



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 4LSP / pdb_00004lsp
Title : Crystal structure of broadly and potently neutralizing antibody VRC-CH31 in complex with HIV-1 clade A/E gp120 93TH057
Authors : Zhou, T.; Moquin, S.; Kwong, P.D.
Deposited on : 2013-07-23
Resolution : 2.15 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

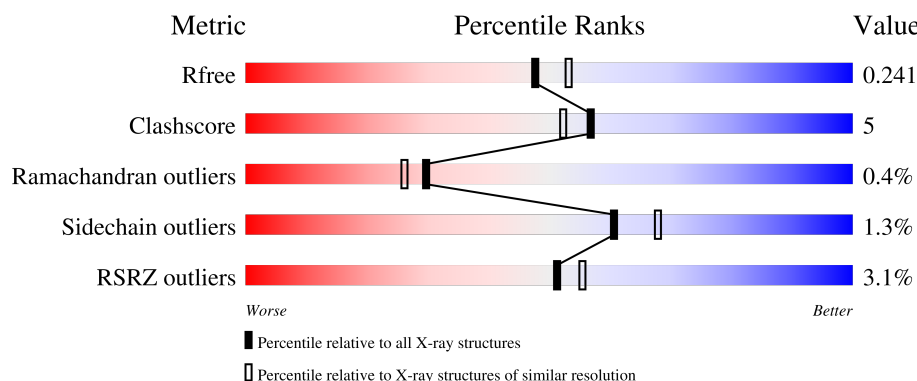
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

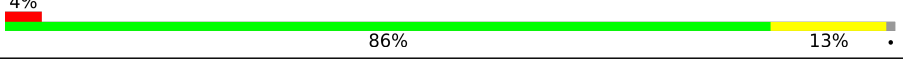
The reported resolution of this entry is 2.15 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	G	353	
2	H	236	
3	L	210	
4	A	3	

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
5	NAG	G	511	-	-	X	-
7	EDO	G	516	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12393 atoms, of which 5895 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 HIV-1 CLADE A/E STRAIN 93TH057 GP120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	347	Total	C	H	N	O	S	0	0	0
			5363	1700	2650	472	518	23			

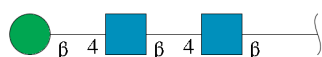
- Molecule 2 is a protein called HEAVY CHAIN OF ANTIBODY VRC-CH31.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	216	Total	C	H	N	O	S	0	0	0
			3261	1043	1614	287	311	6			

- Molecule 3 is a protein called LIGHT CHAIN OF ANTIBODY VRC-CH31.

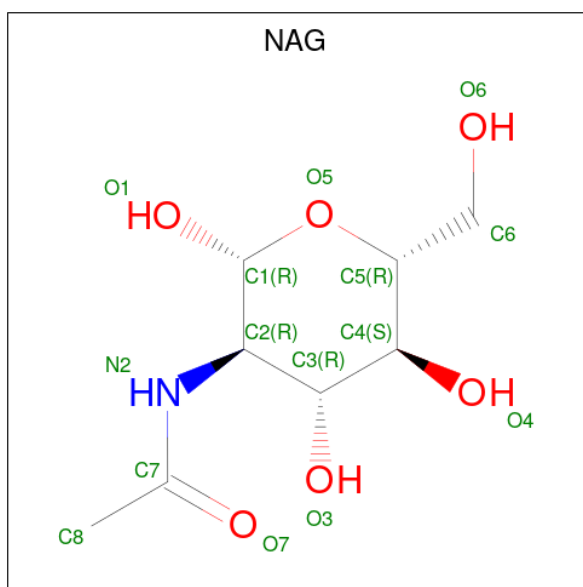
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	208	Total	C	H	N	O	S	0	0	0
			3134	989	1545	271	324	5			

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



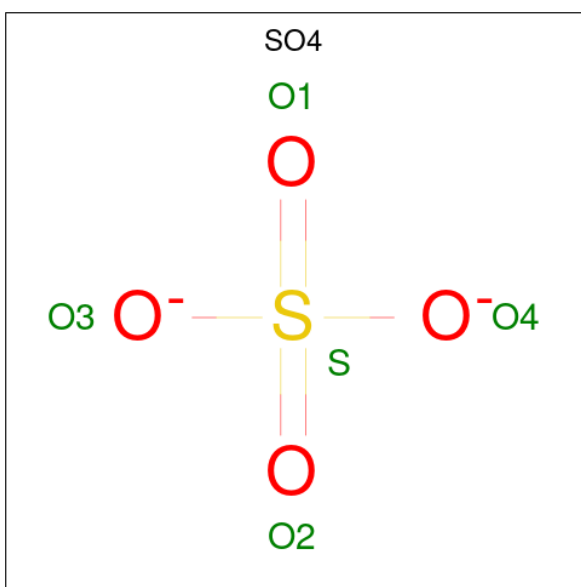
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



