



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:53 AM UTC

PDB ID : 7T6W / pdb_00007t6w
Title : Crystal structure of Chaetomium Glucosidase I (apo)
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2021-12-14
Resolution : 2.60 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

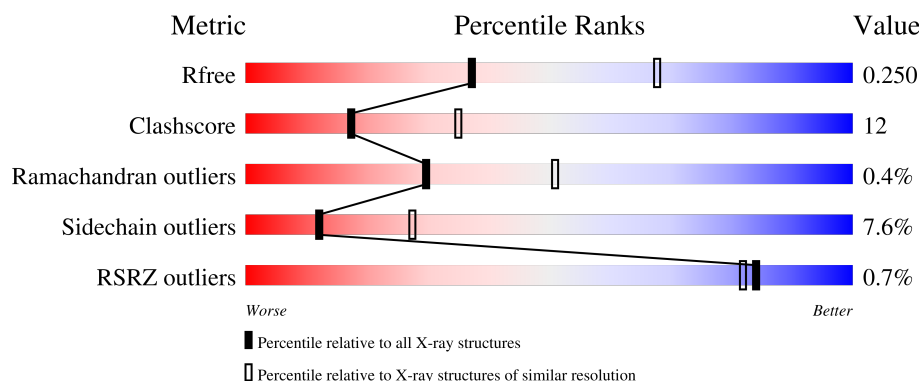
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

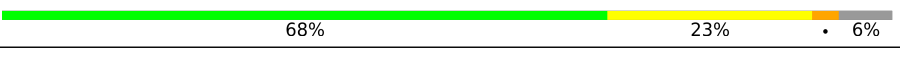
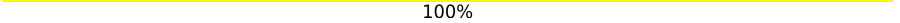
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	819	 69% 22% • 7%
1	B	819	 68% 23% • 6%
2	C	2	 100%

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
3	GOL	B	1203	-	-	X	-
4	SO4	B	1205	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12174 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 Chaetomium alpha glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	0	4	0
			6025	3864	1020	1128	13			
1	B	767	Total	C	N	O	S	0	1	0
			6023	3863	1017	1130	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP G0SFD1
A	0	GLY	-	expression tag	UNP G0SFD1
A	1	ILE	-	expression tag	UNP G0SFD1
A	2	LEU	-	expression tag	UNP G0SFD1
A	3	PRO	-	expression tag	UNP G0SFD1
A	4	SER	-	expression tag	UNP G0SFD1
A	5	PRO	-	expression tag	UNP G0SFD1
A	6	GLY	-	expression tag	UNP G0SFD1
A	7	MET	-	expression tag	UNP G0SFD1
A	8	PRO	-	expression tag	UNP G0SFD1
A	9	ALA	-	expression tag	UNP G0SFD1
A	10	LEU	-	expression tag	UNP G0SFD1
A	11	LEU	-	expression tag	UNP G0SFD1
A	12	SER	-	expression tag	UNP G0SFD1
A	13	LEU	-	expression tag	UNP G0SFD1
A	14	VAL	-	expression tag	UNP G0SFD1
A	15	SER	-	expression tag	UNP G0SFD1
A	16	LEU	-	expression tag	UNP G0SFD1
A	17	LEU	-	expression tag	UNP G0SFD1
A	18	SER	-	expression tag	UNP G0SFD1
A	19	VAL	-	expression tag	UNP G0SFD1
A	20	LEU	-	expression tag	UNP G0SFD1
A	21	LEU	-	expression tag	UNP G0SFD1
A	22	MET	-	expression tag	UNP G0SFD1
A	23	GLY	-	expression tag	UNP G0SFD1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	CYS	-	expression tag	UNP G0SFD1
A	25	VAL	-	expression tag	UNP G0SFD1
A	26	ALA	-	expression tag	UNP G0SFD1
A	27	GLU	-	expression tag	UNP G0SFD1
A	28	THR	-	expression tag	UNP G0SFD1
A	29	GLY	-	expression tag	UNP G0SFD1
A	810	SER	-	expression tag	UNP G0SFD1
A	811	GLY	-	expression tag	UNP G0SFD1
A	812	HIS	-	expression tag	UNP G0SFD1
A	813	HIS	-	expression tag	UNP G0SFD1
A	814	HIS	-	expression tag	UNP G0SFD1
A	815	HIS	-	expression tag	UNP G0SFD1
A	816	HIS	-	expression tag	UNP G0SFD1
A	817	HIS	-	expression tag	UNP G0SFD1
B	-1	MET	-	initiating methionine	UNP G0SFD1
B	0	GLY	-	expression tag	UNP G0SFD1
B	1	ILE	-	expression tag	UNP G0SFD1
B	2	LEU	-	expression tag	UNP G0SFD1
B	3	PRO	-	expression tag	UNP G0SFD1
B	4	SER	-	expression tag	UNP G0SFD1
B	5	PRO	-	expression tag	UNP G0SFD1
B	6	GLY	-	expression tag	UNP G0SFD1
B	7	MET	-	expression tag	UNP G0SFD1
B	8	PRO	-	expression tag	UNP G0SFD1
B	9	ALA	-	expression tag	UNP G0SFD1
B	10	LEU	-	expression tag	UNP G0SFD1
B	11	LEU	-	expression tag	UNP G0SFD1
B	12	SER	-	expression tag	UNP G0SFD1
B	13	LEU	-	expression tag	UNP G0SFD1
B	14	VAL	-	expression tag	UNP G0SFD1
B	15	SER	-	expression tag	UNP G0SFD1
B	16	LEU	-	expression tag	UNP G0SFD1
B	17	LEU	-	expression tag	UNP G0SFD1
B	18	SER	-	expression tag	UNP G0SFD1
B	19	VAL	-	expression tag	UNP G0SFD1
B	20	LEU	-	expression tag	UNP G0SFD1
B	21	LEU	-	expression tag	UNP G0SFD1
B	22	MET	-	expression tag	UNP G0SFD1
B	23	GLY	-	expression tag	UNP G0SFD1
B	24	CYS	-	expression tag	UNP G0SFD1
B	25	VAL	-	expression tag	UNP G0SFD1
B	26	ALA	-	expression tag	UNP G0SFD1

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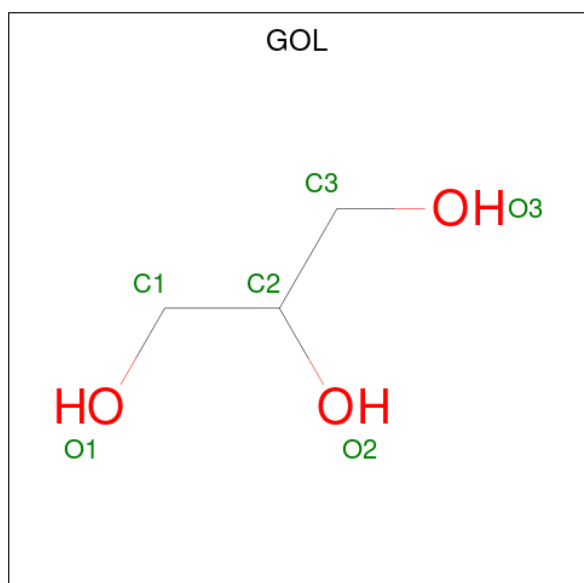
Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLU	-	expression tag	UNP G0SFD1
B	28	THR	-	expression tag	UNP G0SFD1
B	29	GLY	-	expression tag	UNP G0SFD1
B	810	SER	-	expression tag	UNP G0SFD1
B	811	GLY	-	expression tag	UNP G0SFD1
B	812	HIS	-	expression tag	UNP G0SFD1
B	813	HIS	-	expression tag	UNP G0SFD1
B	814	HIS	-	expression tag	UNP G0SFD1
B	815	HIS	-	expression tag	UNP G0SFD1
B	816	HIS	-	expression tag	UNP G0SFD1
B	817	HIS	-	expression tag	UNP G0SFD1

