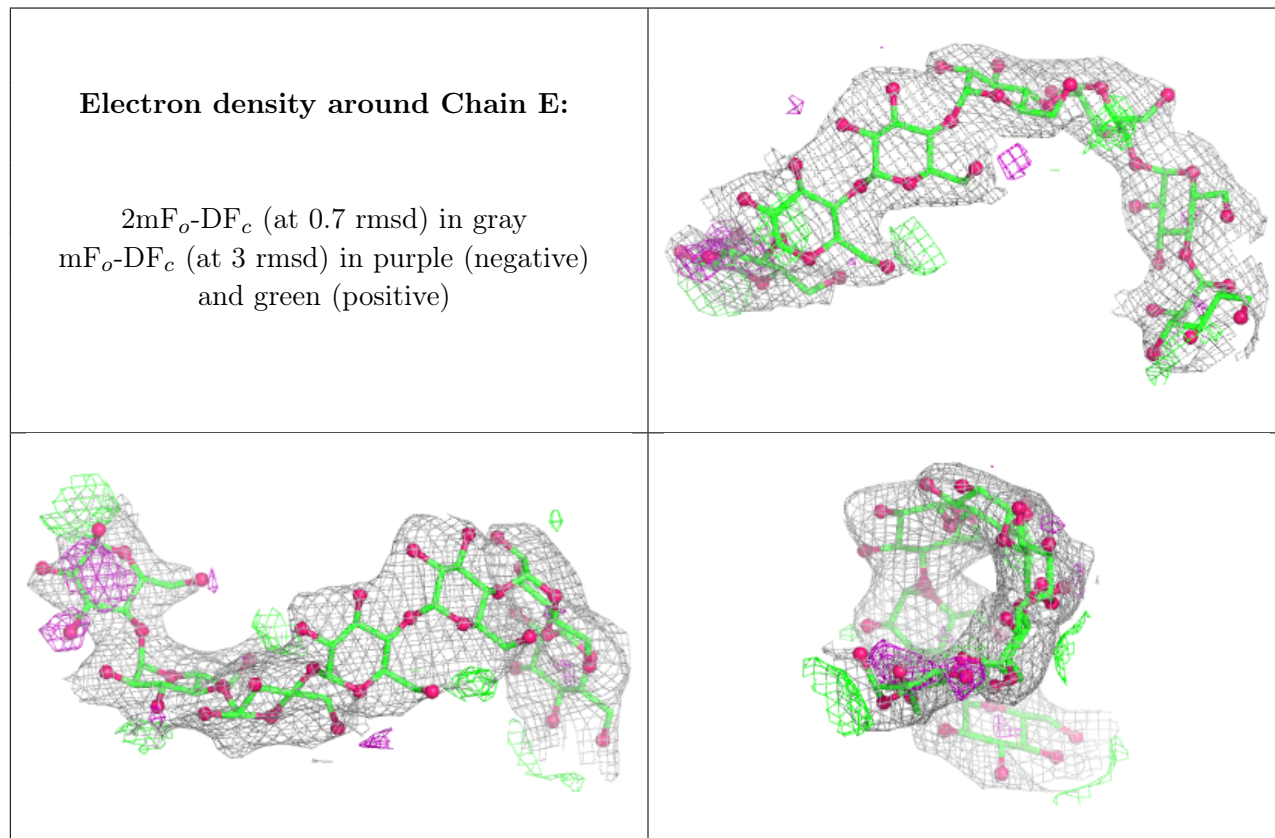
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	E	1	1/12	0.20	0.24	76,76,76,76	0
5	GLC	I	1	1/12	0.49	0.17	78,78,78,78	0
4	GLC	G	4	11/12	0.52	0.15	111,113,115,116	0
3	GLC	F	1	1/12	0.62	0.16	64,64,64,64	0
4	GLC	G	1	1/12	0.62	0.09	105,105,105,105	0
5	GLC	I	5	11/12	0.63	0.13	84,94,99,99	0
2	GLC	E	2	11/12	0.66	0.19	61,70,74,76	0
2	GLC	E	8	11/12	0.67	0.15	70,80,85,86	0