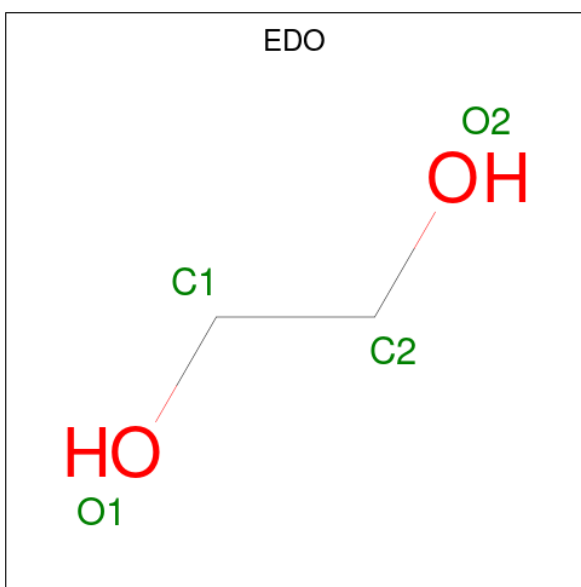
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



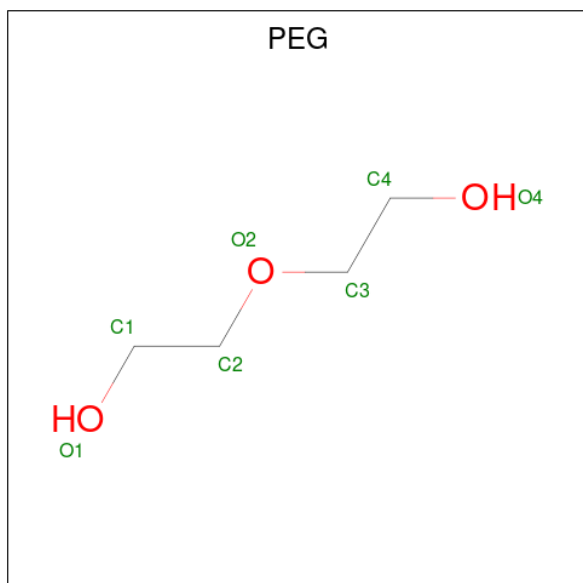
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	H	O	0	0
			10	2	6	2		
7	G	1	Total	C	H	O	0	0
			10	2	6	2		
7	G	1	Total	C	H	O	0	0
			10	2	6	2		
7	G	1	Total	C	H	O	0	0
			10	2	6	2		
7	H	1	Total	C	H	O	0	0
			10	2	6	2		
7	H	1	Total	C	H	O	0	0
			10	2	6	2		
7	H	1	Total	C	H	O	0	0
			10	2	6	2		
7	H	1	Total	C	H	O	0	0
			10	2	6	2		
7	L	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	H	O	0	0
			17	4	10	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	2	Total	Na	0	0
			2	2		
9	H	1	Total	Na	0	0
			1	1		

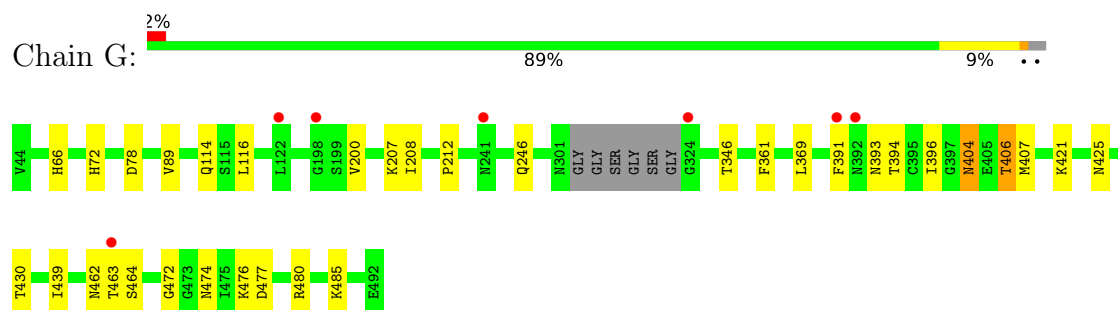
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	142	Total	O	0	0
			142	142		
10	H	78	Total	O	0	0
			78	78		
10	L	46	Total	O	0	0
			46	46		