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



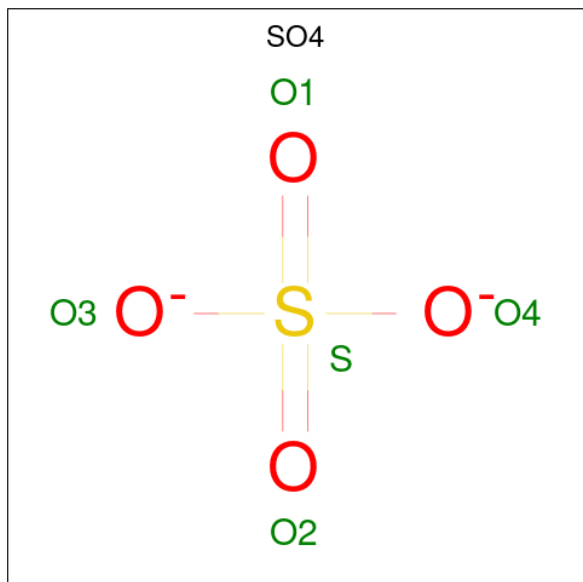
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

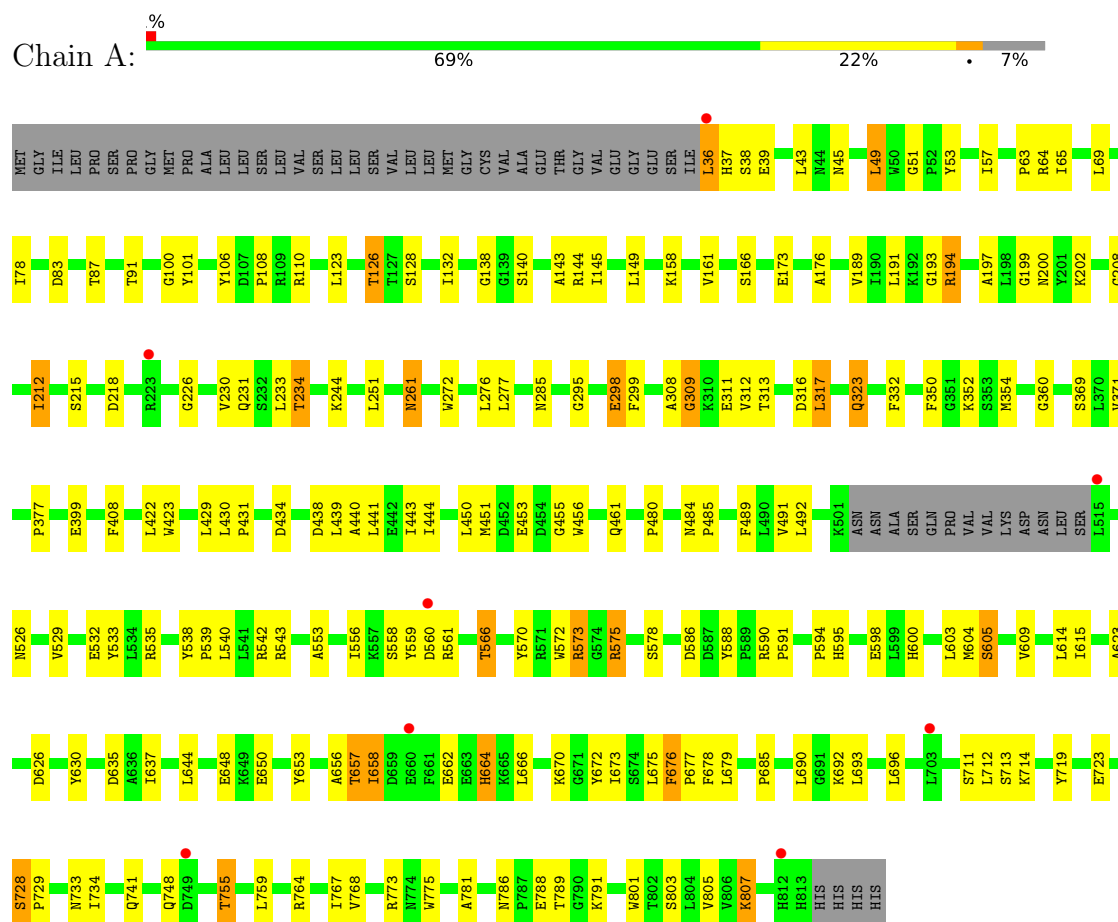
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	8	Total	O	0	0
			8	8		

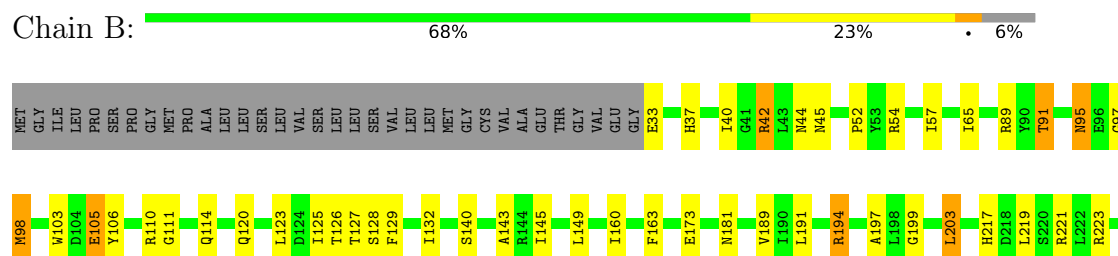
3 Residue-property plots

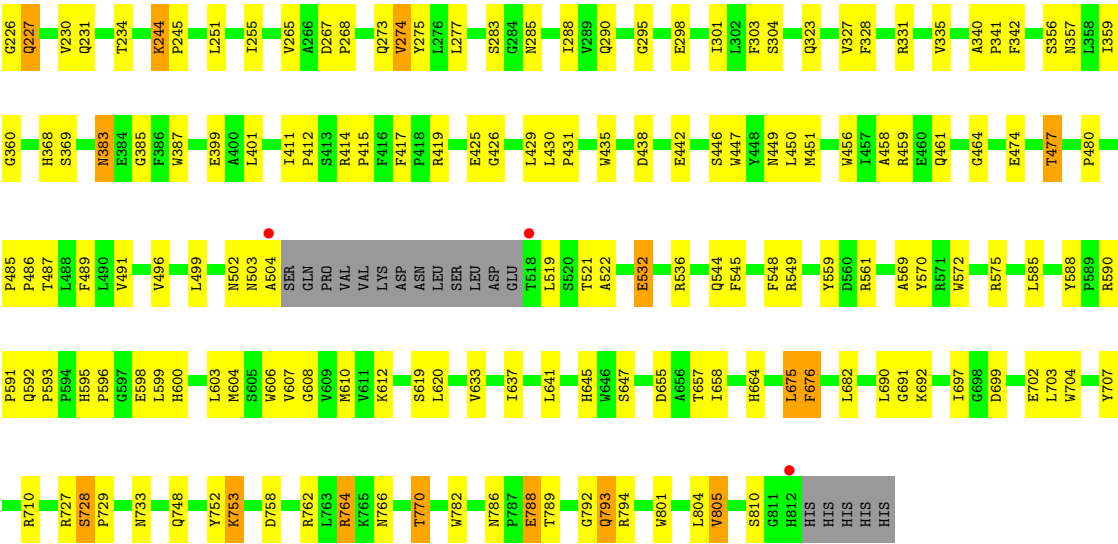
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Chaetomium alpha glucosidase



