



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:20 PM UTC

PDB ID : 2Z1K / pdb_00002z1k
Title : Crystal Structure of Ttha1563 from *Thermus thermophilus* HB8
Authors : Niwa, H.; Shimada, A.; Matsunaga, E.; Kuramitsu, S.; Yokoyama, S.; RIKEN
Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-05-08
Resolution : 2.30 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:

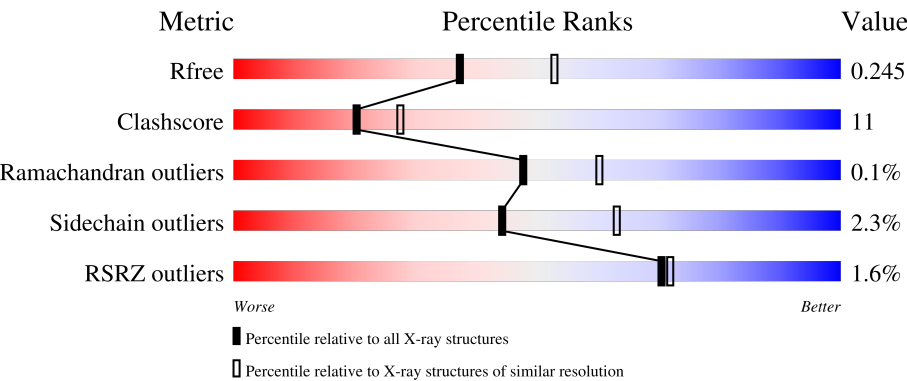
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.30 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.



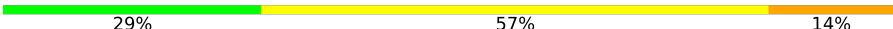
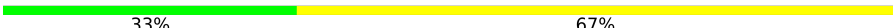
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	475	% 77% 21% .
1	B	475	2% 77% 21% .
1	C	475	% 75% 23% .
1	D	475	3% 72% 26% .
2	E	7	57% 43%

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Mol	Chain	Length	Quality of chain
2	G	7	 57% 43%
2	I	7	 57% 43%
2	K	7	 29% 57% 14%
3	F	3	 67% 33%
3	H	3	 67% 33%
3	J	3	 33% 67%
3	L	3	 67% 33%

2 Entry composition [i](#)

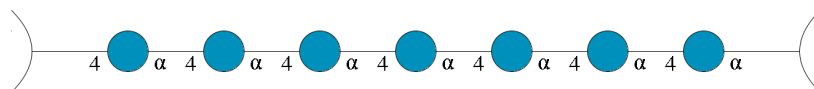
There are 5 unique types of molecules in this entry. The entry contains 16422 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (Neo)pullulanase.

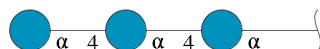
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	Se	0	0	0
			3803	2464	675	655	2	7			
1	B	474	Total	C	N	O	S	Se	0	1	0
			3801	2462	672	658	2	7			
1	C	474	Total	C	N	O	S	Se	0	0	0
			3789	2456	670	654	2	7			
1	D	474	Total	C	N	O	S	Se	0	0	0
			3803	2464	675	655	2	7			

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



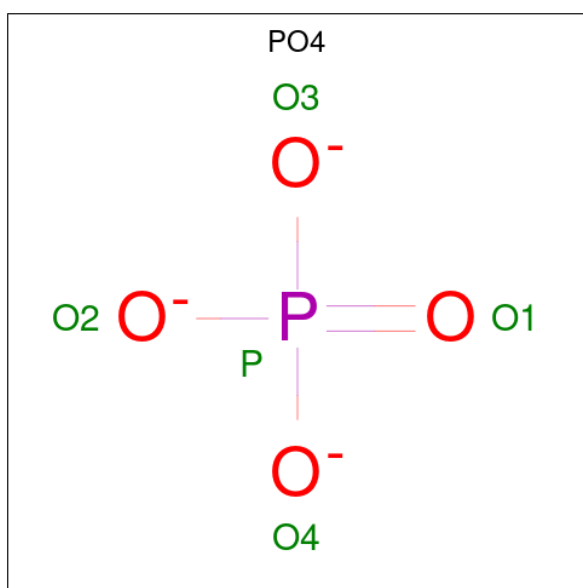
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	7	Total	C	O	0	0	0
			77	42	35			
2	G	7	Total	C	O	0	0	0
			77	42	35			
2	I	7	Total	C	O	0	0	0
			77	42	35			
2	K	7	Total	C	O	0	0	0
			77	42	35			

- 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
3	F	3	Total	C	O	0	0	0
			33	18	15			
3	H	3	Total	C	O	0	0	0
			33	18	15			
3	J	3	Total	C	O	0	0	0
			33	18	15			
3	L	3	Total	C	O	0	0	0
			33	18	15			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		

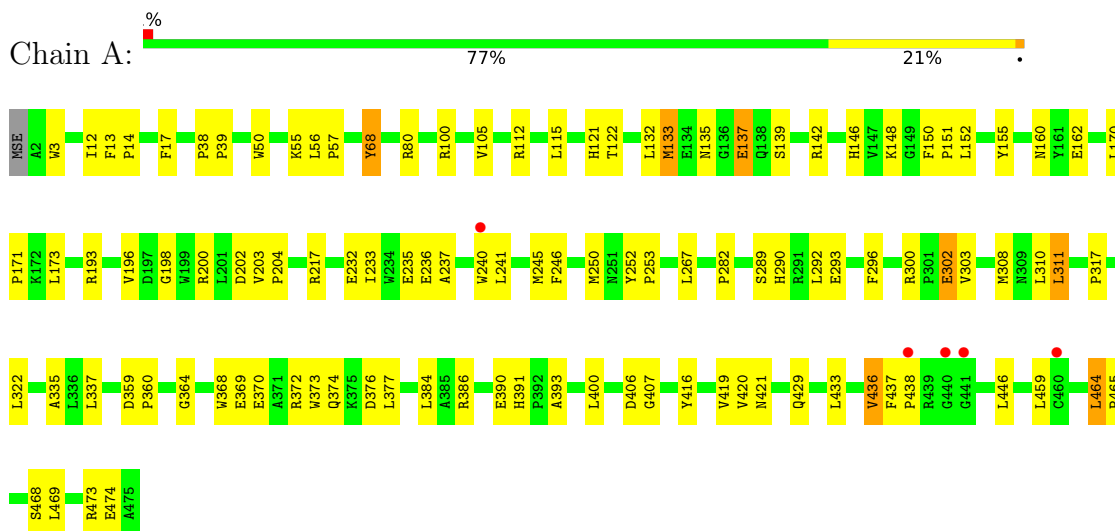
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		
5	B	227	Total	O	0	0
			227	227		
5	C	197	Total	O	0	0
			197	197		
5	D	191	Total	O	0	0
			191	191		

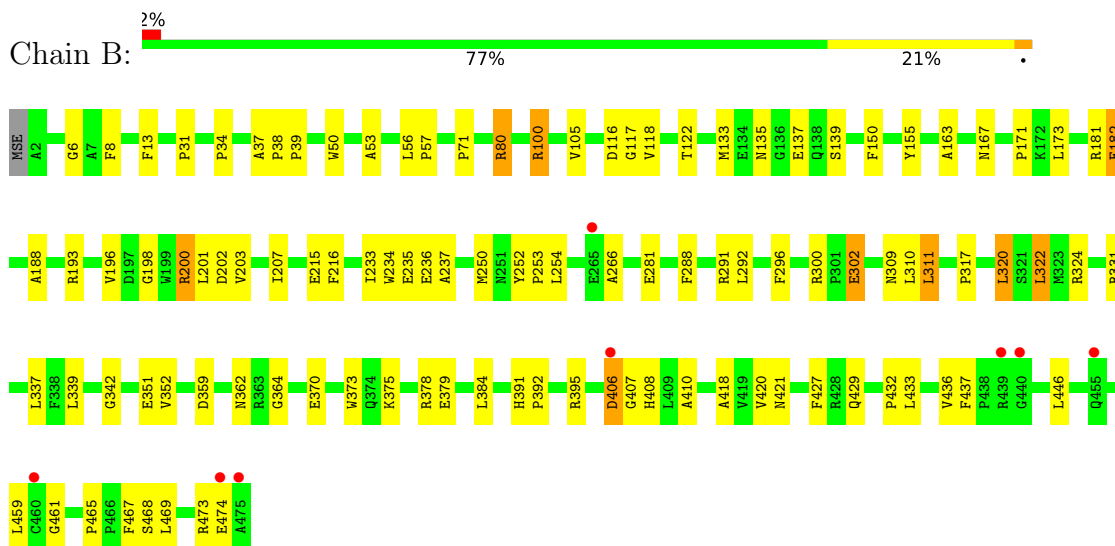
3 Residue-property plots [i](#)

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: (Neo)pullulanase

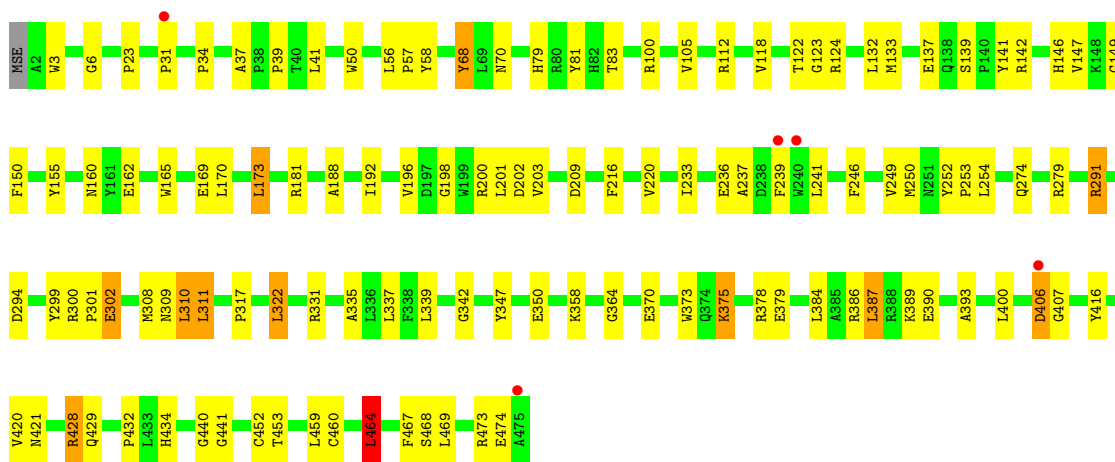


• Molecule 1: (Neo)pullulanase

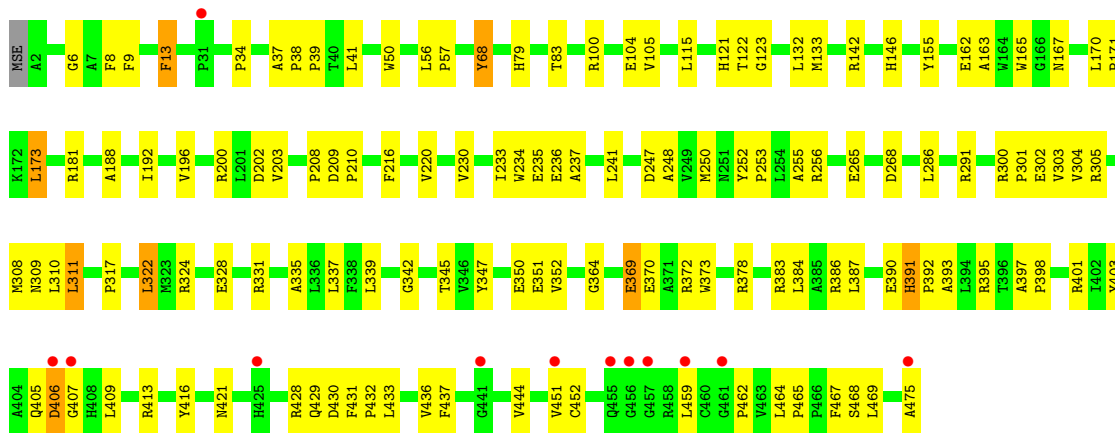


• Molecule 1: (Neo)pullulanase





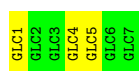
• Molecule 1: (Neo)pullulanase



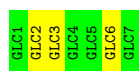
• Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



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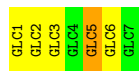


