



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:02 AM UTC

PDB ID : 5FOB / pdb_00005fob
Title : Crystal Structure of Human Complement C3b in complex with Smallpox Inhibitor of Complement (SPICE)
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
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

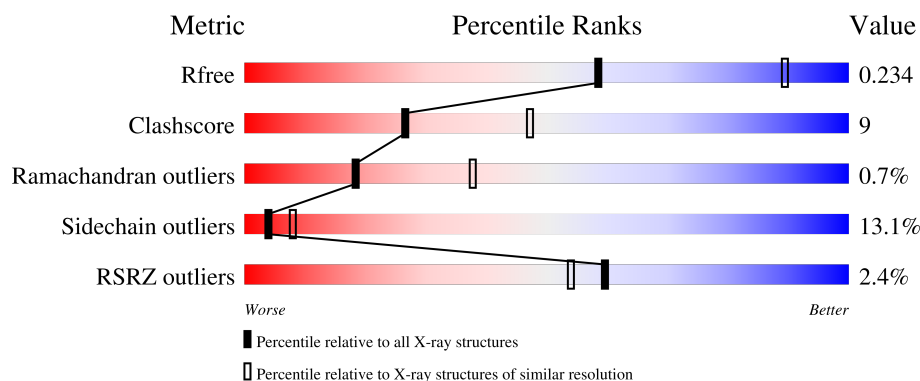
1 Overall quality at a glance

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	645	3% 70% 25% .
2	B	915	% 73% 22% ..
3	C	245	6% 62% 27% 9% .
4	D	4	75% 25%
5	E	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
4	NAG	D	1	X	-	-	-
9	IOD	B	2678	-	-	X	-
9	IOD	B	2679	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 14474 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	3	0
			5011	3193	846	956	16			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	902	Total	C	N	O	S	0	0	0
			7199	4563	1210	1388	38			

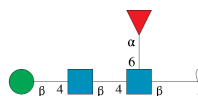
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is a protein called SMALLPOX INHIBITOR OF COMPLEMENT SPICE, D15L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	2	0
			1822	1138	309	356	19			

- Molecule 4 is an oligosaccharide called 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	D	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

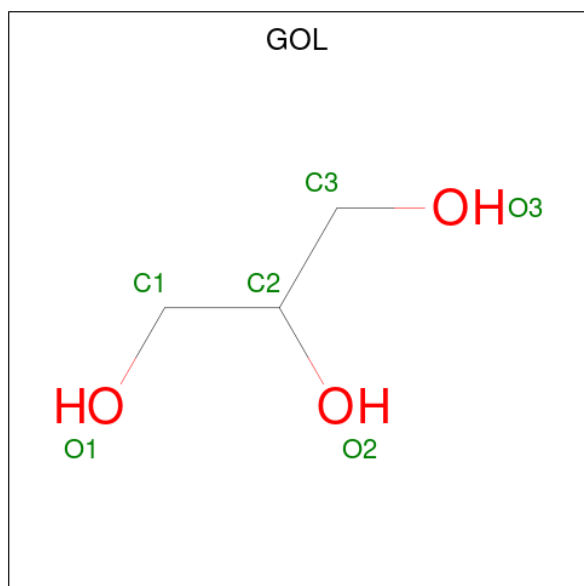


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	2	Total	Cl	0	0
			2	2		
6	C	2	Total	Cl	0	0
			2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		
8	B	1	Total	Na	0	0
			1	1		

- Molecule 9 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	I	0	0
			3	3		
9	B	4	Total	I	0	0
			4	4		