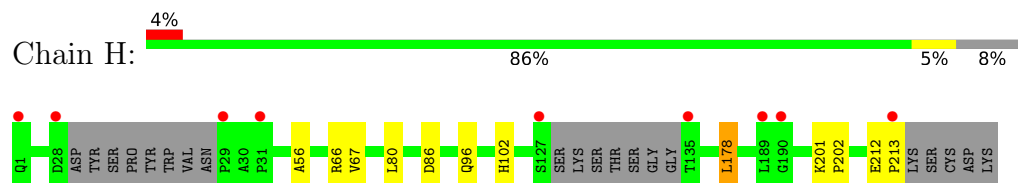
3 Residue-property plots [i](#)

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.

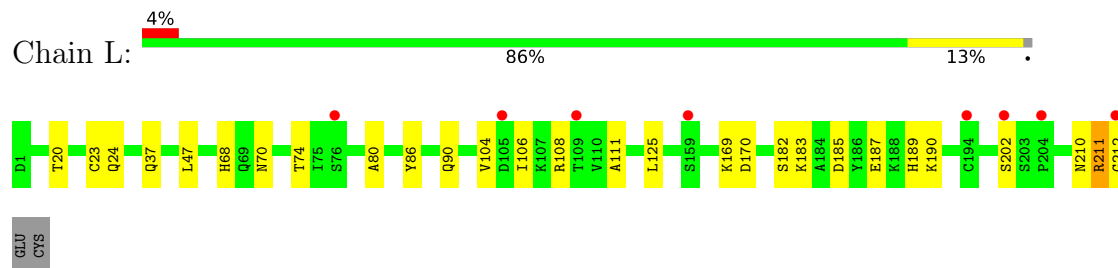
- Molecule 1: HIV-1 CLADE A/E STRAIN 93TH057 GP120



- Molecule 2: HEAVY CHAIN OF ANTIBODY VRC-CH31



- Molecule 3: LIGHT CHAIN OF ANTIBODY VRC-CH31



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.39Å 83.96Å 175.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.04 – 2.15 48.04 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.04-2.15) 95.3 (48.04-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.16Å)	Xtriage
Refinement program	PHENIX dev_1317	Depositor
R, R_{free}	0.180 , 0.214 (Not available) , 0.241	Depositor DCC
R_{free} test set	2669 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12393	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: SO4, NA, NAG, PEG, EDO, BMA

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	G	0.36	0/2770	0.66	0/3760
2	H	0.36	0/1691	0.62	0/2309
3	L	0.34	0/1619	0.63	0/2192
All	All	0.35	0/6080	0.64	0/8261

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2713	2650	2641	22	1
2	H	1647	1614	1609	9	0
3	L	1589	1545	1546	16	0
4	A	39	0	34	2	0
5	G	168	0	156	11	0
6	G	10	0	0	0	0
6	L	5	0	0	0	0
7	G	20	30	29	5	0
7	H	20	30	30	0	0
7	L	4	6	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	14	20	20	3	0
9	G	2	0	0	0	0
9	H	1	0	0	0	0
10	G	142	0	0	6	1
10	H	78	0	0	0	0
10	L	46	0	0	1	0
All	All	6498	5895	6071	57	1

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 5.

