



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:40 AM UTC

PDB ID : 4A5T / pdb_00004a5t
Title : STRUCTURAL BASIS FOR THE CONFORMATIONAL MODULATION
Authors : Xue, Y.; Bodin, C.; Olsson, K.
Deposited on : 2011-10-28
Resolution : 3.49 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

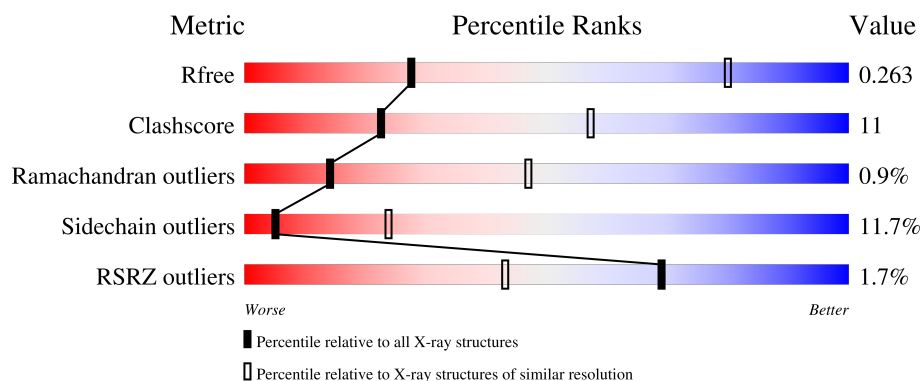
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	S	791	2% 68% 25% . .
2	A	3	67% 33%

2 Entry composition [i](#)

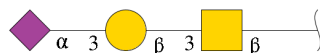
There are 3 unique types of molecules in this entry. The entry contains 6073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PLASMINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	767	Total	C	N	O	S	0	0	0
			6026	3742	1075	1151	58			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	3	Total	C	N	O	0	0	0
			45	25	2	18			

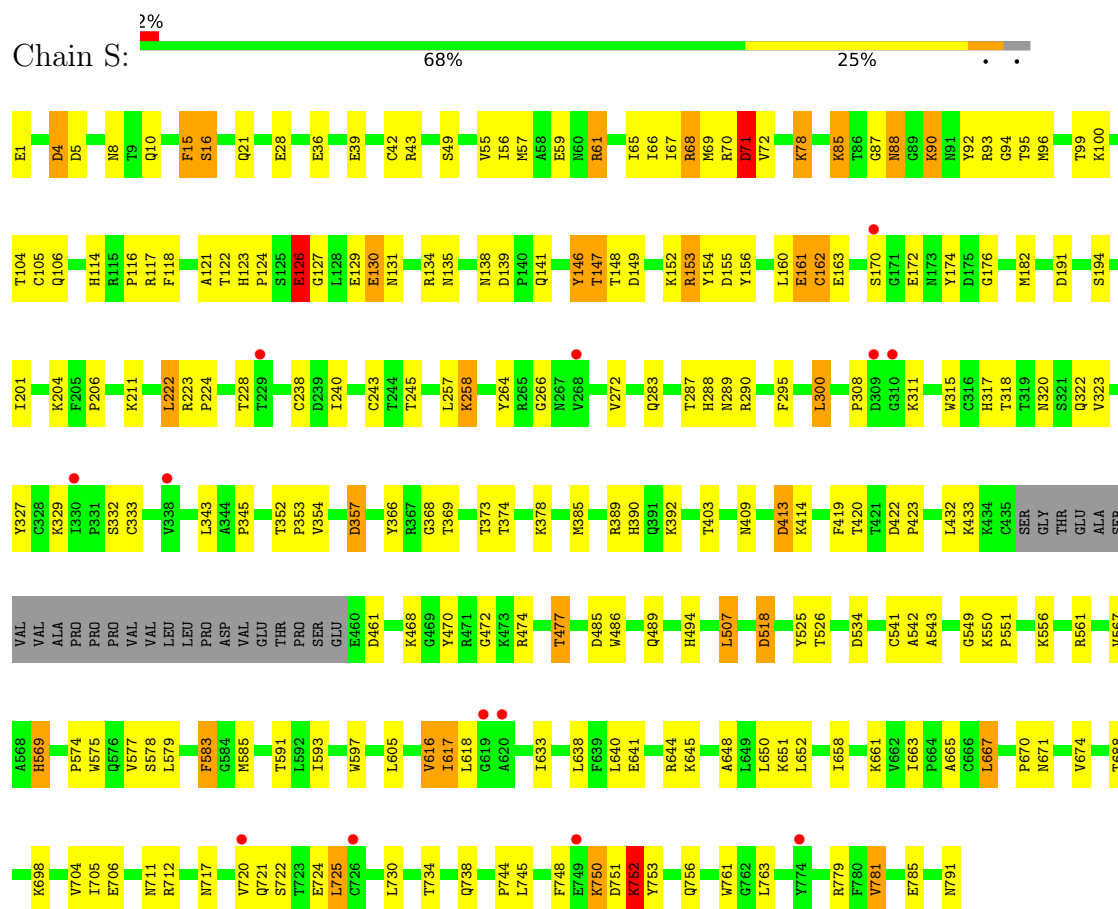
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	2	Total	Cl	0	0
			2	2		

