



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:45 PM UTC

PDB ID : 7A3T / pdb_00007a3t
Title : Crystal structure of dengue 3 virus envelope glycoprotein in complex with the Fab fragment of the broadly neutralizing human antibody EDE1 C8
Authors : Sharma, A.; Vaney, M.C.; Guardado-Calvo, P.; Duquerroy, S.; Rouvinski, A.; Rey, F.A.
Deposited on : 2020-08-18
Resolution : 2.65 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

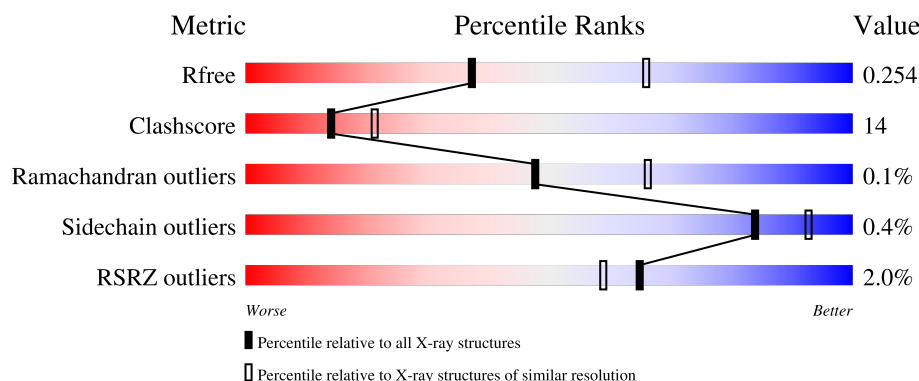
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	428	
2	H	272	
3	L	217	
4	B	5	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6403 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 Core protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2949	1856	509	561	23	0	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	CYS	LEU	engineered mutation	UNP A0A481XTQ0
A	311	CYS	SER	engineered mutation	UNP A0A481XTQ0
A	394	LEU	-	expression tag	UNP A0A481XTQ0
A	395	VAL	-	expression tag	UNP A0A481XTQ0
A	396	PRO	-	expression tag	UNP A0A481XTQ0
A	397	ARG	-	expression tag	UNP A0A481XTQ0
A	398	GLY	-	expression tag	UNP A0A481XTQ0
A	399	SER	-	expression tag	UNP A0A481XTQ0
A	400	SER	-	expression tag	UNP A0A481XTQ0
A	401	ALA	-	expression tag	UNP A0A481XTQ0
A	402	TRP	-	expression tag	UNP A0A481XTQ0
A	403	SER	-	expression tag	UNP A0A481XTQ0
A	404	HIS	-	expression tag	UNP A0A481XTQ0
A	405	PRO	-	expression tag	UNP A0A481XTQ0
A	406	GLN	-	expression tag	UNP A0A481XTQ0
A	407	PHE	-	expression tag	UNP A0A481XTQ0
A	408	GLU	-	expression tag	UNP A0A481XTQ0
A	409	LYS	-	expression tag	UNP A0A481XTQ0
A	410	GLY	-	expression tag	UNP A0A481XTQ0
A	411	GLY	-	expression tag	UNP A0A481XTQ0
A	412	SER	-	expression tag	UNP A0A481XTQ0
A	413	GLY	-	expression tag	UNP A0A481XTQ0
A	414	GLY	-	expression tag	UNP A0A481XTQ0
A	415	GLY	-	expression tag	UNP A0A481XTQ0
A	416	SER	-	expression tag	UNP A0A481XTQ0
A	417	GLY	-	expression tag	UNP A0A481XTQ0
A	418	GLY	-	expression tag	UNP A0A481XTQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	SER	-	expression tag	UNP A0A481XTQ0
A	420	ALA	-	expression tag	UNP A0A481XTQ0
A	421	TRP	-	expression tag	UNP A0A481XTQ0
A	422	SER	-	expression tag	UNP A0A481XTQ0
A	423	HIS	-	expression tag	UNP A0A481XTQ0
A	424	PRO	-	expression tag	UNP A0A481XTQ0
A	425	GLN	-	expression tag	UNP A0A481XTQ0
A	426	PHE	-	expression tag	UNP A0A481XTQ0
A	427	GLU	-	expression tag	UNP A0A481XTQ0
A	428	LYS	-	expression tag	UNP A0A481XTQ0

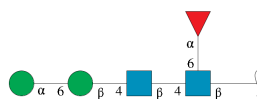
- Molecule 2 is a protein called EDE1 C8 antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	1	0
			1653	1047	269	329	8			

- Molecule 3 is a protein called EDE1 C8 antibody Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	215	Total	C	N	O	S	0	2	0
			1689	1061	288	336	4			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	B	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

