



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2026 – 12:14 AM UTC

PDB ID : 8XRX / pdb_00008xrx
Title : The crystal structure of a GH3 enzyme CcBgl3B with glucose and gentiobiose
Authors : Su, J.Y.
Deposited on : 2024-01-08
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

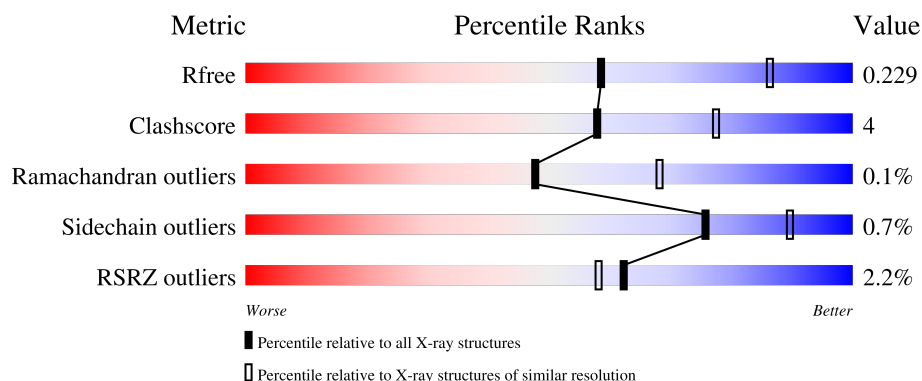
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	768	% 90% 7% % %
1	B	768	% 91% 6% % %
1	C	768	3% 83% 14% % %
1	D	768	% 88% 9% % %
1	E	768	5% 70% 10% 20%

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Mol	Chain	Length	Quality of chain
1	F	768	
2	G	2	
2	J	2	
2	K	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	K	2	-	-	X	-
4	BGC	C	801	-	-	X	-
5	GLC	B	802	-	-	X	-

2 Entry composition [i](#)

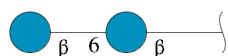
There are 6 unique types of molecules in this entry. The entry contains 33122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GH3 enzyme CcBgl3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			5631	3545	998	1073	15			
1	B	750	Total	C	N	O	S	0	0	0
			5617	3536	998	1068	15			
1	C	741	Total	C	N	O	S	0	0	0
			5555	3500	982	1058	15			
1	D	749	Total	C	N	O	S	0	0	0
			5617	3536	996	1070	15			
1	E	611	Total	C	N	O	S	0	0	0
			4566	2876	806	873	11			
1	F	750	Total	C	N	O	S	0	0	0
			5623	3541	998	1069	15			

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-6)-beta-D-glucopyranose.



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

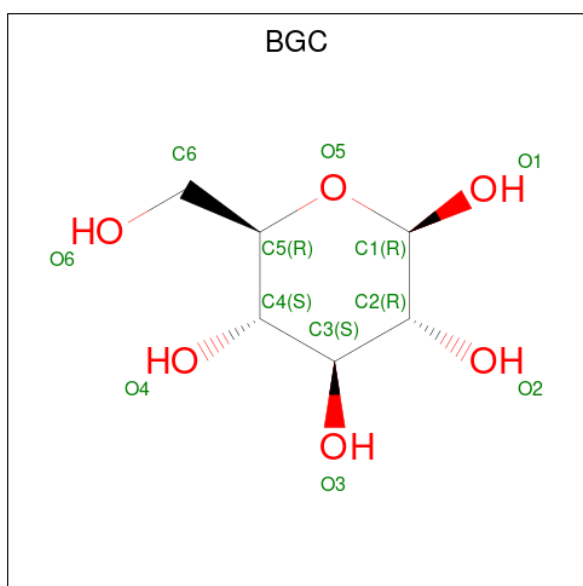
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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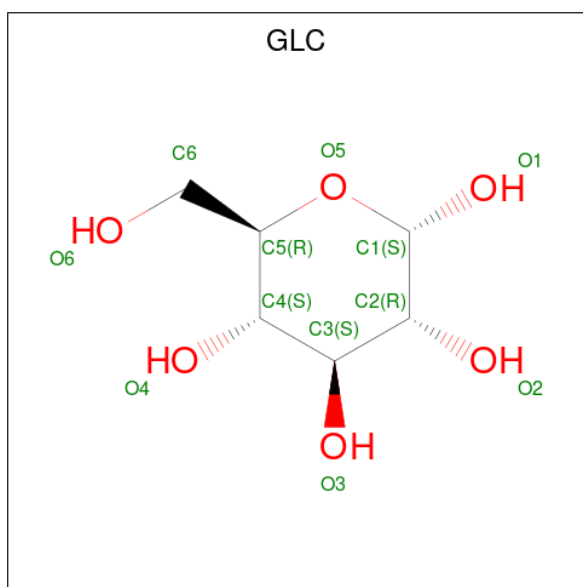
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		
4	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			11	6	5		

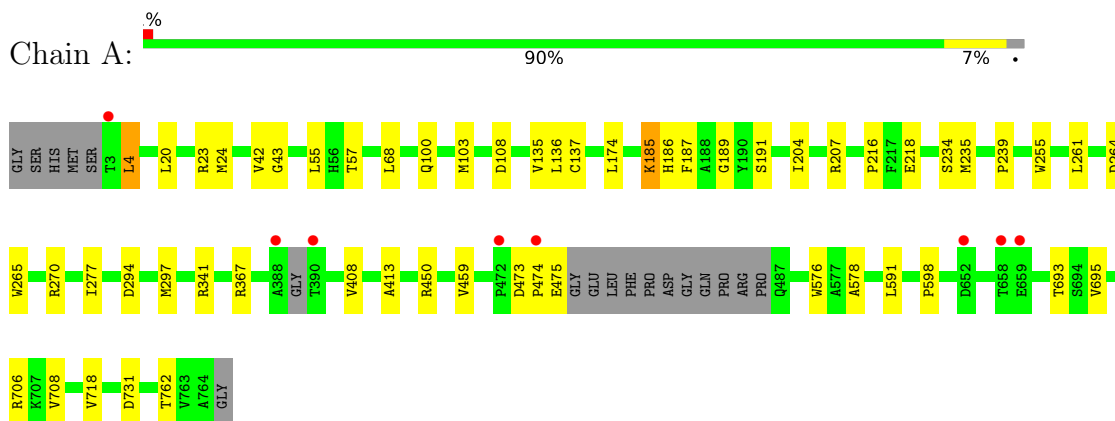
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	144	Total	O	0	0
			144	144		
6	B	155	Total	O	0	0
			155	155		
6	C	18	Total	O	0	0
			18	18		
6	D	38	Total	O	0	0
			38	38		
6	E	14	Total	O	0	0
			14	14		
6	F	34	Total	O	0	0
			34	34		

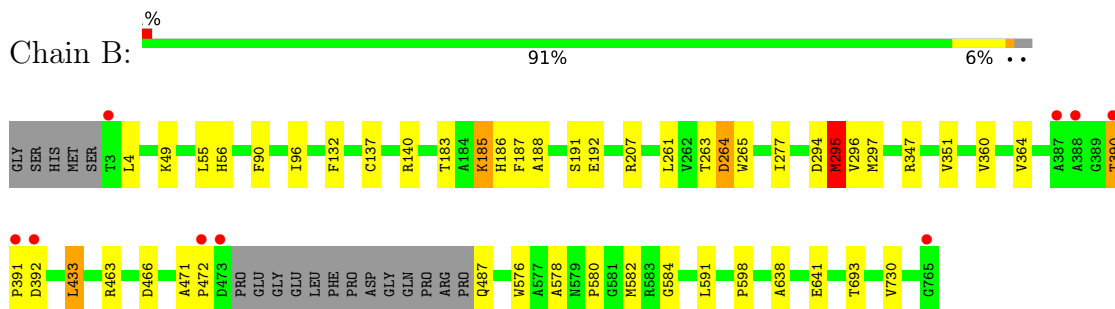
3 Residue-property plots [i](#)

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.