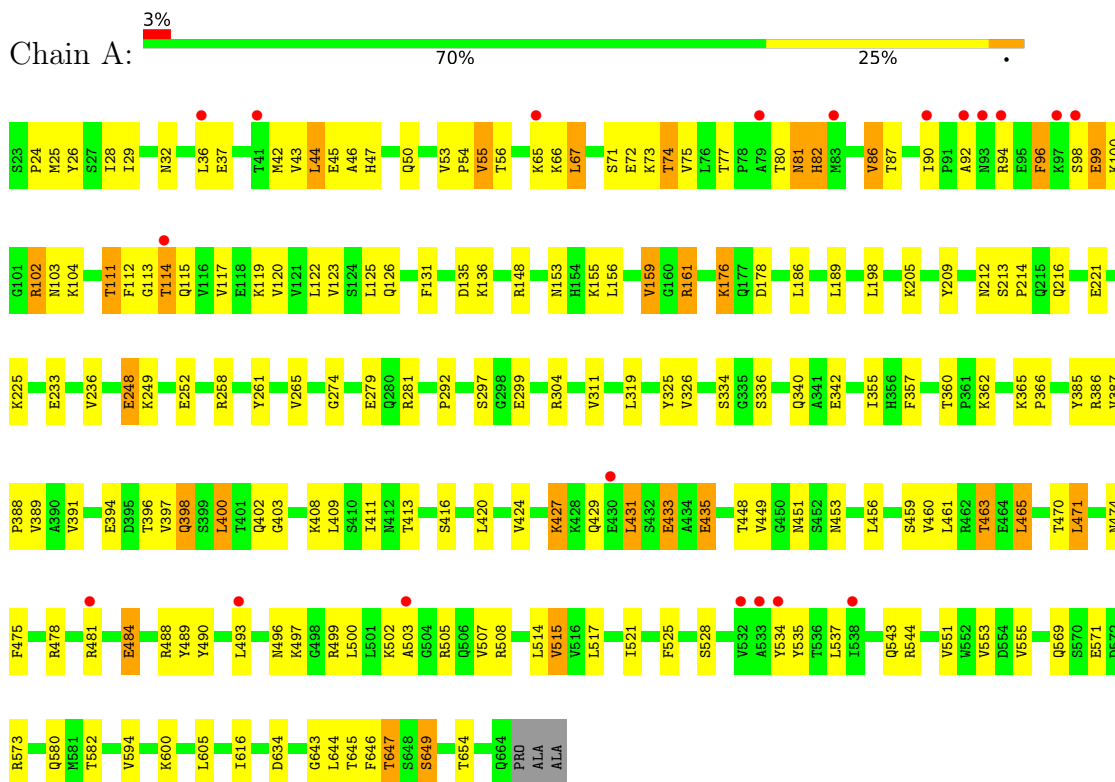
- Molecule 10 is water.

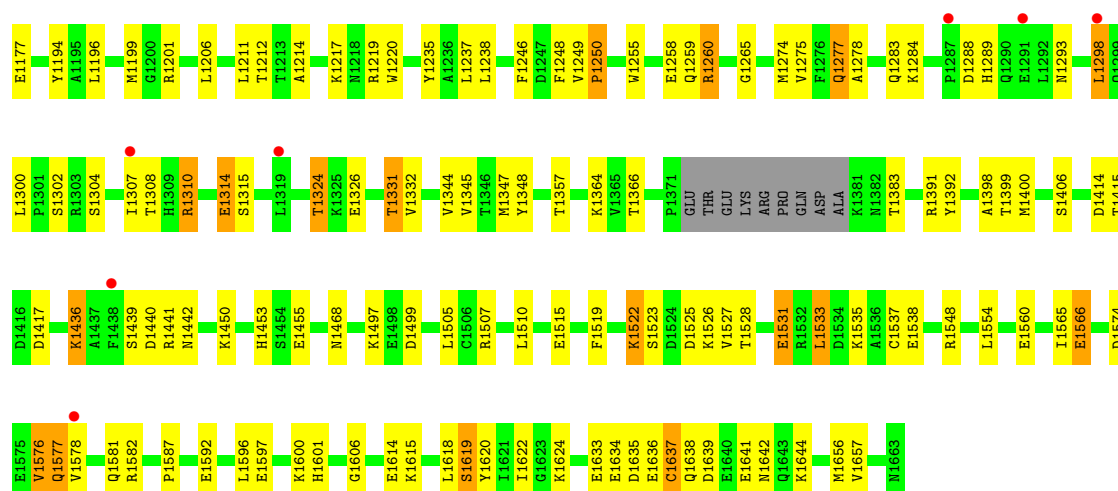
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	98	Total	O	0	0
			98	98		
10	B	92	Total	O	0	0
			92	92		
10	C	17	Total	O	0	0
			17	17		

3 Residue-property plots

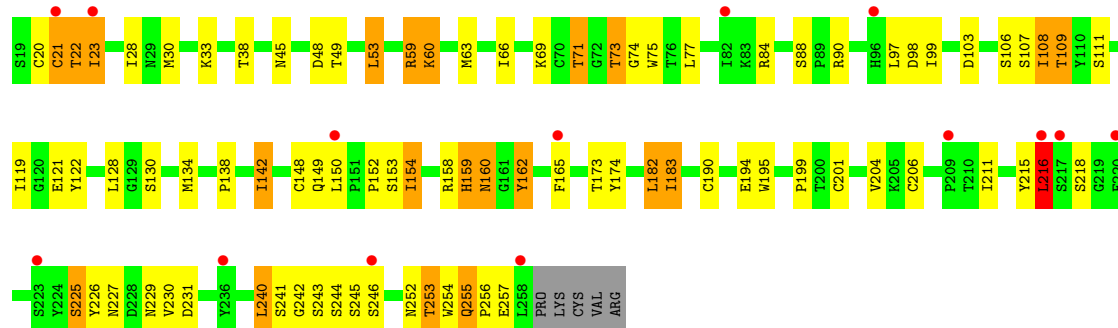
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: COMPLEMENT C3 BETA CHAIN