• Molecule 2: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



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

Chain K:  29% 57% 14%



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

Chain F:  67% 33%

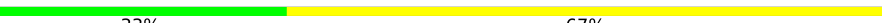


- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:  67% 33%



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

Chain J:  33% 67%



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

Chain L:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.14Å 95.90Å 140.60Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	46.66 – 2.30 46.66 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.66-2.30) 99.8 (46.66-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.32 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.236 0.198 , 0.245	Depositor DCC
R_{free} test set	3980 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16422	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6636e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.39	0/3926	0.91	8/5339 (0.1%)
1	B	0.41	0/3924	0.92	12/5339 (0.2%)
1	C	0.40	0/3912	0.91	10/5323 (0.2%)
1	D	0.39	0/3926	0.89	10/5339 (0.2%)
All	All	0.40	0/15688	0.91	40/21340 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	311	LEU	N-CA-C	-6.75	105.05	113.55
1	D	13	PHE	CA-C-N	6.14	127.51	119.84
1	D	13	PHE	C-N-CA	6.14	127.51	119.84
1	B	31	PRO	N-CA-C	6.12	120.11	110.50
1	A	311	LEU	N-CA-C	-6.11	105.73	113.43
1	B	207	ILE	CA-C-N	5.94	127.26	119.84
1	B	207	ILE	C-N-CA	5.94	127.26	119.84
1	B	311	LEU	N-CA-C	-5.88	106.03	113.43
1	D	406	ASP	CB-CA-C	-5.82	109.88	116.63
1	D	83	THR	N-CA-C	5.77	118.70	110.10
1	C	464	LEU	N-CA-C	-5.73	101.27	109.24
1	B	200	ARG	N-CA-C	-5.70	99.22	108.52
1	B	80	ARG	N-CA-C	5.69	120.17	113.23
1	D	247	ASP	N-CA-C	-5.66	106.22	113.23
1	A	13	PHE	CA-C-N	5.65	126.90	119.84
1	A	13	PHE	C-N-CA	5.65	126.90	119.84
1	B	50	TRP	N-CA-C	-5.63	105.14	111.28
1	B	406	ASP	CB-CA-C	-5.63	110.07	116.54
1	C	83	THR	N-CA-C	5.63	118.48	110.10
1	A	80	ARG	N-CA-C	5.59	120.05	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	440	GLY	N-CA-C	5.53	122.47	114.67
1	D	311	LEU	N-CA-C	-5.48	107.14	113.88
1	D	123	GLY	N-CA-C	-5.42	104.33	112.89
1	C	70	ASN	N-CA-C	-5.41	102.42	110.20
1	D	50	TRP	N-CA-C	-5.37	105.43	111.28
1	C	375	LYS	N-CA-C	5.33	117.09	111.28
1	D	391	HIS	CA-C-N	5.27	125.59	119.47
1	D	391	HIS	C-N-CA	5.27	125.59	119.47
1	C	406	ASP	CB-CA-C	-5.15	110.65	116.63
1	C	200	ARG	N-CA-C	-5.15	98.87	107.99
1	C	50	TRP	N-CA-C	-5.12	105.69	111.28
1	B	13	PHE	CA-C-N	5.11	126.23	119.84
1	B	13	PHE	C-N-CA	5.11	126.23	119.84
1	C	123	GLY	N-CA-C	-5.09	104.85	112.89
1	A	436	VAL	N-CA-C	5.08	115.80	110.62
1	B	391	HIS	CA-C-N	5.03	126.13	119.84
1	B	391	HIS	C-N-CA	5.03	126.13	119.84
1	A	391	HIS	CA-C-N	5.02	126.12	119.84
1	A	391	HIS	C-N-CA	5.02	126.12	119.84
1	A	50	TRP	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3803	0	3682	83	0
1	B	3801	0	3663	79	0
1	C	3789	0	3654	86	0
1	D	3803	0	3682	98	0
2	E	77	0	63	1	0
2	G	77	0	63	3	0
2	I	77	0	63	1	0
2	K	77	0	63	3	0
3	F	33	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	33	0	28	1	0
3	J	33	0	28	2	0
3	L	33	0	28	1	0
4	D	5	0	0	0	0
5	A	166	0	0	3	0
5	B	227	0	0	8	0
5	C	197	0	0	7	0
5	D	191	0	0	5	0
All	All	16422	0	15045	347	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 11.