All (57) 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)
5:G:501:NAG:H82	5:G:501:NAG:O3	1.63	0.95
3:L:189:HIS:O	3:L:211:ARG:NH1	2.17	0.78
1:G:391:PHE:O	10:G:706:HOH:O	2.05	0.73
5:G:511:NAG:C3	5:G:511:NAG:H83	2.19	0.73
5:G:511:NAG:C3	5:G:511:NAG:C8	2.69	0.71
1:G:406:THR:HA	5:G:511:NAG:H62	1.73	0.69
5:G:511:NAG:C8	5:G:511:NAG:H3	2.22	0.69
5:G:511:NAG:H83	5:G:511:NAG:O3	1.95	0.67
7:G:516:EDO:O1	10:G:677:HOH:O	2.13	0.67
3:L:70:ASN:ND2	4:A:1:NAG:H83	2.11	0.65
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.32	0.63
3:L:24:GLN:NE2	3:L:70:ASN:OD1	2.33	0.61
1:G:407:MET:O	5:G:511:NAG:O6	2.19	0.60
5:G:501:NAG:O3	5:G:501:NAG:C8	2.45	0.59
1:G:369:LEU:HB2	8:G:521:PEG:H31	1.85	0.59
5:G:512:NAG:H83	10:G:639:HOH:O	2.04	0.57
1:G:246:GLN:NE2	10:G:681:HOH:O	2.39	0.55
5:G:511:NAG:H83	5:G:511:NAG:H3	1.83	0.53
3:L:182:SER:OG	3:L:185:ASP:OD1	2.25	0.53
2:H:96:GLN:OE1	2:H:102:HIS:NE2	2.41	0.52
1:G:485:LYS:NZ	10:G:732:HOH:O	2.40	0.52
3:L:210:ASN:O	3:L:212:GLY:N	2.43	0.52
7:G:516:EDO:H22	2:H:56:ALA:HB1	1.92	0.52
3:L:183:LYS:NZ	3:L:187:GLU:OE2	2.44	0.50
3:L:70:ASN:HD22	4:A:1:NAG:H83	1.76	0.50
1:G:425:ASN:CG	8:G:521:PEG:H11	2.37	0.49
1:G:472:GLY:HA2	7:G:516:EDO:H21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:LYS:HE2	1:G:439:ILE:HG23	1.94	0.49
1:G:394:THR:CG2	1:G:407:MET:SD	3.01	0.49
3:L:190:LYS:NZ	10:L:431:HOH:O	2.44	0.48
1:G:421:LYS:NZ	8:G:521:PEG:H21	2.29	0.47
1:G:114:GLN:NE2	10:G:709:HOH:O	2.38	0.47
1:G:393:ASN:HA	1:G:396:ILE:HD13	1.96	0.47
2:H:67:VAL:CG1	2:H:80:LEU:HD11	2.44	0.47
1:G:462:ASN:O	1:G:464:SER:N	2.47	0.46
5:G:511:NAG:H3	5:G:511:NAG:H82	1.94	0.46
3:L:80:ALA:HA	3:L:106:ILE:HD11	1.98	0.46
3:L:20:THR:HG22	3:L:74:THR:HG23	1.98	0.46
2:H:178:LEU:C	2:H:178:LEU:HD12	2.41	0.46
1:G:346:THR:HG21	1:G:396:ILE:HG21	1.97	0.45
1:G:477:ASP:OD1	1:G:480:ARG:NH1	2.43	0.45
1:G:474:ASN:OD1	1:G:476:LYS:HB2	2.16	0.45
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.24	0.45
3:L:169:LYS:HG3	3:L:170:ASP:N	2.33	0.44
7:G:516:EDO:H22	2:H:56:ALA:CB	2.47	0.43
1:G:396:ILE:C	1:G:404:ASN:H	2.25	0.43
1:G:346:THR:HG22	1:G:361:PHE:HE2	1.82	0.43
3:L:86:TYR:HE1	3:L:104:VAL:CG1	2.32	0.42
1:G:66:HIS:CG	1:G:212:PRO:HA	2.54	0.42
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.00	0.42
1:G:78:ASP:HB3	7:G:518:EDO:H12	2.02	0.42
3:L:86:TYR:HE1	3:L:104:VAL:HG11	1.85	0.42
2:H:212:GLU:HB2	2:H:213:PRO:HD2	2.01	0.41
1:G:116:LEU:HD21	1:G:208:ILE:HD11	2.03	0.41
3:L:108:ARG:NH2	3:L:111:ALA:HB2	2.36	0.41
3:L:125:LEU:O	3:L:183:LYS:HD2	2.21	0.41
2:H:201:LYS:N	2:H:202:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:HIS:O	10:G:738:HOH:O[4_555]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	343/353 (97%)	327 (95%)	15 (4%)	1 (0%)	36	34
2	H	210/236 (89%)	206 (98%)	4 (2%)	0	100	100
3	L	206/210 (98%)	199 (97%)	5 (2%)	2 (1%)	12	8
All	All	759/799 (95%)	732 (96%)	24 (3%)	3 (0%)	30	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	463	THR
3	L	211	ARG
3	L	68	HIS

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	G	309/311 (99%)	304 (98%)	5 (2%)	55	61
2	H	180/198 (91%)	179 (99%)	1 (1%)	78	84
3	L	180/182 (99%)	177 (98%)	3 (2%)	53	60
All	All	669/691 (97%)	660 (99%)	9 (1%)	61	68

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	89	VAL
1	G	200	VAL
1	G	404	ASN
1	G	406	THR
1	G	430	THR
2	H	178	LEU
3	L	23	CYS
3	L	90	GLN
3	L	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	85	HIS
1	G	229	ASN
1	G	339	ASN
2	H	43	GLN
3	L	90	GLN
3	L	147	GLN
3	L	160	GLN
3	L	189	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 ⓘ