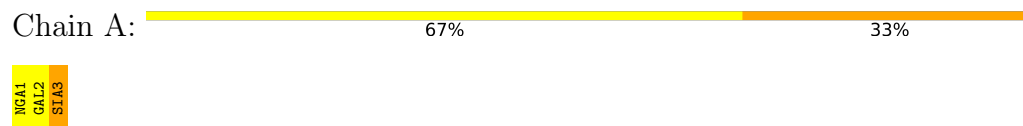
3 Residue-property plots

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: PLASMINOGEN



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.46Å 118.46Å 179.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.80 – 3.49 50.80 – 3.49	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.80-3.49) 95.2 (50.80-3.49)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.208 , 0.250 0.228 , 0.263	Depositor DCC
R_{free} test set	811 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: CL, SIA, GAL, NGA

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	S	0.65	0/6199	1.20	31/8428 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	518	ASP	CA-CB-CG	9.73	122.33	112.60
1	S	542	ALA	N-CA-C	7.79	120.46	111.11
1	S	373	THR	CA-C-N	6.88	130.42	120.38
1	S	373	THR	C-N-CA	6.88	130.42	120.38
1	S	106	GLN	N-CA-C	-6.51	99.56	109.85
1	S	706	GLU	CB-CG-CD	6.44	123.55	112.60
1	S	752	LYS	N-CA-C	6.38	118.64	109.14
1	S	121	ALA	CA-C-N	6.35	131.43	120.58
1	S	121	ALA	C-N-CA	6.35	131.43	120.58
1	S	71	ASP	CA-CB-CG	6.10	118.70	112.60
1	S	153	ARG	N-CA-C	6.04	117.53	111.07
1	S	413	ASP	CA-CB-CG	6.01	118.61	112.60
1	S	78	LYS	CA-C-N	5.99	128.98	120.53
1	S	78	LYS	C-N-CA	5.99	128.98	120.53
1	S	139	ASP	CA-CB-CG	5.90	118.50	112.60
1	S	569	HIS	N-CA-C	-5.89	100.84	109.50
1	S	422	ASP	CA-CB-CG	5.78	118.38	112.60
1	S	485	ASP	CA-CB-CG	5.71	118.31	112.60
1	S	541	CYS	CA-C-N	5.68	128.20	120.54
1	S	541	CYS	C-N-CA	5.68	128.20	120.54
1	S	419	PHE	N-CA-C	-5.32	102.41	110.28
1	S	317	HIS	N-CA-C	-5.24	102.72	110.48
1	S	583	PHE	CA-CB-CG	5.24	119.04	113.80
1	S	161	GLU	N-CA-C	5.14	117.75	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	126	GLU	N-CA-C	5.13	119.39	113.18
1	S	525	TYR	N-CA-C	-5.10	102.14	110.20
1	S	15	PHE	CA-CB-CG	-5.08	108.72	113.80
1	S	146	TYR	CA-C-N	5.08	131.28	122.64
1	S	146	TYR	C-N-CA	5.08	131.28	122.64
1	S	567	VAL	N-CA-C	-5.02	102.27	108.89
1	S	357	ASP	CA-CB-CG	5.00	117.60	112.60