All (347) 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:406:ASP:CG	1:C:407:GLY:H	1.63	1.04
1:D:406:ASP:CG	1:D:407:GLY:H	1.69	1.00
1:B:100:ARG:HG2	1:B:100:ARG:HH11	1.28	0.98
1:A:406:ASP:CG	1:A:407:GLY:H	1.74	0.94
1:D:311:LEU:HG	1:D:337:LEU:HD11	1.49	0.92
1:B:406:ASP:CG	1:B:407:GLY:H	1.75	0.90
1:D:429:GLN:HB3	1:D:459:LEU:HD23	1.54	0.90
1:C:100:ARG:HG2	1:C:100:ARG:HH11	1.46	0.80
1:C:311:LEU:HG	1:C:337:LEU:HD11	1.65	0.79
1:D:406:ASP:CG	1:D:407:GLY:N	2.39	0.79
1:B:34:PRO:HG2	1:B:37:ALA:HB2	1.64	0.78
1:A:406:ASP:CG	1:A:407:GLY:N	2.39	0.76
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.49	0.76
1:B:465:PRO:HG2	1:B:468:SER:OG	1.86	0.75
1:B:118:VAL:HG22	1:B:202[B]:ASP:OD2	1.88	0.72
1:B:235:GLU:HG2	1:C:301:PRO:HG3	1.73	0.71
1:D:202:ASP:OD1	3:L:1:GLC:C1	2.39	0.70
1:A:429:GLN:HB3	1:A:459:LEU:HD23	1.74	0.70
1:A:56:LEU:HD22	1:A:105:VAL:HG12	1.74	0.70
1:B:406:ASP:CG	1:B:407:GLY:N	2.41	0.69
1:D:132:LEU:HD21	1:D:142:ARG:HA	1.74	0.69
1:D:465:PRO:HG2	1:D:468:SER:OG	1.92	0.69
1:B:200:ARG:NH1	1:B:202[B]:ASP:OD1	2.26	0.68
1:C:233:ILE:HG21	1:C:237:ALA:HB2	1.76	0.68
1:D:100:ARG:HG2	1:D:100:ARG:HH11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ASP:CG	1:C:407:GLY:N	2.35	0.67
1:B:311:LEU:HG	1:B:337:LEU:HD11	1.76	0.67
1:B:302:GLU:CD	1:B:302:GLU:H	2.03	0.67
1:B:433:LEU:O	1:B:436:VAL:HG23	1.96	0.66
1:A:393:ALA:HB3	1:A:416:TYR:HE2	1.61	0.66
1:C:429:GLN:HB3	1:C:459:LEU:HD23	1.77	0.66
1:A:133:MSE:HE1	1:A:155:TYR:HE2	1.61	0.66
1:C:317:PRO:HB2	1:C:322:LEU:HD13	1.76	0.65
1:D:339:LEU:HD11	1:D:469:LEU:HD21	1.77	0.65
1:C:300:ARG:HB3	1:C:302:GLU:OE2	1.97	0.64
1:A:282:PRO:HG3	5:A:658:HOH:O	1.96	0.64
1:A:122:THR:O	1:A:171:PRO:HD2	1.98	0.64
1:A:464:LEU:CD2	1:A:468:SER:HB2	2.28	0.64
1:C:241:LEU:HD21	1:C:249:VAL:HG13	1.79	0.64
1:B:100:ARG:HG2	1:B:100:ARG:NH1	2.07	0.63
1:B:370:GLU:HG2	1:B:373:TRP:CH2	2.34	0.63
1:A:132:LEU:HD21	1:A:142:ARG:HA	1.80	0.63
1:A:289:SER:O	1:A:293:GLU:HG3	1.98	0.62
1:A:386:ARG:O	1:A:390:GLU:HG3	1.99	0.62
1:B:202[A]:ASP:OD1	3:H:1:GLC:C1	2.47	0.62
1:C:132:LEU:HD21	1:C:142:ARG:HA	1.80	0.62
1:A:446:LEU:HD21	1:A:473:ARG:HD3	1.82	0.62
1:C:370:GLU:HG2	1:C:373:TRP:CZ3	2.35	0.61
1:C:464:LEU:HD22	1:C:468:SER:HB2	1.83	0.61
1:C:339:LEU:HD11	1:C:469:LEU:HD21	1.83	0.61
1:C:56:LEU:N	1:C:57:PRO:HD2	2.16	0.61
1:B:56:LEU:HD22	1:B:105:VAL:HG12	1.83	0.60
1:D:433:LEU:O	1:D:436:VAL:HG23	2.02	0.59
1:C:389:LYS:HE3	5:C:617:HOH:O	2.02	0.59
1:A:311:LEU:HG	1:A:337:LEU:HD11	1.84	0.59
1:D:236:GLU:CD	1:D:236:GLU:H	2.10	0.59
1:B:122:THR:O	1:B:171:PRO:HD2	2.02	0.59
1:B:317:PRO:HB2	1:B:322:LEU:HD13	1.84	0.58
1:D:392:PRO:HA	1:D:395:ARG:NH1	2.18	0.58
1:A:56:LEU:N	1:A:57:PRO:HD2	2.18	0.58
1:C:56:LEU:HD23	1:C:105:VAL:HG12	1.84	0.58
1:D:208:PRO:O	1:D:210:PRO:HD3	2.03	0.58
1:D:369:GLU:HG2	1:D:372:ARG:HG3	1.84	0.58
1:C:375:LYS:O	1:C:379:GLU:HG3	2.03	0.58
1:A:236:GLU:CD	1:A:236:GLU:H	2.10	0.58
1:C:302:GLU:CD	1:C:302:GLU:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PRO:HB2	1:A:322:LEU:HD13	1.85	0.57
1:B:100:ARG:HH11	1:B:100:ARG:CG	2.07	0.57
1:C:146:HIS:HB2	1:C:162:GLU:HB2	1.86	0.57
1:D:265:GLU:CD	1:D:265:GLU:H	2.13	0.57
1:A:370:GLU:HG2	1:A:373:TRP:CZ3	2.40	0.57
1:B:432:PRO:HG2	5:B:718:HOH:O	2.03	0.57
1:C:39:PRO:HG3	1:C:364:GLY:HA2	1.87	0.57
1:A:146:HIS:HB2	1:A:162:GLU:HB2	1.86	0.57
1:D:122:THR:O	1:D:171:PRO:HD2	2.05	0.57
1:A:290:HIS:HA	1:A:293:GLU:OE1	2.04	0.57
1:B:292:LEU:HB3	1:B:296:PHE:CE2	2.39	0.57
1:A:121:HIS:CD2	1:A:170:LEU:HD23	2.40	0.56
1:A:302:GLU:H	1:A:302:GLU:CD	2.12	0.56
1:A:121:HIS:NE2	1:A:170:LEU:HD23	2.20	0.56
1:D:34:PRO:HG2	1:D:37:ALA:HB2	1.86	0.56
5:B:784:HOH:O	1:C:434:HIS:HD2	1.87	0.56
1:C:56:LEU:CD2	1:C:105:VAL:HG12	2.36	0.56
1:A:421:ASN:HB2	1:A:464:LEU:HD13	1.88	0.56
1:D:309:ASN:ND2	1:D:342:GLY:HA3	2.21	0.55
1:A:202:ASP:OD1	3:F:1:GLC:C1	2.54	0.55
1:B:429:GLN:HB3	1:B:459:LEU:HD23	1.88	0.55
1:C:441:GLY:O	1:C:453:THR:HG23	2.07	0.55
1:D:328:GLU:HG2	5:D:920:HOH:O	2.05	0.55
1:B:56:LEU:CD2	1:B:105:VAL:HG12	2.37	0.55
1:D:250:MSE:HE2	1:D:310:LEU:HD13	1.89	0.55
1:C:188:ALA:HB2	1:C:216:PHE:CE1	2.42	0.55
1:D:56:LEU:CD2	1:D:105:VAL:HG12	2.35	0.55
1:D:317:PRO:HB2	1:D:322:LEU:HD13	1.88	0.55
1:A:465:PRO:HG2	1:A:468:SER:OG	2.06	0.55
1:C:170:LEU:N	1:C:170:LEU:HD12	2.22	0.54
1:C:370:GLU:HG2	1:C:373:TRP:CH2	2.43	0.54
1:A:137:GLU:HG2	1:A:150:PHE:CE2	2.43	0.54
1:C:420:VAL:HG22	1:C:469:LEU:CD1	2.36	0.54
1:D:146:HIS:HB2	1:D:162:GLU:HB2	1.88	0.54
1:C:122:THR:HG23	1:C:173:LEU:HD13	1.88	0.54
1:D:317:PRO:HB2	1:D:322:LEU:CD1	2.38	0.54
1:C:6:GLY:HA2	1:C:342:GLY:O	2.08	0.54
1:D:310:LEU:HD23	1:D:310:LEU:H	1.72	0.54
1:C:100:ARG:HH11	1:C:100:ARG:CG	2.19	0.54
1:C:309:ASN:ND2	1:C:342:GLY:HA3	2.23	0.54
1:D:234:TRP:CE2	2:K:1:GLC:H2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:N	1:B:57:PRO:HD2	2.23	0.53
1:B:351:GLU:HG2	1:B:352:VAL:HG13	1.91	0.53
1:C:241:LEU:HD12	1:C:299:TYR:CE1	2.43	0.53
1:B:181:ARG:NH1	1:B:215:GLU:OE1	2.41	0.53
1:B:421:ASN:O	1:B:467:PHE:HA	2.08	0.53
1:D:339:LEU:CD1	1:D:469:LEU:HD21	2.39	0.53
1:C:34:PRO:HG2	1:C:37:ALA:HB2	1.91	0.53
1:D:39:PRO:HG3	1:D:364:GLY:HA2	1.90	0.53
1:D:133:MSE:HE1	1:D:155:TYR:HE2	1.73	0.53
1:C:3:TRP:CE3	1:C:112:ARG:HG3	2.43	0.53
1:C:147:VAL:HG12	1:C:149:GLY:H	1.72	0.53
1:D:192:ILE:HG13	1:D:220:VAL:HG13	1.91	0.53
1:A:203:VAL:HG23	1:A:203:VAL:O	2.10	0.52
1:A:3:TRP:CE3	1:A:112:ARG:HG3	2.44	0.52
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.22	0.52
1:A:39:PRO:HG3	1:A:364:GLY:HA2	1.91	0.52
1:B:196:VAL:HG12	1:B:198:GLY:H	1.75	0.52
1:B:39:PRO:HG3	1:B:364:GLY:HA2	1.91	0.52
1:D:6:GLY:HA3	1:D:395:ARG:HD2	1.92	0.52
1:C:331:ARG:NH1	5:C:659:HOH:O	2.42	0.51
1:D:56:LEU:HD22	1:D:105:VAL:HG12	1.91	0.51
1:D:309:ASN:HD21	1:D:342:GLY:HA3	1.73	0.51
1:D:421:ASN:O	1:D:467:PHE:HA	2.10	0.51
1:A:437:PHE:CD1	1:A:474:GLU:HG3	2.44	0.51
1:C:31:PRO:HA	5:C:763:HOH:O	2.09	0.51
1:C:100:ARG:HG2	1:C:100:ARG:NH1	2.22	0.51
1:C:254:LEU:HD23	1:C:309:ASN:OD1	2.11	0.51
1:A:133:MSE:HE1	1:A:155:TYR:CE2	2.44	0.51
1:D:444:VAL:HG12	1:D:475:ALA:HB2	1.91	0.51
1:A:56:LEU:CD2	1:A:105:VAL:HG12	2.39	0.51
1:B:100:ARG:NH1	1:B:100:ARG:CG	2.71	0.51
1:C:335:ALA:HB1	1:C:384:LEU:HD22	1.92	0.51
1:D:370:GLU:HG2	1:D:373:TRP:CZ3	2.45	0.51
1:D:252:TYR:N	1:D:253:PRO:CD	2.74	0.51
1:D:429:GLN:HB3	1:D:459:LEU:CD2	2.35	0.50
1:C:181:ARG:NH2	1:C:209:ASP:OD1	2.44	0.50
1:B:233:ILE:HG21	1:B:237:ALA:HB2	1.93	0.50
1:C:68:TYR:CD1	1:C:68:TYR:C	2.89	0.50
2:E:3:GLC:H61	2:E:4:GLC:O5	2.11	0.50
1:B:116:ASP:OD2	1:B:202[B]:ASP:OD1	2.29	0.50
1:D:203:VAL:HG23	1:D:203:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLY:HA2	1:B:342:GLY:O	2.12	0.50
1:C:274:GLN:HE21	1:C:358:LYS:HD3	1.77	0.50
1:A:39:PRO:CG	1:A:364:GLY:HA2	2.43	0.49
1:A:100:ARG:HG2	1:A:100:ARG:NH1	2.24	0.49
1:B:310:LEU:H	1:B:310:LEU:HD23	1.78	0.49
1:B:375:LYS:O	1:B:379:GLU:HG3	2.12	0.49
1:C:192:ILE:HG13	1:C:220:VAL:HG13	1.95	0.49
1:C:202:ASP:O	1:C:203:VAL:C	2.55	0.49
1:B:410:ALA:HA	1:B:418:ALA:O	2.13	0.49
1:C:23:PRO:HB3	5:C:777:HOH:O	2.12	0.49
1:C:58:TYR:CE1	1:C:378:ARG:NH2	2.81	0.49
1:A:335:ALA:HA	1:A:384:LEU:HD22	1.95	0.49
1:B:234:TRP:CE2	2:G:1:GLC:H2	2.48	0.49
5:C:723:HOH:O	1:D:301:PRO:HG2	2.12	0.49
1:D:268:ASP:HA	1:D:324:ARG:NH2	2.28	0.49
1:C:165:TRP:HZ3	2:I:3:GLC:H5	1.77	0.48
1:D:8:PHE:CD1	1:D:8:PHE:C	2.90	0.48
1:A:200:ARG:HD3	1:A:200:ARG:C	2.38	0.48
1:C:201:LEU:HD12	1:C:246:PHE:CE1	2.48	0.48
1:C:473:ARG:HG2	1:C:473:ARG:HH11	1.78	0.48
1:D:200:ARG:HD3	1:D:200:ARG:C	2.38	0.48
1:A:235:GLU:HB3	1:A:236:GLU:OE2	2.14	0.48
1:B:266:ALA:O	1:B:324:ARG:HD2	2.13	0.48
1:C:252:TYR:N	1:C:253:PRO:CD	2.77	0.48
1:D:122:THR:HG23	1:D:173:LEU:HD13	1.95	0.48
1:D:405:GLN:O	1:D:406:ASP:HB3	2.12	0.48
1:A:233:ILE:HG21	1:A:237:ALA:HB2	1.96	0.48
1:B:34:PRO:HG2	1:B:37:ALA:CB	2.41	0.48
1:D:369:GLU:HB3	1:D:372:ARG:HD3	1.94	0.48
1:D:378:ARG:HG2	1:D:378:ARG:HH11	1.79	0.48
1:D:393:ALA:HB3	1:D:416:TYR:HE2	1.79	0.48
1:A:12:ILE:O	1:A:14:PRO:HD3	2.14	0.47
1:A:250:MSE:HE2	1:A:310:LEU:HD13	1.96	0.47
1:A:300:ARG:HB3	1:A:302:GLU:OE2	2.14	0.47
1:B:331:ARG:HG2	1:B:331:ARG:HH11	1.79	0.47
1:B:202[B]:ASP:O	1:B:203:VAL:C	2.56	0.47
1:B:236:GLU:H	1:B:236:GLU:CD	2.21	0.47
1:D:100:ARG:O	1:D:104:GLU:HG3	2.15	0.47
1:D:121:HIS:CD2	1:D:170:LEU:HD23	2.49	0.47
1:D:56:LEU:N	1:D:57:PRO:HD2	2.30	0.47
1:D:235:GLU:HB3	1:D:236:GLU:OE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ARG:HG2	1:C:279:ARG:HH11	1.79	0.47
1:D:403:TYR:O	1:D:409:LEU:HD12	2.15	0.47
1:B:71:PRO:HB2	1:B:80:ARG:HB3	1.96	0.47
1:A:193:ARG:HD3	5:A:737:HOH:O	2.14	0.47
1:A:433:LEU:O	1:A:436:VAL:HG23	2.15	0.47
1:D:115:LEU:HD11	1:D:196:VAL:HG21	1.96	0.47
1:D:335:ALA:HA	1:D:384:LEU:HD22	1.97	0.47
1:D:451:VAL:O	1:D:452:CYS:HB3	2.15	0.47
1:C:202:ASP:OD1	3:J:1:GLC:C1	2.63	0.47
1:A:252:TYR:N	1:A:253:PRO:CD	2.78	0.47
1:B:420:VAL:HG22	1:B:469:LEU:CD1	2.46	0.46
1:C:137:GLU:HG2	1:C:150:PHE:CE2	2.50	0.46
1:D:13:PHE:CZ	1:D:79:HIS:HA	2.50	0.46
1:B:408:HIS:HB3	1:B:427:PHE:CZ	2.51	0.46
1:B:252:TYR:N	1:B:253:PRO:CD	2.78	0.46
1:A:150:PHE:HA	1:A:151:PRO:C	2.40	0.46
1:B:39:PRO:HD2	5:B:740:HOH:O	2.15	0.46
1:A:420:VAL:HG22	1:A:469:LEU:CD1	2.45	0.46
1:B:201:LEU:HD21	1:B:216:PHE:CZ	2.51	0.46
1:A:436:VAL:C	1:A:438:PRO:HD3	2.41	0.46
1:B:300:ARG:HB3	1:B:302:GLU:OE2	2.16	0.46
2:G:4:GLC:H61	2:G:5:GLC:O5	2.16	0.46
1:A:135:ASN:HB2	1:A:139:SER:HB2	1.97	0.45
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.79	0.45
1:B:281:GLU:HG2	5:B:798:HOH:O	2.15	0.45
1:B:437:PHE:HB3	1:B:474:GLU:OE2	2.16	0.45
1:D:331:ARG:HH11	1:D:331:ARG:HG2	1.80	0.45
1:A:55:LYS:HE3	1:A:368:TRP:CE2	2.52	0.45
1:B:163:ALA:HB1	1:B:167:ASN:O	2.16	0.45
1:D:300:ARG:O	1:D:304:VAL:HG23	2.16	0.45
1:A:115:LEU:HD11	1:A:196:VAL:HG21	1.99	0.45
1:A:369:GLU:HB3	1:A:372:ARG:HD3	1.98	0.45
1:B:310:LEU:H	1:B:310:LEU:CD2	2.29	0.45
1:C:239:PHE:CD1	1:C:239:PHE:C	2.94	0.45
1:D:431:PHE:HB2	1:D:432:PRO:HD2	1.99	0.45
1:A:202:ASP:O	1:A:203:VAL:C	2.59	0.45
1:A:310:LEU:HD23	1:A:310:LEU:H	1.80	0.45
1:C:386:ARG:O	1:C:390:GLU:HG3	2.16	0.45
1:A:374:GLN:HG3	1:A:377:LEU:H	1.82	0.45
1:B:182:GLU:HG2	5:B:796:HOH:O	2.17	0.45
5:C:723:HOH:O	1:D:302:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:VAL:HA	1:D:248:ALA:O	2.17	0.45
1:D:241:LEU:HD13	1:D:303:VAL:HG11	1.99	0.45
1:C:233:ILE:CG2	1:C:237:ALA:HB2	2.45	0.44
1:C:347:TYR:O	1:C:350:GLU:HG2	2.17	0.44
1:D:286:LEU:HD11	1:D:401:ARG:NH1	2.31	0.44
1:C:139:SER:C	1:C:141:TYR:H	2.25	0.44
1:D:163:ALA:HB1	1:D:167:ASN:O	2.17	0.44
1:A:335:ALA:CA	1:A:384:LEU:HD22	2.48	0.44
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.80	0.44
1:B:8:PHE:C	1:B:8:PHE:CD1	2.95	0.44
1:C:79:HIS:CE1	1:C:81:TYR:HB2	2.53	0.44
1:D:370:GLU:HG2	1:D:373:TRP:CH2	2.53	0.44
1:D:428:ARG:HD2	1:D:430:ASP:OD2	2.18	0.44
1:A:17:PHE:HB3	5:A:608:HOH:O	2.18	0.44
1:C:100:ARG:CG	1:C:100:ARG:NH1	2.79	0.44
1:C:428:ARG:CD	1:C:428:ARG:H	2.29	0.44
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.92	0.44
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.81	0.44
1:B:202[A]:ASP:O	1:B:203:VAL:C	2.61	0.44
1:B:446:LEU:HD21	1:B:473:ARG:HD2	2.00	0.44
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.86	0.44
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.30	0.44
1:A:420:VAL:HG22	1:A:469:LEU:HD11	2.00	0.44
1:B:291:ARG:HD2	5:B:787:HOH:O	2.18	0.44
1:C:124:ARG:NH2	1:C:169:GLU:HG2	2.33	0.44
1:C:203:VAL:HG23	1:C:203:VAL:O	2.18	0.44
1:B:133:MSE:HE1	1:B:155:TYR:HE2	1.83	0.43
1:A:359:ASP:OD1	1:A:360:PRO:HA	2.17	0.43
1:D:165:TRP:HZ3	2:K:3:GLC:H5	1.84	0.43
1:D:369:GLU:HG2	1:D:372:ARG:CD	2.49	0.43
1:A:68:TYR:CD1	1:A:68:TYR:C	2.96	0.43
1:D:209:ASP:HB2	5:D:926:HOH:O	2.17	0.43
1:A:240:TRP:HB3	1:A:246:PHE:CD2	2.54	0.43
1:B:203:VAL:O	1:B:203:VAL:HG23	2.18	0.43
1:B:370:GLU:HG2	1:B:373:TRP:CZ3	2.54	0.43
1:A:250:MSE:HE3	1:A:308:MSE:SE	2.69	0.43
1:A:393:ALA:HB3	1:A:416:TYR:CE2	2.47	0.43
1:A:419:VAL:HG12	1:A:464:LEU:HD12	2.00	0.43
1:A:465:PRO:HG2	1:A:468:SER:CB	2.49	0.43
1:A:217:ARG:HD2	1:A:245:MSE:O	2.18	0.43
1:C:133:MSE:HE1	1:C:155:TYR:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:PRO:HG2	1:D:468:SER:HG	1.82	0.43
1:C:56:LEU:N	1:C:57:PRO:CD	2.81	0.43
1:B:38:PRO:HA	1:B:39:PRO:HD3	1.92	0.42
1:B:200:ARG:HE	1:B:250:MSE:SE	2.52	0.42
1:A:370:GLU:HG2	1:A:373:TRP:CH2	2.53	0.42
1:C:331:ARG:HG2	1:C:331:ARG:HH11	1.84	0.42
1:D:68:TYR:CD1	1:D:68:TYR:C	2.95	0.42
1:C:250:MSE:HA	1:C:308:MSE:HB3	2.01	0.42
1:C:335:ALA:CA	1:C:384:LEU:HD22	2.49	0.42
1:D:433:LEU:HD13	1:D:437:PHE:HD2	1.85	0.42
1:B:188:ALA:HB2	1:B:216:PHE:CE1	2.54	0.42
1:D:301:PRO:O	1:D:305:ARG:HG3	2.20	0.42
1:D:391:HIS:HA	1:D:392:PRO:HD2	1.86	0.42
1:A:267:LEU:HD12	1:A:322:LEU:O	2.19	0.42
1:A:292:LEU:HB3	1:A:296:PHE:CE2	2.55	0.42
1:A:446:LEU:HD21	1:A:473:ARG:CD	2.49	0.42
1:C:393:ALA:HB3	1:C:416:TYR:HE2	1.84	0.42
1:C:416:TYR:CE1	1:C:473:ARG:HD3	2.54	0.42
1:D:347:TYR:O	1:D:350:GLU:HG2	2.20	0.42
1:A:232:GLU:O	1:A:232:GLU:HG2	2.20	0.42
1:A:137:GLU:HG2	1:A:150:PHE:CD2	2.54	0.42
1:D:188:ALA:HB2	1:D:216:PHE:CE1	2.54	0.42
1:B:117:GLY:HA2	5:B:614:HOH:O	2.19	0.42
1:B:137:GLU:HG2	1:B:150:PHE:CD2	2.54	0.42
1:B:288:PHE:CE2	1:B:292:LEU:HD11	2.55	0.42
1:D:252:TYR:O	1:D:256:ARG:HG3	2.20	0.42
1:D:305:ARG:NH2	5:D:917:HOH:O	2.53	0.42
1:D:383:ARG:HG2	1:D:383:ARG:HH11	1.85	0.42
1:D:250:MSE:HA	1:D:308:MSE:HB3	2.02	0.41
1:D:351:GLU:HG2	1:D:352:VAL:HG13	2.02	0.41
1:D:115:LEU:CD1	1:D:196:VAL:HG21	2.50	0.41
1:A:204:PRO:HG2	1:A:233:ILE:HD11	2.02	0.41
1:A:241:LEU:HD13	1:A:303:VAL:HG11	2.02	0.41
1:B:254:LEU:HD23	1:B:309:ASN:CG	2.45	0.41
1:B:352:VAL:HG12	1:B:378:ARG:HD2	2.02	0.41
1:C:310:LEU:H	1:C:310:LEU:HD23	1.85	0.41
1:C:473:ARG:NH1	1:C:474:GLU:O	2.53	0.41
1:D:39:PRO:CG	1:D:364:GLY:HA2	2.49	0.41
1:D:444:VAL:CG1	1:D:475:ALA:HB2	2.50	0.41
1:A:133:MSE:HG2	1:A:152:LEU:HD12	2.01	0.41
1:C:236:GLU:OE1	1:D:301:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:PRO:HG2	5:D:921:HOH:O	2.19	0.41
1:D:386:ARG:O	1:D:390:GLU:HG3	2.20	0.41
1:D:397:ALA:HA	1:D:398:PRO:HD3	1.90	0.41
1:A:250:MSE:HA	1:A:308:MSE:HB3	2.03	0.41
1:B:254:LEU:HD23	1:B:309:ASN:OD1	2.21	0.41
1:D:133:MSE:HE2	5:D:823:HOH:O	2.20	0.41
1:A:148:LYS:HB2	1:A:160:ASN:OD1	2.21	0.41
1:B:53:ALA:HB3	5:B:715:HOH:O	2.20	0.41
1:B:234:TRP:CD2	2:G:1:GLC:H2	2.55	0.41
1:C:196:VAL:HG12	1:C:198:GLY:H	1.85	0.41
1:C:335:ALA:CB	1:C:384:LEU:HD22	2.50	0.41
1:D:233:ILE:HG21	1:D:237:ALA:HB2	2.03	0.41
1:A:374:GLN:OE1	1:A:376:ASP:HB3	2.21	0.41
1:D:335:ALA:CA	1:D:384:LEU:HD22	2.51	0.41
2:K:5:GLC:H61	2:K:6:GLC:O5	2.21	0.41
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.36	0.41
1:C:79:HIS:CD2	3:J:2:GLC:H2	2.56	0.41
1:C:149:GLY:N	1:C:160:ASN:OD1	2.54	0.41
1:C:236:GLU:CD	1:C:236:GLU:H	2.29	0.41
1:D:255:ALA:HB2	1:D:310:LEU:O	2.21	0.41
1:B:302:GLU:CD	1:B:302:GLU:N	2.77	0.41
1:D:181:ARG:NH2	1:D:209:ASP:OD2	2.54	0.41
1:B:359:ASP:HA	1:B:362:ASN:OD1	2.21	0.40
1:D:38:PRO:HA	1:D:39:PRO:HD3	1.92	0.40
1:A:196:VAL:HG12	1:A:198:GLY:H	1.85	0.40
1:B:392:PRO:HA	1:B:395:ARG:NH1	2.37	0.40
1:C:254:LEU:HD23	1:C:309:ASN:CG	2.46	0.40
1:C:291:ARG:NH1	1:C:294:ASP:OD2	2.54	0.40
1:B:339:LEU:HD11	1:B:469:LEU:HD21	2.03	0.40
1:D:9:PHE:HB3	1:D:345:THR:HG23	2.01	0.40
1:D:413:ARG:HH11	1:D:413:ARG:HG3	1.86	0.40
1:C:421:ASN:O	1:C:467:PHE:HA	2.22	0.40
1:C:432:PRO:HG2	5:C:653:HOH:O	2.21	0.40
1:C:452:CYS:SG	1:C:460:CYS:C	3.04	0.40
1:B:135:ASN:HB2	1:B:139:SER:HB2	2.03	0.40