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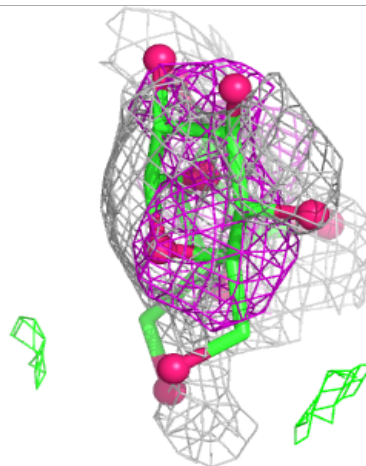
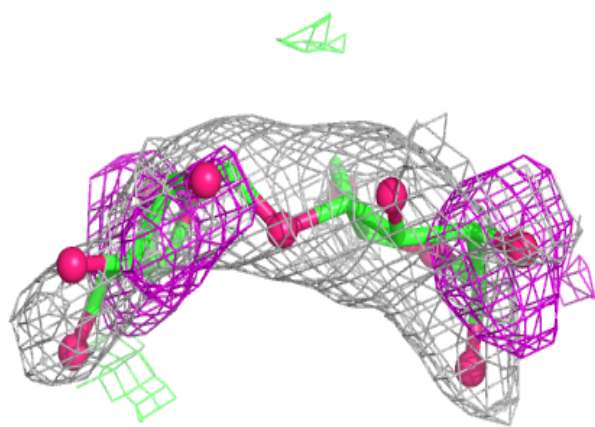
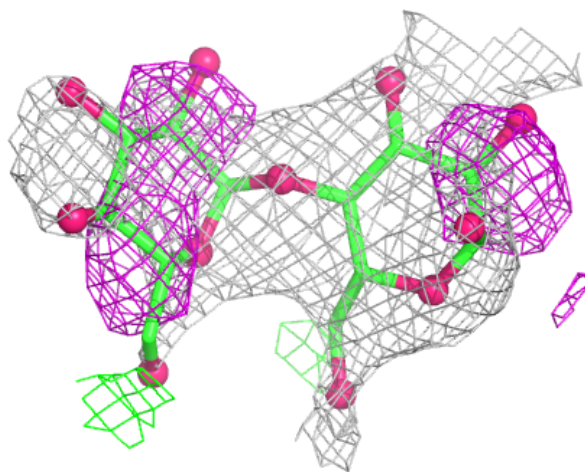
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GLC	G	2	11/12	0.70	0.13	103,106,109,110	0
4	GLC	G	3	11/12	0.72	0.12	108,110,113,113	0
5	GLC	H	1	1/12	0.72	0.10	52,52,52,52	0
5	GLC	H	5	11/12	0.77	0.11	78,85,87,87	0
5	GLC	I	2	11/12	0.78	0.12	66,71,75,77	0
2	GLC	E	6	11/12	0.80	0.10	68,77,83,86	0
3	GLC	F	3	11/12	0.82	0.16	66,71,75,75	0
2	GLC	E	7	11/12	0.83	0.13	76,82,87,88	0
3	GLC	F	2	11/12	0.83	0.12	60,62,69,69	0
5	GLC	H	2	11/12	0.84	0.13	46,56,60,63	0
5	GLC	I	4	11/12	0.86	0.11	65,71,75,80	0
2	GLC	E	5	11/12	0.90	0.09	64,65,71,75	0
2	GLC	E	3	11/12	0.90	0.08	54,61,66,67	0
5	GLC	H	4	11/12	0.92	0.09	58,63,69,75	0
2	GLC	E	4	11/12	0.93	0.07	53,60,63,66	0
5	GLC	I	3	11/12	0.93	0.08	57,60,65,69	0
5	GLC	H	3	11/12	0.95	0.06	49,53,56,56	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.