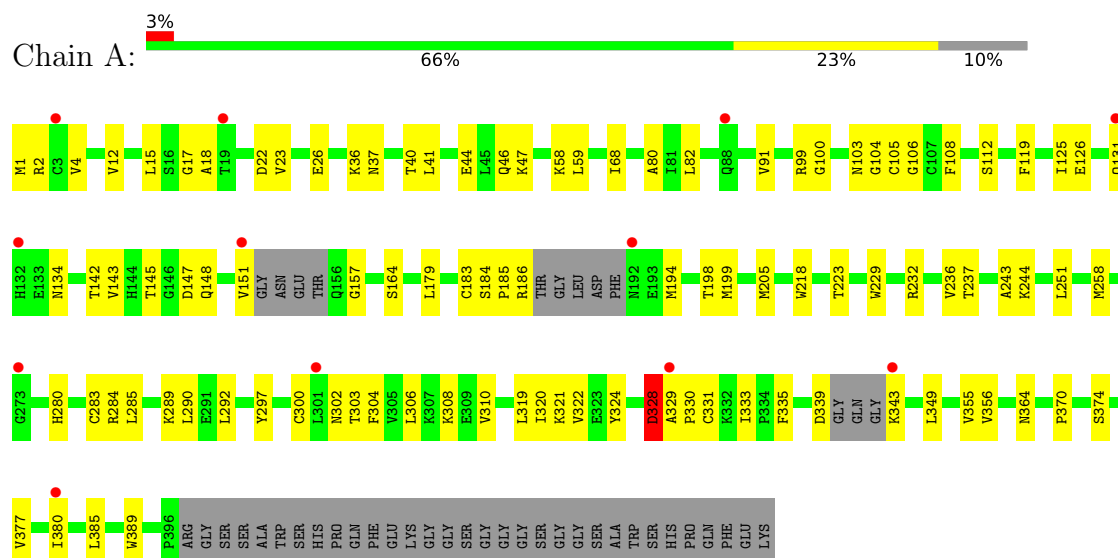
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	O	0	0
			2	2		
7	H	1	Total	O	0	0
			1	1		
7	L	5	Total	O	0	0
			5	5		

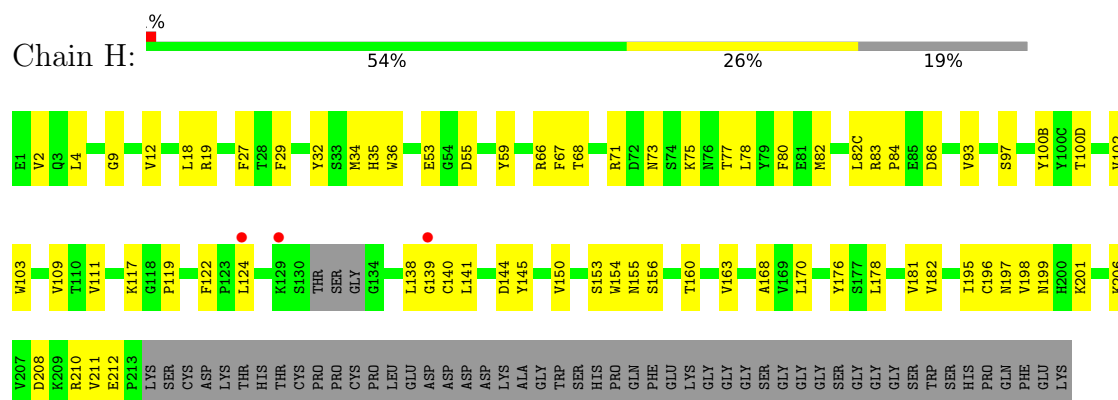
3 Residue-property plots [i](#)

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.

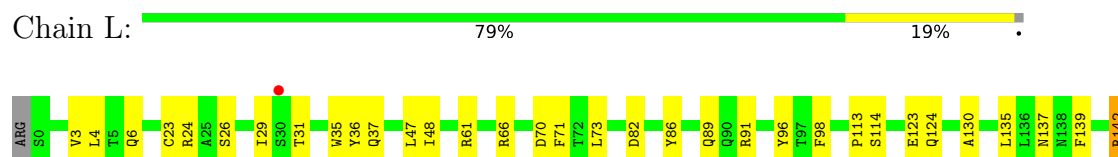
• Molecule 1: Core protein

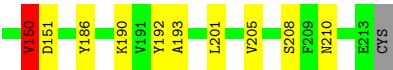


• Molecule 2: EDE1 C8 antibody Fab fragment



• Molecule 3: EDE1 C8 antibody Fab fragment





- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.31Å 110.31Å 217.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.53 – 2.65 29.53 – 2.66	Depositor EDS
% Data completeness (in resolution range)	74.0 (29.53-2.65) 73.9 (29.53-2.66)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.64Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.207 , 0.254 0.209 , 0.254	Depositor DCC
R_{free} test set	2031 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: BMA, FUC, NAG, SO4, GOL, MAN