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	S	6026	0	5690	122	0
2	A	45	0	38	2	0
3	S	2	0	0	2	0
All	All	6073	0	5728	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (124) 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:S:409:ASN:HD21	1:S:413:ASP:H	1.14	0.95
1:S:206:PRO:HB2	1:S:423:PRO:HD2	1.54	0.90
1:S:224:PRO:HD2	1:S:240:ILE:HD13	1.55	0.86
1:S:147:THR:HG23	1:S:149:ASP:H	1.42	0.85
1:S:354:VAL:HG21	1:S:753:TYR:HE2	1.42	0.84
1:S:320:ASN:HB3	1:S:323:VAL:HG22	1.61	0.83
1:S:206:PRO:HB2	1:S:423:PRO:CD	2.09	0.81
1:S:99:THR:HG21	1:S:155:ASP:HB3	1.66	0.76
1:S:283:GLN:HE22	1:S:288:HIS:H	1.33	0.76
1:S:105:CYS:O	1:S:148:THR:HG23	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:711:ASN:HD21	1:S:720:VAL:H	1.34	0.75
1:S:354:VAL:HG21	1:S:753:TYR:CE2	2.22	0.74
1:S:147:THR:CG2	1:S:149:ASP:H	2.00	0.73
1:S:390:HIS:HD2	1:S:392:LYS:H	1.37	0.73
1:S:318:THR:OG1	1:S:323:VAL:HG23	1.91	0.70
1:S:222:LEU:HD22	1:S:295:PHE:CZ	2.27	0.69
1:S:597:TRP:CZ2	1:S:651:LYS:HD2	2.27	0.69
1:S:671:ASN:HD22	1:S:779:ARG:HD2	1.59	0.68
1:S:489:GLN:HE22	1:S:494:HIS:H	1.41	0.68
1:S:385:MET:HB3	1:S:389:ARG:HG2	1.78	0.65
1:S:90:LYS:HG2	1:S:138:ASN:HD22	1.62	0.64
1:S:114:HIS:CE1	1:S:153:ARG:HA	2.33	0.63
1:S:671:ASN:ND2	1:S:779:ARG:HD2	2.14	0.62
1:S:122:THR:HG22	1:S:123:HIS:CE1	2.35	0.62
1:S:122:THR:C	1:S:124:PRO:HD3	2.24	0.61
1:S:311:LYS:HD3	1:S:315:TRP:NE1	2.14	0.61
1:S:160:LEU:N	1:S:160:LEU:HD12	2.16	0.61
1:S:352:THR:HG23	1:S:748:PHE:HE2	1.68	0.59
1:S:238:CYS:HB2	1:S:240:ILE:HD11	1.86	0.58
1:S:141:GLN:HB2	1:S:156:TYR:CE2	2.38	0.57
1:S:222:LEU:CD2	1:S:295:PHE:CZ	2.87	0.57
1:S:641:GLU:O	1:S:645:LYS:HA	2.05	0.57
1:S:147:THR:CG2	1:S:149:ASP:HB3	2.36	0.56
1:S:272:VAL:HG22	1:S:329:LYS:HB2	1.86	0.56
1:S:222:LEU:CD2	1:S:295:PHE:HZ	2.20	0.55
1:S:550:LYS:HG3	1:S:752:LYS:HB3	1.89	0.55
1:S:68:ARG:HB3	3:S:1001:CL:CL	2.45	0.54
1:S:409:ASN:ND2	1:S:413:ASP:H	1.94	0.54
1:S:725:LEU:C	1:S:725:LEU:HD23	2.32	0.54
1:S:122:THR:CG2	1:S:123:HIS:CE1	2.90	0.53
1:S:1:GLU:HB3	1:S:4:ASP:HB2	1.90	0.53
1:S:272:VAL:HG23	1:S:327:TYR:O	2.09	0.53
1:S:781:VAL:O	1:S:785:GLU:HG2	2.08	0.53
1:S:123:HIS:HB3	1:S:126:GLU:HG2	1.91	0.53
1:S:85:LYS:O	1:S:162:CYS:HB2	2.09	0.52
1:S:92:TYR:CZ	1:S:94:GLY:HA3	2.45	0.51
1:S:21:GLN:HG3	1:S:55:VAL:HG22	1.92	0.51
1:S:409:ASN:HD21	1:S:413:ASP:N	1.95	0.51
1:S:605:LEU:HD13	1:S:638:LEU:HG	1.93	0.51
1:S:357:ASP:HB3	1:S:432:LEU:HD21	1.92	0.51
1:S:257:LEU:HB3	1:S:332:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:288:HIS:HD2	1:S:290:ARG:H	1.59	0.50
1:S:633:ILE:HG21	1:S:652:LEU:HB3	1.94	0.50
1:S:705:ILE:HD12	1:S:730:LEU:HD11	1.92	0.50
1:S:118:PHE:CD1	1:S:123:HIS:CE1	3.00	0.49
1:S:651:LYS:NZ	1:S:791:ASN:O	2.45	0.49
1:S:674:VAL:HG11	1:S:704:VAL:HG21	1.94	0.49
1:S:320:ASN:HB3	1:S:323:VAL:CG2	2.40	0.49
1:S:138:ASN:O	1:S:138:ASN:CG	2.55	0.49
1:S:160:LEU:N	1:S:160:LEU:CD1	2.75	0.48
1:S:152:LYS:HD2	1:S:154:TYR:O	2.14	0.47