3 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	A	1	3,4	14,14,15	0.77	0	17,19,21	0.66	0
4	NAG	A	2	4	14,14,15	0.89	1 (7%)	17,19,21	0.77	0
4	BMA	A	3	4	11,11,12	0.79	0	15,15,17	0.77	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	A	1	3,4	-	5/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2	NAG	O5-C1	-3.07	1.38	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

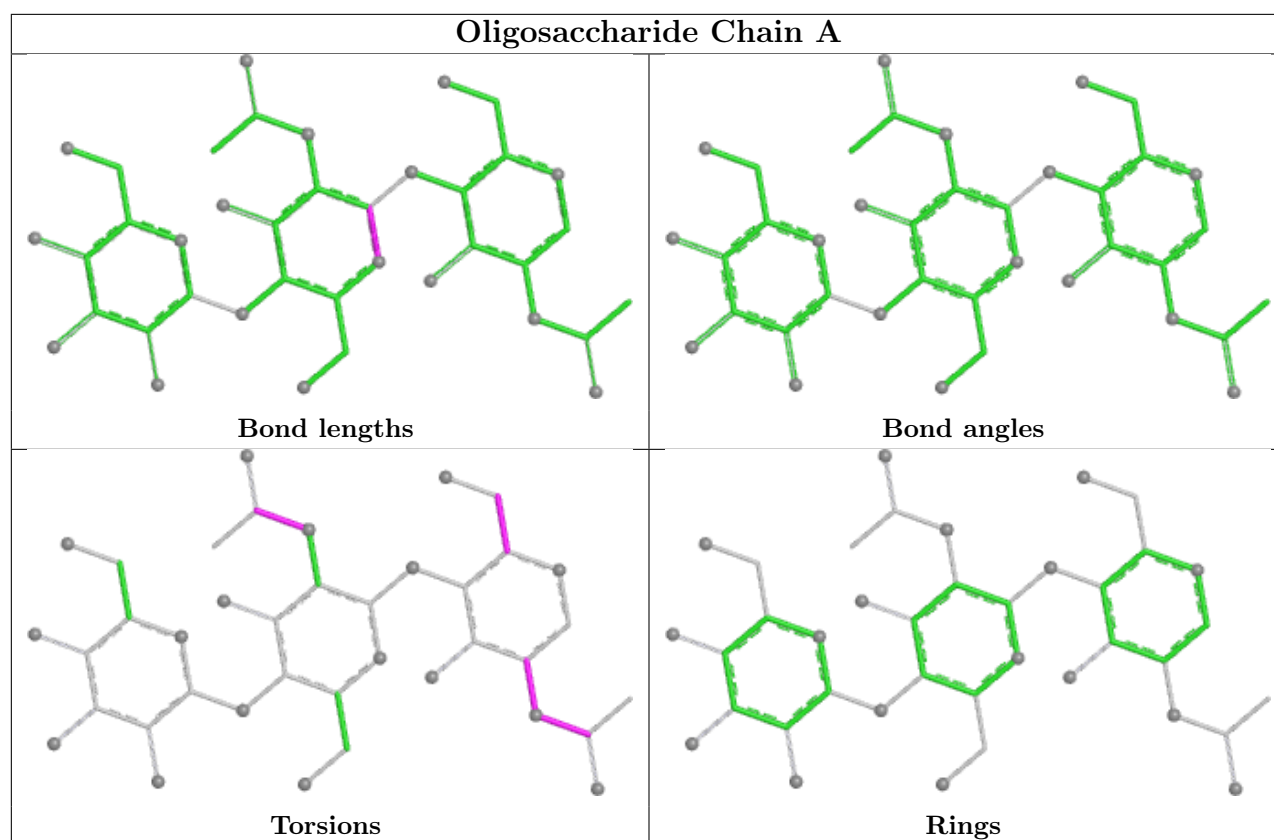
Mol	Chain	Res	Type	Atoms
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
4	A	1	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	1	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	NAG	2	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 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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	NAG	G	507	1	14,14,15	0.26	0	17,19,21	0.37	0
8	PEG	G	521	-	6,6,6	0.57	0	5,5,5	1.14	0
8	PEG	G	520	-	6,6,6	0.66	0	5,5,5	0.96	1 (20%)
7	EDO	H	303	-	3,3,3	0.43	0	2,2,2	0.37	0
7	EDO	H	304	-	3,3,3	0.42	0	2,2,2	0.46	0
7	EDO	G	519	-	3,3,3	0.44	0	2,2,2	0.27	0
7	EDO	H	302	-	3,3,3	0.45	0	2,2,2	0.23	0
5	NAG	G	502	1	14,14,15	0.38	0	17,19,21	0.58	0
7	EDO	G	515	-	3,3,3	0.40	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	H	301	-	3,3,3	0.45	0	2,2,2	0.33	0
5	NAG	G	501	1	14,14,15	1.20	1 (7%)	17,19,21	1.38	2 (11%)
5	NAG	G	505	1	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	G	506	1	14,14,15	0.29	0	17,19,21	0.35	0
5	NAG	G	510	1	14,14,15	1.02	1 (7%)	17,19,21	0.82	0
6	SO4	G	513	-	4,4,4	0.25	0	6,6,6	0.15	0
7	EDO	H	305	-	3,3,3	0.35	0	2,2,2	0.56	0
6	SO4	L	304	-	4,4,4	0.23	0	6,6,6	0.10	0
5	NAG	G	509	1	14,14,15	0.61	1 (7%)	17,19,21	0.43	0
5	NAG	G	511	1	14,14,15	0.56	0	17,19,21	1.70	4 (23%)
7	EDO	G	516	-	3,3,3	0.38	0	2,2,2	0.40	0