There are no symmetry-related clashes.

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	472/475 (99%)	446 (94%)	26 (6%)	0	100	100
1	B	473/475 (100%)	451 (95%)	21 (4%)	1 (0%)	43	55
1	C	472/475 (99%)	450 (95%)	22 (5%)	0	100	100
1	D	472/475 (99%)	444 (94%)	27 (6%)	1 (0%)	43	55
All	All	1889/1900 (99%)	1791 (95%)	96 (5%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	461	GLY
1	D	462	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	379/373 (102%)	372 (98%)	7 (2%)	51	70
1	B	378/373 (101%)	371 (98%)	7 (2%)	50	69
1	C	376/373 (101%)	364 (97%)	12 (3%)	34	51
1	D	379/373 (102%)	371 (98%)	8 (2%)	47	66
All	All	1512/1492 (101%)	1478 (98%)	34 (2%)	44	65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	TYR
1	A	133	MSE
1	A	137	GLU
1	A	173	LEU
1	A	302	GLU
1	A	400	LEU
1	A	464	LEU
1	B	100	ARG
1	B	173	LEU
1	B	182	GLU
1	B	302	GLU
1	B	320	LEU
1	B	322	LEU
1	B	384	LEU
1	C	41	LEU
1	C	68	TYR
1	C	118	VAL
1	C	173	LEU
1	C	291	ARG
1	C	302	GLU
1	C	310	LEU
1	C	322	LEU
1	C	387	LEU
1	C	400	LEU
1	C	428	ARG
1	C	464	LEU
1	D	41	LEU
1	D	68	TYR
1	D	173	LEU
1	D	291	ARG
1	D	322	LEU
1	D	369	GLU
1	D	387	LEU
1	D	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	274	GLN
1	A	284	GLN
1	B	11	GLN
1	B	70	ASN

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Mol	Chain	Res	Type
1	B	88	GLN
1	B	146	HIS
1	B	274	GLN
1	B	284	GLN
1	C	11	GLN
1	C	70	ASN
1	C	88	GLN
1	C	274	GLN
1	C	391	HIS
1	D	11	GLN
1	D	70	ASN
1	D	88	GLN
1	D	218	GLN
1	D	251	ASN
1	D	309	ASN
1	D	374	GLN
1	D	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

40 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	E	1	2	11,11,12	0.53	0	15,15,17	0.56	0
2	GLC	E	2	2	11,11,12	0.61	0	15,15,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	E	3	2	11,11,12	0.61	0	15,15,17	0.62	0
2	GLC	E	4	2	11,11,12	0.59	0	15,15,17	0.57	0
2	GLC	E	5	2	11,11,12	0.53	0	15,15,17	0.58	1 (6%)
2	GLC	E	6	2	11,11,12	0.60	0	15,15,17	0.57	0
2	GLC	E	7	2	11,11,12	0.61	0	15,15,17	0.67	0
3	GLC	F	1	3	11,11,12	0.47	0	15,15,17	0.57	0
3	GLC	F	2	3	11,11,12	0.55	0	15,15,17	0.54	0
3	GLC	F	3	3	11,11,12	0.47	0	15,15,17	0.51	0
2	GLC	G	1	2	11,11,12	0.52	0	15,15,17	0.52	0
2	GLC	G	2	2	11,11,12	0.56	0	15,15,17	0.54	0
2	GLC	G	3	2	11,11,12	0.53	0	15,15,17	0.62	0
2	GLC	G	4	2	11,11,12	0.42	0	15,15,17	0.52	0
2	GLC	G	5	2	11,11,12	0.54	0	15,15,17	0.53	0
2	GLC	G	6	2	11,11,12	0.54	0	15,15,17	0.69	0
2	GLC	G	7	2	11,11,12	0.62	0	15,15,17	0.52	0
3	GLC	H	1	3	11,11,12	0.49	0	15,15,17	0.82	1 (6%)
3	GLC	H	2	3	11,11,12	0.60	0	15,15,17	0.49	0
3	GLC	H	3	3	11,11,12	0.51	0	15,15,17	0.46	0
2	GLC	I	1	2	11,11,12	0.56	0	15,15,17	0.52	0
2	GLC	I	2	2	11,11,12	0.61	0	15,15,17	0.70	1 (6%)
2	GLC	I	3	2	11,11,12	0.63	0	15,15,17	0.56	0
2	GLC	I	4	2	11,11,12	0.52	0	15,15,17	0.55	0
2	GLC	I	5	2	11,11,12	0.54	0	15,15,17	0.55	0
2	GLC	I	6	2	11,11,12	0.54	0	15,15,17	0.60	1 (6%)
2	GLC	I	7	2	11,11,12	0.67	0	15,15,17	0.75	0
3	GLC	J	1	3	11,11,12	0.48	0	15,15,17	0.54	0
3	GLC	J	2	3	11,11,12	0.55	0	15,15,17	0.54	0
3	GLC	J	3	3	11,11,12	0.54	0	15,15,17	0.45	0
2	GLC	K	1	2	11,11,12	0.53	0	15,15,17	0.62	0
2	GLC	K	2	2	11,11,12	0.62	0	15,15,17	0.65	1 (6%)
2	GLC	K	3	2	11,11,12	0.58	0	15,15,17	0.53	0
2	GLC	K	4	2	11,11,12	0.56	0	15,15,17	0.56	0
2	GLC	K	5	2	11,11,12	0.52	0	15,15,17	0.60	1 (6%)
2	GLC	K	6	2	11,11,12	0.60	0	15,15,17	0.60	0
2	GLC	K	7	2	11,11,12	0.69	0	15,15,17	0.60	0
3	GLC	L	1	3	11,11,12	0.42	0	15,15,17	0.64	0
3	GLC	L	2	3	11,11,12	0.55	0	15,15,17	0.54	0
3	GLC	L	3	3	11,11,12	0.59	0	15,15,17	0.52	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	E	1	2	-	0/2/19/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	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	-	2/2/19/22	0/1/1/1
2	GLC	E	7	2	-	2/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/19/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	3	3	-	1/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/19/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	2/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	G	6	2	-	0/2/19/22	0/1/1/1
2	GLC	G	7	2	-	0/2/19/22	0/1/1/1
3	GLC	H	1	3	-	0/2/19/22	0/1/1/1
3	GLC	H	2	3	-	0/2/19/22	0/1/1/1
3	GLC	H	3	3	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	2/2/19/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	1/2/19/22	0/1/1/1
2	GLC	I	5	2	-	0/2/19/22	0/1/1/1
2	GLC	I	6	2	-	2/2/19/22	0/1/1/1
2	GLC	I	7	2	-	2/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/19/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	3	3	-	1/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/19/22	0/1/1/1
2	GLC	K	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	0/2/19/22	0/1/1/1
2	GLC	K	5	2	-	2/2/19/22	0/1/1/1
2	GLC	K	6	2	-	0/2/19/22	0/1/1/1
2	GLC	K	7	2	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/19/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	GLC	C1-O5-C5	2.20	115.13	112.19
3	H	1	GLC	C2-C3-C4	-2.18	107.03	110.86
2	K	5	GLC	C1-O5-C5	2.12	115.03	112.19
2	K	2	GLC	C1-O5-C5	2.09	114.98	112.19
2	I	6	GLC	C1-O5-C5	2.05	114.94	112.19
2	E	5	GLC	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	6	GLC	O5-C5-C6-O6
2	I	6	GLC	C4-C5-C6-O6
2	E	6	GLC	C4-C5-C6-O6
2	K	5	GLC	O5-C5-C6-O6
2	K	5	GLC	C4-C5-C6-O6
2	E	7	GLC	C4-C5-C6-O6
2	E	6	GLC	O5-C5-C6-O6
2	I	7	GLC	C4-C5-C6-O6
2	E	7	GLC	O5-C5-C6-O6
2	I	1	GLC	C4-C5-C6-O6
3	J	3	GLC	O5-C5-C6-O6
2	I	7	GLC	O5-C5-C6-O6
2	G	4	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	G	4	GLC	O5-C5-C6-O6
2	I	4	GLC	C4-C5-C6-O6
3	F	3	GLC	O5-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	GLC	1	0
2	I	3	GLC	1	0
2	K	1	GLC	1	0
2	G	5	GLC	1	0
2	E	3	GLC	1	0
2	G	4	GLC	1	0