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	0.27	0/3002	0.64	4/4063 (0.1%)
2	H	0.27	0/1698	0.57	0/2312
3	L	0.30	1/1732 (0.1%)	0.66	5/2356 (0.2%)
All	All	0.28	1/6432 (0.0%)	0.63	9/8731 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	150	VAL	CA-CB	-5.61	1.46	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASP	N-CA-C	-10.23	94.86	110.10
3	L	150	VAL	CA-C-N	-8.95	104.45	121.54
3	L	150	VAL	C-N-CA	-8.95	104.45	121.54
3	L	29	ILE	CA-C-N	7.63	136.12	121.54
3	L	29	ILE	C-N-CA	7.63	136.12	121.54
1	A	105	CYS	CA-CB-SG	-6.00	100.59	114.40
3	L	150	VAL	O-C-N	-5.90	115.19	122.57
1	A	104	GLY	CA-C-N	-5.30	113.59	122.92
1	A	104	GLY	C-N-CA	-5.30	113.59	122.92

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	2949	0	2940	81	0
2	H	1653	0	1591	64	0
3	L	1689	0	1643	42	0
4	B	60	0	52	1	0
5	A	10	0	0	1	0
5	H	10	0	0	0	0
6	A	18	0	24	1	0
6	L	6	0	8	0	0
7	A	2	0	0	0	0
7	H	1	0	0	0	0
7	L	5	0	0	0	0
All	All	6403	0	6258	181	0