6	SO4	G	514	-	4,4,4	0.25	0	6,6,6	0.07	0
7	EDO	G	518	-	3,3,3	0.38	0	2,2,2	0.35	0
5	NAG	G	508	1	14,14,15	0.43	0	17,19,21	1.01	3 (17%)
5	NAG	G	503	1	14,14,15	0.58	0	17,19,21	0.48	0
5	NAG	G	512	1	14,14,15	0.44	0	17,19,21	0.60	0
7	EDO	L	305	-	3,3,3	0.41	0	2,2,2	0.37	0
5	NAG	G	504	1	14,14,15	0.65	0	17,19,21	0.50	0
7	EDO	G	517	9	3,3,3	0.38	0	2,2,2	0.41	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
5	NAG	G	507	1	-	2/6/23/26	0/1/1/1
8	PEG	G	521	-	-	2/4/4/4	-
8	PEG	G	520	-	-	2/4/4/4	-
7	EDO	H	303	-	-	0/1/1/1	-
7	EDO	H	304	-	-	0/1/1/1	-
7	EDO	G	519	-	-	0/1/1/1	-
7	EDO	H	302	-	-	0/1/1/1	-
5	NAG	G	502	1	-	2/6/23/26	0/1/1/1
7	EDO	G	515	-	-	0/1/1/1	-
7	EDO	H	301	-	-	0/1/1/1	-
5	NAG	G	501	1	-	6/6/23/26	0/1/1/1
5	NAG	G	505	1	-	0/6/23/26	0/1/1/1
5	NAG	G	506	1	-	0/6/23/26	0/1/1/1
5	NAG	G	510	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	H	305	-	-	1/1/1/1	-
7	EDO	G	516	-	-	0/1/1/1	-
5	NAG	G	509	1	-	2/6/23/26	0/1/1/1
5	NAG	G	511	1	-	3/6/23/26	0/1/1/1
7	EDO	G	518	-	-	0/1/1/1	-
5	NAG	G	508	1	-	2/6/23/26	0/1/1/1
5	NAG	G	503	1	-	0/6/23/26	0/1/1/1
5	NAG	G	512	1	-	3/6/23/26	0/1/1/1
7	EDO	L	305	-	-	0/1/1/1	-
5	NAG	G	504	1	-	2/6/23/26	0/1/1/1
7	EDO	G	517	9	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	501	NAG	O5-C1	-4.22	1.36	1.43
5	G	510	NAG	C1-C2	2.87	1.56	1.52
5	G	509	NAG	C1-C2	2.05	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	511	NAG	C2-N2-C7	4.58	129.04	122.90
5	G	501	NAG	C2-N2-C7	3.74	127.92	122.90
5	G	511	NAG	C1-C2-N2	3.07	115.27	110.43
5	G	501	NAG	O3-C3-C2	2.87	115.36	109.40
5	G	511	NAG	C4-C3-C2	-2.44	107.45	111.02
5	G	511	NAG	C1-O5-C5	2.38	115.37	112.19
5	G	508	NAG	C4-C3-C2	-2.15	107.86	111.02
5	G	508	NAG	C1-C2-N2	2.08	113.71	110.43