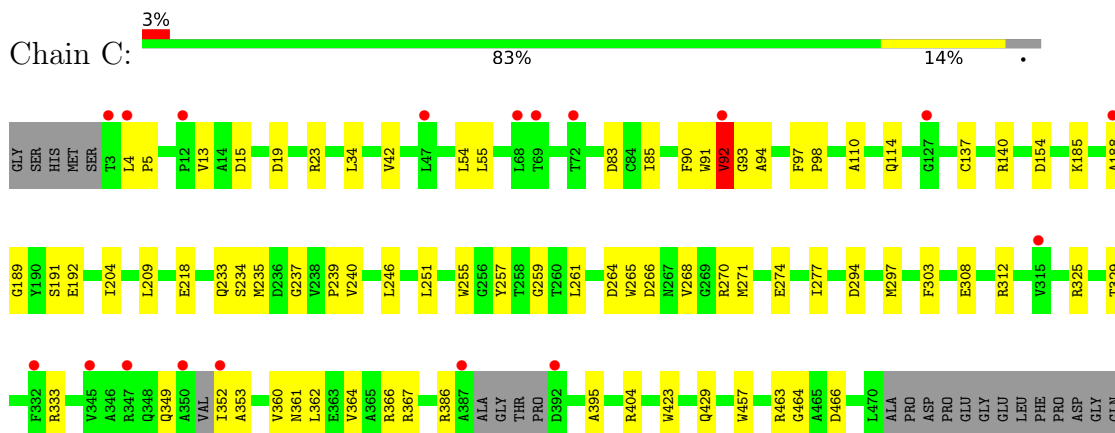
• Molecule 1: GH3 enzyme CcBgl3B



• Molecule 1: GH3 enzyme CcBgl3B

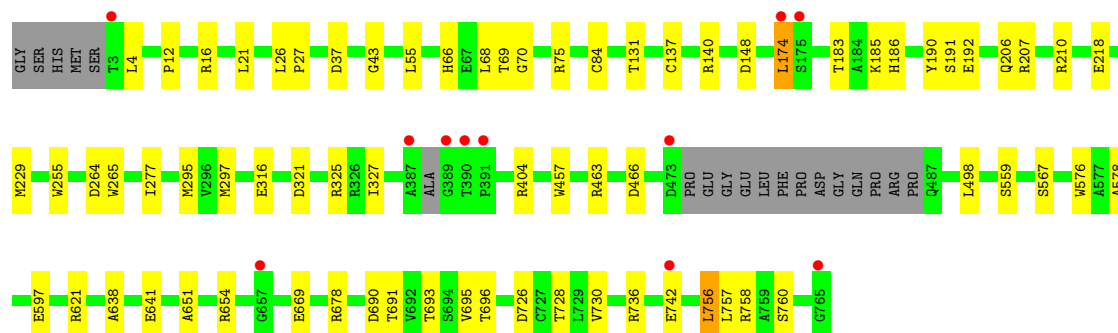
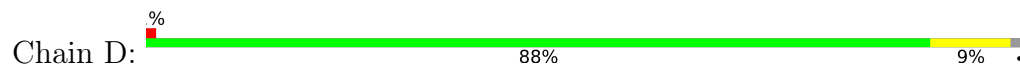


• Molecule 1: GH3 enzyme CcBgl3B

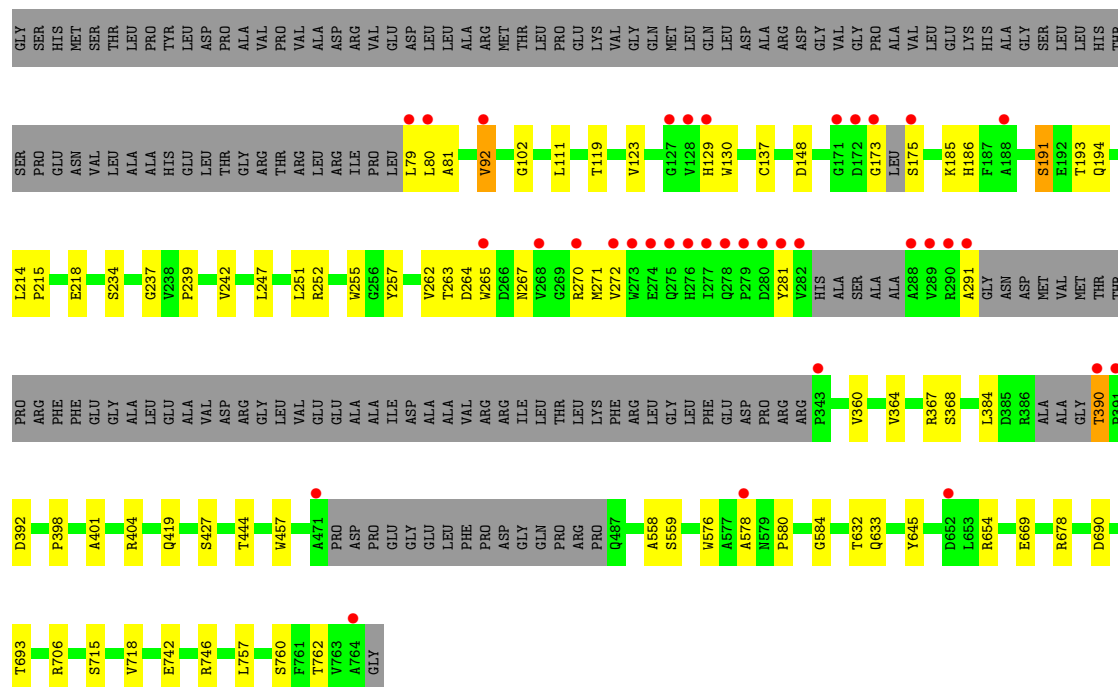




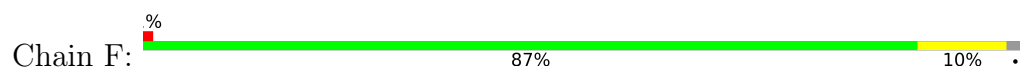
• Molecule 1: GH3 enzyme CcBgl3B

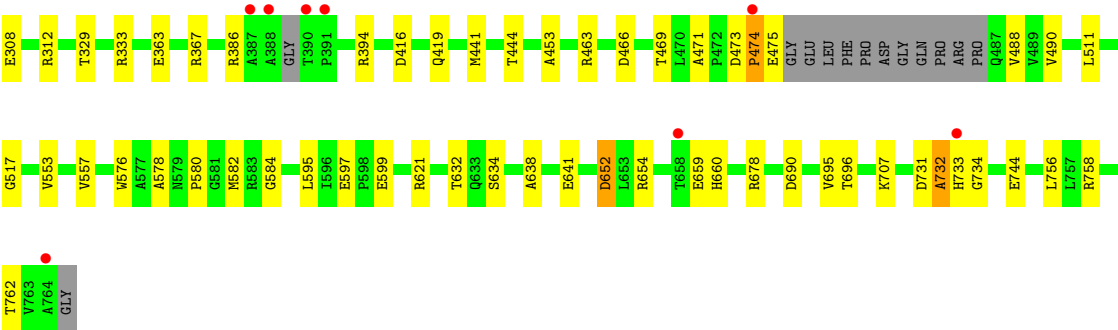


• Molecule 1: GH3 enzyme CcBgl3B



• Molecule 1: GH3 enzyme CcBgl3B





• Molecule 2: beta-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain G: 100%



• Molecule 2: beta-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain J: 50% 50%



• Molecule 2: beta-D-glucopyranose-(1-6)-beta-D-glucopyranose

Chain K: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.09Å 183.01Å 269.15Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	19.95 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.95-2.50) 99.1 (19.95-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.50Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.230 0.198 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (0.75%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33122	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% 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: CA, GLC, BGC

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	0.54	2/5754 (0.0%)	0.63	3/7870 (0.0%)
1	B	0.63	5/5739 (0.1%)	0.72	10/7848 (0.1%)
1	C	0.43	1/5674 (0.0%)	0.58	4/7756 (0.1%)
1	D	0.52	1/5739 (0.0%)	0.58	1/7847 (0.0%)
1	E	0.48	0/4666	0.56	0/6383
1	F	0.46	0/5746	0.59	4/7860 (0.1%)
All	All	0.52	9/33318 (0.0%)	0.62	22/45564 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	ASP	N-CA	-15.67	1.27	1.45
1	B	183	THR	C-O	-6.74	1.15	1.23
1	B	295	MET	C-O	-6.44	1.16	1.24
1	B	296	VAL	C-O	-5.94	1.17	1.24
1	A	187	PHE	C-O	-5.80	1.17	1.24
1	B	264	ASP	CG-OD1	-5.59	1.14	1.25
1	A	762	THR	C-O	-5.36	1.17	1.24
1	D	190	TYR	C-O	-5.17	1.17	1.24
1	C	688	VAL	C-O	-5.04	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	THR	CA-C-N	15.48	149.44	122.67
1	B	263	THR	C-N-CA	15.48	149.44	122.67
1	B	263	THR	O-C-N	-9.97	108.97	122.23
1	B	264	ASP	CA-CB-CG	-9.87	102.73	112.60
1	B	185	LYS	N-CA-C	9.26	124.33	109.24
1	B	390	THR	N-CA-C	7.54	121.74	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	756	LEU	N-CA-C	7.40	120.79	108.73
1	C	13	VAL	N-CA-C	7.38	118.15	110.62
1	B	264	ASP	CB-CG-OD1	6.76	133.95	118.40
1	A	185	LYS	N-CA-C	6.75	120.66	109.46
1	F	732	ALA	N-CA-C	-6.18	101.79	110.50
1	F	734	GLY	N-CA-C	5.85	123.43	115.30
1	B	49	LYS	CA-C-N	-5.70	110.65	121.54
1	B	49	LYS	C-N-CA	-5.70	110.65	121.54
1	B	4	LEU	N-CA-C	5.70	116.16	109.60
1	F	652	ASP	N-CA-C	5.58	119.39	112.24
1	C	658	THR	N-CA-C	5.32	116.89	111.14
1	C	349	GLN	N-CA-C	5.31	117.06	111.28
1	A	185	LYS	CA-C-N	5.30	130.26	122.63
1	A	185	LYS	C-N-CA	5.30	130.26	122.63
1	C	91	TRP	N-CA-C	-5.21	103.81	110.53
1	F	652	ASP	N-CA-CB	-5.16	104.46	112.30

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	5631	0	5543	40	0
1	B	5617	0	5529	41	0
1	C	5555	0	5462	67	0
1	D	5617	0	5529	43	0
1	E	4566	0	4456	47	0
1	F	5623	0	5535	53	0
2	G	23	0	21	4	0
2	J	23	0	21	2	0
2	K	23	0	21	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	B	12	0	10	2	0
4	C	12	0	12	6	0
5	B	11	0	10	6	0
6	A	144	0	0	2	0
6	B	155	0	0	2	0
6	C	18	0	0	1	0
6	D	38	0	0	0	0
6	E	14	0	0	0	0
6	F	34	0	0	0	0
All	All	33122	0	32149	290	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 4.