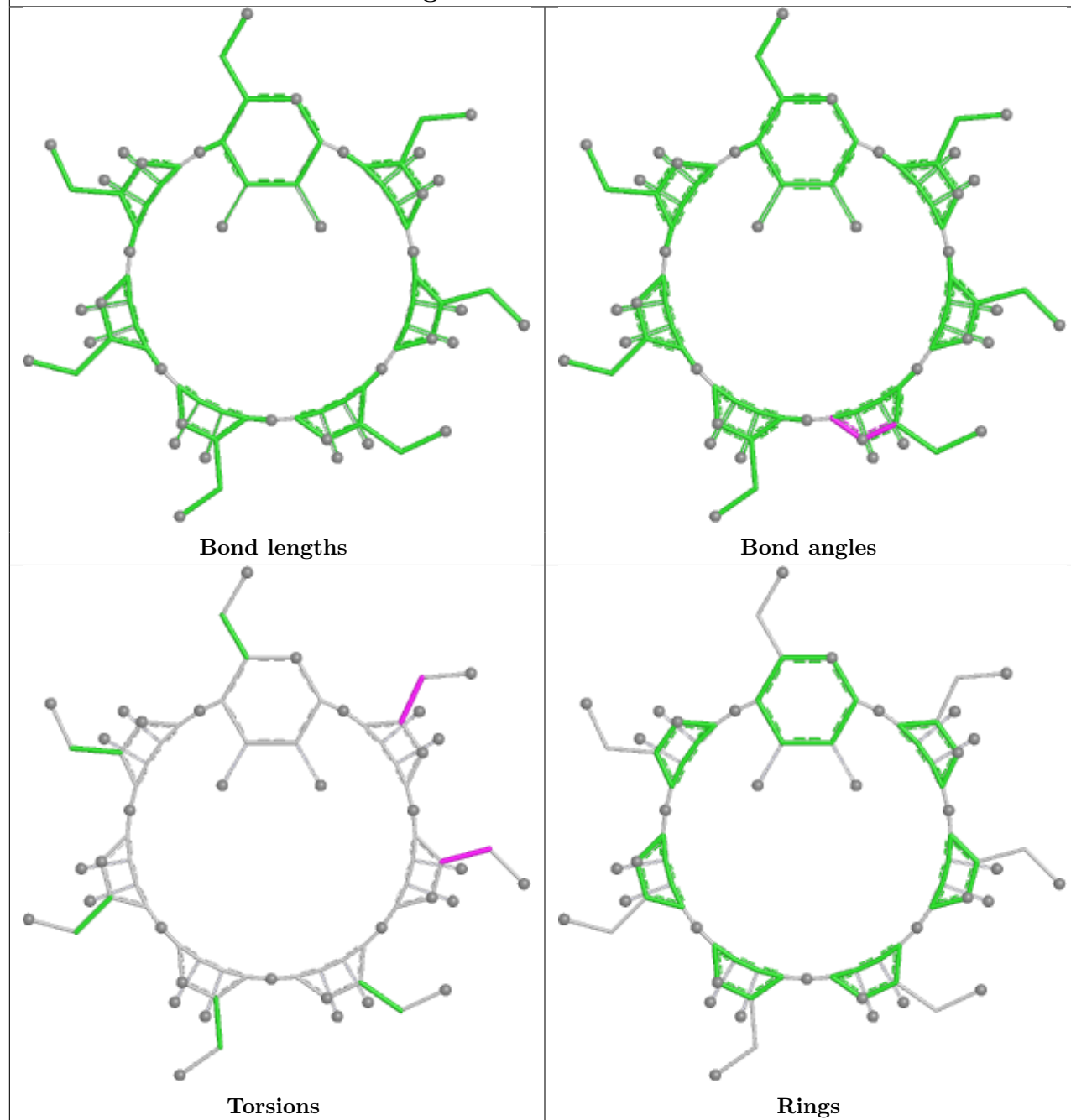
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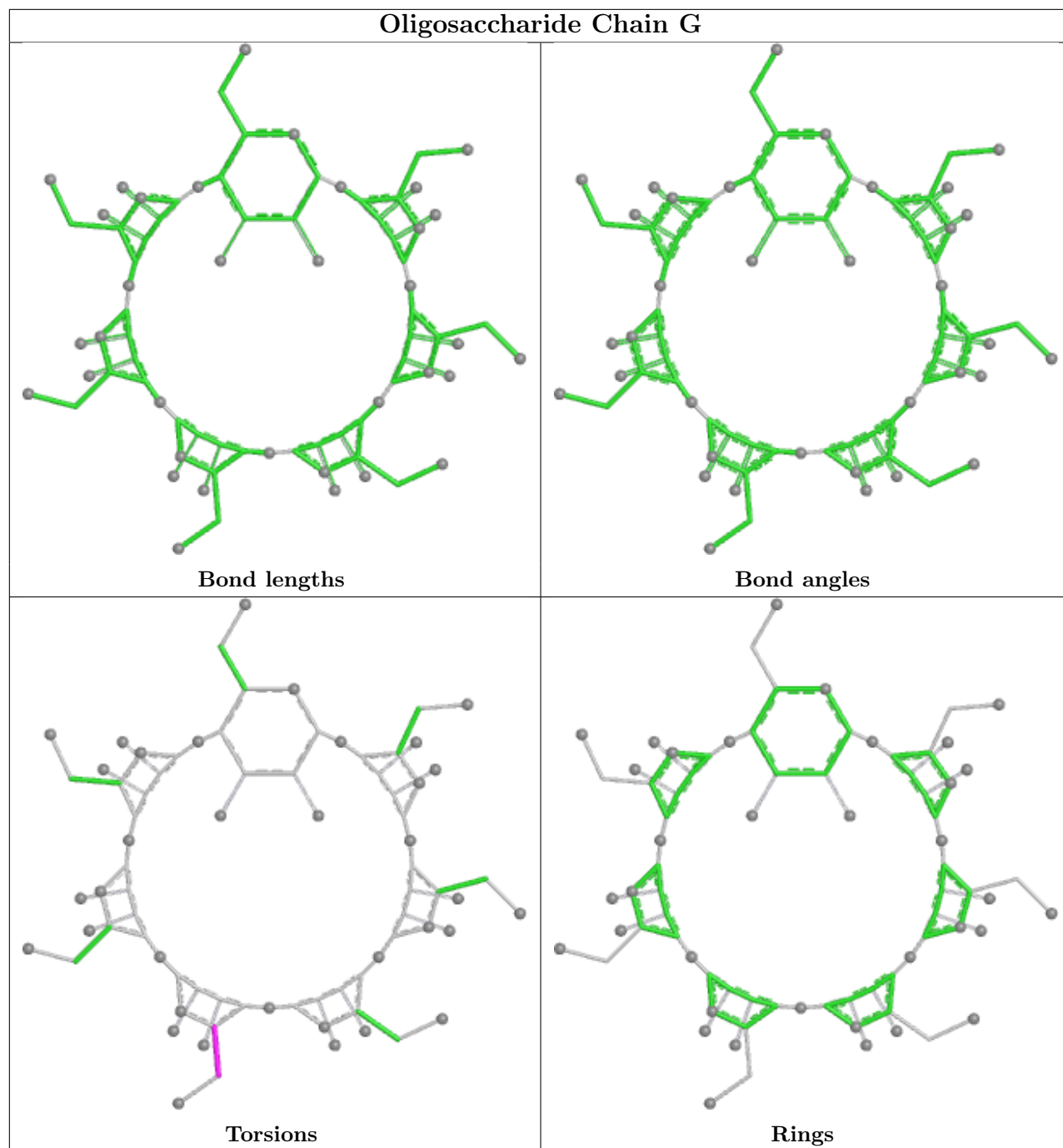
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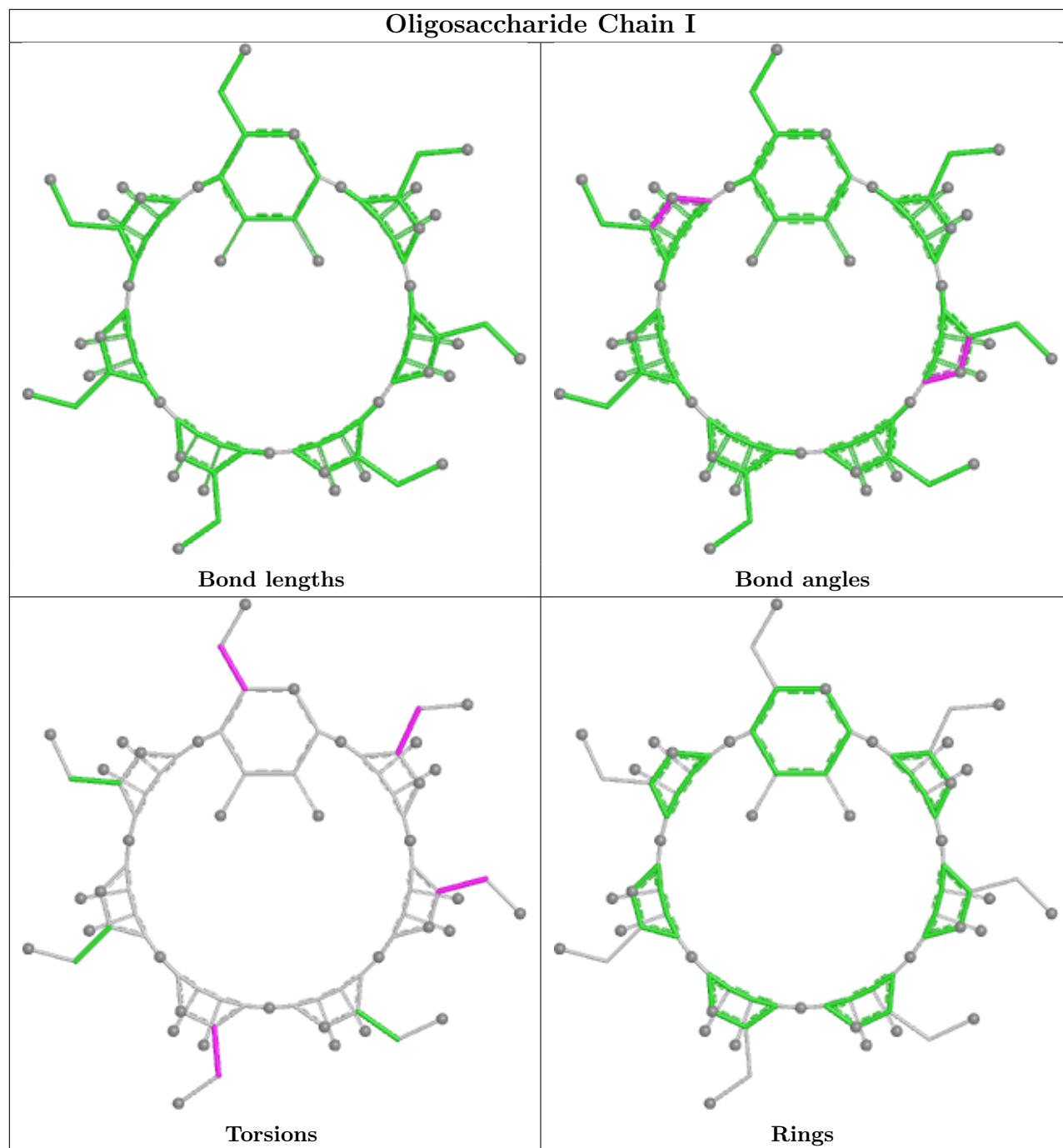
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	6	GLC	1	0
3	J	1	GLC	1	0
2	K	5	GLC	1	0
2	K	3	GLC	1	0
3	H	1	GLC	1	0
3	F	1	GLC	1	0
2	G	1	GLC	2	0
2	E	4	GLC	1	0
3	J	2	GLC	1	0