1:S:116:PRO:HB3	1:S:146:TYR:CE2	2.48	0.47
1:S:127:GLY:O	1:S:129:GLU:HG2	2.15	0.47
1:S:489:GLN:NE2	1:S:494:HIS:H	2.09	0.47
1:S:734:THR:HG21	1:S:738:GLN:HE22	1.80	0.47
1:S:578:SER:HB3	1:S:617:ILE:HG22	1.97	0.47
1:S:354:VAL:HG11	1:S:551:PRO:HD2	1.95	0.47
1:S:670:PRO:HA	1:S:781:VAL:CG1	2.45	0.47
1:S:16:SER:HB2	1:S:59:GLU:CD	2.40	0.47
1:S:549:GLY:HA2	1:S:575:TRP:CZ3	2.49	0.47
1:S:42:CYS:SG	1:S:56:ILE:HG23	2.56	0.46
1:S:222:LEU:HD11	1:S:289:ASN:HB3	1.97	0.46
1:S:147:THR:HG22	1:S:149:ASP:O	2.16	0.46
1:S:390:HIS:HD2	1:S:392:LYS:N	2.08	0.45
1:S:722:SER:C	1:S:724:GLU:H	2.23	0.45
1:S:118:PHE:HD1	1:S:123:HIS:CE1	2.34	0.45
1:S:323:VAL:HG23	1:S:323:VAL:O	2.16	0.45
1:S:300:LEU:HD11	1:S:308:PRO:HB3	1.98	0.45
1:S:138:ASN:O	1:S:138:ASN:OD1	2.34	0.45
1:S:390:HIS:CD2	1:S:392:LYS:H	2.27	0.45
1:S:352:THR:HA	1:S:353:PRO:HD3	1.94	0.45
1:S:477:THR:OG1	1:S:534:ASP:HB3	2.17	0.44
1:S:591:THR:OG1	1:S:744:PRO:HB3	2.17	0.44
1:S:88:ASN:OD1	1:S:135:ASN:ND2	2.51	0.44
2:A:3:SIA:H32	2:A:3:SIA:H8	2.00	0.44
1:S:577:VAL:HG22	1:S:618:LEU:CD2	2.48	0.44
1:S:174:TYR:CZ	1:S:176:GLY:HA3	2.52	0.44
1:S:470:TYR:CZ	1:S:472:GLY:HA3	2.52	0.44
1:S:104:THR:HG22	1:S:105:CYS:O	2.18	0.44
1:S:206:PRO:CB	1:S:423:PRO:HD2	2.36	0.44
1:S:61:ARG:HB3	1:S:66:ILE:HD11	2.00	0.43
1:S:147:THR:CG2	1:S:149:ASP:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:366:TYR:CZ	1:S:368:GLY:HA3	2.53	0.43
1:S:670:PRO:HA	1:S:781:VAL:HG11	2.01	0.43
1:S:574:PRO:HB2	1:S:663:ILE:H	1.83	0.43
1:S:577:VAL:CG1	1:S:616:VAL:HG13	2.48	0.43
1:S:153:ARG:NH2	3:S:1002:CL:CL	2.82	0.43
1:S:264:TYR:CZ	1:S:266:GLY:HA3	2.54	0.43
1:S:577:VAL:HG13	1:S:616:VAL:HG13	1.99	0.43
1:S:756:GLN:HE21	1:S:756:GLN:HA	1.84	0.43
1:S:258:LYS:HG2	1:S:333:CYS:SG	2.59	0.43
1:S:461:ASP:O	1:S:474:ARG:NH1	2.52	0.42
1:S:575:TRP:CG	1:S:665:ALA:HB2	2.53	0.42
1:S:551:PRO:HD3	1:S:575:TRP:CH2	2.55	0.42
1:S:413:ASP:OD1	1:S:414:LYS:N	2.37	0.42
1:S:616:VAL:HG11	1:S:652:LEU:HD21	2.02	0.42
2:A:3:SIA:H112	2:A:3:SIA:H4	2.00	0.42
1:S:71:ASP:OD1	1:S:72:VAL:N	2.53	0.42
1:S:711:ASN:ND2	1:S:720:VAL:H	2.10	0.42
1:S:93:ARG:HE	1:S:134:ARG:HD2	1.84	0.42
1:S:182:MET:HE3	1:S:223:ARG:HH22	1.84	0.42
1:S:318:THR:HG1	1:S:323:VAL:HG23	1.83	0.42
1:S:201:ILE:HG23	1:S:204:LYS:HG3	2.02	0.41
1:S:147:THR:HG21	1:S:149:ASP:HB3	2.01	0.41
1:S:288:HIS:HD2	1:S:290:ARG:N	2.19	0.41
1:S:667:LEU:HD12	1:S:667:LEU:HA	1.89	0.41
1:S:640:LEU:HD23	1:S:648:ALA:HB2	2.02	0.41
1:S:90:LYS:HA	1:S:90:LYS:HD2	1.72	0.41
1:S:486:TRP:CD2	1:S:507:LEU:HG	2.56	0.41
1:S:357:ASP:HB3	1:S:432:LEU:CD2	2.50	0.40
1:S:129:GLU:HG2	1:S:129:GLU:H	1.69	0.40
1:S:130:GLU:HB3	1:S:131:ASN:H	1.72	0.40
1:S:283:GLN:NE2	1:S:287:THR:HA	2.37	0.40
1:S:579:LEU:HD21	1:S:650:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	763/791 (96%)	700 (92%)	56 (7%)	7 (1%)	14	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	717	ASN
1	S	163	GLU
1	S	750	LYS
1	S	345	PRO
1	S	761	TRP
1	S	87	GLY
1	S	543	ALA