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

All (181) 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:A:131:GLN:HE21	1:A:134:ASN:HB3	1.24	1.01
3:L:150:VAL:HG13	3:L:151:ASP:H	1.23	1.00
3:L:142[A]:ARG:HH11	3:L:142[A]:ARG:HG3	1.30	0.95
3:L:150:VAL:CG1	3:L:151:ASP:N	2.38	0.87
3:L:24:ARG:HH21	3:L:70:ASP:HB2	1.40	0.84
3:L:150:VAL:HG13	3:L:151:ASP:N	1.89	0.81
3:L:150:VAL:O	3:L:151:ASP:C	2.17	0.80
1:A:99:ARG:HA	1:A:103:ASN:HD21	1.46	0.80
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.15	0.80
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.14	0.79
1:A:179:LEU:HD11	1:A:285:LEU:HB3	1.64	0.79
3:L:150:VAL:CG1	3:L:151:ASP:H	1.94	0.77
2:H:163:VAL:HG12	2:H:182:VAL:HB	1.64	0.77
2:H:4:LEU:HD21	2:H:34[B]:MET:HE1	1.69	0.75
2:H:84:PRO:HA	2:H:111:VAL:HG23	1.69	0.74
3:L:36:TYR:OH	3:L:91:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HG11	1:A:319:LEU:HD22	1.69	0.72
1:A:328:ASP:OD2	1:A:328:ASP:N	2.11	0.71
1:A:12:VAL:HG11	1:A:23:VAL:HG12	1.73	0.71
2:H:201:LYS:HZ1	2:H:206:LYS:HE2	1.56	0.70
2:H:181:VAL:HG21	3:L:135:LEU:HD13	1.72	0.70
1:A:164:SER:HA	1:A:185:PRO:HG2	1.74	0.70
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.74	0.69
1:A:91:VAL:HG11	1:A:236:VAL:HG21	1.75	0.69
1:A:339:ASP:HB3	1:A:343:LYS:HB2	1.77	0.67
1:A:22:ASP:HA	1:A:284:ARG:HB3	1.77	0.66
2:H:12:VAL:HG11	2:H:82(C):LEU:HD12	1.78	0.66
1:A:26:GLU:HG2	1:A:280:HIS:ND1	2.10	0.66
2:H:29:PHE:HE1	2:H:34[B]:MET:HE2	1.61	0.66
1:A:292:LEU:H	1:A:292:LEU:HD12	1.60	0.65
2:H:139:GLY:O	2:H:211:VAL:HG21	1.96	0.65
2:H:12:VAL:HB	2:H:111:VAL:HG12	1.80	0.64
1:A:300:CYS:SG	1:A:324:TYR:CZ	2.92	0.63
1:A:183:CYS:HA	1:A:283:CYS:HA	1.81	0.62
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.81	0.62
1:A:1:MET:HB3	1:A:151:VAL:HG11	1.82	0.61
2:H:124:LEU:CD1	2:H:181:VAL:HG22	2.30	0.61
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.36	0.61
2:H:9:GLY:HA2	2:H:109:VAL:HG12	1.83	0.61
3:L:150:VAL:O	3:L:151:ASP:O	2.18	0.60
3:L:193:ALA:HB2	3:L:208:SER:HB3	1.84	0.60
1:A:142:THR:HG22	1:A:157:GLY:HA3	1.84	0.60
2:H:181:VAL:HG21	3:L:135:LEU:CD1	2.31	0.59
1:A:339:ASP:HB3	1:A:343:LYS:CB	2.33	0.59
1:A:297:TYR:HD1	1:A:355:VAL:HG21	1.68	0.58
2:H:32:TYR:O	2:H:71:ARG:NH2	2.34	0.58
2:H:170:LEU:HD12	2:H:176:TYR:CZ	2.38	0.58
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.85	0.58
1:A:46:GLN:HG2	1:A:47:LYS:HG2	1.86	0.58
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.39	0.58
2:H:124:LEU:HG	2:H:139:GLY:C	2.30	0.57
2:H:160:THR:O	2:H:163:VAL:HG22	2.05	0.57
3:L:123[A]:GLU:OE1	3:L:123[A]:GLU:N	2.35	0.57
3:L:123[B]:GLU:OE1	3:L:123[B]:GLU:N	2.35	0.57
1:A:37:ASN:C	1:A:292:LEU:HD11	2.29	0.56
2:H:97:SER:OG	2:H:100(B):TYR:O	2.14	0.55
1:A:308:LYS:HE2	3:L:31:THR:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82(C):LEU:HB3	2:H:111:VAL:HG11	1.89	0.55
1:A:308:LYS:HE2	3:L:31:THR:HG21	1.89	0.54
2:H:124:LEU:HD11	2:H:181:VAL:HG22	1.90	0.54
3:L:61:ARG:HH12	3:L:82:ASP:CG	2.15	0.54
1:A:125:ILE:HG21	1:A:199:MET:HE2	1.91	0.53
1:A:335:PHE:CE1	1:A:349:LEU:HD21	2.43	0.53
2:H:4:LEU:HD11	2:H:102:VAL:HG13	1.91	0.53
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.44	0.52
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.91	0.52
1:A:184:SER:O	1:A:186:ARG:N	2.44	0.51
2:H:156:SER:HA	2:H:197:ASN:HD21	1.76	0.51
1:A:2:ARG:HH21	1:A:44:GLU:CD	2.18	0.51
2:H:18:LEU:HD12	2:H:19:ARG:H	1.75	0.51
1:A:306:LEU:HD23	1:A:306:LEU:H	1.75	0.51
2:H:83:ARG:O	2:H:111:VAL:HG21	2.10	0.51
3:L:142[A]:ARG:HG3	3:L:142[A]:ARG:NH1	2.09	0.51
2:H:71:ARG:HD3	2:H:73:ASN:OD1	2.12	0.50
2:H:156:SER:HA	2:H:197:ASN:ND2	2.26	0.50
2:H:124:LEU:HG	2:H:140:CYS:N	2.26	0.50
1:A:297:TYR:CD1	1:A:355:VAL:HG21	2.46	0.50
3:L:6:GLN:NE2	3:L:86:TYR:O	2.41	0.50
3:L:190:LYS:HE2	3:L:210:ASN:OD1	2.12	0.50
1:A:145:THR:HG21	1:A:147:ASP:HB2	1.94	0.49
2:H:34[B]:MET:HG2	2:H:71:ARG:NH2	2.28	0.49
2:H:117:LYS:HD3	2:H:144:ASP:O	2.12	0.49
1:A:329:ALA:HB3	1:A:330:PRO:HD3	1.95	0.48
3:L:186:TYR:O	3:L:192:TYR:OH	2.30	0.48
1:A:68:ILE:N	6:A:504:GOL:O1	2.46	0.48
1:A:119:PHE:CD2	1:A:232:ARG:HG2	2.49	0.48
2:H:75:LYS:O	2:H:77:THR:HG23	2.13	0.48
2:H:124:LEU:HB2	2:H:139:GLY:N	2.29	0.48
1:A:58:LYS:C	1:A:59:LEU:HD23	2.39	0.48
1:A:370:PRO:HG2	1:A:374:SER:HB2	1.96	0.48
1:A:205:MET:HB3	1:A:205:MET:HE3	1.78	0.48
2:H:93:VAL:HG22	2:H:103:TRP:CD2	2.49	0.47
2:H:210:ARG:HH21	2:H:212:GLU:CD	2.22	0.47
1:A:310:VAL:HG12	1:A:320:ILE:HG12	1.95	0.47
2:H:196:CYS:O	2:H:208:ASP:HA	2.14	0.47
2:H:53:GLU:HB2	2:H:55:ASP:OD1	2.14	0.47
1:A:289:LYS:HD3	1:A:289:LYS:O	2.14	0.47
2:H:155:ASN:HA	2:H:195:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:HG23	1:A:147:ASP:H	1.79	0.47
1:A:100:GLY:HA3	1:A:108:PHE:CE1	2.50	0.46
1:A:330:PRO:HA	1:A:356:VAL:O	2.15	0.46
2:H:67:PHE:HD2	2:H:80:PHE:CZ	2.33	0.46
3:L:3:VAL:HG22	3:L:26:SER:HB2	1.98	0.46
1:A:199:MET:HE1	1:A:258:MET:CB	2.45	0.46
1:A:302:ASN:HB3	1:A:324:TYR:CE2	2.50	0.46
2:H:59:TYR:CE1	2:H:68:THR:HA	2.50	0.46
3:L:124:GLN:OE1	3:L:130:ALA:HA	2.16	0.46
1:A:15:LEU:O	1:A:18:ALA:N	2.49	0.46
3:L:3:VAL:H	3:L:26:SER:HB3	1.80	0.46
1:A:302:ASN:ND2	1:A:303:THR:H	2.13	0.46
1:A:131:GLN:H	1:A:131:GLN:CD	2.25	0.46