• Molecule 1: Chaetomium alpha glucosidase





● Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	139.15Å 178.80Å 180.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.06 – 2.60 47.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.06-2.60) 99.3 (47.06-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.190 , 0.250 0.190 , 0.250	Depositor DCC
R_{free} test set	3515 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12174	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/6209	1.00	2/8465 (0.0%)
1	B	0.65	1/6199 (0.0%)	0.99	1/8455 (0.0%)
All	All	0.64	1/12408 (0.0%)	0.99	3/16920 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	645	HIS	CE1-NE2	5.11	1.37	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ARG	CB-CA-C	6.32	120.21	109.53
1	B	45	ASN	CB-CA-C	5.66	120.18	110.79
1	A	126	THR	CA-CB-OG1	-5.58	101.22	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	585	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6025	0	5618	144	0
1	B	6023	0	5597	152	0
2	C	28	0	25	0	0
3	A	18	0	24	3	0
3	B	18	0	24	5	0
4	A	30	0	0	2	0
4	B	15	0	0	3	0
5	A	9	0	0	0	0
5	B	8	0	0	0	0
All	All	12174	0	11288	292	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 12.

All (292) 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:91:THR:HG23	3:B:1203:GOL:H31	1.28	1.11
1:B:764:ARG:HH11	1:B:764:ARG:HG2	1.24	0.99
1:B:572:TRP:H	1:B:600:HIS:HD2	1.11	0.99
1:A:451:MET:HE3	1:A:540:LEU:HD22	1.48	0.92
1:B:464:GLY:HA2	4:B:1205:SO4:O4	1.72	0.90
1:B:766:ASN:O	1:B:770:THR:HG23	1.74	0.87
1:B:561:ARG:HE	1:B:664:HIS:HD2	1.23	0.87
1:B:572:TRP:H	1:B:600:HIS:CD2	1.92	0.86
1:A:451:MET:CE	1:A:540:LEU:HB3	2.06	0.85
1:A:572:TRP:H	1:A:600:HIS:HD2	1.24	0.84
1:B:217:HIS:HD2	1:B:219:LEU:H	1.26	0.84
1:B:91:THR:CG2	3:B:1203:GOL:H31	2.09	0.81
1:A:451:MET:HE1	1:A:540:LEU:HB3	1.63	0.80
1:A:685:PRO:HG3	1:A:748:GLN:HE22	1.47	0.80
1:B:244:LYS:HB3	1:B:245:PRO:HD3	1.62	0.80
1:B:786:ASN:HD22	1:B:789:THR:H	1.28	0.77
1:A:728:SER:OG	1:A:729:PRO:HD3	1.83	0.77
1:B:128:SER:O	1:B:143:ALA:HA	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:VAL:HG12	1:B:637:ILE:HD12	1.69	0.74
1:B:764:ARG:HG2	1:B:764:ARG:NH1	2.00	0.74
1:B:91:THR:HG23	3:B:1203:GOL:C3	2.15	0.74
1:A:673:ILE:HA	1:A:676:PHE:HD2	1.53	0.73
1:B:217:HIS:HE1	1:B:267:ASP:O	1.71	0.73
1:B:561:ARG:HE	1:B:664:HIS:CD2	2.07	0.73
1:B:590:ARG:HB3	1:B:591:PRO:CD	2.19	0.72
1:A:598:GLU:OE2	1:A:600:HIS:HE1	1.71	0.72
1:B:430:LEU:HB2	1:B:431:PRO:HD3	1.73	0.71
1:B:163:PHE:CE1	1:B:301:ILE:HD13	2.26	0.71
1:B:368:HIS:HD2	4:B:1205:SO4:O3	1.74	0.71
1:B:33:GLU:HB2	1:B:536:ARG:HH12	1.53	0.71
1:A:456:TRP:CE2	1:A:480:PRO:HA	2.26	0.70
1:B:604:MET:HE3	1:B:641:LEU:HD23	1.74	0.70
1:B:604:MET:CE	1:B:641:LEU:HD23	2.23	0.68
1:A:559:TYR:CE1	1:A:658:ILE:HD13	2.28	0.68
1:A:588:TYR:CD2	1:A:673:ILE:HG13	2.27	0.68
1:B:559:TYR:CE2	1:B:658:ILE:HG13	2.29	0.68
1:B:575:ARG:NH1	1:B:598:GLU:OE2	2.28	0.67
1:B:40:ILE:HD12	1:B:522:ALA:HB1	1.75	0.67
1:A:108:PRO:HG3	1:A:439:LEU:HD22	1.77	0.66
1:B:707:TYR:HA	1:B:770:THR:HG21	1.76	0.66
1:A:144:ARG:HB2	1:A:317:LEU:HD21	1.78	0.66
1:B:733:ASN:HB3	1:B:801:TRP:CG	2.30	0.66
1:B:748:GLN:O	1:B:753:LYS:HD3	1.96	0.65
1:A:234[A]:THR:HA	1:A:285:ASN:OD1	1.97	0.65
1:A:234[B]:THR:HA	1:A:285:ASN:OD1	1.97	0.65
1:A:672:TYR:CE2	1:A:711:SER:HA	2.32	0.65
1:A:434:ASP:OD2	1:A:807:LYS:HD3	1.97	0.65
1:A:451:MET:HE3	1:A:540:LEU:CD2	2.26	0.65
1:B:95:ASN:HD22	1:B:97:GLY:H	1.45	0.65
1:A:598:GLU:OE2	1:A:600:HIS:CE1	2.50	0.64
1:A:451:MET:SD	1:A:455:GLY:HA2	2.38	0.64
1:B:103:TRP:H	1:B:357:ASN:ND2	1.96	0.64
1:A:208:GLY:HA2	3:A:901:GOL:H12	1.81	0.63
1:B:385:GLY:HA2	1:B:387:TRP:CZ3	2.34	0.63
1:B:458:ALA:N	3:B:1202:GOL:O2	2.17	0.63
1:B:590:ARG:HB3	1:B:591:PRO:HD2	1.81	0.62
1:B:600:HIS:HA	1:B:655:ASP:OD1	1.99	0.62
1:A:572:TRP:H	1:A:600:HIS:CD2	2.12	0.62
1:A:354:MET:HE1	1:A:781:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HB3	1:A:484:ASN:HD22	1.64	0.61
1:A:110:ARG:NH2	1:A:323:GLN:HG3	2.16	0.61
1:B:699:ASP:HB3	1:B:702:GLU:HB2	1.82	0.61
1:A:39:GLU:OE2	1:A:39:GLU:HA	2.00	0.61
1:A:685:PRO:HG3	1:A:748:GLN:NE2	2.16	0.60
1:A:313:THR:O	1:A:316:ASP:HB2	2.00	0.60
1:A:786:ASN:HD22	1:A:789:THR:H	1.50	0.60
1:B:633:VAL:HG12	1:B:637:ILE:CD1	2.31	0.60
1:B:149:LEU:HD11	1:B:295:GLY:HA2	1.84	0.60
1:B:331:ARG:NH1	1:B:435:TRP:O	2.35	0.60
1:A:234[A]:THR:HG21	1:B:268:PRO:HG3	1.84	0.60
1:A:234[B]:THR:HG21	1:B:268:PRO:HG3	1.84	0.59
1:A:650:GLU:OE1	1:A:650:GLU:HA	2.03	0.59
1:B:786:ASN:ND2	1:B:789:THR:H	2.00	0.59
1:B:595:HIS:ND1	1:B:596:PRO:HD2	2.18	0.59
1:B:114:GLN:NE2	1:B:414:ARG:HH12	2.01	0.58
1:B:575:ARG:NH1	1:B:591:PRO:HD2	2.18	0.58
1:A:108:PRO:HG3	1:A:439:LEU:CD2	2.33	0.58
1:A:588:TYR:CE2	1:A:673:ILE:HG13	2.39	0.58
1:B:608:GLY:HA3	1:B:682:LEU:HD11	1.85	0.57