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	S	673/694 (97%)	594 (88%)	79 (12%)	5	24

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	4	ASP
1	S	5	ASP
1	S	8	ASN
1	S	10	GLN
1	S	15	PHE
1	S	16	SER
1	S	28	GLU
1	S	36	GLU
1	S	39	GLU
1	S	43	ARG

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Mol	Chain	Res	Type
1	S	49	SER
1	S	57	MET
1	S	61	ARG
1	S	65	ILE
1	S	67	ILE
1	S	68	ARG
1	S	69	MET
1	S	70	ARG
1	S	71	ASP
1	S	78	LYS
1	S	85	LYS
1	S	88	ASN
1	S	90	LYS
1	S	95	THR
1	S	96	MET
1	S	100	LYS
1	S	117	ARG
1	S	126	GLU
1	S	130	GLU
1	S	147	THR
1	S	161	GLU
1	S	162	CYS
1	S	170	SER
1	S	172	GLU
1	S	191	ASP
1	S	194	SER
1	S	211	LYS
1	S	222	LEU
1	S	228	THR
1	S	243	CYS
1	S	245	THR
1	S	258	LYS
1	S	300	LEU
1	S	322	GLN
1	S	343	LEU
1	S	369	THR
1	S	374	THR
1	S	378	LYS
1	S	403	THR
1	S	420	THR
1	S	433	LYS
1	S	468	LYS