1:A:237:THR:HG23	1:A:251:LEU:HD21	1.98	0.46
1:A:377:VAL:HA	1:A:385:LEU:O	2.16	0.46
3:L:89:GLN:HB2	3:L:98:PHE:CD1	2.51	0.45
1:A:59:LEU:HD22	1:A:218:TRP:HB3	1.97	0.45
1:A:148:GLN:CD	1:A:321:LYS:HZ1	2.24	0.45
1:A:199:MET:HE1	1:A:258:MET:HB3	1.99	0.45
3:L:35:TRP:HD1	3:L:48:ILE:HD11	1.82	0.45
1:A:1:MET:HG2	1:A:145:THR:O	2.16	0.45
1:A:304:PHE:CE2	1:A:324:TYR:HB2	2.52	0.45
3:L:201:LEU:HD13	3:L:205:VAL:HG13	1.98	0.45
1:A:179:LEU:HB2	1:A:290:LEU:HD11	1.98	0.45
2:H:201:LYS:NZ	2:H:206:LYS:HE2	2.31	0.45
1:A:333:ILE:HG12	1:A:356:VAL:HG23	1.99	0.45
2:H:36:TRP:CE2	2:H:80:PHE:HB2	2.51	0.45
2:H:67:PHE:CD1	2:H:67:PHE:N	2.85	0.45
3:L:150:VAL:HG12	3:L:151:ASP:N	2.26	0.45
2:H:170:LEU:HD12	2:H:176:TYR:CE2	2.53	0.44
3:L:89:GLN:HB2	3:L:98:PHE:CE1	2.51	0.44
1:A:223:THR:O	1:A:223:THR:HG22	2.17	0.44
1:A:2:ARG:HD3	1:A:142:THR:HG21	1.98	0.44
1:A:331:CYS:O	1:A:355:VAL:HG23	2.16	0.44
1:A:17:GLY:H	1:A:36:LYS:HZ1	1.65	0.44
1:A:80:ALA:H	1:A:112:SER:HB3	1.82	0.44
1:A:335:PHE:CD1	1:A:349:LEU:HD21	2.52	0.44
1:A:292:LEU:HD12	1:A:292:LEU:N	2.29	0.44
1:A:306:LEU:H	1:A:306:LEU:CD2	2.31	0.44
3:L:114:SER:HB2	3:L:137:ASN:HB3	2.00	0.44
2:H:100(D):THR:O	3:L:91:ARG:NH1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3:BMA:C5	4:B:4:MAN:H2	2.47	0.44
1:A:320:ILE:HG22	1:A:322:VAL:HG13	1.99	0.44
2:H:153:SER:OG	2:H:197:ASN:HB2	2.18	0.44
1:A:126:GLU:HB2	1:A:198:THR:CG2	2.48	0.43
1:A:229:TRP:O	1:A:232:ARG:HG3	2.18	0.43
2:H:12:VAL:O	2:H:111:VAL:HA	2.18	0.43
2:H:67:PHE:CD2	2:H:82:MET:HG2	2.53	0.43
1:A:40:THR:O	1:A:41:LEU:HD23	2.18	0.43
2:H:150:VAL:HG11	2:H:198:VAL:HG13	2.01	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.77	0.43
1:A:310:VAL:HG23	1:A:389:TRP:HZ3	1.84	0.43
2:H:199:ASN:HD21	2:H:201:LYS:NZ	2.16	0.43
3:L:24:ARG:NH2	3:L:70:ASP:HB2	2.19	0.43
1:A:1:MET:HE2	1:A:364:ASN:HB3	2.01	0.42
1:A:1:MET:CB	1:A:151:VAL:HG11	2.48	0.42
1:A:329:ALA:CB	1:A:330:PRO:HD3	2.49	0.42
2:H:34[B]:MET:HB3	2:H:78:LEU:HD22	2.00	0.42
2:H:122:PHE:CE2	3:L:124:GLN:HG3	2.54	0.42
3:L:4:LEU:HB3	3:L:23:CYS:SG	2.59	0.42
1:A:17:GLY:H	1:A:36:LYS:NZ	2.17	0.42
3:L:66:ARG:HG3	3:L:71:PHE:CE2	2.55	0.42
2:H:138:LEU:N	2:H:138:LEU:HD23	2.34	0.42
1:A:12:VAL:HG11	1:A:23:VAL:CG1	2.46	0.42
1:A:179:LEU:HD21	1:A:285:LEU:HD12	2.00	0.42
1:A:106:GLY:N	5:A:501:SO4:O3	2.53	0.42
1:A:243:ALA:C	1:A:244:LYS:HD2	2.44	0.42
1:A:310:VAL:CG1	1:A:320:ILE:HG12	2.50	0.41
1:A:380:ILE:HA	1:A:380:ILE:HD12	1.80	0.41
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.26	0.41
3:L:35:TRP:CD1	3:L:48:ILE:HD11	2.56	0.41
3:L:91:ARG:HA	3:L:96:TYR:CD1	2.56	0.41
1:A:143:VAL:O	1:A:145:THR:N	2.54	0.41
2:H:141:LEU:HD12	2:H:178:LEU:O	2.21	0.41
2:H:168:ALA:HA	2:H:178:LEU:HB3	2.03	0.41
2:H:181:VAL:HG11	3:L:135:LEU:HD13	2.03	0.41
1:A:292:LEU:H	1:A:292:LEU:CD1	2.33	0.40
2:H:4:LEU:HD12	2:H:102:VAL:HG22	2.02	0.40
3:L:35:TRP:CD2	3:L:73:LEU:HB2	2.56	0.40
2:H:199:ASN:CG	2:H:201:LYS:HZ2	2.28	0.40
1:A:194:MET:HE3	1:A:205:MET:HE3	2.03	0.40
2:H:67:PHE:N	2:H:67:PHE:HD1	2.19	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	376/428 (88%)	358 (95%)	18 (5%)	0	100	100
2	H	216/272 (79%)	207 (96%)	9 (4%)	0	100	100
3	L	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	24	39
All	All	807/917 (88%)	770 (95%)	36 (4%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	150	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/355 (91%)	322 (100%)	1 (0%)	86	94
2	H	186/226 (82%)	186 (100%)	0	100	100
3	L	190/190 (100%)	187 (98%)	3 (2%)	55	74
All	All	699/771 (91%)	695 (99%)	4 (1%)	84	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	ASP
3	L	142[A]	ARG
3	L	142[B]	ARG
3	L	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	246	GLN
1	A	346	ASN
1	A	353	ASN
2	H	171	GLN
2	H	197	ASN
3	L	137	ASN
3	L	152	ASN
3	L	189	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 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	$\# Z > 2$
4	NAG	B	1	1,4	14,14,15	1.27	2 (14%)	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	2	4	14,14,15	0.96	1 (7%)	17,19,21	1.35	2 (11%)
4	BMA	B	3	4	11,11,12	0.92	0	15,15,17	0.85	1 (6%)
4	MAN	B	4	4	11,11,12	1.47	2 (18%)	15,15,17	1.34	2 (13%)
4	FUC	B	5	4	10,10,11	1.51	2 (20%)	14,14,16	0.88	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
4	NAG	B	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	BMA	B	3	4	-	2/2/19/22	1/1/1/1
4	MAN	B	4	4	-	2/2/19/22	1/1/1/1
4	FUC	B	5	4	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	O5-C1	3.61	1.49	1.43
4	B	2	NAG	O5-C1	3.45	1.49	1.43
4	B	4	MAN	O5-C5	3.40	1.50	1.43
4	B	1	NAG	C1-C2	2.96	1.56	1.52
4	B	5	FUC	C4-C3	2.61	1.59	1.52
4	B	5	FUC	C4-C5	2.43	1.58	1.52
4	B	4	MAN	C1-C2	2.26	1.57	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C1-O5-C5	4.90	118.76	112.19
4	B	4	MAN	C1-O5-C5	3.62	117.03	112.19
4	B	4	MAN	O2-C2-C3	-2.32	105.34	110.15
4	B	3	BMA	C1-O5-C5	2.11	115.02	112.19
4	B	2	NAG	C4-C3-C2	-2.01	108.08	111.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3	BMA	O5-C5-C6-O6
4	B	3	BMA	C4-C5-C6-O6
4	B	1	NAG	C8-C7-N2-C2
4	B	1	NAG	O7-C7-N2-C2
4	B	2	NAG	C8-C7-N2-C2
4	B	2	NAG	O7-C7-N2-C2
4	B	4	MAN	O5-C5-C6-O6
4	B	1	NAG	C4-C5-C6-O6
4	B	4	MAN	C4-C5-C6-O6