8	G	520	PEG	C3-O2-C2	2.02	122.11	113.26
5	G	508	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	508	NAG	C1-C2-N2-C7
5	G	511	NAG	C3-C2-N2-C7
5	G	509	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	G	502	NAG	O5-C5-C6-O6
5	G	502	NAG	C4-C5-C6-O6
8	G	520	PEG	O2-C3-C4-O4
5	G	501	NAG	O5-C5-C6-O6
5	G	509	NAG	C4-C5-C6-O6
5	G	501	NAG	C8-C7-N2-C2
5	G	501	NAG	O7-C7-N2-C2
5	G	507	NAG	C8-C7-N2-C2
5	G	507	NAG	O7-C7-N2-C2
5	G	510	NAG	C8-C7-N2-C2
5	G	510	NAG	O7-C7-N2-C2
5	G	511	NAG	C8-C7-N2-C2
5	G	511	NAG	O7-C7-N2-C2
5	G	512	NAG	C8-C7-N2-C2
5	G	512	NAG	O7-C7-N2-C2
8	G	521	PEG	O1-C1-C2-O2
5	G	501	NAG	C4-C5-C6-O6
8	G	521	PEG	C1-C2-O2-C3
5	G	508	NAG	C4-C5-C6-O6
5	G	512	NAG	O5-C5-C6-O6
8	G	520	PEG	C1-C2-O2-C3
5	G	504	NAG	C4-C5-C6-O6
5	G	501	NAG	C1-C2-N2-C7
5	G	501	NAG	C3-C2-N2-C7
7	H	305	EDO	O1-C1-C2-O2
5	G	504	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	521	PEG	3	0
5	G	501	NAG	2	0
5	G	511	NAG	8	0
7	G	516	EDO	4	0
7	G	518	EDO	1	0
5	G	512	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	G	347/353 (98%)	-0.02	7 (2%) 65 69	38, 59, 115, 150	0
2	H	216/236 (91%)	-0.04	9 (4%) 40 45	37, 56, 108, 131	0
3	L	208/210 (99%)	0.26	8 (3%) 44 49	41, 74, 117, 137	0
All	All	771/799 (96%)	0.05	24 (3%) 51 55	37, 62, 116, 150	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	29	PRO	3.7
2	H	31	PRO	3.4
1	G	324	GLY	3.4
3	L	212	GLY	3.3
1	G	122	LEU	3.3
2	H	1	GLN	2.8
2	H	213	PRO	2.6
2	H	127	SER	2.5
3	L	76	SER	2.5
3	L	202	SER	2.5
3	L	105	ASP	2.4
1	G	463	THR	2.3
2	H	28	ASP	2.2
1	G	391	PHE	2.2
3	L	109	THR	2.2
2	H	189	LEU	2.2
3	L	159	SER	2.1
3	L	194	CYS	2.1
1	G	241	ASN	2.1
1	G	392	ASN	2.0
2	H	135	THR	2.0
2	H	190	GLY	2.0
3	L	204	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	198	GLY	2.0