1:A:37:HIS:CD2	1:A:532:GLU:CG	2.87	0.57
1:A:132:ILE:N	1:A:132:ILE:HD12	2.19	0.56
1:A:786:ASN:ND2	1:A:788:GLU:H	2.03	0.56
1:B:728:SER:N	1:B:729:PRO:HD3	2.20	0.56
1:A:176:ALA:HA	1:A:191:LEU:HD23	1.88	0.56
1:B:65:ILE:HD13	1:B:197:ALA:HB1	1.87	0.56
1:B:114:GLN:HB3	1:B:127:THR:OG1	2.05	0.56
1:A:202:LYS:CE	1:A:311:GLU:OE1	2.53	0.56
1:A:623:ALA:HB1	1:A:626:ASP:HB2	1.86	0.56
1:B:766:ASN:O	1:B:770:THR:CG2	2.53	0.56
1:A:371:VAL:O	1:A:399:GLU:HA	2.05	0.55
1:B:189:VAL:HG11	1:B:230:VAL:HG21	1.88	0.55
1:B:690:LEU:HD12	1:B:690:LEU:O	2.07	0.55
1:B:368:HIS:CD2	4:B:1205:SO4:O3	2.57	0.55
1:B:57:ILE:HA	1:B:91:THR:HA	1.89	0.54
1:A:553:ALA:O	1:A:573:ARG:NH2	2.36	0.54
1:B:106:TYR:HD2	1:B:359:ILE:HG23	1.72	0.54
1:A:36:LEU:O	1:A:36:LEU:HG	2.07	0.54
1:A:578:SER:HB2	4:A:909:SO4:O1	2.08	0.54
1:B:451:MET:CE	1:B:544:GLN:HB2	2.38	0.54
1:B:707:TYR:HE2	1:B:788:GLU:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LYS:HB3	1:B:245:PRO:CD	2.35	0.54
1:A:664:HIS:C	1:A:664:HIS:CD2	2.86	0.54
1:B:226:GLY:H	1:B:227:GLN:HE22	1.54	0.53
1:B:786:ASN:HB2	1:B:793:GLN:NE2	2.23	0.53
1:B:503:ASN:O	1:B:504:ALA:HB2	2.07	0.53
1:A:561:ARG:NH2	1:A:657:THR:O	2.41	0.53
1:A:733:ASN:HB3	1:A:801:TRP:CG	2.44	0.53
1:A:590:ARG:HB3	1:A:591:PRO:HD2	1.91	0.53
1:A:51:GLY:HA3	1:A:53:TYR:CZ	2.44	0.53
1:A:251:LEU:HD23	1:A:277:LEU:HD21	1.91	0.53
1:A:672:TYR:CZ	1:A:711:SER:HA	2.44	0.53
1:B:549:ARG:HG2	1:B:570:TYR:OH	2.08	0.52
1:A:140:SER:HB3	1:A:312:VAL:HG21	1.91	0.52
1:A:308:ALA:O	1:A:309:GLY:O	2.28	0.52
1:B:456:TRP:CE2	1:B:480:PRO:HA	2.45	0.52
1:A:678:PHE:CE1	1:A:741:GLN:HB3	2.45	0.52
1:B:37:HIS:CG	1:B:532:GLU:HG2	2.44	0.52
1:A:803:SER:C	1:A:805[B]:VAL:H	2.17	0.52
1:B:194:ARG:HH11	1:B:194:ARG:CG	2.23	0.52
1:B:103:TRP:H	1:B:357:ASN:HD21	1.58	0.51
1:B:451:MET:HE1	1:B:544:GLN:HB2	1.91	0.51
1:B:37:HIS:CD2	1:B:532:GLU:HG2	2.46	0.51
1:B:149:LEU:CD1	1:B:295:GLY:HA2	2.40	0.51
1:B:728:SER:N	1:B:729:PRO:CD	2.73	0.51
1:A:145:ILE:O	1:A:298:GLU:HA	2.10	0.51
1:A:653:TYR:CD2	1:A:677:PRO:HG2	2.44	0.51
1:B:697:ILE:O	1:B:704:TRP:HB2	2.11	0.51
1:A:64:ARG:HD3	1:A:408:PHE:CE1	2.46	0.51
1:B:612:LYS:HD2	1:B:682:LEU:CD2	2.41	0.51
1:B:450:LEU:HD13	1:B:461:GLN:NE2	2.24	0.51
1:A:350:PHE:HB2	1:A:775:TRP:CZ3	2.46	0.51
1:A:430:LEU:HB2	1:A:431:PRO:HD3	1.93	0.51
1:B:532:GLU:O	1:B:532:GLU:HG3	2.11	0.51
1:A:489:PHE:HA	1:A:492:LEU:HD12	1.92	0.51
1:A:423:TRP:CE3	1:A:485:PRO:HG2	2.46	0.51
1:A:128:SER:O	1:A:143:ALA:HA	2.11	0.50
1:B:575:ARG:HH12	1:B:591:PRO:HD2	1.76	0.50
1:A:149:LEU:HD11	1:A:295:GLY:HA2	1.94	0.50
1:B:707:TYR:CA	1:B:770:THR:HG21	2.42	0.50
1:A:594:PRO:HA	1:A:598:GLU:OE1	2.12	0.50
1:A:673:ILE:HA	1:A:676:PHE:CD2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:TRP:CH2	1:B:603:LEU:HD13	2.47	0.49
1:A:672:TYR:CD2	1:A:711:SER:HA	2.47	0.49
1:A:441:LEU:HD22	1:A:533:TYR:CE1	2.47	0.49
1:B:561:ARG:NE	1:B:664:HIS:HD2	2.01	0.49
1:A:298:GLU:OE2	3:A:901:GOL:O1	2.28	0.49
1:B:414:ARG:N	1:B:415:PRO:HD2	2.27	0.49
1:B:604:MET:HE3	1:B:641:LEU:CD2	2.41	0.49
1:A:588:TYR:CE2	1:A:673:ILE:CG1	2.96	0.49
1:A:161:VAL:HG11	1:A:299:PHE:CE2	2.47	0.49
1:B:106:TYR:CD2	1:B:360:GLY:HA2	2.48	0.49
1:A:803:SER:C	1:A:805[A]:VAL:H	2.17	0.49
1:B:274:VAL:HG12	1:B:275:TYR:CD1	2.47	0.49
1:B:105:GLU:HA	1:B:356:SER:OG	2.12	0.48
1:B:545:PHE:CZ	1:B:549:ARG:HD2	2.47	0.48
1:A:51:GLY:HA3	1:A:53:TYR:CE2	2.48	0.48
1:A:598:GLU:HA	1:A:656:ALA:O	2.13	0.48
1:A:37:HIS:CD2	1:A:532:GLU:HG3	2.48	0.48
1:A:161:VAL:HG11	1:A:299:PHE:HE2	1.79	0.48
1:A:233:LEU:HD22	1:B:265:VAL:HG23	1.96	0.48
1:B:728:SER:H	1:B:729:PRO:CD	2.25	0.48
1:A:231:GLN:OE1	1:A:277:LEU:HB3	2.14	0.48
1:A:672:TYR:CG	1:A:734:ILE:HG21	2.49	0.48
1:B:603:LEU:O	1:B:607:VAL:HG23	2.14	0.48
1:B:485:PRO:HB3	1:B:606:TRP:CE2	2.49	0.48
1:A:106:TYR:CD2	1:A:360:GLY:HA2	2.49	0.47
1:A:451:MET:HE3	1:A:540:LEU:HB3	1.92	0.47
1:A:542:ARG:HG3	4:A:908:SO4:O2	2.14	0.47
1:B:160:ILE:CG2	1:B:290:GLN:HE21	2.27	0.47
1:A:566:THR:HG1	3:A:903:GOL:HO3	1.57	0.47
1:A:83:ASP:O	1:A:87:THR:HG23	2.14	0.47
1:A:108:PRO:CG	1:A:439:LEU:HD22	2.43	0.47
1:B:194:ARG:HA	1:B:199:GLY:O	2.15	0.47
1:B:675:LEU:O	1:B:676:PHE:C	2.57	0.47
1:A:37:HIS:CD2	1:A:532:GLU:HG2	2.50	0.47
1:B:105:GLU:HG3	1:B:328:PHE:CG	2.50	0.47
1:A:559:TYR:HE1	1:A:658:ILE:HD13	1.75	0.47
1:A:453:GLU:O	1:A:543:ARG:HD3	2.14	0.47
1:B:140:SER:HB3	1:B:303:PHE:O	2.15	0.46
1:A:194:ARG:HG3	1:A:200:ASN:OD1	2.14	0.46
1:B:42:ARG:HE	1:B:42:ARG:HB2	1.15	0.46
1:A:423:TRP:H	1:A:484:ASN:ND2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:MET:HE1	1:A:781:ALA:CB	2.44	0.46
1:A:556:ILE:HD12	1:A:566:THR:O	2.16	0.46
1:B:521:THR:O	1:B:522:ALA:C	2.59	0.46
1:A:377:PRO:HG3	1:B:401:LEU:HG	1.98	0.46
1:A:65:ILE:HD13	1:A:197:ALA:HB1	1.97	0.46
1:A:538:TYR:HB3	1:A:539:PRO:HD3	1.97	0.46
1:A:570:TYR:HB3	1:A:603:LEU:HG	1.98	0.45