All (290) 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:B:264:ASP:OD1	5:B:802:GLC:C1	1.97	1.12
1:F:297:MET:HE1	2:K:2:BGC:H6C1	1.41	0.99
1:B:297:MET:HE1	5:B:802:GLC:H62	1.42	0.98
1:A:473:ASP:OD1	1:A:474:PRO:HD2	1.73	0.89
1:A:473:ASP:OD1	1:A:474:PRO:CD	2.24	0.84
1:B:297:MET:HE1	5:B:802:GLC:C6	2.08	0.82
1:F:297:MET:CE	2:K:2:BGC:H6C1	2.12	0.80
1:C:598:PRO:HG2	1:C:644:SER:HA	1.68	0.75
1:F:473:ASP:HB2	1:F:474:PRO:HD2	1.71	0.73
1:F:597:GLU:OE2	1:F:678:ARG:NH1	2.21	0.72
1:A:591:LEU:HD11	1:A:598:PRO:HG3	1.71	0.72
1:D:654:ARG:NH2	1:D:669:GLU:OE1	2.22	0.71
1:B:591:LEU:HD11	1:B:598:PRO:HG3	1.73	0.71
1:C:700:LYS:CE	1:C:753:GLU:OE2	2.38	0.71
1:F:83:ASP:OD2	2:K:2:BGC:O6	2.09	0.70
1:D:207:ARG:NH1	1:D:730:VAL:O	2.24	0.69
1:E:263:THR:HG22	1:E:264:ASP:O	1.92	0.69
1:D:463:ARG:NH1	1:D:466:ASP:OD1	2.24	0.68
1:E:263:THR:HG23	1:E:267:ASN:HB2	1.76	0.68
1:D:70:GLY:HA2	1:D:75:ARG:HD2	1.76	0.68
1:C:83:ASP:OD2	4:C:801:BGC:H6C1	1.93	0.67
1:E:130:TRP:CZ2	1:E:262:VAL:HG21	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:MET:HE1	2:K:2:BGC:C6	2.23	0.67
1:F:756:LEU:O	1:F:758:ARG:NH2	2.26	0.67
1:A:185:LYS:HE3	2:G:2:BGC:O3	1.95	0.67
1:B:297:MET:CE	5:B:802:GLC:H62	2.24	0.65
1:D:576:TRP:CE2	1:D:578:ALA:HB2	2.33	0.64
2:K:1:BGC:H6C2	2:K:2:BGC:H6C2	1.79	0.63
1:D:316:GLU:N	1:D:316:GLU:OE1	2.33	0.62
1:C:188:ALA:HB1	1:C:209:LEU:HD21	1.82	0.61
1:C:297:MET:HE1	4:C:801:BGC:O5	2.01	0.60
1:E:576:TRP:CZ2	1:E:578:ALA:HB2	2.36	0.60
1:C:266:ASP:O	1:C:270:ARG:HG3	2.02	0.60
1:E:390:THR:O	1:E:390:THR:OG1	2.16	0.60
1:B:390:THR:HG23	1:B:390:THR:O	2.02	0.59
1:F:137:CYS:HB3	1:F:191:SER:HB3	1.84	0.59
1:B:207:ARG:NH2	6:B:906:HOH:O	2.35	0.59
1:B:137:CYS:HB3	1:B:191:SER:HB3	1.84	0.59
1:A:265:TRP:O	1:A:270:ARG:NH2	2.36	0.59
1:F:185:LYS:HE2	2:K:2:BGC:O3	2.04	0.58
1:B:137:CYS:SG	1:B:186:HIS:HB2	2.42	0.58
1:A:576:TRP:CZ2	1:A:578:ALA:HB2	2.38	0.58
1:F:744:GLU:OE2	1:F:758:ARG:HG2	2.02	0.58
1:C:576:TRP:CE2	1:C:578:ALA:HB2	2.39	0.58
1:C:590:GLU:HA	1:C:595:LEU:HD12	1.85	0.58
1:F:463:ARG:NH1	1:F:466:ASP:OD1	2.32	0.58
1:C:233:GLN:HE21	1:C:235:MET:HE3	1.68	0.57
1:E:252:ARG:NH2	1:E:257:TYR:O	2.36	0.57
1:F:265:TRP:HE3	1:F:297:MET:HE2	1.68	0.57
1:E:137:CYS:HB3	1:E:191:SER:HB2	1.85	0.57
1:F:265:TRP:CE3	1:F:297:MET:HE2	2.39	0.57
1:C:576:TRP:CZ2	1:C:578:ALA:HB2	2.40	0.57
1:E:247:LEU:HD12	1:E:291:ALA:HB3	1.87	0.57
1:D:137:CYS:HB3	1:D:191:SER:HB3	1.86	0.57
1:B:140:ARG:HD3	1:B:192:GLU:OE1	2.04	0.57
1:E:130:TRP:HZ2	1:E:262:VAL:HG21	1.67	0.57
1:B:265:TRP:HE3	1:B:297:MET:HE2	1.70	0.57
1:A:189:GLY:HA3	1:A:235:MET:HE1	1.86	0.56
1:B:261:LEU:O	1:B:294:ASP:HB2	2.04	0.56
4:C:801:BGC:O1	4:C:801:BGC:O6	2.20	0.56
1:F:580:PRO:HG2	1:F:584:GLY:HA3	1.88	0.56
1:B:265:TRP:CE3	1:B:297:MET:HE2	2.40	0.56
1:E:80:LEU:HD12	1:E:129:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:GLY:HA3	1:F:235:MET:HE1	1.87	0.56
1:E:576:TRP:CE2	1:E:578:ALA:HB2	2.40	0.56
1:E:654:ARG:NH1	1:E:669:GLU:OE1	2.34	0.56
1:C:268:VAL:HA	1:C:271:MET:HE2	1.88	0.56
1:F:576:TRP:CE2	1:F:578:ALA:HB2	2.40	0.56
4:B:801:BGC:O6	5:B:802:GLC:O6	2.23	0.55
1:A:136:LEU:HD23	1:A:216:PRO:HB2	1.88	0.55
1:A:297:MET:HE1	2:G:2:BGC:C5	2.37	0.55
1:E:80:LEU:HD12	1:E:129:HIS:HE1	1.71	0.55
1:B:55:LEU:CD2	1:B:297:MET:HE3	2.37	0.55
1:C:140:ARG:NH2	6:C:903:HOH:O	2.40	0.55
1:C:137:CYS:HB3	1:C:191:SER:HB3	1.87	0.54
1:B:132:PHE:HB3	1:B:185:LYS:HE3	1.90	0.54
1:C:42:VAL:HG23	1:C:54:LEU:HD11	1.89	0.54
1:F:135:VAL:HG22	1:F:185:LYS:HD3	1.89	0.54
1:A:277:ILE:HA	1:B:693:THR:O	2.08	0.54
1:F:638:ALA:O	1:F:641:GLU:HG2	2.08	0.54
1:C:366:ARG:HE	1:C:596:ILE:HG21	1.72	0.54
1:D:140:ARG:HD3	1:D:192:GLU:OE1	2.08	0.54
1:E:234:SER:HA	1:E:239:PRO:HA	1.89	0.54
1:F:108:ASP:OD2	1:F:367:ARG:NH2	2.41	0.54
1:F:394:ARG:NH1	1:F:453:ALA:O	2.35	0.54
1:C:154:ASP:OD1	1:C:617:TYR:OH	2.25	0.54
1:D:756:LEU:O	1:D:758:ARG:NH1	2.40	0.54
1:F:60:GLU:CD	1:F:60:GLU:H	2.15	0.54
1:F:471:ALA:O	1:F:488:VAL:HG22	2.08	0.53
1:F:659:GLU:OE1	1:F:659:GLU:N	2.31	0.53
1:F:140:ARG:HD3	1:F:192:GLU:OE2	2.08	0.53
1:A:137:CYS:HB3	1:A:191:SER:HB3	1.88	0.53
1:C:140:ARG:HD3	1:C:192:GLU:OE1	2.09	0.53
1:E:173:GLY:C	1:E:175:SER:N	2.66	0.53
1:C:240:VAL:HG13	1:C:246:LEU:HD23	1.90	0.53
1:C:234:SER:HA	1:C:239:PRO:HA	1.90	0.52
1:C:360:VAL:O	1:C:364:VAL:HG23	2.09	0.52
1:B:463:ARG:NH1	1:B:466:ASP:OD1	2.38	0.52
1:F:204:ILE:HB	1:F:235:MET:HE2	1.91	0.52
1:C:693:THR:OG1	1:C:695:VAL:O	2.20	0.51
1:C:657:GLY:O	1:C:660:HIS:HE1	1.92	0.51
1:E:392:ASP:OD1	1:E:392:ASP:N	2.44	0.51
1:B:638:ALA:O	1:B:641:GLU:HG2	2.11	0.51
1:C:188:ALA:HB3	1:C:246:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:VAL:O	1:B:364:VAL:HG23	2.11	0.51
1:C:92:VAL:O	1:C:94:ALA:N	2.43	0.51
1:D:218:GLU:HB2	1:D:255:TRP:CZ2	2.46	0.51
1:C:261:LEU:O	1:C:294:ASP:HB2	2.11	0.51
1:E:272:VAL:HG21	1:E:281:TYR:CZ	2.46	0.51
1:A:264:ASP:OD1	1:A:265:TRP:N	2.40	0.50
1:A:450:ARG:NH1	1:A:459:VAL:O	2.40	0.50
1:C:55:LEU:HD21	1:C:297:MET:HE3	1.94	0.50
1:A:204:ILE:HB	1:A:235:MET:HE2	1.92	0.50
1:A:261:LEU:O	1:A:294:ASP:HB2	2.11	0.50
1:E:218:GLU:OE1	1:E:255:TRP:NE1	2.44	0.50
1:E:706:ARG:NH1	1:E:718:VAL:HG13	2.27	0.50
1:C:270:ARG:HD3	1:C:274:GLU:OE1	2.12	0.50
1:C:597:GLU:OE1	1:C:678:ARG:NH1	2.45	0.49
1:E:632:THR:O	1:E:633:GLN:HB2	2.11	0.49
1:F:363:GLU:O	1:F:367:ARG:HG3	2.12	0.49
1:A:693:THR:O	1:B:277:ILE:HA	2.13	0.49
1:A:20:LEU:O	1:A:24:MET:HG3	2.11	0.49
1:C:110:ALA:O	1:C:114:GLN:HG3	2.13	0.49
1:F:621:ARG:NH2	1:F:690:ASP:O	2.45	0.49
1:E:218:GLU:HB2	1:E:255:TRP:CZ2	2.48	0.49
1:C:34:LEU:HD11	1:C:303:PHE:HB2	1.94	0.49
1:B:433:LEU:N	1:B:433:LEU:HD12	2.28	0.49
1:B:471:ALA:O	1:B:487:GLN:N	2.46	0.49
1:C:257:TYR:CZ	1:C:259:GLY:HA3	2.47	0.49
1:A:265:TRP:HB2	1:A:297:MET:HE2	1.93	0.48
1:C:185:LYS:HE2	4:C:801:BGC:O3	2.14	0.48
1:A:265:TRP:CA	1:A:297:MET:HE2	2.43	0.48
1:C:325:ARG:O	1:C:329:THR:OG1	2.25	0.48
1:B:471:ALA:HB1	1:B:472:PRO:CD	2.44	0.48
1:D:264:ASP:OD1	2:J:2:BGC:O5	2.31	0.48
1:B:55:LEU:HD21	1:B:297:MET:HE3	1.96	0.48
1:C:362:LEU:HD22	1:C:583:ARG:NH2	2.28	0.48
1:D:84:CYS:HB2	1:D:131:THR:OG1	2.14	0.48
1:B:56:HIS:NE2	4:B:801:BGC:H6C1	2.29	0.48
1:A:174:LEU:O	1:A:341:ARG:NH2	2.46	0.47
1:C:189:GLY:HA3	1:C:235:MET:HE1	1.96	0.47
1:C:329:THR:HG22	1:C:333:ARG:HE	1.79	0.47
1:E:580:PRO:HG2	1:E:584:GLY:HA3	1.96	0.47
1:B:187:PHE:CD1	1:B:188:ALA:HB2	2.49	0.47
1:E:185:LYS:HG2	1:E:186:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:GLU:HB2	1:F:255:TRP:CZ2	2.50	0.47
1:D:638:ALA:O	1:D:641:GLU:HB2	2.15	0.47
1:D:691:THR:HB	1:D:742:GLU:HG2	1.97	0.47
1:E:185:LYS:HG2	1:E:186:HIS:ND1	2.30	0.47
1:F:329:THR:O	1:F:333:ARG:HG3	2.15	0.47