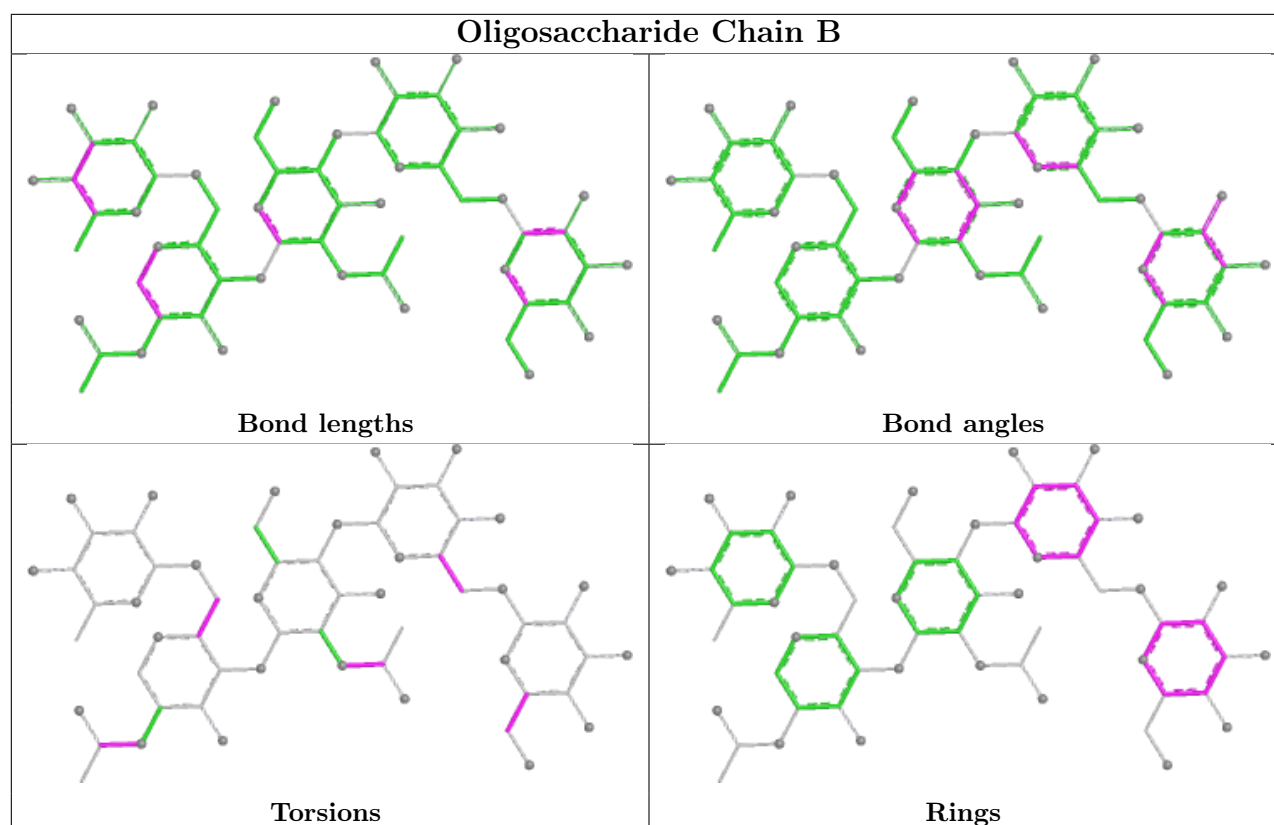
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4	MAN	C1-C2-C3-C4-C5-O5
4	B	3	BMA	C1-C2-C3-C4-C5-O5