1:A:215:SER:HB2	1:A:272:TRP:CH2	2.51	0.45
1:B:425:GLU:HG2	1:B:447:TRP:NE1	2.32	0.45
1:B:569:ALA:HB1	1:B:599:LEU:HD22	1.98	0.45
1:B:419:ARG:HH11	1:B:419:ARG:HG2	1.81	0.45
1:A:166:SER:HA	1:A:285:ASN:O	2.16	0.45
1:B:103:TRP:N	1:B:357:ASN:HD21	2.14	0.45
1:A:408:PHE:O	1:A:443:ILE:HG23	2.16	0.45
1:A:526:ASN:O	1:A:529:VAL:HB	2.17	0.45
1:B:727:ARG:O	1:B:728:SER:HB3	2.17	0.45
1:A:755:THR:O	1:A:759:LEU:HG	2.16	0.45
1:B:572:TRP:N	1:B:600:HIS:CD2	2.74	0.44
1:B:219:LEU:HD23	1:B:273:GLN:HG2	1.97	0.44
1:B:251:LEU:O	1:B:255:ILE:HG13	2.16	0.44
1:B:230:VAL:HA	1:B:288:ILE:O	2.17	0.44
1:A:648:GLU:OE2	1:A:648:GLU:HA	2.16	0.44
1:B:489:PHE:CE1	1:B:610:MET:HE3	2.53	0.44
1:A:670:LYS:O	1:A:712:LEU:HD12	2.18	0.44
1:B:244:LYS:HE3	3:B:1203:GOL:H2	1.99	0.44
1:B:429:LEU:HB2	1:B:491:VAL:HG21	2.00	0.44
1:B:559:TYR:CD2	1:B:658:ILE:HG13	2.52	0.44
1:A:57:ILE:HA	1:A:91:THR:HA	2.00	0.44
1:A:189:VAL:HG11	1:A:230:VAL:HG21	1.99	0.44
1:B:399:GLU:HB3	1:B:477:THR:CG2	2.47	0.44
1:A:595:HIS:CE1	1:A:658:ILE:HG12	2.52	0.44
1:B:33:GLU:CB	1:B:536:ARG:HH12	2.24	0.44
1:A:261:ASN:N	1:A:261:ASN:HD22	2.15	0.44
1:B:385:GLY:HA2	1:B:387:TRP:CH2	2.53	0.44
1:A:106:TYR:CE2	1:A:360:GLY:HA2	2.53	0.43
1:A:764:ARG:O	1:A:768:VAL:HG23	2.17	0.43
1:B:786:ASN:CB	1:B:793:GLN:HE22	2.30	0.43
1:A:532:GLU:OE1	1:A:535:ARG:NH1	2.51	0.43
1:B:223:ARG:NH1	1:B:223:ARG:HG3	2.32	0.43
1:A:422:LEU:HB3	1:A:484:ASN:ND2	2.31	0.43
1:A:538:TYR:N	1:A:539:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:MET:HE2	1:B:641:LEU:HD23	1.98	0.43
1:A:456:TRP:CD2	1:A:480:PRO:HA	2.53	0.43
1:A:194:ARG:HA	1:A:199:GLY:O	2.18	0.43
1:B:804:LEU:O	1:B:805:VAL:C	2.62	0.43
1:A:644:LEU:O	1:A:666:LEU:HD21	2.18	0.43
1:A:49:LEU:O	1:A:63:PRO:HA	2.19	0.43
1:A:714:LYS:HA	1:A:719:TYR:CG	2.54	0.43
1:B:549:ARG:HA	1:B:570:TYR:HE1	1.84	0.43
1:A:786:ASN:HD22	1:A:788:GLU:H	1.66	0.42
1:A:173:GLU:O	1:A:193:GLY:HA2	2.19	0.42
1:B:341:PRO:HD2	1:B:342:PHE:CE2	2.54	0.42
1:A:110:ARG:HH22	1:A:323:GLN:HG3	1.83	0.42
1:A:658:ILE:HD12	1:A:662:GLU:HA	2.00	0.42
1:B:231:GLN:NE2	1:B:277:LEU:HB3	2.34	0.42
1:B:474:GLU:H	1:B:474:GLU:HG3	1.62	0.42
1:A:110:ARG:NH2	1:A:323:GLN:CG	2.81	0.42
1:B:111:GLY:HA3	1:B:129:PHE:O	2.19	0.42
1:A:49:LEU:HD22	1:A:138:GLY:HA3	2.00	0.42
1:A:675:LEU:HB2	1:A:679:LEU:HD11	2.01	0.42
1:B:703:LEU:O	1:B:710:ARG:N	2.37	0.42
1:B:369:SER:O	1:B:401:LEU:HA	2.19	0.42
1:B:572:TRP:N	1:B:600:HIS:HD2	1.95	0.42
1:A:332:PHE:CD2	1:A:352:LYS:HE2	2.55	0.42
1:B:163:PHE:CZ	1:B:301:ILE:HD13	2.54	0.42
1:B:217:HIS:CD2	1:B:219:LEU:H	2.18	0.42
1:B:383:ASN:H	1:B:383:ASN:ND2	2.17	0.42
1:B:52:PRO:HD3	1:B:129:PHE:CE2	2.54	0.42
1:B:145:ILE:O	1:B:298:GLU:HA	2.20	0.42
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.75	0.42
1:A:450:LEU:HD13	1:A:461:GLN:CD	2.45	0.41
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.84	0.41
1:A:251:LEU:HD23	1:A:277:LEU:CD2	2.50	0.41
1:A:614:LEU:HB3	1:A:630:TYR:CE2	2.55	0.41
1:B:110:ARG:NH1	1:B:327:VAL:HG11	2.35	0.41
1:B:114:GLN:HE21	1:B:414:ARG:HH12	1.68	0.41
1:A:350:PHE:HB2	1:A:775:TRP:CE3	2.56	0.41
1:B:499:LEU:HD23	1:B:499:LEU:HA	1.94	0.41
1:B:503:ASN:O	1:B:504:ALA:CB	2.69	0.41
1:A:69:LEU:HD12	1:A:166:SER:O	2.19	0.41
1:B:234:THR:HA	1:B:285:ASN:OD1	2.21	0.41
1:B:691:GLY:HA3	1:B:752:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:HIS:CG	1:A:532:GLU:HG2	2.56	0.41
1:B:89:ARG:NH2	1:B:98:MET:CE	2.84	0.41
1:B:426:GLY:HA3	1:B:487:THR:OG1	2.20	0.41
1:B:592:GLN:HA	1:B:593:PRO:HA	1.91	0.41
1:A:100:GLY:O	1:A:101:TYR:HB3	2.21	0.41
1:A:212:ILE:HD11	1:A:226:GLY:C	2.46	0.41
1:A:605:SER:O	1:A:609:VAL:HG23	2.20	0.41
1:B:340:ALA:HA	1:B:341:PRO:HA	1.88	0.41
1:B:486:PRO:CD	1:B:606:TRP:HB3	2.51	0.41
1:B:782:TRP:CG	1:B:792:GLY:HA3	2.56	0.41
1:A:675:LEU:O	1:A:676:PHE:C	2.64	0.41
1:B:191:LEU:HB2	1:B:203:LEU:HB3	2.03	0.41
1:B:412:PRO:HD2	1:B:417:PHE:O	2.21	0.41
1:B:588:TYR:O	1:B:590:ARG:HG2	2.21	0.41
1:A:276:LEU:HD12	1:A:276:LEU:HA	1.88	0.41
1:A:429:LEU:HB2	1:A:491:VAL:HG21	2.02	0.41
1:A:440:ALA:O	1:A:444:ILE:HG13	2.21	0.41
1:B:120:GLN:HE21	1:B:120:GLN:HB3	1.73	0.41
1:B:194:ARG:CG	1:B:194:ARG:NH1	2.82	0.41
1:B:114:GLN:HE22	1:B:414:ARG:HH22	1.68	0.40
1:A:595:HIS:N	1:A:598:GLU:OE1	2.53	0.40
1:A:678:PHE:O	1:A:741:GLN:HG3	2.21	0.40
1:B:251:LEU:HD23	1:B:251:LEU:HA	1.95	0.40
1:B:690:LEU:HD12	1:B:690:LEU:C	2.46	0.40
1:A:441:LEU:HD23	1:A:444:ILE:HD12	2.04	0.40
1:A:693:LEU:O	1:A:696:LEU:N	2.54	0.40
1:B:244:LYS:CB	1:B:245:PRO:HD3	2.43	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	765/819 (93%)	729 (95%)	33 (4%)	3 (0%)	30	51
1	B	764/819 (93%)	731 (96%)	30 (4%)	3 (0%)	30	51
All	All	1529/1638 (93%)	1460 (96%)	63 (4%)	6 (0%)	30	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	GLY
1	A	728	SER
1	B	728	SER
1	B	805	VAL
1	A	560	ASP
1	B	794	ARG