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

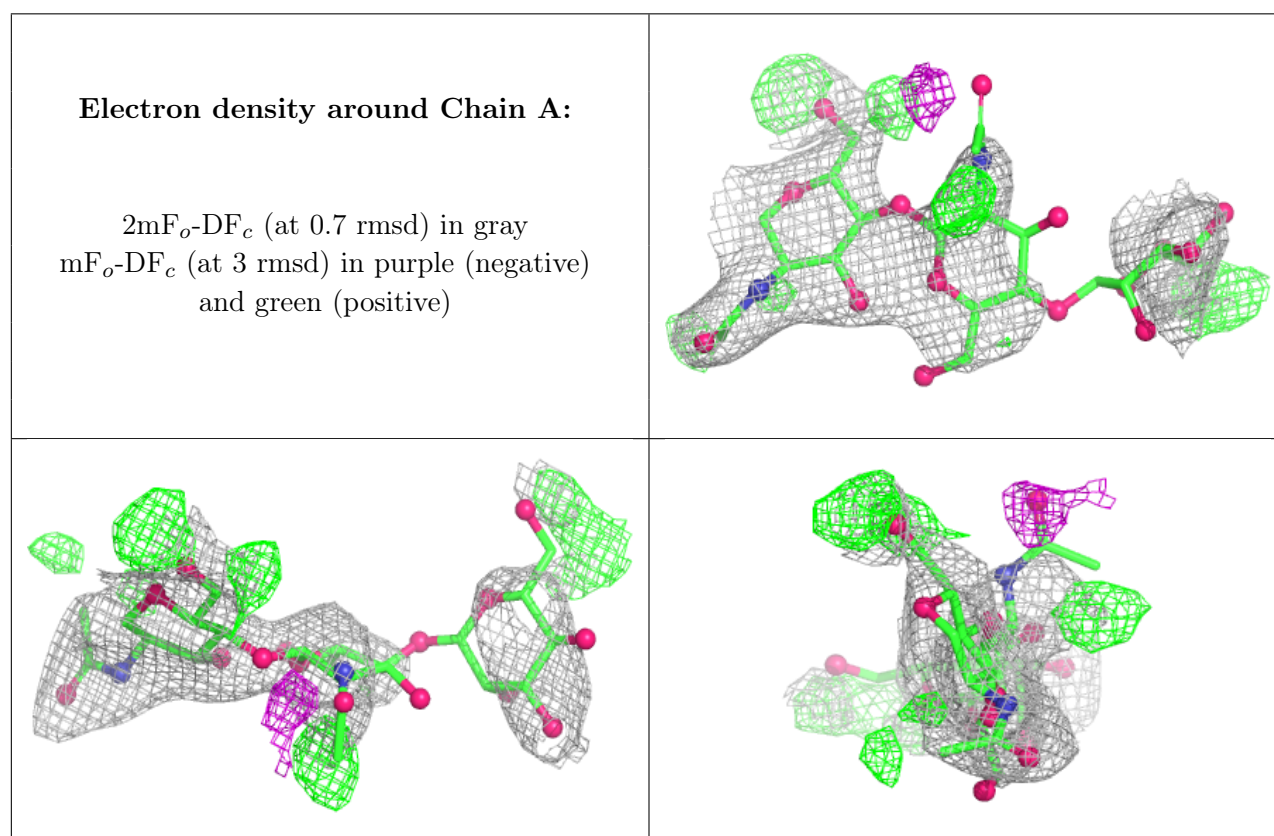
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	A	1	14/15	-	-	59,82,97,123	0
4	NAG	A	2	14/15	-	-	127,137,160,162	0
4	BMA	A	3	11/12	-	-	134,153,160,162	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(Å ²)	Q<0.9
5	NAG	G	511	14/15	0.29	0.17	108,119,146,152	0
5	NAG	G	510	14/15	0.60	0.15	105,129,138,143	0
5	NAG	G	508	14/15	0.60	0.17	79,108,114,121	0
5	NAG	G	512	14/15	0.62	0.18	95,110,127,138	0
5	NAG	G	501	14/15	0.68	0.16	100,115,126,128	0
5	NAG	G	507	14/15	0.71	0.14	66,78,97,106	0
8	PEG	G	521	7/7	0.71	0.20	56,86,104,104	0
8	PEG	G	520	7/7	0.79	0.20	49,67,82,82	0
5	NAG	G	506	14/15	0.82	0.11	61,76,81,87	0
7	EDO	G	516	4/4	0.83	0.22	59,85,92,102	0
7	EDO	L	305	4/4	0.83	0.15	79,95,103,114	0
5	NAG	G	504	14/15	0.87	0.11	37,60,76,86	0
7	EDO	H	301	4/4	0.87	0.16	46,70,83,84	0
7	EDO	H	305	4/4	0.87	0.21	78,94,109,109	0
9	NA	H	306	1/1	0.88	0.35	81,81,81,81	0
9	NA	G	523	1/1	0.89	0.23	83,83,83,83	0
6	SO4	G	514	5/5	0.89	0.10	95,98,103,112	0
7	EDO	H	303	4/4	0.90	0.15	86,104,108,116	0
7	EDO	H	304	4/4	0.90	0.13	46,63,84,91	0
7	EDO	G	519	4/4	0.90	0.13	49,66,79,90	0
5	NAG	G	509	14/15	0.90	0.11	56,68,78,81	0
5	NAG	G	505	14/15	0.91	0.09	53,67,73,77	0
5	NAG	G	502	14/15	0.91	0.10	44,58,65,80	0
6	SO4	L	304	5/5	0.92	0.16	115,118,119,122	0
6	SO4	G	513	5/5	0.93	0.08	63,66,81,83	0
5	NAG	G	503	14/15	0.93	0.09	26,45,52,62	0
7	EDO	H	302	4/4	0.94	0.11	37,52,71,85	0
7	EDO	G	517	4/4	0.94	0.14	48,60,72,73	0
7	EDO	G	518	4/4	0.94	0.13	63,78,94,94	0
7	EDO	G	515	4/4	0.96	0.10	43,52,56,56	0
9	NA	G	522	1/1	0.97	0.10	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.