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3	BMA	1	0
4	B	4	MAN	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](#)

8 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	$\# Z > 2$
6	GOL	A	504	-	5,5,5	0.92	0	5,5,5	1.06	0
6	GOL	A	505	-	5,5,5	0.91	0	5,5,5	1.06	0
5	SO4	H	301	-	4,4,4	0.38	0	6,6,6	0.11	0
6	GOL	L	301	-	5,5,5	1.01	0	5,5,5	1.04	0
6	GOL	A	503	-	5,5,5	1.15	0	5,5,5	0.94	0
5	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.16	0
5	SO4	A	501	-	4,4,4	0.28	0	6,6,6	0.08	0
5	SO4	H	302	-	4,4,4	0.41	0	6,6,6	0.25	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
6	GOL	A	504	-	-	0/4/4/4	-
6	GOL	A	505	-	-	0/4/4/4	-
6	GOL	L	301	-	-	2/4/4/4	-
6	GOL	A	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	301	GOL	O1-C1-C2-C3
6	L	301	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	504	GOL	1	0
5	A	501	SO4	1	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	384/428 (89%)	0.28	12 (3%) 51 43	50, 75, 115, 139	0
2	H	219/272 (80%)	-0.03	3 (1%) 73 69	33, 64, 102, 118	1 (0%)
3	L	215/217 (99%)	-0.36	1 (0%) 87 85	26, 56, 80, 107	2 (0%)
All	All	818/917 (89%)	0.03	16 (1%) 65 59	26, 66, 107, 139	3 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	139	GLY	4.6
2	H	124	LEU	3.3
1	A	132	HIS	3.0
1	A	329	ALA	2.8
1	A	273	GLY	2.8
1	A	380	ILE	2.6
1	A	131	GLN	2.6
1	A	192	ASN	2.5
3	L	30	SER	2.3
1	A	88	GLN	2.2
1	A	301	LEU	2.2
2	H	129	LYS	2.2
1	A	151	VAL	2.2
1	A	19	THR	2.2
1	A	343	LYS	2.1
1	A	3	CYS	2.1