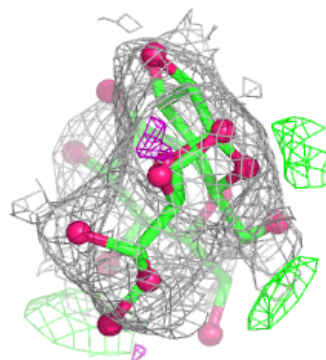
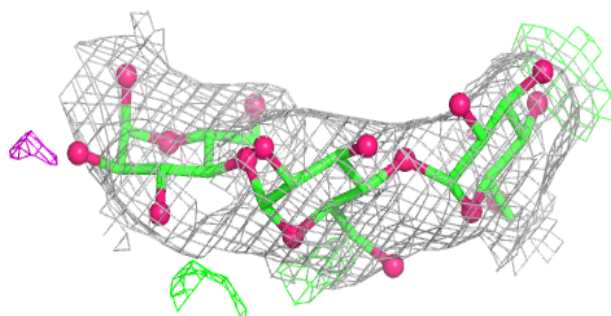
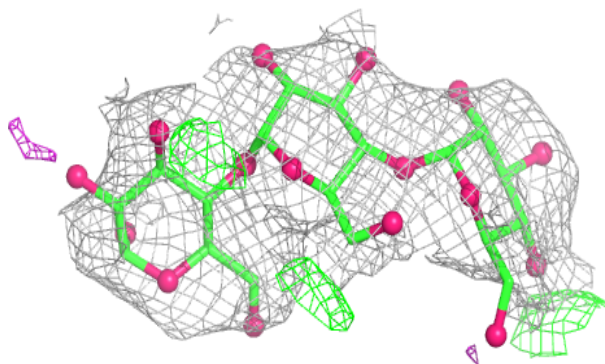
Electron density around Chain F:

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

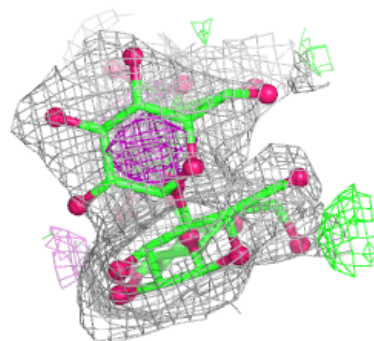
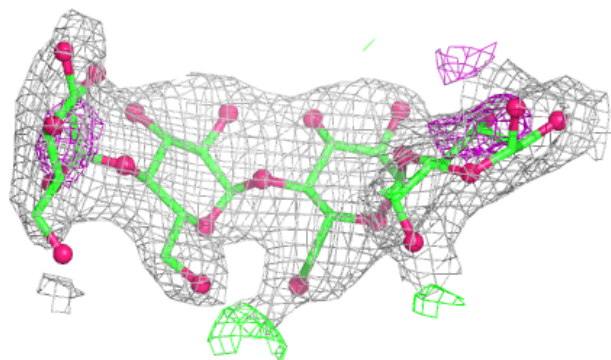
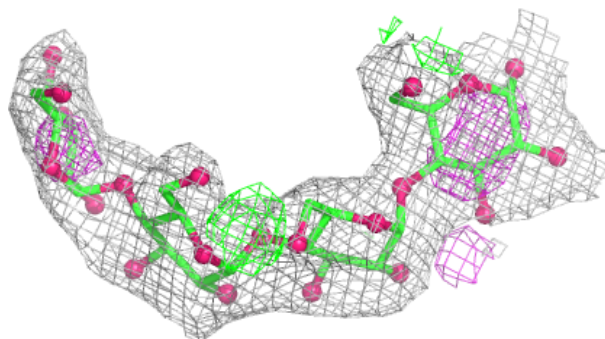