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

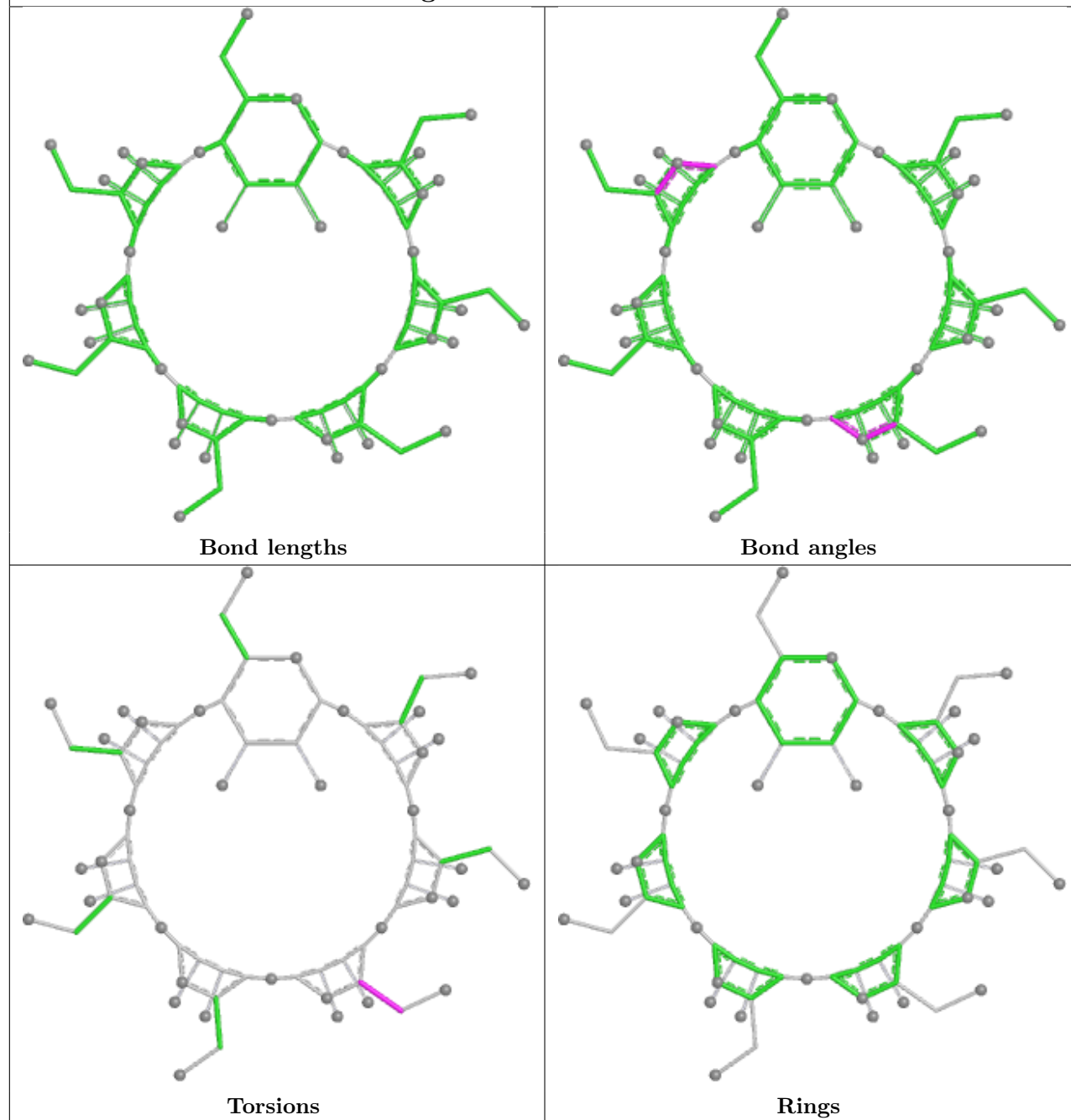
Oligosaccharide Chain E

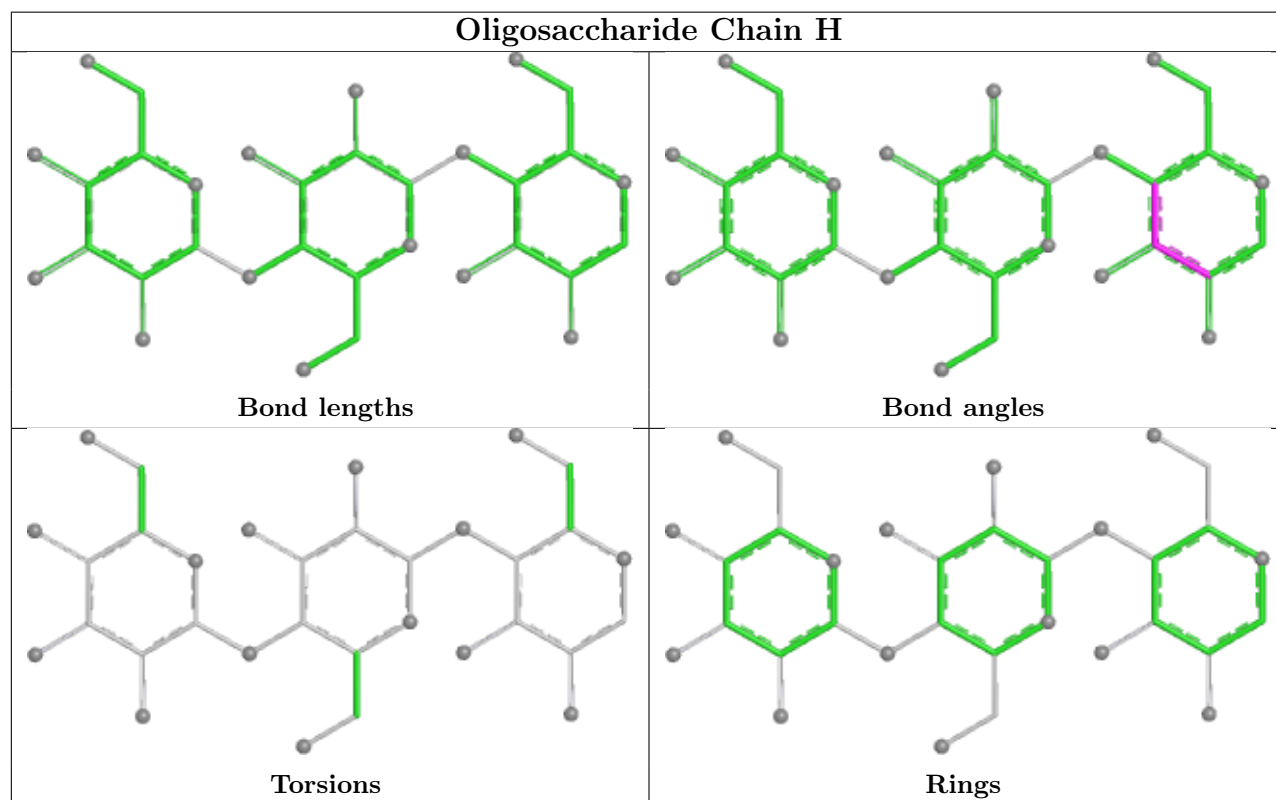
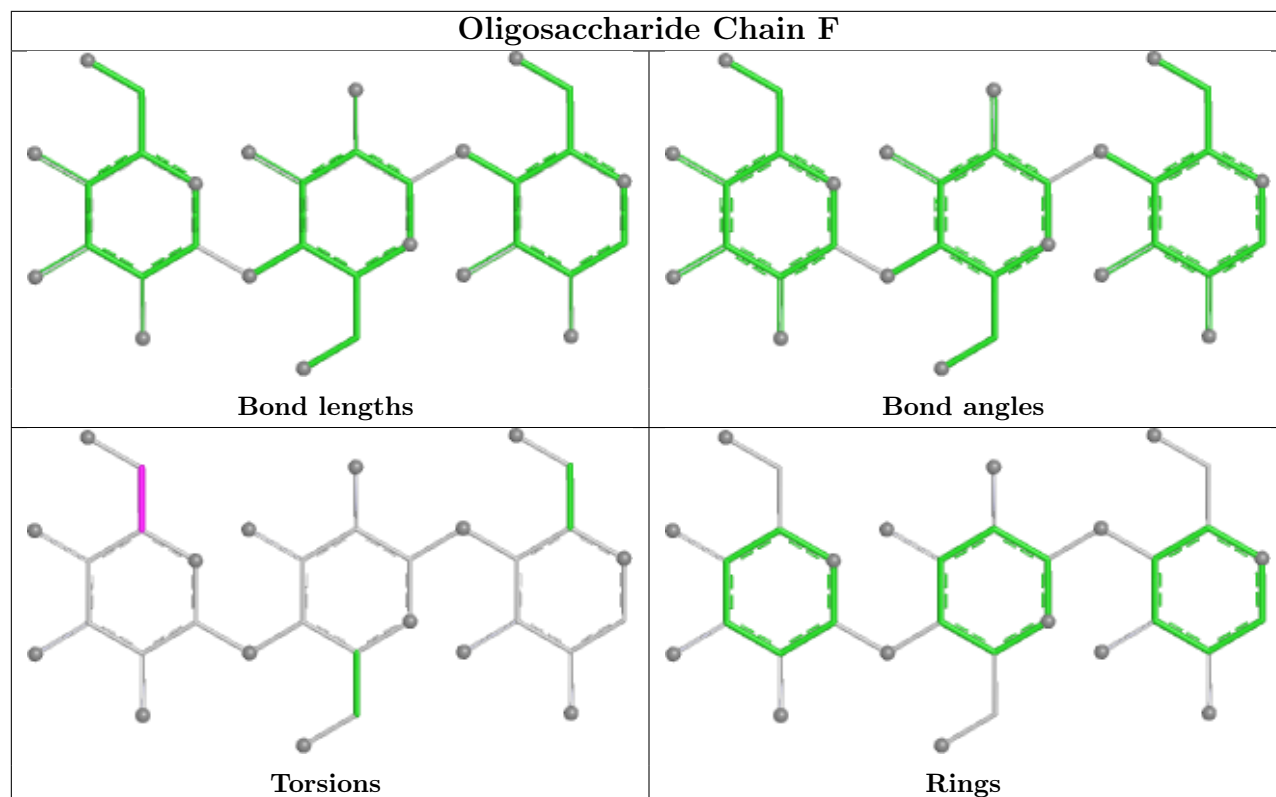