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Mol	Chain	Res	Type
1	S	477	THR
1	S	507	LEU
1	S	518	ASP
1	S	526	THR
1	S	556	LYS
1	S	561	ARG
1	S	569	HIS
1	S	583	PHE
1	S	585	MET
1	S	593	ILE
1	S	616	VAL
1	S	617	ILE
1	S	644	ARG
1	S	658	ILE
1	S	661	LYS
1	S	667	LEU
1	S	688	THR
1	S	698	LYS
1	S	712	ARG
1	S	721	GLN
1	S	725	LEU
1	S	745	LEU
1	S	750	LYS
1	S	751	ASP
1	S	752	LYS
1	S	763	LEU
1	S	781	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	8	ASN
1	S	46	GLN
1	S	48	HIS
1	S	91	ASN
1	S	114	HIS
1	S	138	ASN
1	S	196	HIS
1	S	275	HIS
1	S	283	GLN
1	S	288	HIS
1	S	360	HIS

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Mol	Chain	Res	Type
1	S	390	HIS
1	S	405	ASN
1	S	409	ASN
1	S	431	ASN
1	S	484	GLN
1	S	489	GLN
1	S	492	HIS
1	S	502	ASN
1	S	552	GLN
1	S	571	HIS
1	S	671	ASN
1	S	711	ASN
1	S	738	GLN
1	S	756	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 ⓘ

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$
2	NGA	A	1	1,2	14,14,15	1.12	1 (7%)	17,19,21	2.83	8 (47%)
2	GAL	A	2	2	11,11,12	1.31	1 (9%)	15,15,17	2.67	8 (53%)
2	SIA	A	3	2	20,20,21	2.06	4 (20%)	21,28,31	1.90	7 (33%)

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	NGA	A	1	1,2	-	2/6/23/26	0/1/1/1
2	GAL	A	2	2	-	0/2/19/22	0/1/1/1
2	SIA	A	3	2	-	9/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	SIA	C2-C1	6.20	1.59	1.52
2	A	3	SIA	C4-C5	4.00	1.56	1.53
2	A	3	SIA	C11-C10	2.76	1.56	1.50
2	A	2	GAL	C4-C3	2.56	1.59	1.52
2	A	1	NGA	C4-C3	2.07	1.57	1.52
2	A	3	SIA	O10-C10	2.06	1.27	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NGA	C1-O5-C5	-8.00	101.46	112.19
2	A	2	GAL	C1-C2-C3	-6.49	100.19	109.64
2	A	1	NGA	C2-N2-C7	3.91	128.14	122.90
2	A	1	NGA	O3-C3-C2	3.85	117.39	109.40
2	A	2	GAL	O2-C2-C1	3.77	117.86	109.22
2	A	3	SIA	C5-N5-C10	3.65	131.65	123.11
2	A	1	NGA	C6-C5-C4	3.41	121.39	113.02
2	A	3	SIA	C6-C5-N5	3.28	116.13	110.91
2	A	2	GAL	O5-C1-C2	-3.03	103.56	110.79
2	A	1	NGA	C1-C2-N2	-2.93	105.82	110.43
2	A	3	SIA	O6-C2-C3	2.83	114.37	110.56
2	A	2	GAL	O4-C4-C5	2.70	115.97	109.32
2	A	3	SIA	O7-C7-C8	2.62	114.89	108.93
2	A	3	SIA	C4-C5-N5	-2.43	105.65	110.44
2	A	3	SIA	O10-C10-N5	-2.39	117.76	121.98
2	A	2	GAL	C2-C3-C4	2.37	115.03	110.86
2	A	2	GAL	O3-C3-C4	2.37	115.96	110.38
2	A	3	SIA	O8-C8-C9	2.36	114.40	109.03
2	A	1	NGA	O7-C7-C8	2.35	126.23	122.05
2	A	2	GAL	O4-C4-C3	2.23	115.64	110.38
2	A	1	NGA	C4-C3-C2	2.20	114.25	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	GAL	C6-C5-C4	2.20	118.42	113.02
2	A	1	NGA	O7-C7-N2	-2.05	118.35	121.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