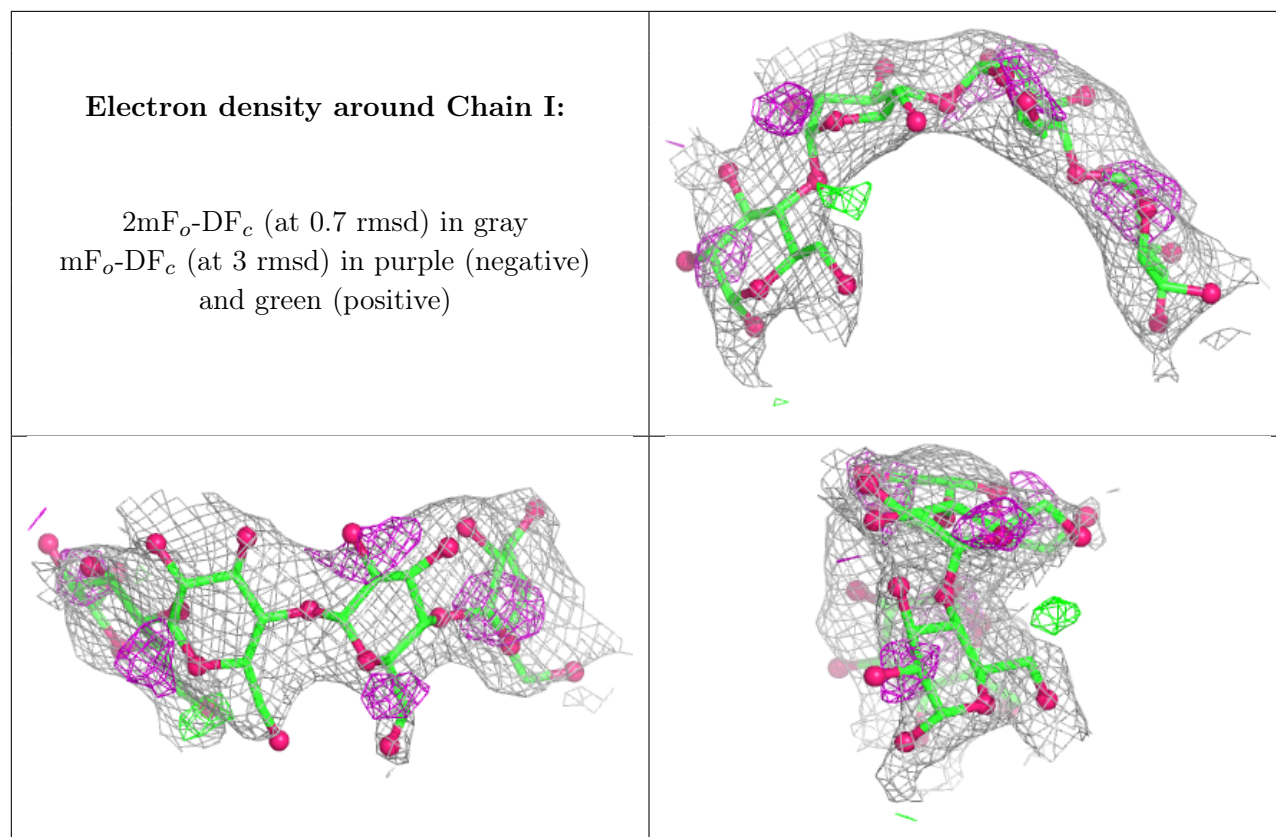
Electron density around Chain G:

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

**Electron density around Chain H:**

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





6.4 Ligands [i](#)

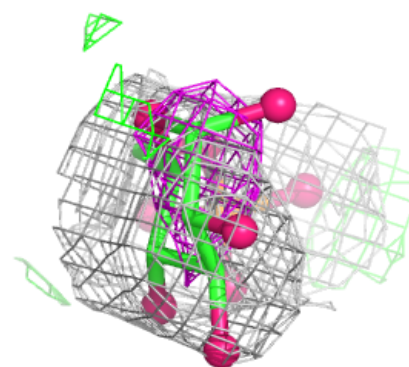
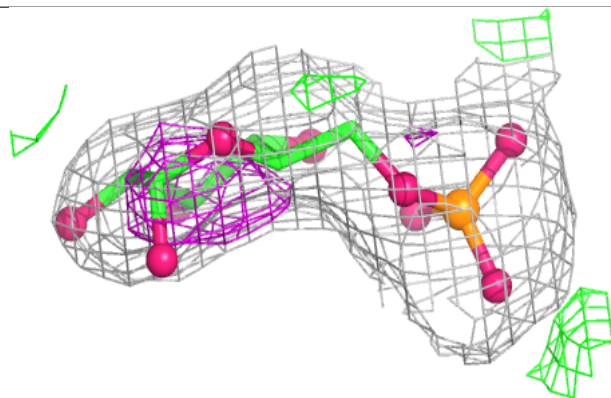
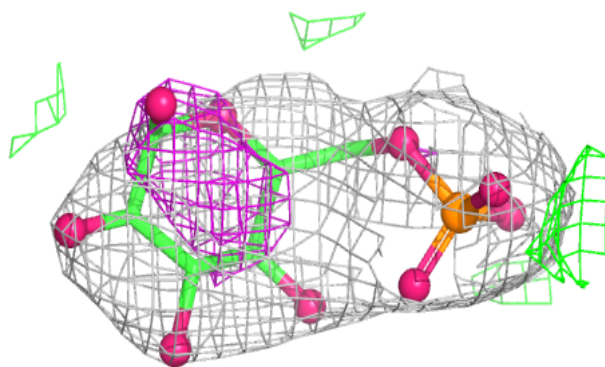
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	G6P	B	902	16/16	0.79	0.14	78,83,88,89	0
7	PEG	B	706	7/7	0.86	0.15	51,56,63,63	0
7	PEG	C	1004	7/7	0.93	0.10	48,51,58,60	0
7	PEG	A	1009	7/7	0.94	0.11	58,60,62,62	0
7	PEG	B	1001	7/7	0.95	0.08	50,52,55,55	0
6	G6P	C	901	16/16	0.97	0.07	46,50,52,52	0
6	G6P	D	901	16/16	0.97	0.06	35,37,40,41	0
6	G6P	B	901	16/16	0.98	0.05	42,45,48,50	0
6	G6P	A	901	16/16	0.98	0.06	34,36,41,43	0

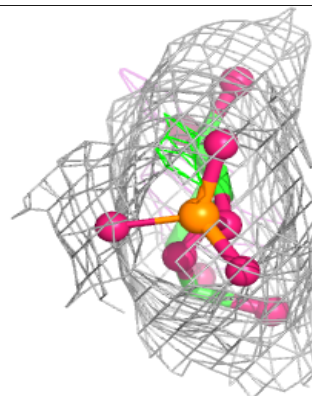
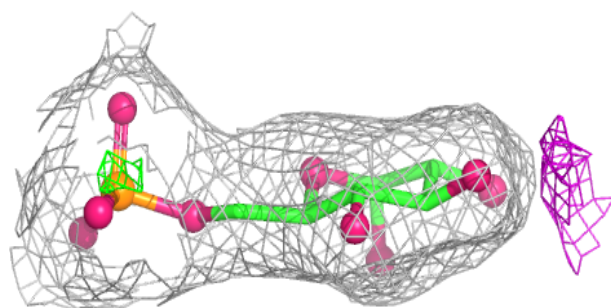
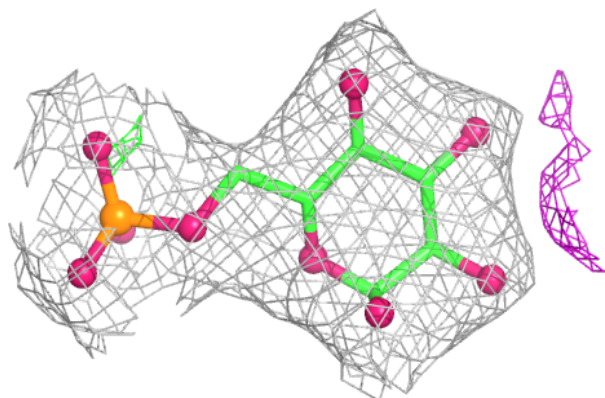
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G6P B 902:

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

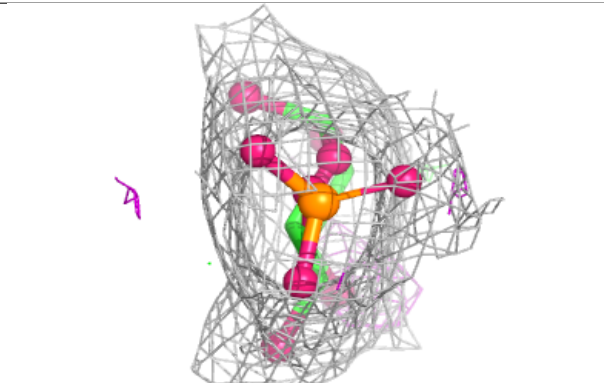
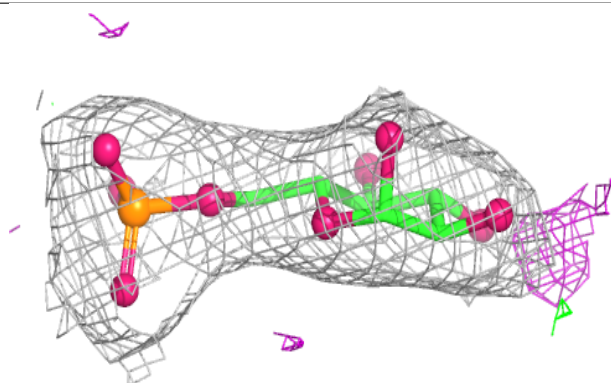
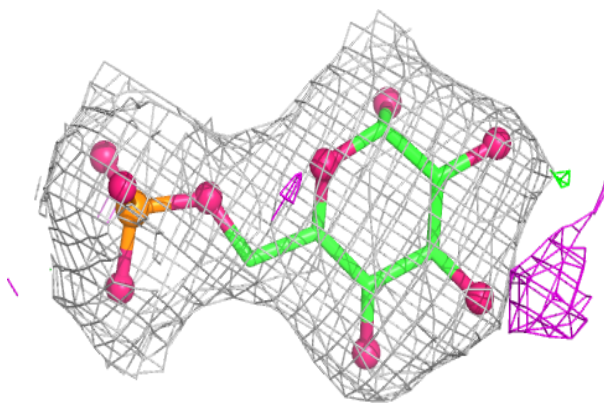
**Electron density around G6P C 901:**

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

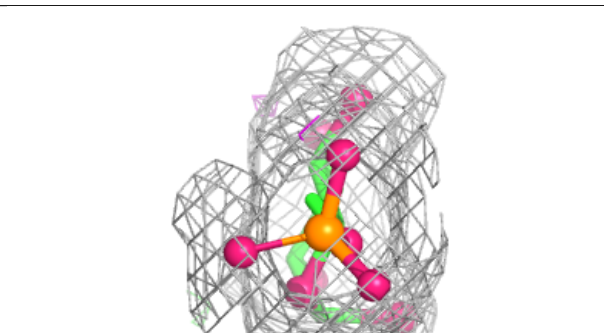
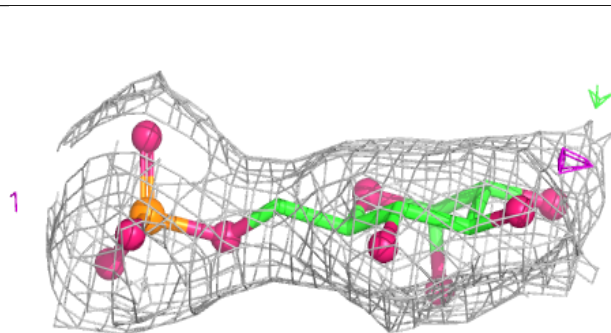
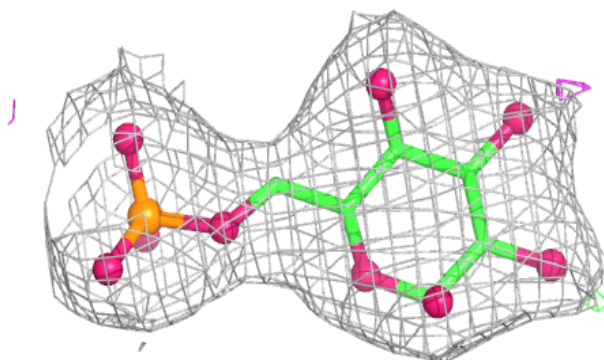


Electron density around G6P D 901:

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

**Electron density around G6P B 901:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.