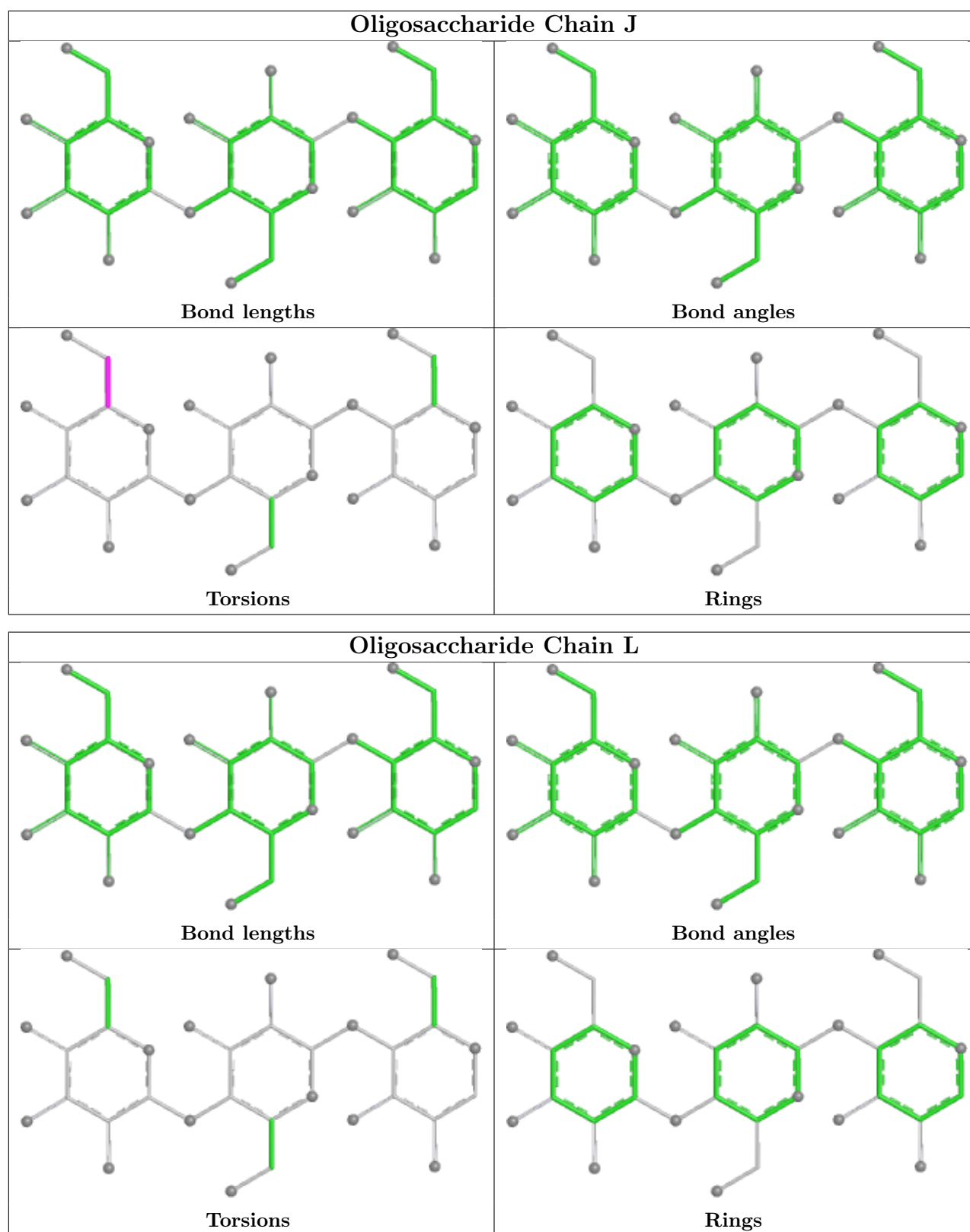




Oligosaccharide Chain K







5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PO4	D	800	-	4,4,4	1.77	2 (50%)	6,6,6	0.45	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	800	PO4	P-O4	-2.06	1.48	1.54
4	D	800	PO4	P-O2	-2.02	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	467/475 (98%)	0.05	5 (1%) 78 79	16, 31, 46, 59	0
1	B	467/475 (98%)	-0.21	8 (1%) 69 70	9, 25, 44, 64	1 (0%)
1	C	467/475 (98%)	0.01	5 (1%) 78 79	15, 27, 52, 65	0
1	D	467/475 (98%)	0.07	12 (2%) 57 59	12, 29, 63, 80	0
All	All	1868/1900 (98%)	-0.02	30 (1%) 70 72	9, 28, 52, 80	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	460	CYS	4.1
1	C	239	PHE	4.0
1	A	441	GLY	3.3
1	D	475	ALA	3.2
1	B	265	GLU	3.0
1	C	240	TRP	3.0
1	D	406	ASP	2.9
1	D	407	GLY	2.8
1	C	31	PRO	2.8
1	B	475	ALA	2.6
1	D	441	GLY	2.6
1	B	474	GLU	2.5
1	D	459	LEU	2.5
1	D	451	VAL	2.5
1	B	406	ASP	2.5
1	C	475	ALA	2.5
1	D	455	GLN	2.4
1	D	31	PRO	2.3
1	B	455	GLN	2.3
1	D	461	GLY	2.2
1	D	425	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	460	CYS	2.2
1	D	456	GLY	2.2
1	A	240	TRP	2.2
1	D	457	GLY	2.2
1	C	406	ASP	2.1
1	B	440	GLY	2.1
1	B	439	ARG	2.1
1	A	440	GLY	2.0
1	A	438	PRO	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
3	GLC	J	3	11/12	0.65	0.13	55,56,57,57	0
2	GLC	I	6	11/12	0.72	0.14	70,72,73,73	0
2	GLC	I	3	11/12	0.75	0.13	65,67,69,71	0
3	GLC	F	3	11/12	0.78	0.12	52,53,55,55	0
2	GLC	E	6	11/12	0.79	0.13	50,56,56,57	0
2	GLC	I	7	11/12	0.79	0.14	59,63,66,67	0
2	GLC	E	3	11/12	0.81	0.11	54,55,58,59	0
3	GLC	L	3	11/12	0.81	0.10	39,41,41,43	0
2	GLC	I	5	11/12	0.82	0.11	74,76,77,78	0
3	GLC	J	2	11/12	0.83	0.14	43,47,49,52	0
3	GLC	F	2	11/12	0.83	0.12	40,44,47,50	0
2	GLC	E	4	11/12	0.83	0.11	54,56,57,57	0
2	GLC	G	5	11/12	0.84	0.10	37,39,40,44	0
2	GLC	I	4	11/12	0.84	0.11	72,73,74,75	0
2	GLC	K	6	11/12	0.86	0.10	42,45,47,48	0
3	GLC	J	1	11/12	0.87	0.11	43,45,46,46	0
2	GLC	E	5	11/12	0.87	0.10	54,56,56,57	0
3	GLC	F	1	11/12	0.87	0.11	36,41,42,42	0
3	GLC	H	3	11/12	0.87	0.09	31,32,35,36	0

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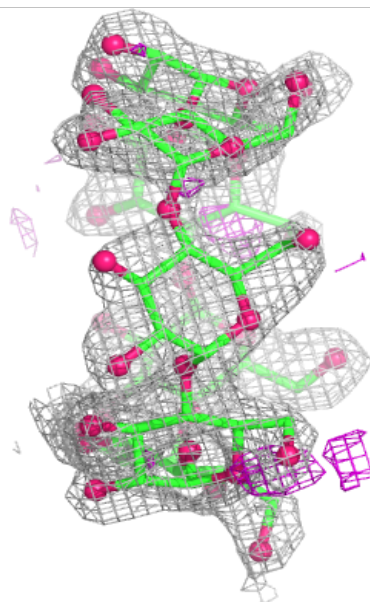
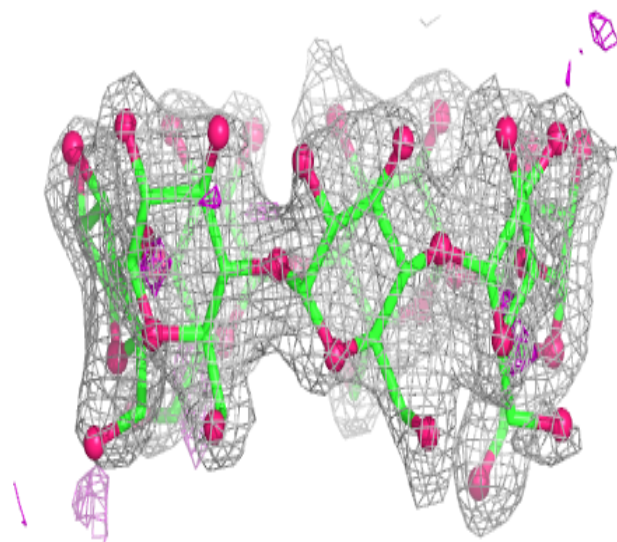
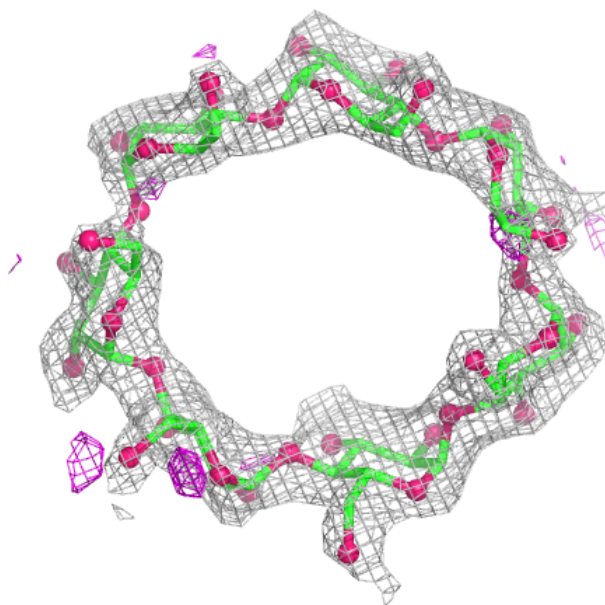
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	H	1	11/12	0.88	0.11	23,27,29,31	0
2	GLC	I	2	11/12	0.89	0.11	56,58,60,62	0
2	GLC	E	2	11/12	0.89	0.10	43,45,46,51	0
2	GLC	K	4	11/12	0.90	0.08	44,45,46,47	0
2	GLC	K	5	11/12	0.90	0.08	45,46,48,49	0
2	GLC	E	1	11/12	0.90	0.09	37,41,42,43	0
2	GLC	G	6	11/12	0.90	0.08	31,33,36,38	0
2	GLC	K	2	11/12	0.90	0.10	40,40,42,43	0
2	GLC	K	3	11/12	0.90	0.08	41,42,44,45	0
3	GLC	L	2	11/12	0.91	0.09	30,33,35,37	0
2	GLC	K	1	11/12	0.91	0.09	37,40,42,44	0
2	GLC	G	4	11/12	0.92	0.08	31,33,36,37	0
2	GLC	E	7	11/12	0.92	0.07	41,43,47,48	0
2	GLC	G	3	11/12	0.92	0.07	31,33,34,34	0
2	GLC	I	1	11/12	0.92	0.09	45,53,55,55	0
2	GLC	K	7	11/12	0.92	0.08	38,42,44,44	0
3	GLC	L	1	11/12	0.93	0.09	28,32,34,35	0
3	GLC	H	2	11/12	0.95	0.06	20,26,27,31	0
2	GLC	G	1	11/12	0.95	0.07	22,23,26,26	0
2	GLC	G	2	11/12	0.96	0.05	22,24,25,29	0
2	GLC	G	7	11/12	0.96	0.05	23,25,28,30	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.

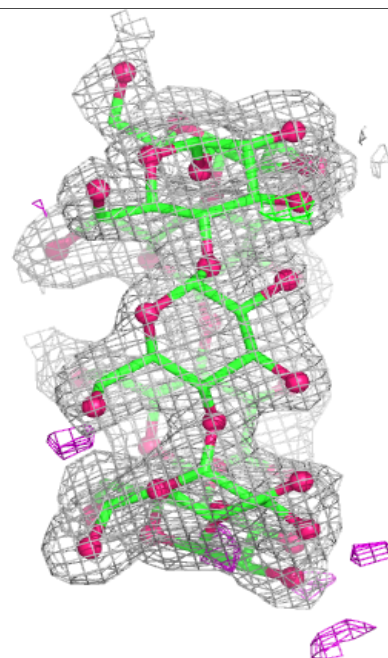
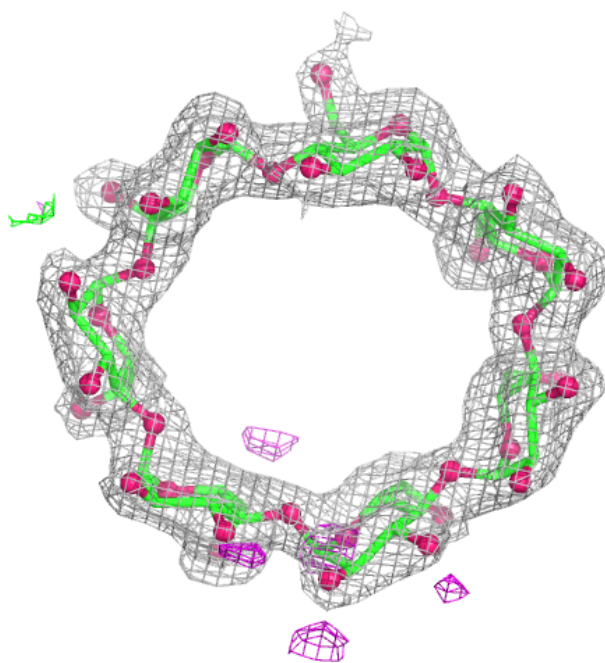
Electron density around Chain E:

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



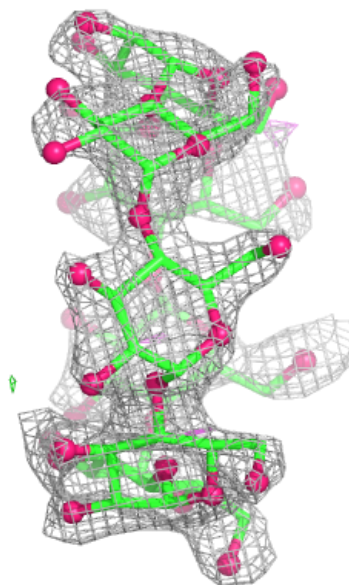
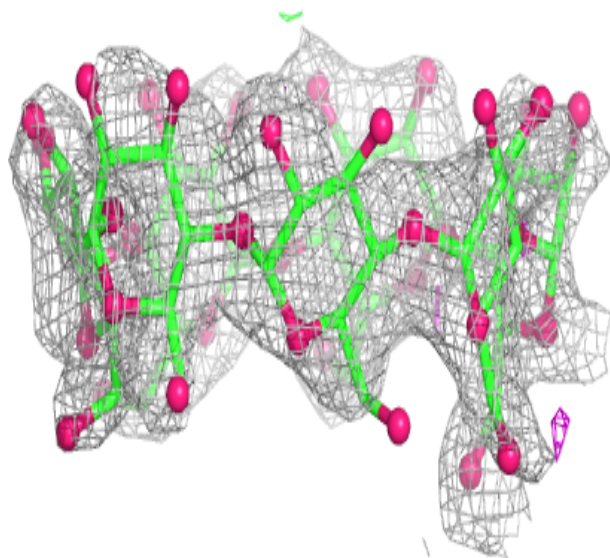
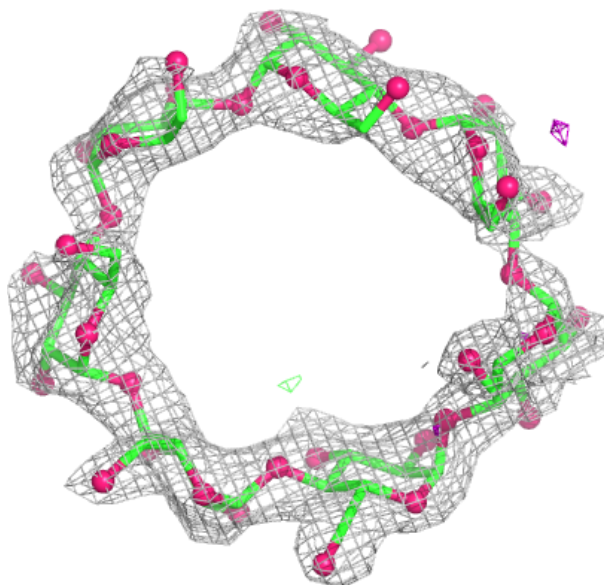
Electron density around Chain G:

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



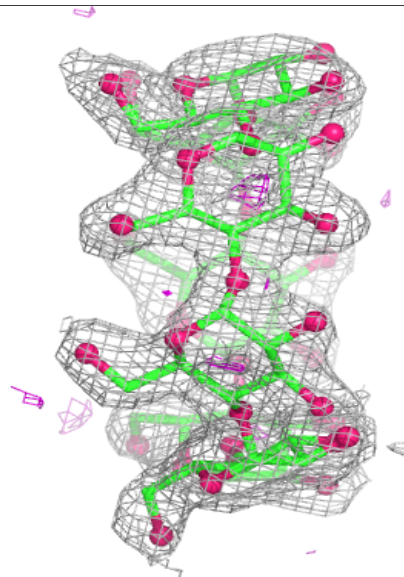
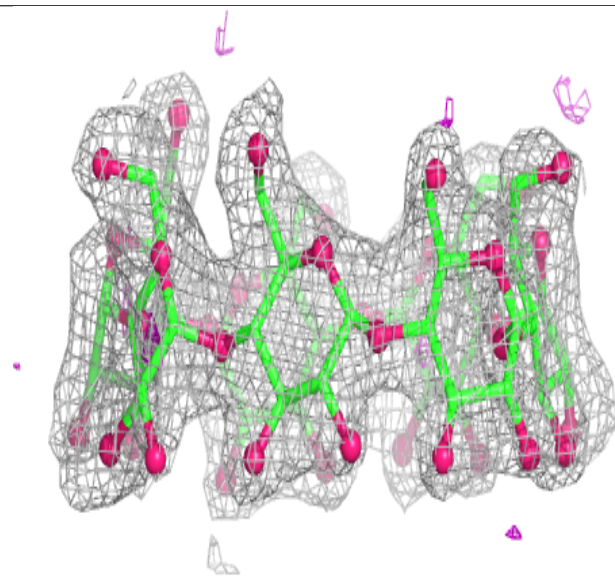
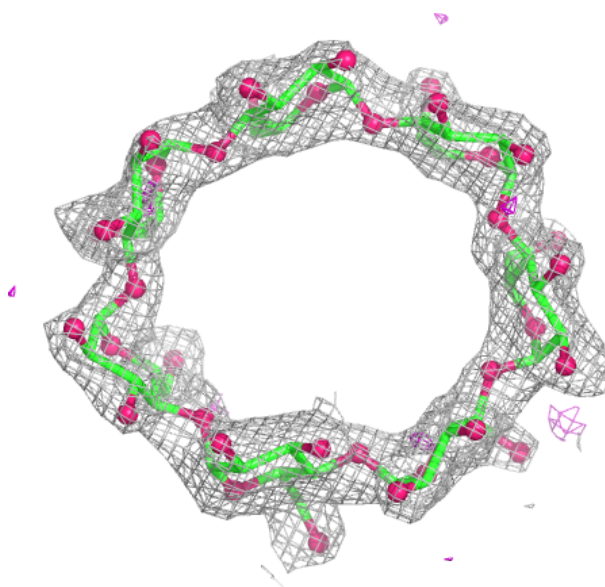
Electron density around Chain I:

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



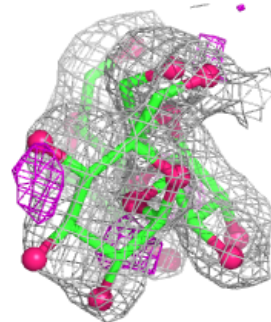
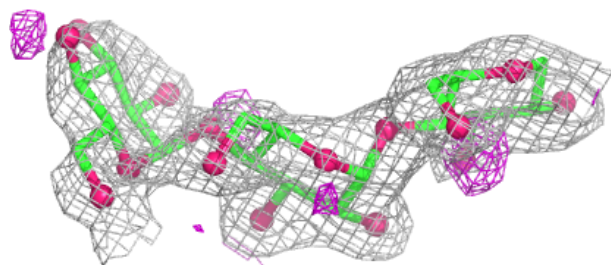
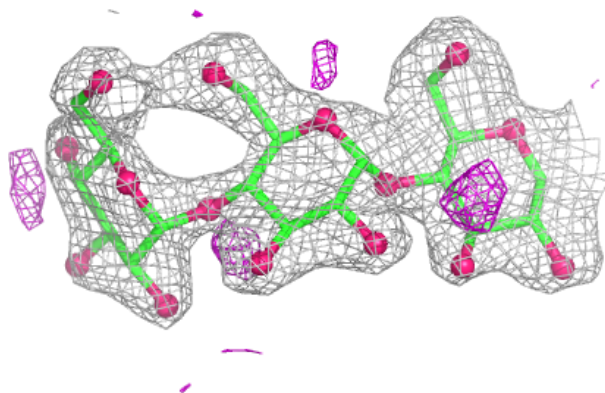
Electron density around Chain K:

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

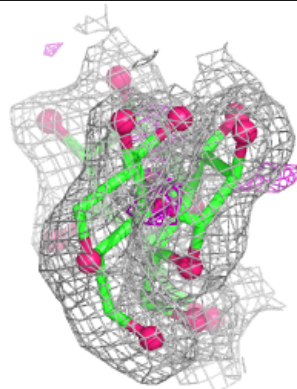
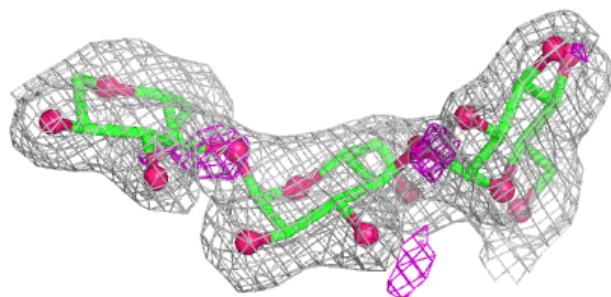
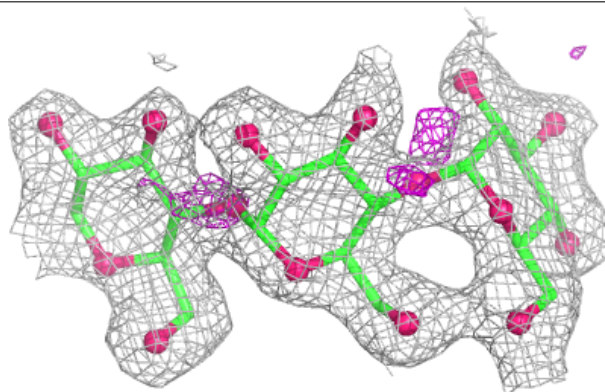


Electron density around Chain F:

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

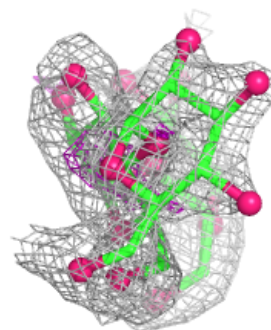
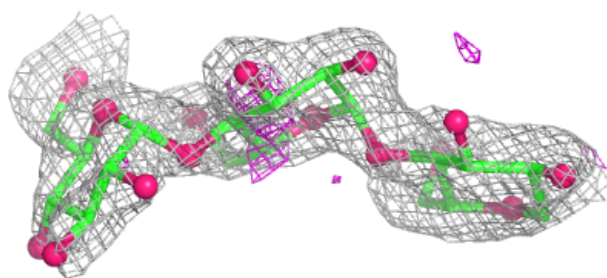
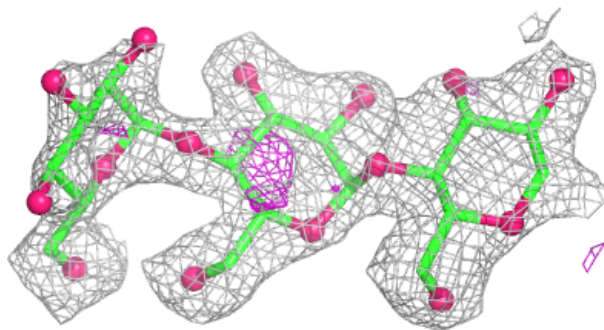
**Electron density around Chain H:**

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

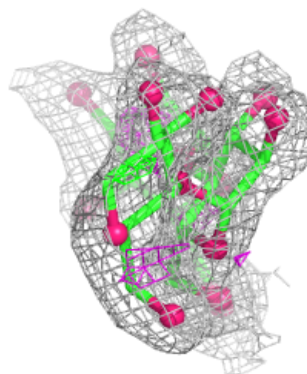
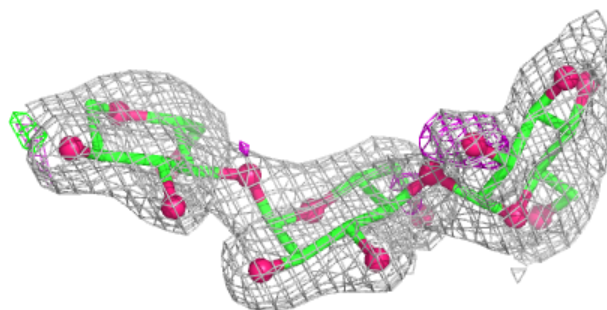
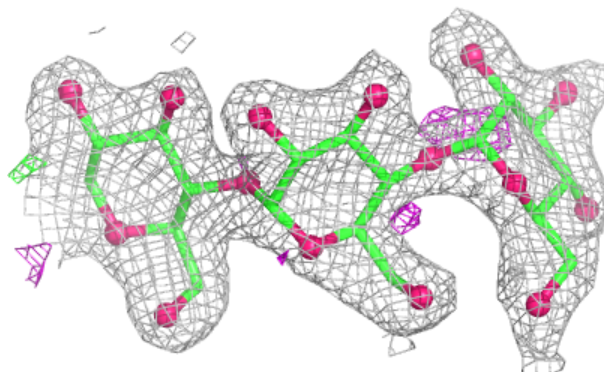


Electron density around Chain J:

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

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	D	800	5/5	0.94	0.09	55,55,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.