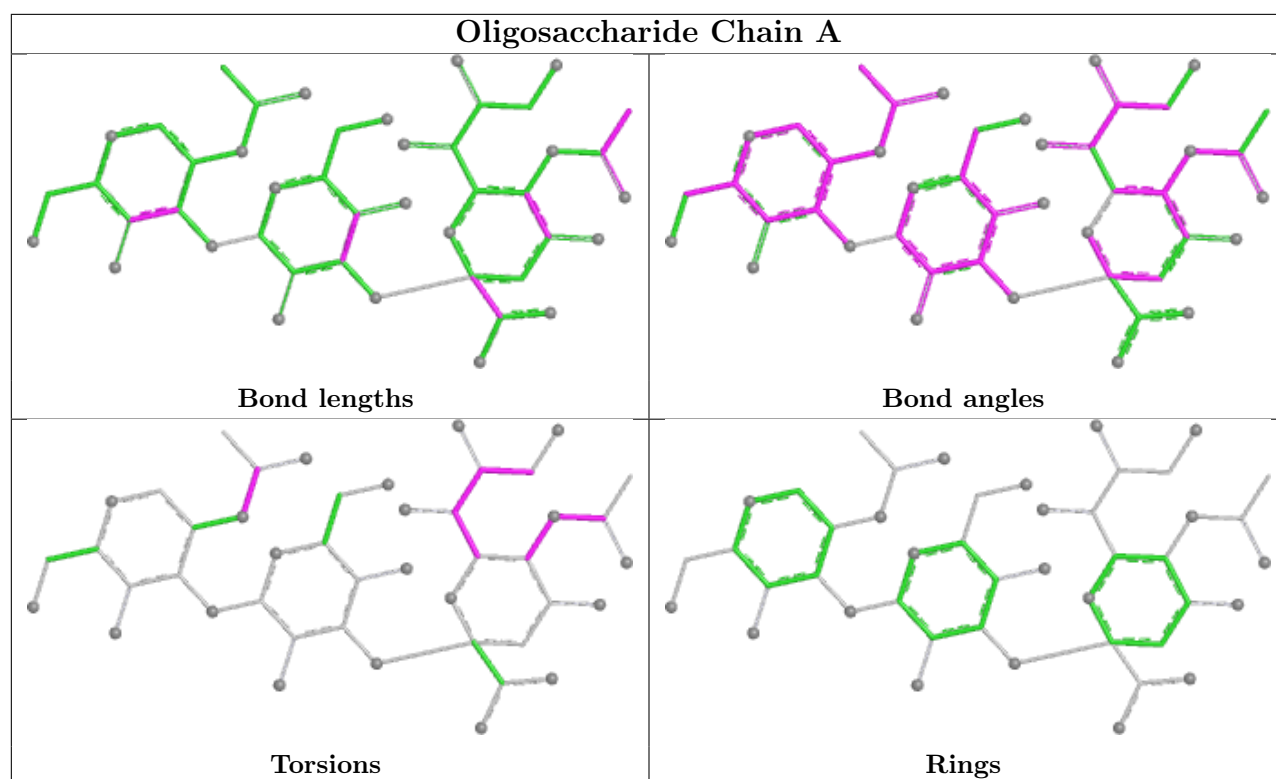
Mol	Chain	Res	Type	Atoms
2	A	3	SIA	C5-C6-C7-C8
2	A	3	SIA	C7-C8-C9-O9
2	A	1	NGA	C8-C7-N2-C2
2	A	1	NGA	O7-C7-N2-C2
2	A	3	SIA	C11-C10-N5-C5
2	A	3	SIA	O10-C10-N5-C5
2	A	3	SIA	O8-C8-C9-O9
2	A	3	SIA	C6-C5-N5-C10
2	A	3	SIA	O7-C7-C8-C9
2	A	3	SIA	C4-C5-N5-C10
2	A	3	SIA	C6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	SIA	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	S	767/791 (96%)	0.20	13 (1%) 69 43	38, 90, 189, 215	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	749	GLU	3.3
1	S	309	ASP	2.4
1	S	726	CYS	2.3
1	S	310	GLY	2.3
1	S	330	ILE	2.2
1	S	229	THR	2.2
1	S	268	VAL	2.2
1	S	620	ALA	2.2
1	S	619	GLY	2.1
1	S	720	VAL	2.1
1	S	338	VAL	2.1
1	S	774	TYR	2.0
1	S	170	SER	2.0