1:F:695:VAL:HG21	1:F:731:ASP:HA	1.95	0.47
1:B:207:ARG:NH1	1:B:730:VAL:O	2.47	0.47
1:C:97:PHE:HA	1:C:361:ASN:OD1	2.15	0.47
1:C:218:GLU:HB2	1:C:255:TRP:CZ2	2.50	0.47
1:C:700:LYS:NZ	1:C:753:GLU:OE2	2.47	0.47
1:F:44:PRO:O	1:F:48:GLU:HB3	2.15	0.47
1:F:576:TRP:CZ2	1:F:578:ALA:HB2	2.49	0.47
1:C:423:TRP:CZ3	1:C:429:GLN:HG2	2.50	0.47
1:F:55:LEU:CD2	1:F:297:MET:HE3	2.44	0.47
1:F:441:MET:HE2	1:F:582:MET:HE1	1.96	0.47
1:D:66:HIS:O	1:D:69:THR:O	2.33	0.46
1:D:264:ASP:OD1	1:D:265:TRP:N	2.46	0.46
1:D:728:THR:HG23	1:D:736:ARG:HH21	1.80	0.46
1:E:558:ALA:O	1:E:578:ALA:HA	2.16	0.46
1:D:728:THR:OG1	1:D:736:ARG:HG2	2.14	0.46
1:A:297:MET:HE1	2:G:2:BGC:C6	2.46	0.46
1:E:265:TRP:O	1:E:270:ARG:NH1	2.34	0.46
1:E:148:ASP:HB3	1:E:559:SER:HB2	1.97	0.46
1:F:416:ASP:OD1	1:F:416:ASP:N	2.44	0.46
1:E:742:GLU:OE2	1:E:762:THR:OG1	2.23	0.45
1:B:90:PHE:HA	1:B:433:LEU:HD21	1.98	0.45
1:D:726:ASP:O	1:D:728:THR:HG22	2.17	0.45
1:A:218:GLU:HB2	1:A:255:TRP:CZ2	2.51	0.45
1:C:308:GLU:HG2	1:C:312:ARG:HD3	1.98	0.45
1:F:732:ALA:O	1:F:733:HIS:CG	2.70	0.45
1:C:83:ASP:OD1	4:C:801:BGC:O4	2.29	0.45
1:F:659:GLU:O	1:F:659:GLU:HG2	2.17	0.45
1:D:651:ALA:O	1:D:757:LEU:HD13	2.17	0.45
1:F:517:GLY:HA3	1:F:557:VAL:O	2.17	0.45
1:D:43:GLY:HA2	1:D:68:LEU:HD13	1.99	0.45
1:B:265:TRP:HE3	1:B:297:MET:CE	2.30	0.45
1:C:657:GLY:O	1:C:660:HIS:CE1	2.69	0.45
1:F:469:THR:HG23	1:F:490:VAL:HB	1.99	0.45
1:B:55:LEU:C	1:B:55:LEU:HD12	2.42	0.44
1:B:96:ILE:H	1:B:582:MET:HE2	1.82	0.44
1:E:263:THR:CG2	1:E:267:ASN:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:PRO:HG2	1:B:584:GLY:HA3	2.00	0.44
1:C:83:ASP:HB3	1:C:85:ILE:HD11	1.98	0.44
1:A:137:CYS:SG	1:A:186:HIS:HB2	2.58	0.44
1:A:265:TRP:CB	1:A:297:MET:HE2	2.48	0.44
1:A:408:VAL:HG12	1:A:413:ALA:HB1	1.98	0.44
1:C:90:PHE:CZ	1:C:429:GLN:HB2	2.53	0.44
1:F:261:LEU:HD23	1:F:293:ASN:HA	1.98	0.44
1:E:193:THR:O	1:E:194:GLN:C	2.59	0.44
1:C:654:ARG:NH2	1:C:669:GLU:OE2	2.51	0.44
1:C:463:ARG:NH1	1:C:466:ASP:OD1	2.50	0.44
1:D:70:GLY:HA2	1:D:75:ARG:CD	2.47	0.44
2:G:1:BGC:H6C2	2:G:2:BGC:H6C2	2.00	0.44
1:F:202:ALA:HB1	1:F:204:ILE:HG13	1.99	0.44
1:D:597:GLU:OE1	1:D:678:ARG:NH1	2.51	0.43
1:C:700:LYS:HE3	1:C:753:GLU:OE2	2.16	0.43
1:B:576:TRP:CZ2	1:B:578:ALA:HB2	2.54	0.43
1:E:81:ALA:HB2	1:E:130:TRP:CE3	2.52	0.43
1:A:4:LEU:HD22	1:A:23:ARG:CZ	2.48	0.43
1:A:234:SER:HA	1:A:239:PRO:HA	2.00	0.43
1:F:308:GLU:HG2	1:F:312:ARG:HD3	2.00	0.43
1:B:295:MET:HE2	1:B:295:MET:HB2	1.67	0.43
1:C:386:ARG:HA	1:C:395:ALA:HA	2.00	0.43
1:D:185:LYS:HG2	1:D:186:HIS:CE1	2.54	0.43
1:E:360:VAL:O	1:E:364:VAL:HG23	2.19	0.43
1:F:632:THR:C	1:F:634:SER:H	2.26	0.43
1:C:15:ASP:N	1:C:15:ASP:OD1	2.50	0.43
1:C:264:ASP:OD1	1:C:265:TRP:N	2.41	0.43
1:E:384:LEU:HD22	1:E:398:PRO:HD3	2.01	0.43
1:D:12:PRO:O	1:D:16:ARG:HG3	2.19	0.43
1:D:576:TRP:CZ2	1:D:578:ALA:HB2	2.54	0.43
1:D:26:LEU:HB3	1:D:27:PRO:HD3	2.01	0.43
1:D:404:ARG:HB2	1:D:457:TRP:CD2	2.54	0.43
1:D:693:THR:OG1	1:D:695:VAL:O	2.26	0.43
1:F:732:ALA:C	1:F:733:HIS:CG	2.96	0.43
1:B:347:ARG:O	1:B:351:VAL:HG22	2.19	0.42
1:D:321:ASP:O	1:D:325:ARG:HG3	2.19	0.42
1:E:111:LEU:HD22	1:E:367:ARG:HH11	1.84	0.42
1:F:660:HIS:HB2	1:F:762:THR:O	2.19	0.42
1:A:693:THR:OG1	1:A:695:VAL:O	2.29	0.42
1:C:5:PRO:HD2	1:C:23:ARG:HH21	1.85	0.42
1:E:102:GLY:O	1:E:368:SER:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:645:TYR:HB3	1:E:678:ARG:HD2	2.01	0.42
1:C:237:GLY:HA2	1:D:696:THR:OG1	2.19	0.42
1:D:21:LEU:HD21	1:D:321:ASP:HB2	2.01	0.42
1:F:130:TRP:CZ2	1:F:227:THR:HG21	2.54	0.42
1:A:207:ARG:NH2	6:A:913:HOH:O	2.53	0.42
1:B:55:LEU:HD22	1:B:297:MET:HE3	2.02	0.42
1:C:658:THR:O	1:C:660:HIS:ND1	2.48	0.42
1:D:316:GLU:H	1:D:316:GLU:CD	2.27	0.42
1:E:242:VAL:HG13	1:E:271:MET:HE1	2.02	0.42
1:E:119:THR:O	1:E:123:VAL:HG23	2.20	0.41
1:F:419:GLN:OE1	1:F:444:THR:HA	2.20	0.41
1:A:100:GLN:HA	1:A:103:MET:HE3	2.01	0.41
1:C:4:LEU:HB3	1:C:5:PRO:CD	2.50	0.41
1:C:464:GLY:HA3	1:C:541:LEU:HD22	2.02	0.41
1:E:247:LEU:O	1:E:251:LEU:HB3	2.20	0.41
1:C:638:ALA:O	1:C:641:GLU:HG2	2.20	0.41
1:D:295:MET:HE3	1:D:327:ILE:HD13	2.02	0.41
1:A:576:TRP:CE2	1:A:578:ALA:HB2	2.55	0.41
1:F:386:ARG:HG3	1:F:595:LEU:HD22	2.02	0.41
1:A:108:ASP:OD2	1:A:367:ARG:NH1	2.50	0.41
1:B:140:ARG:NH2	6:B:908:HOH:O	2.40	0.41
1:B:391:PRO:O	1:B:392:ASP:CB	2.68	0.41
1:B:297:MET:HE1	5:B:802:GLC:C5	2.49	0.41
1:C:352:ILE:HG22	1:C:353:ALA:N	2.34	0.41
1:F:9:PRO:HA	1:F:16:ARG:NH2	2.35	0.41
1:D:621:ARG:NH2	1:D:690:ASP:O	2.51	0.41
1:E:79:LEU:HD23	1:E:79:LEU:HA	1.75	0.41
1:E:404:ARG:HB2	1:E:457:TRP:CD2	2.56	0.41
1:E:746:ARG:HA	1:E:757:LEU:O	2.21	0.41
1:A:4:LEU:HD22	1:A:23:ARG:NH2	2.36	0.41
1:A:473:ASP:HA	1:A:474:PRO:HD3	1.81	0.41
1:C:19:ASP:O	1:C:23:ARG:HG3	2.20	0.41
1:C:251:LEU:O	1:C:255:TRP:HB2	2.21	0.41
1:A:43:GLY:HA2	1:A:68:LEU:HD13	2.03	0.41
1:B:576:TRP:CE2	1:B:578:ALA:HB2	2.56	0.41
1:C:185:LYS:CE	4:C:801:BGC:O3	2.69	0.41
1:D:148:ASP:HB3	1:D:559:SER:HB2	2.02	0.41
1:D:206:GLN:O	1:D:210:ARG:HG3	2.21	0.41
1:F:599:GLU:OE1	1:F:707:LYS:HE3	2.20	0.41
1:C:277:ILE:HA	1:D:693:THR:O	2.21	0.41
1:D:183:THR:HG21	1:D:229:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:VAL:HG22	1:A:185:LYS:HE2	2.03	0.40
1:A:708:VAL:HG21	1:A:718:VAL:HG21	2.04	0.40
1:B:187:PHE:HA	1:B:188:ALA:HA	1.85	0.40
1:C:92:VAL:HB	1:C:93:GLY:H	1.81	0.40
1:C:204:ILE:HD12	1:C:235:MET:HE2	2.02	0.40
1:D:137:CYS:SG	1:D:186:HIS:HB2	2.61	0.40
1:D:297:MET:HE1	2:J:2:BGC:C6	2.51	0.40
1:E:214:LEU:N	1:E:215:PRO:CD	2.85	0.40
1:F:511:LEU:HD11	1:F:553:VAL:HG23	2.02	0.40
1:A:42:VAL:HG12	1:A:68:LEU:HD12	2.03	0.40
1:E:419:GLN:OE1	1:E:444:THR:HA	2.21	0.40
1:E:690:ASP:OD2	1:E:693:THR:HG22	2.21	0.40
1:C:367:ARG:NE	1:C:599:GLU:OE2	2.45	0.40
1:E:398:PRO:HG2	1:E:401:ALA:HB3	2.02	0.40
1:F:83:ASP:CG	2:K:2:BGC:O6	2.64	0.40
1:C:97:PHE:HB3	1:C:98:PRO:HD2	2.02	0.40
1:D:37:ASP:HA	1:D:55:LEU:HD12	2.02	0.40
1:D:498:LEU:HD12	1:D:498:LEU:HA	1.87	0.40
1:A:706:ARG:NH1	1:A:718:VAL:HG13	2.37	0.40
1:A:731:ASP:HB2	6:A:943:HOH:O	2.20	0.40
1:C:404:ARG:HB2	1:C:457:TRP:CD2	2.56	0.40
1:E:237:GLY:HA2	1:F:696:THR:OG1	2.21	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	744/768 (97%)	713 (96%)	30 (4%)	1 (0%)	48	68
1	B	746/768 (97%)	717 (96%)	29 (4%)	0	100	100
1	C	733/768 (95%)	696 (95%)	36 (5%)	1 (0%)	48	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	743/768 (97%)	714 (96%)	28 (4%)	1 (0%)	48	68
1	E	599/768 (78%)	557 (93%)	41 (7%)	1 (0%)	43	63
1	F	744/768 (97%)	715 (96%)	28 (4%)	1 (0%)	48	68
All	All	4309/4608 (94%)	4112 (95%)	192 (4%)	5 (0%)	48	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	92	VAL
1	A	4	LEU
1	D	174	LEU
1	F	474	PRO
1	E	92	VAL