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	613/707 (87%)	570 (93%)	43 (7%)	14	31
1	B	612/707 (87%)	561 (92%)	51 (8%)	10	23
All	All	1225/1414 (87%)	1131 (92%)	94 (8%)	12	27

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	38	SER
1	A	43	LEU
1	A	45	ASN
1	A	49	LEU
1	A	78	ILE
1	A	126	THR
1	A	158	LYS
1	A	194	ARG
1	A	212	ILE

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Mol	Chain	Res	Type
1	A	218	ASP
1	A	234[A]	THR
1	A	234[B]	THR
1	A	244	LYS
1	A	261	ASN
1	A	298	GLU
1	A	317	LEU
1	A	323	GLN
1	A	369	SER
1	A	438	ASP
1	A	558	SER
1	A	566	THR
1	A	573	ARG
1	A	575	ARG
1	A	586	ASP
1	A	604	MET
1	A	605	SER
1	A	615	ILE
1	A	635	ASP
1	A	637	ILE
1	A	657	THR
1	A	658	ILE
1	A	664	HIS
1	A	676	PHE
1	A	690	LEU
1	A	692	LYS
1	A	713	SER
1	A	723	GLU
1	A	755	THR
1	A	767	ILE
1	A	773	ARG
1	A	791	LYS
1	A	807	LYS
1	B	42	ARG
1	B	44	ASN
1	B	54	ARG
1	B	91	THR
1	B	95	ASN
1	B	98	MET
1	B	105	GLU
1	B	123	LEU
1	B	125	ILE