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

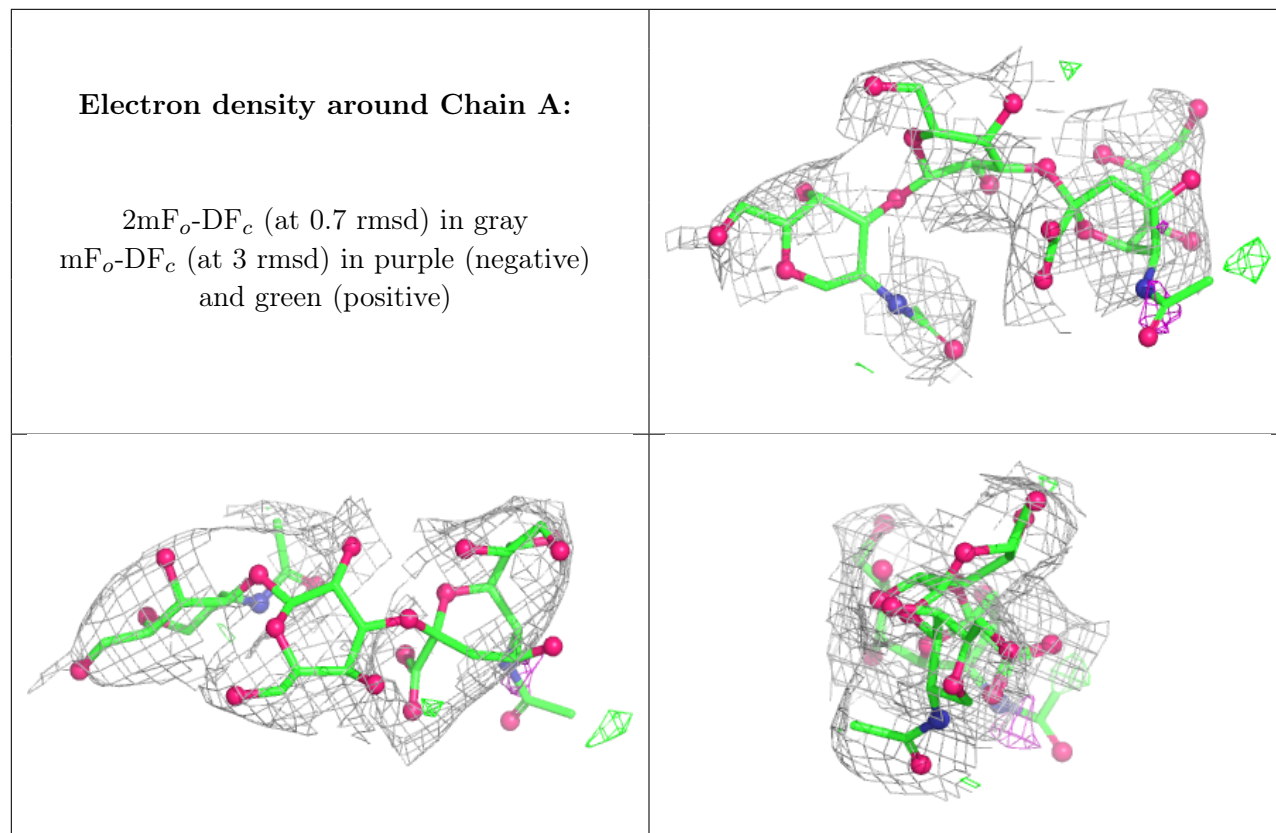
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	NGA	A	1	14/15	-	-	104,104,106,106	0
2	GAL	A	2	11/12	-	-	103,106,112,116	0
2	SIA	A	3	20/21	-	-	112,112,114,114	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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
3	CL	S	1002	1/1	0.96	0.16	37,37,37,37	0
3	CL	S	1001	1/1	0.97	0.12	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.