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	575/589 (98%)	572 (100%)	3 (0%)	81	92
1	B	571/589 (97%)	569 (100%)	2 (0%)	84	93
1	C	565/589 (96%)	561 (99%)	4 (1%)	76	89
1	D	573/589 (97%)	568 (99%)	5 (1%)	70	87
1	E	464/589 (79%)	458 (99%)	6 (1%)	61	82
1	F	573/589 (97%)	569 (99%)	4 (1%)	76	89
All	All	3321/3534 (94%)	3297 (99%)	24 (1%)	76	89

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	57	THR
1	A	475	GLU

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Mol	Chain	Res	Type
1	B	295	MET
1	B	433	LEU
1	C	92	VAL
1	C	659	GLU
1	C	686	VAL
1	C	715	SER
1	D	4	LEU
1	D	174	LEU
1	D	277	ILE
1	D	567	SER
1	D	760	SER
1	E	92	VAL
1	E	191	SER
1	E	390	THR
1	E	427	SER
1	E	715	SER
1	E	760	SER
1	F	92	VAL
1	F	475	GLU
1	F	652	ASP
1	F	654	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	66	HIS
1	A	275	GLN
1	A	276	HIS
1	A	461	HIS
1	B	66	HIS
1	B	117	HIS
1	B	293	ASN
1	C	35	GLN
1	C	86	HIS
1	C	267	ASN
1	C	276	HIS
1	C	623	GLN
1	C	633	GLN
1	D	66	HIS
1	D	275	GLN
1	E	114	GLN

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Mol	Chain	Res	Type
1	E	129	HIS
1	E	170	GLN
1	E	623	GLN
1	E	633	GLN
1	F	276	HIS
1	F	733	HIS

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 ⓘ

6 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	BGC	G	1	2	12,12,12	1.21	2 (16%)	17,17,17	1.62	5 (29%)
2	BGC	G	2	2	11,11,12	1.82	2 (18%)	15,15,17	1.56	3 (20%)
2	BGC	J	1	2	12,12,12	1.39	2 (16%)	17,17,17	1.83	3 (17%)
2	BGC	J	2	2	11,11,12	1.69	2 (18%)	15,15,17	0.98	0
2	BGC	K	1	2	12,12,12	1.31	2 (16%)	17,17,17	1.64	3 (17%)
2	BGC	K	2	2	11,11,12	1.88	2 (18%)	15,15,17	1.30	1 (6%)