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Mol	Chain	Res	Type
1	B	126	THR
1	B	132	ILE
1	B	173	GLU
1	B	181	ASN
1	B	194	ARG
1	B	203	LEU
1	B	221	ARG
1	B	227	GLN
1	B	244	LYS
1	B	274	VAL
1	B	283	SER
1	B	304	SER
1	B	323	GLN
1	B	335	VAL
1	B	383	ASN
1	B	411	ILE
1	B	438	ASP
1	B	442	GLU
1	B	446	SER
1	B	449	ASN
1	B	459	ARG
1	B	477	THR
1	B	496	VAL
1	B	502	ASN
1	B	519	LEU
1	B	532	GLU
1	B	548	PHE
1	B	619	SER
1	B	620	LEU
1	B	647	SER
1	B	657	THR
1	B	675	LEU
1	B	676	PHE
1	B	692	LYS
1	B	753	LYS
1	B	758	ASP
1	B	762	ARG
1	B	764	ARG
1	B	770	THR
1	B	788	GLU
1	B	793	GLN
1	B	810	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	85	GLN
1	A	120	GLN
1	A	157	GLN
1	A	167	GLN
1	A	227	GLN
1	A	231	GLN
1	A	242	GLN
1	A	250	GLN
1	A	397	HIS
1	A	398	GLN
1	A	461	GLN
1	A	484	ASN
1	A	579	HIS
1	A	592	GLN
1	A	600	HIS
1	A	639	HIS
1	A	664	HIS
1	A	748	GLN
1	A	786	ASN
1	A	793	GLN
1	B	37	HIS
1	B	85	GLN
1	B	95	ASN
1	B	114	GLN
1	B	120	GLN
1	B	137	HIS
1	B	167	GLN
1	B	181	ASN
1	B	217	HIS
1	B	227	GLN
1	B	231	GLN
1	B	242	GLN
1	B	249	GLN
1	B	250	GLN
1	B	290	GLN
1	B	323	GLN
1	B	357	ASN
1	B	368	HIS
1	B	383	ASN
1	B	398	GLN

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Mol	Chain	Res	Type
1	B	478	GLN
1	B	484	ASN
1	B	502	ASN
1	B	544	GLN
1	B	600	HIS
1	B	664	HIS
1	B	748	GLN
1	B	766	ASN
1	B	786	ASN
1	B	793	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 ⓘ

2 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	NAG	C	1	1,2	14,14,15	0.68	0	17,19,21	2.27	2 (11%)
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	1.37	4 (23%)

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	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	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	C	1	NAG	C1-O5-C5	8.14	123.10	112.19
2	C	2	NAG	C3-C4-C5	-3.32	104.20	110.23
2	C	2	NAG	O5-C5-C6	2.81	113.12	107.66
2	C	2	NAG	O5-C5-C4	-2.50	104.75	110.83
2	C	1	NAG	O5-C5-C4	2.49	116.87	110.83
2	C	2	NAG	C2-N2-C7	-2.05	120.16	122.90

There are no chirality outliers.

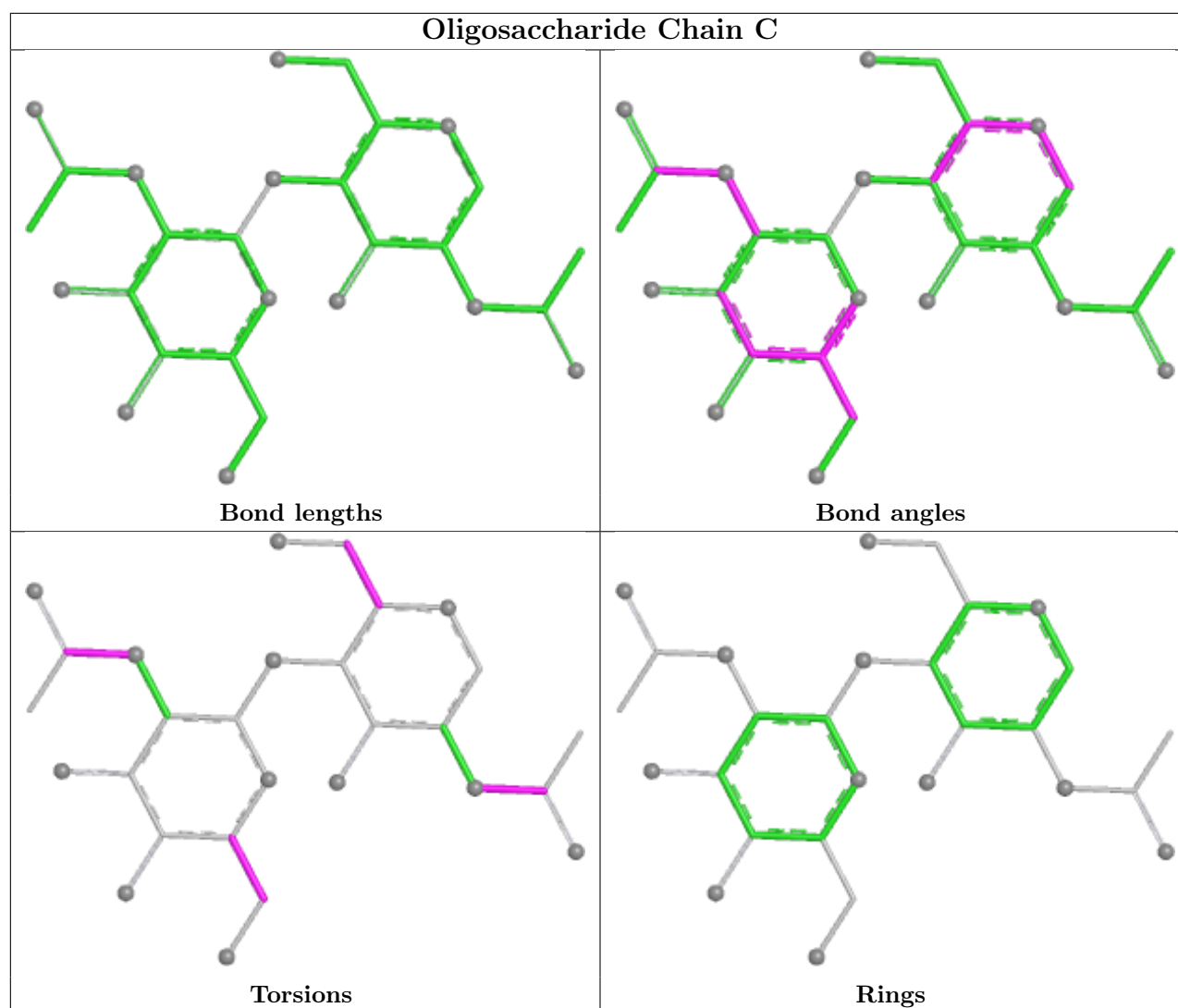
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