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

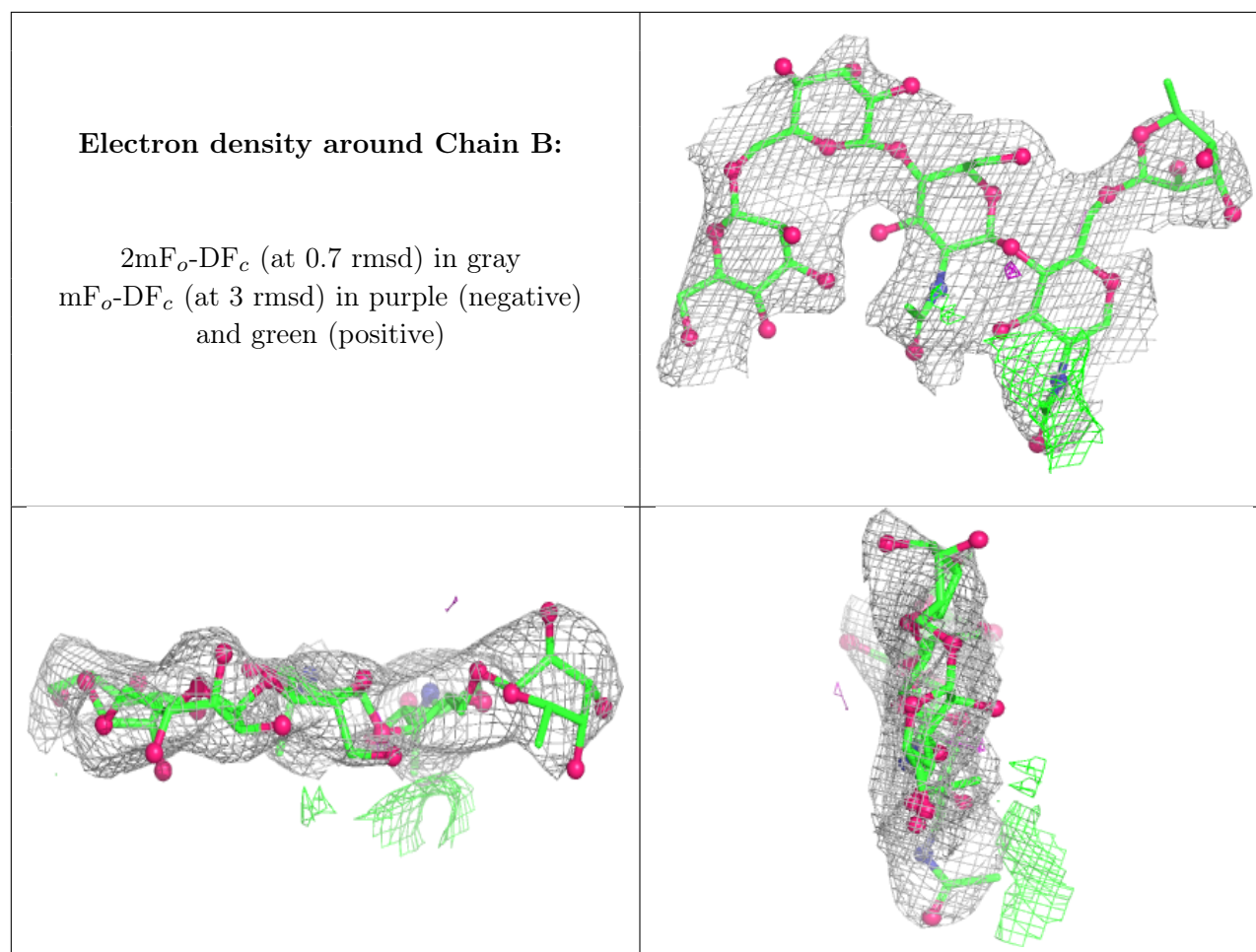
There are no non-standard protein/DNA/RNA residues in this entry.

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(Å ²)	Q<0.9
4	NAG	B	1	14/15	-	-	78,94,113,128	0
4	NAG	B	2	14/15	-	-	90,124,138,138	0
4	BMA	B	3	11/12	-	-	116,122,133,133	0
4	MAN	B	4	11/12	-	-	91,116,130,134	0
4	FUC	B	5	10/11	-	-	104,110,131,144	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 [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
5	SO4	H	301	5/5	0.77	0.29	96,108,110,130	0
6	GOL	A	503	6/6	0.77	0.26	86,91,96,99	0
6	GOL	A	504	6/6	0.85	0.15	53,68,75,97	0
5	SO4	A	502	5/5	0.86	0.26	91,99,120,121	0
6	GOL	L	301	6/6	0.88	0.14	60,74,75,81	0
5	SO4	H	302	5/5	0.91	0.21	96,105,111,132	0
6	GOL	A	505	6/6	0.93	0.11	72,80,80,81	0
5	SO4	A	501	5/5	0.95	0.14	82,101,103,106	0

6.5 Other polymers [i](#)

There are no such residues in this entry.