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	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	BGC	G	2	2	-	2/2/19/22	0/1/1/1
2	BGC	J	1	2	-	2/2/22/22	0/1/1/1
2	BGC	J	2	2	-	2/2/19/22	0/1/1/1
2	BGC	K	1	2	-	2/2/22/22	0/1/1/1
2	BGC	K	2	2	-	2/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	BGC	O5-C1	4.65	1.51	1.43
2	J	2	BGC	O5-C1	4.23	1.50	1.43
2	G	2	BGC	C2-C3	-4.14	1.46	1.52
2	G	2	BGC	O5-C1	3.70	1.49	1.43
2	K	2	BGC	C2-C3	-3.16	1.47	1.52
2	J	2	BGC	C2-C3	-2.99	1.47	1.52
2	J	1	BGC	O5-C5	2.91	1.51	1.44
2	K	1	BGC	O5-C5	2.81	1.51	1.44
2	G	1	BGC	C4-C3	-2.43	1.46	1.52
2	J	1	BGC	C4-C3	-2.29	1.46	1.52
2	K	1	BGC	C4-C3	-2.22	1.46	1.52
2	G	1	BGC	O5-C5	2.20	1.49	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	BGC	C1-C2-C3	-4.83	100.51	110.36
2	K	1	BGC	C6-C5-C4	-4.51	101.94	113.02
2	K	2	BGC	C1-O5-C5	3.71	117.16	112.19
2	G	2	BGC	O3-C3-C2	-3.40	103.11	110.05
2	J	1	BGC	C4-C3-C2	-3.40	104.87	110.83
2	G	1	BGC	O4-C4-C5	3.16	117.10	109.32
2	K	1	BGC	C4-C3-C2	-3.14	105.32	110.83
2	G	2	BGC	C1-C2-C3	2.54	113.34	109.64
2	G	1	BGC	C4-C3-C2	-2.52	106.41	110.83
2	K	1	BGC	C3-C4-C5	2.40	114.58	110.23
2	J	1	BGC	O5-C5-C4	2.33	113.89	109.70
2	G	1	BGC	O1-C1-O5	-2.30	103.58	110.41
2	G	2	BGC	C1-O5-C5	2.11	115.02	112.19
2	G	1	BGC	C6-C5-C4	-2.11	107.85	113.02
2	G	1	BGC	C3-C4-C5	2.04	113.93	110.23

There are no chirality outliers.

All (12) torsion outliers are listed below:

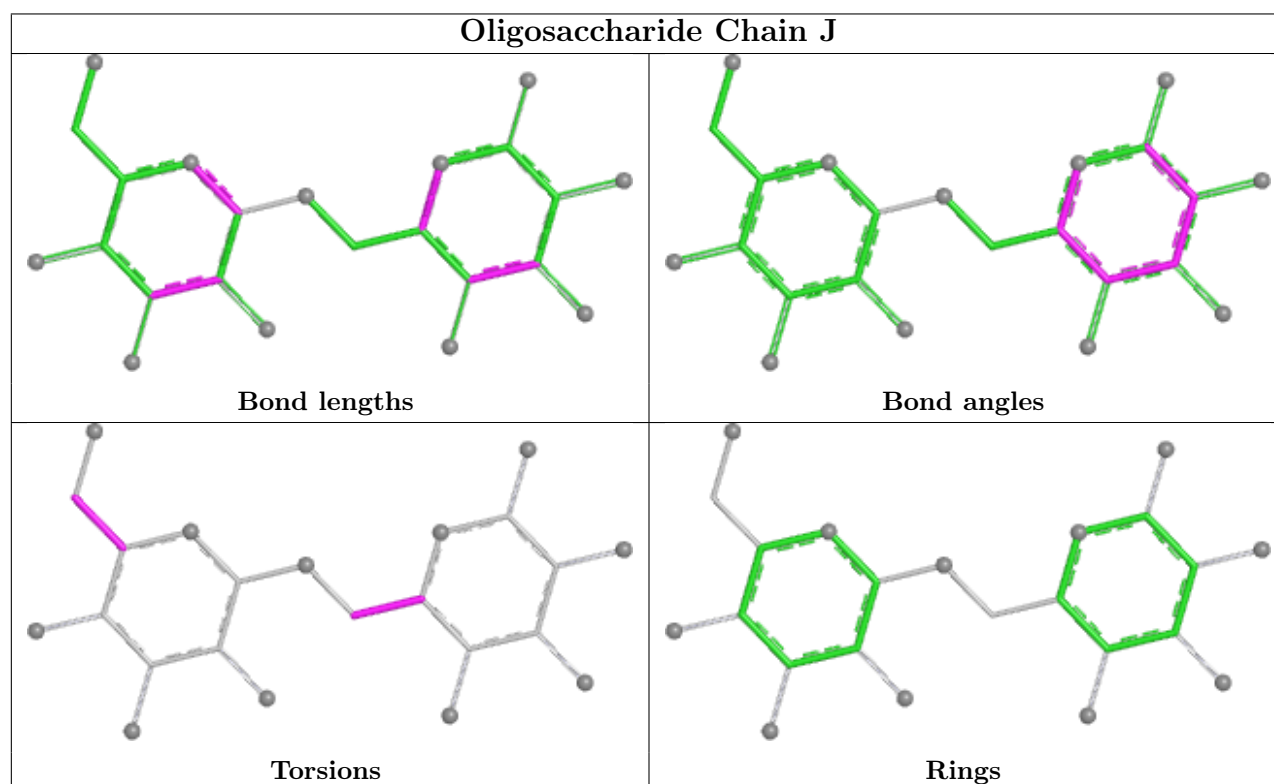
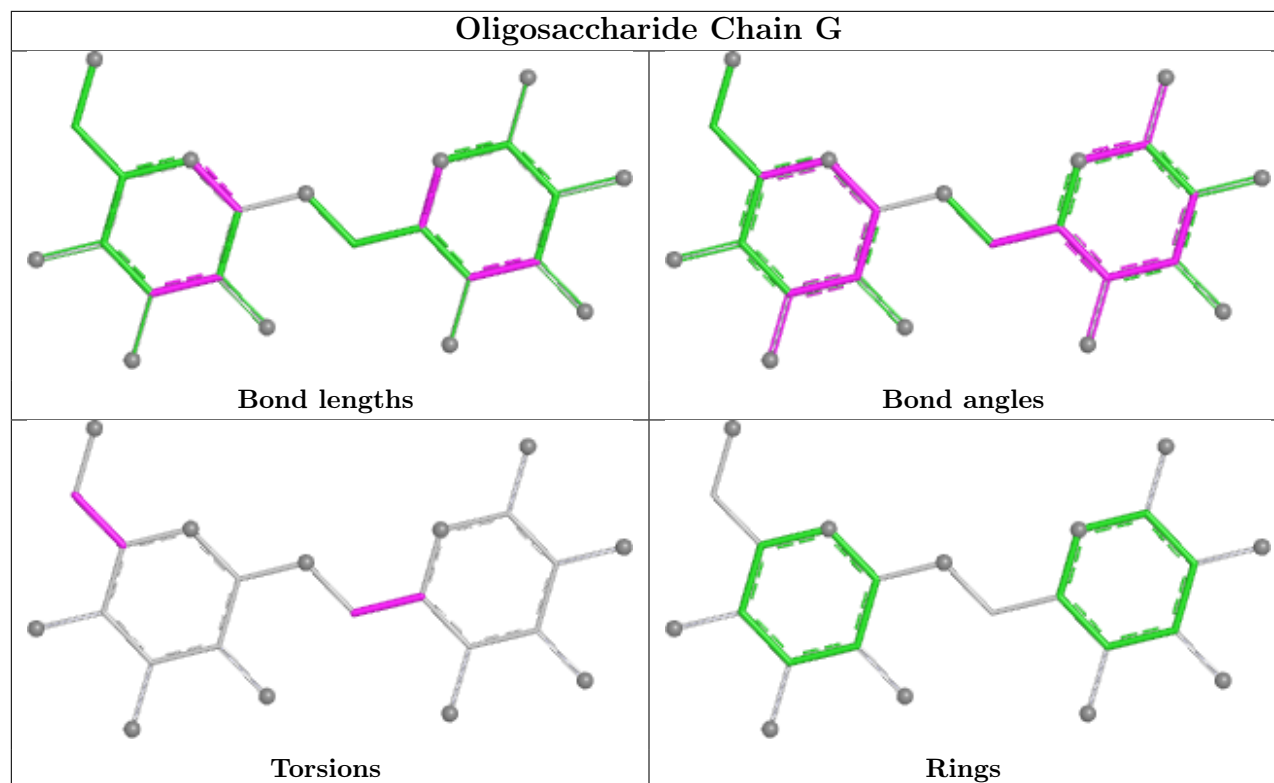
Mol	Chain	Res	Type	Atoms
2	K	2	BGC	O5-C5-C6-O6
2	K	2	BGC	C4-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6
2	J	2	BGC	O5-C5-C6-O6
2	K	1	BGC	O5-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6
2	K	1	BGC	C4-C5-C6-O6
2	J	2	BGC	C4-C5-C6-O6
2	J	1	BGC	O5-C5-C6-O6
2	G	2	BGC	O5-C5-C6-O6
2	G	2	BGC	C4-C5-C6-O6
2	J	1	BGC	C4-C5-C6-O6