15 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	908	-	4,4,4	0.34	0	6,6,6	0.07	0
4	SO4	B	1204	-	4,4,4	0.27	0	6,6,6	0.10	0
3	GOL	A	903	-	5,5,5	0.14	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	1202	-	5,5,5	0.06	0	5,5,5	0.38	0
3	GOL	B	1203	-	5,5,5	0.19	0	5,5,5	0.44	0
4	SO4	A	907	-	4,4,4	0.38	0	6,6,6	0.21	0
4	SO4	B	1205	-	4,4,4	0.49	0	6,6,6	0.17	0
3	GOL	A	902	-	5,5,5	0.13	0	5,5,5	0.36	0
4	SO4	A	909	-	4,4,4	0.27	0	6,6,6	0.10	0
4	SO4	A	905	-	4,4,4	0.32	0	6,6,6	0.11	0
3	GOL	A	901	-	5,5,5	0.24	0	5,5,5	0.67	0
3	GOL	B	1201	-	5,5,5	0.10	0	5,5,5	0.34	0
4	SO4	A	904	-	4,4,4	0.31	0	6,6,6	0.07	0
4	SO4	B	1206	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	A	906	-	4,4,4	0.31	0	6,6,6	0.09	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
3	GOL	A	903	-	-	4/4/4/4	-
3	GOL	B	1202	-	-	2/4/4/4	-
3	GOL	B	1203	-	-	3/4/4/4	-
3	GOL	A	902	-	-	2/4/4/4	-
3	GOL	A	901	-	-	1/4/4/4	-
3	GOL	B	1201	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	GOL	O1-C1-C2-C3
3	A	903	GOL	C1-C2-C3-O3
3	B	1201	GOL	O1-C1-C2-C3
3	B	1201	GOL	C1-C2-C3-O3
3	B	1201	GOL	O1-C1-C2-O2
3	A	901	GOL	C1-C2-C3-O3
3	A	902	GOL	O1-C1-C2-C3
3	B	1202	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1203	GOL	O1-C1-C2-C3
3	B	1203	GOL	C1-C2-C3-O3
3	A	902	GOL	O1-C1-C2-O2
3	A	903	GOL	O1-C1-C2-O2
3	B	1203	GOL	O1-C1-C2-O2
3	A	903	GOL	O2-C2-C3-O3
3	B	1201	GOL	O2-C2-C3-O3
3	B	1202	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	908	SO4	1	0
3	A	903	GOL	1	0
3	B	1202	GOL	1	0
3	B	1203	GOL	4	0
4	B	1205	SO4	3	0
4	A	909	SO4	1	0
3	A	901	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	765/819 (93%)	-0.40	8 (1%) 79 76	30, 67, 97, 132	4 (0%)
1	B	767/819 (93%)	-0.48	3 (0%) 88 86	31, 65, 93, 150	1 (0%)
All	All	1532/1638 (93%)	-0.44	11 (0%) 84 82	30, 66, 96, 150	5 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	504	ALA	3.6
1	B	812	HIS	3.4
1	A	223[A]	ARG	3.1
1	A	36	LEU	3.0
1	A	560	ASP	2.8
1	A	703	LEU	2.7
1	A	812	HIS	2.7
1	B	518	THR	2.6
1	A	749	ASP	2.5
1	A	660	GLU	2.4
1	A	515	LEU	2.1

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

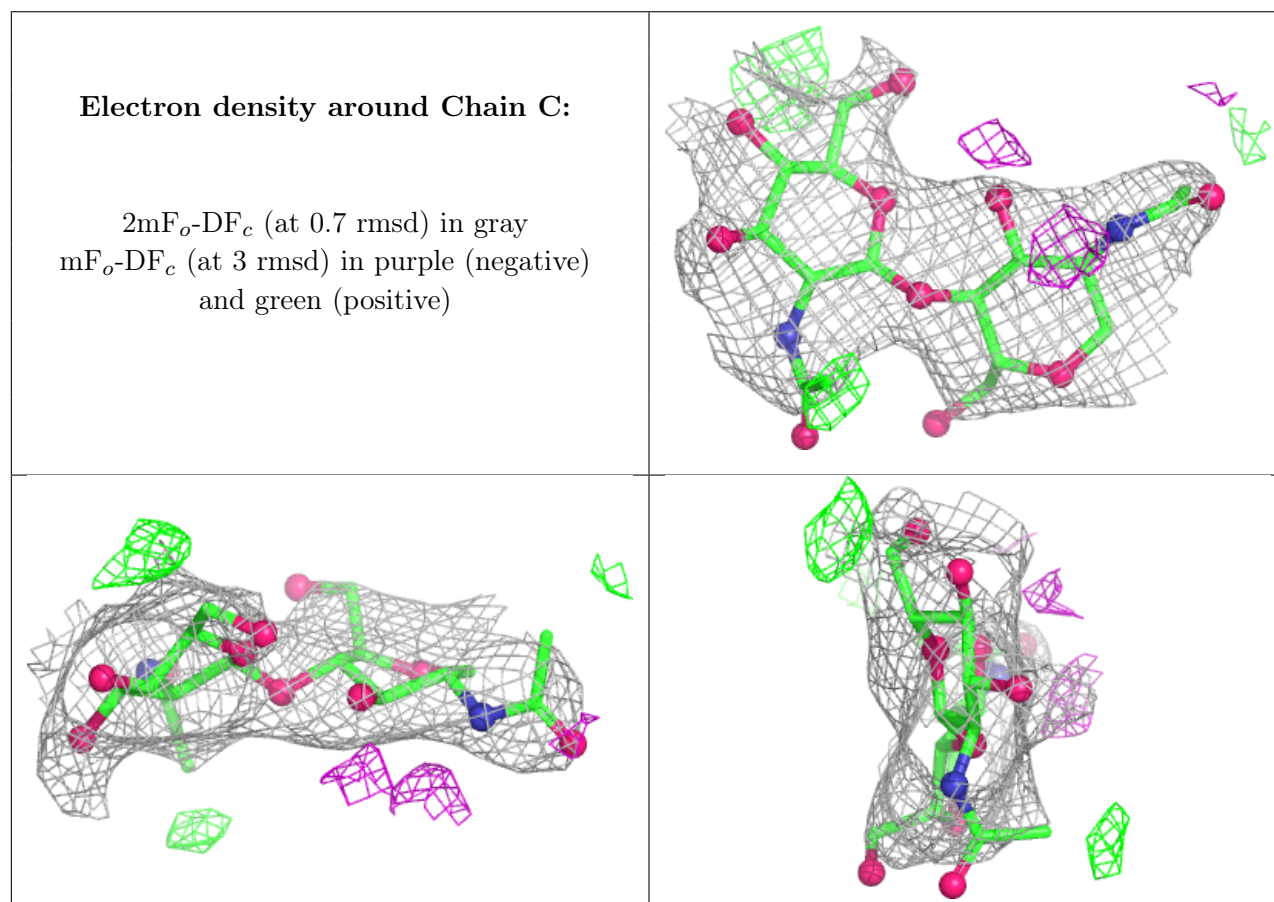
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.35	0.13	106,142,153,158	0
2	NAG	C	1	14/15	0.82	0.12	91,103,124,154	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.



6.4 Ligands ⓘ

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	SO4	A	909	5/5	0.80	0.07	110,132,136,137	0
4	SO4	A	905	5/5	0.81	0.08	112,138,153,161	0
3	GOL	B	1201	6/6	0.84	0.13	88,98,105,105	0
3	GOL	A	903	6/6	0.85	0.11	98,115,116,122	0
4	SO4	A	904	5/5	0.87	0.08	123,129,142,149	0
4	SO4	A	908	5/5	0.88	0.08	134,142,154,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	902	6/6	0.88	0.11	98,103,116,116	0
4	SO4	A	906	5/5	0.89	0.14	77,78,100,120	0
4	SO4	B	1206	5/5	0.89	0.11	75,86,100,119	0
3	GOL	B	1202	6/6	0.91	0.15	63,71,73,73	0
3	GOL	A	901	6/6	0.92	0.10	62,80,88,94	0
3	GOL	B	1203	6/6	0.92	0.10	61,73,81,82	0
4	SO4	B	1204	5/5	0.94	0.07	86,88,97,105	0
4	SO4	A	907	5/5	0.97	0.05	48,66,71,79	0
4	SO4	B	1205	5/5	0.98	0.04	59,62,74,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.