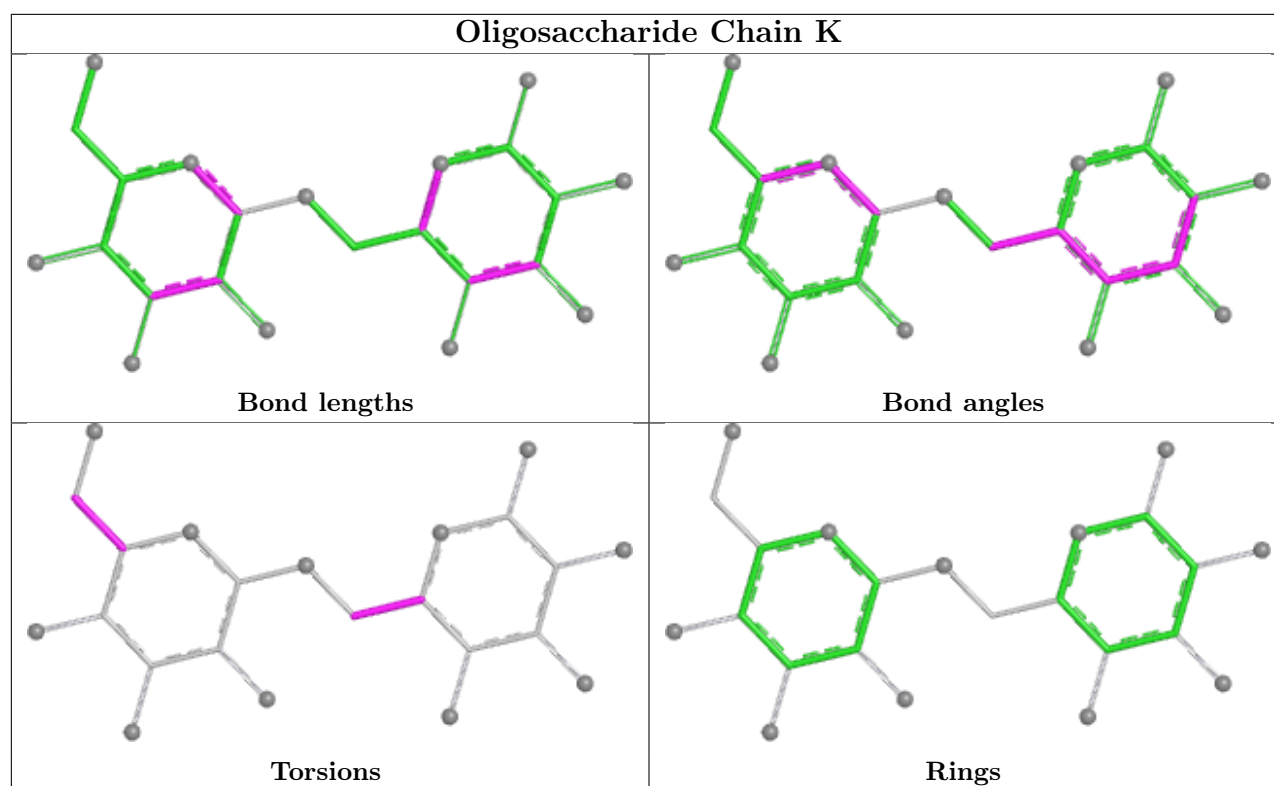
There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	2	BGC	2	0
2	K	1	BGC	1	0
2	G	2	BGC	4	0
2	K	2	BGC	7	0
2	G	1	BGC	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](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
5	GLC	B	802	-	11,11,12	1.61	2 (18%)	15,15,17	0.81	0
4	BGC	C	801	-	12,12,12	1.43	2 (16%)	17,17,17	1.40	3 (17%)
4	BGC	B	801	-	12,12,12	1.54	3 (25%)	17,17,17	1.86	5 (29%)

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
5	GLC	B	802	-	-	2/2/19/22	0/1/1/1
4	BGC	C	801	-	-	0/2/22/22	0/1/1/1
4	BGC	B	801	-	-	2/2/22/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	GLC	C2-C3	-3.10	1.47	1.52
4	C	801	BGC	C3-C2	-2.58	1.45	1.52
4	B	801	BGC	C4-C3	-2.50	1.45	1.52
5	B	802	GLC	O5-C5	2.45	1.48	1.43
4	B	801	BGC	C3-C2	-2.41	1.46	1.52
4	C	801	BGC	C4-C3	-2.14	1.46	1.52
4	B	801	BGC	O5-C5	2.00	1.49	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	BGC	O5-C5-C6	4.34	117.18	106.44
4	B	801	BGC	C4-C3-C2	-3.79	104.17	110.83
4	C	801	BGC	C4-C3-C2	-3.31	105.02	110.83
4	B	801	BGC	C1-O5-C5	-2.73	108.38	113.65
4	C	801	BGC	O5-C1-C2	2.68	115.01	110.30
4	B	801	BGC	C1-C2-C3	-2.64	104.98	110.36
4	C	801	BGC	C6-C5-C4	-2.43	107.05	113.02
4	B	801	BGC	C6-C5-C4	-2.29	107.39	113.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	BGC	O5-C5-C6-O6
4	B	801	BGC	C4-C5-C6-O6
5	B	802	GLC	C4-C5-C6-O6
5	B	802	GLC	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	802	GLC	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	801	BGC	6	0
4	B	801	BGC	2	0

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	750/768 (97%)	-0.63	8 (1%) 78 75	15, 24, 48, 98	0
1	B	750/768 (97%)	-0.69	9 (1%) 76 73	17, 24, 40, 110	0
1	C	741/768 (96%)	0.27	23 (3%) 51 47	25, 49, 74, 103	0
1	D	749/768 (97%)	-0.35	11 (1%) 72 68	24, 35, 59, 116	0
1	E	611/768 (79%)	0.09	36 (5%) 28 24	22, 42, 80, 121	0
1	F	750/768 (97%)	-0.29	10 (1%) 75 71	23, 37, 59, 102	0
All	All	4351/4608 (94%)	-0.28	97 (2%) 62 58	15, 34, 67, 121	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	282	VAL	8.0
1	C	92	VAL	6.7
1	D	389	GLY	6.7
1	B	473	ASP	6.6
1	E	288	ALA	6.4
1	E	281	TYR	5.8
1	F	388	ALA	5.8
1	E	173	GLY	5.8
1	C	387	ALA	5.8
1	D	387	ALA	5.8
1	D	390	THR	5.6
1	B	392	ASP	5.4
1	B	388	ALA	5.4
1	E	92	VAL	5.3
1	E	272	VAL	5.2
1	E	390	THR	4.8
1	B	391	PRO	4.8
1	A	388	ALA	4.7
1	C	3	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	391	PRO	4.6
1	E	175	SER	4.5
1	D	174	LEU	4.5
1	F	474	PRO	4.4
1	D	3	THR	4.4
1	D	765	GLY	4.2
1	B	3	THR	4.2
1	E	279	PRO	4.0
1	E	289	VAL	4.0
1	E	291	ALA	4.0
1	E	471	ALA	3.9
1	C	659	GLU	3.8
1	E	172	ASP	3.8
1	F	390	THR	3.7
1	F	764	ALA	3.7
1	E	127	GLY	3.6
1	E	171	GLY	3.6
1	E	273	TRP	3.6
1	A	3	THR	3.6
1	B	765	GLY	3.6
1	C	69	THR	3.5
1	C	764	ALA	3.5
1	E	188	ALA	3.5
1	C	658	THR	3.4
1	F	92	VAL	3.4
1	C	392	ASP	3.4
1	C	315	VAL	3.4
1	E	343	PRO	3.4
1	E	764	ALA	3.4
1	D	473	ASP	3.4
1	F	3	THR	3.3
1	E	280	ASP	3.3
1	C	352	ILE	3.2
1	D	657	GLY	3.1
1	E	80	LEU	3.1
1	E	391	PRO	3.1
1	E	128	VAL	3.0
1	D	175	SER	3.0
1	B	390	THR	3.0
1	E	276	HIS	2.9
1	D	742	GLU	2.9
1	F	733	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	472	PRO	2.8
1	A	658	THR	2.8
1	E	129	HIS	2.8
1	C	68	LEU	2.8
1	A	390	THR	2.7
1	F	387	ALA	2.6
1	E	265	TRP	2.6
1	B	387	ALA	2.6
1	C	347	ARG	2.6
1	C	350	ALA	2.6
1	F	391	PRO	2.5
1	E	274	GLU	2.5
1	E	275	GLN	2.5
1	B	472	PRO	2.4
1	C	127	GLY	2.4
1	E	278	GLN	2.4
1	C	47	LEU	2.4
1	F	658	THR	2.4
1	E	578	ALA	2.3
1	C	12	PRO	2.3
1	E	79	LEU	2.3
1	E	277	ILE	2.3
1	E	652	ASP	2.2
1	A	659	GLU	2.2
1	C	332	PHE	2.2
1	C	345	VAL	2.1
1	C	188	ALA	2.1
1	C	4	LEU	2.1
1	C	715	SER	2.1
1	E	270	ARG	2.1
1	A	652	ASP	2.1
1	E	268	VAL	2.1
1	A	474	PRO	2.1
1	E	290	ARG	2.0
1	C	72	THR	2.0
1	C	671	THR	2.0

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

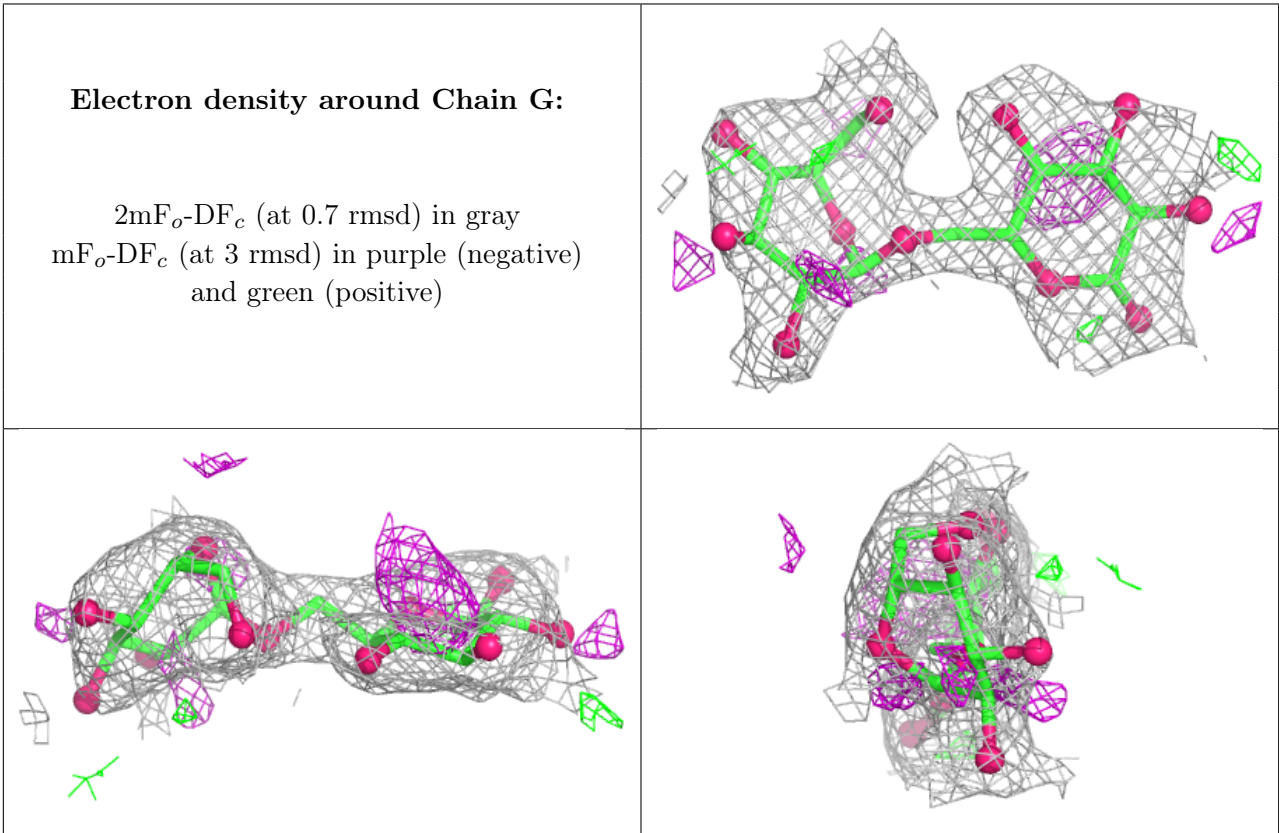
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

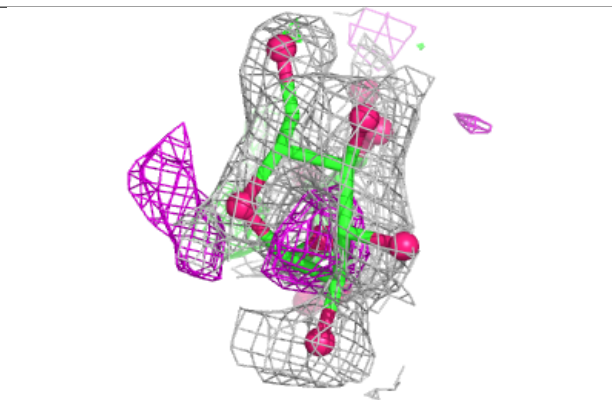
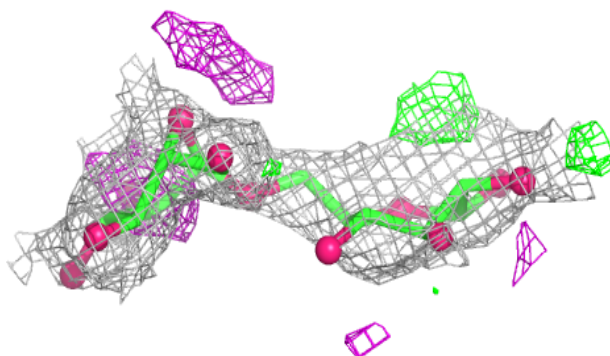
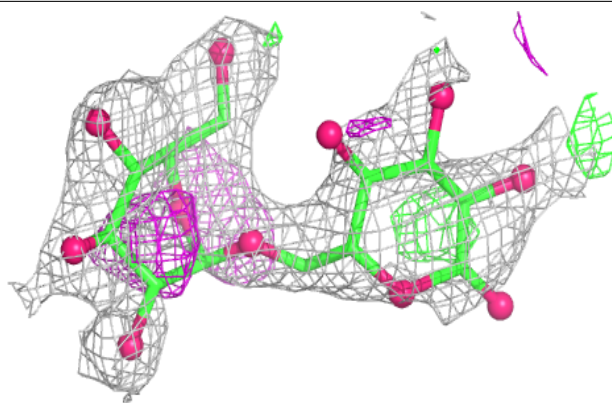
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	G	1	12/12	0.81	0.18	49,69,79,82	0
2	BGC	G	2	11/12	0.86	0.16	45,61,69,76	0
2	BGC	J	1	12/12	-	-	90,113,119,123	0
2	BGC	J	2	11/12	-	-	64,88,103,109	0
2	BGC	K	1	12/12	-	-	85,100,105,107	0
2	BGC	K	2	11/12	-	-	78,92,109,114	0

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.

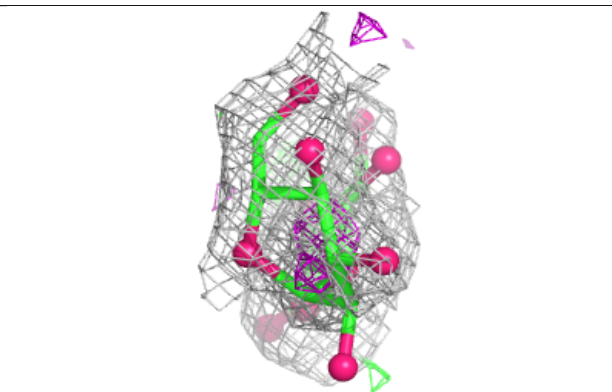
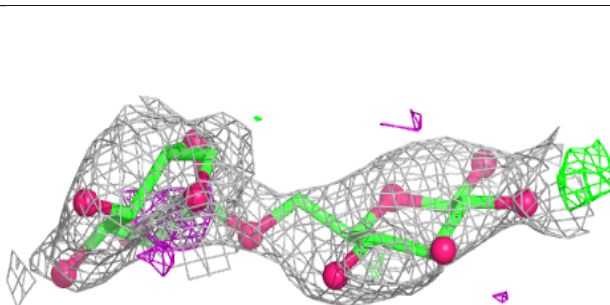
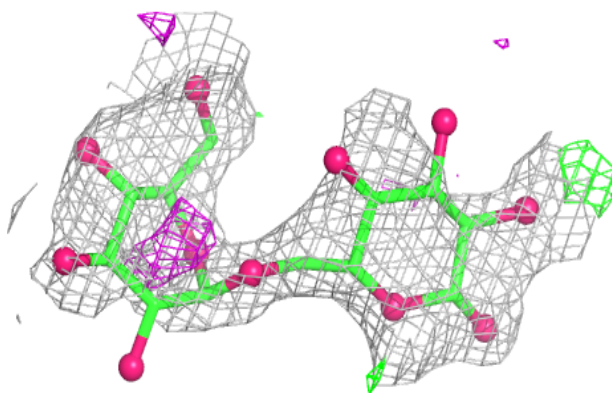


Electron density around Chain J:

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

**Electron density around Chain K:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
4	BGC	C	801	12/12	0.77	0.17	69,86,92,93	0
5	GLC	B	802	11/12	0.79	0.26	45,50,56,59	0
3	CA	F	801	1/1	0.82	0.12	75,75,75,75	0
4	BGC	B	801	12/12	0.85	0.18	66,84,93,110	0
3	CA	C	802	1/1	0.88	0.09	62,62,62,62	0
3	CA	E	801	1/1	0.89	0.10	64,64,64,64	0
3	CA	B	803	1/1	0.90	0.07	44,44,44,44	0
3	CA	A	801	1/1	0.91	0.14	54,54,54,54	0
3	CA	D	801	1/1	0.95	0.06	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.