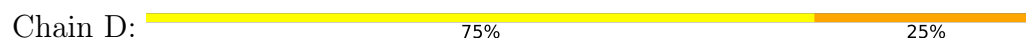




• Molecule 3: SMALLPOX INHIBITOR OF COMPLEMENT SPICE, D15L



• Molecule 4: 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



• Molecule 5: 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 1	Depositor
Cell constants a, b, c, α , β , γ	68.89Å 83.31Å 127.38Å 75.03° 76.20° 68.50°	Depositor
Resolution (Å)	42.36 – 2.60 42.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.36-2.60) 97.3 (42.36-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.230 0.206 , 0.234	Depositor DCC
R_{free} test set	2251 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.9	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	0.94	EDS
Total number of atoms	14474	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: FUC, BMA, NAG, GOL, NA, IOD, CL

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	0.32	0/5121	0.76	0/6958
2	B	0.33	0/7343	0.77	10/9943 (0.1%)
3	C	0.35	0/1877	0.89	3/2550 (0.1%)
All	All	0.33	0/14341	0.78	13/19451 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1009	GLY	CA-C-O	-8.93	113.99	121.76
3	C	255	GLN	CA-C-N	-8.56	109.14	119.84
3	C	255	GLN	C-N-CA	-8.56	109.14	119.84
2	B	1009	GLY	CA-C-N	8.05	136.18	121.70
2	B	1009	GLY	C-N-CA	8.05	136.18	121.70
2	B	1606	GLY	N-CA-C	6.24	119.60	110.80
2	B	783	LYS	N-CA-C	-6.04	102.55	110.53
2	B	948	ASP	CA-C-N	5.52	125.61	119.32
2	B	948	ASP	C-N-CA	5.52	125.61	119.32
3	C	20	CYS	N-CA-C	5.44	117.29	111.36
2	B	1250	PRO	N-CA-C	5.29	117.16	110.70
2	B	1010	CYS	N-CA-CB	5.23	119.39	110.50
2	B	830	PHE	N-CA-C	5.10	116.04	108.60

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	A	5011	0	5068	99	0
2	B	7199	0	7116	123	1
3	C	1822	0	1703	48	1
4	D	49	0	43	3	0
5	E	28	0	25	0	0
6	A	1	0	0	0	0
6	B	2	0	0	1	0
6	C	2	0	0	0	0
7	A	60	0	80	12	0
7	B	72	0	96	13	0
7	C	12	0	16	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
9	A	3	0	0	1	0
9	B	4	0	0	8	0
10	A	98	0	0	1	0
10	B	92	0	0	4	0
10	C	17	0	0	0	0
All	All	14474	0	14147	264	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 9.

All (264) 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)
2:B:760:ASN:ND2	9:B:2679:IOD:I	2.35	1.25
9:B:2679:IOD:I	10:B:2007:HOH:O	2.24	1.25
2:B:1032:GLU:HG3	9:B:2678:IOD:I	2.26	1.04
2:B:1010:CYS:HB3	2:B:1013:GLU:HB2	1.43	0.99
2:B:1105:LYS:HD2	9:B:2681:IOD:I	2.45	0.87
2:B:1032:GLU:CG	9:B:2678:IOD:I	3.03	0.77
3:C:49:THR:HG22	3:C:69:LYS:HG3	1.69	0.75
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.68	0.73
1:A:448:THR:HG21	1:A:453:ASN:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:NZ	1:A:460:VAL:O	2.21	0.72
3:C:99:ILE:HA	3:C:108:ILE:HG22	1.73	0.70
3:C:225:SER:OG	3:C:226:TYR:N	2.22	0.69
2:B:873:CYS:HB2	2:B:901:VAL:HB	1.74	0.69
1:A:99:GLU:HA	1:A:100:LYS:C	2.18	0.69
2:B:1211:LEU:O	2:B:1217:LYS:NZ	2.25	0.69
3:C:98:ASP:HB3	3:C:109:THR:HG23	1.74	0.68
1:A:471:LEU:HB3	1:A:521:ILE:HD11	1.77	0.67
2:B:875:LEU:O	2:B:880:ARG:NH1	2.29	0.66
2:B:766:GLU:OE2	3:C:90:ARG:NH1	2.30	0.65
2:B:1635:ASP:OD1	2:B:1636:GLU:N	2.29	0.65
1:A:571:GLU:HG3	1:A:573:ARG:H	1.62	0.64
2:B:1258:GLU:OE2	2:B:1260:ARG:NH2	2.31	0.64
1:A:42:MET:HB3	1:A:86:VAL:HG23	1.79	0.63
1:A:366:PRO:HB3	1:A:416:SER:H	1.62	0.63
1:A:304:ARG:H	7:A:1668:GOL:H2	1.64	0.63
3:C:206:CYS:HB3	3:C:254:TRP:CZ2	2.34	0.63
1:A:176:LYS:NZ	1:A:178:ASP:OD2	2.28	0.63
2:B:941:THR:HG23	2:B:1345:VAL:HG22	1.80	0.63
2:B:1072:ARG:NH1	7:B:2668:GOL:O3	2.31	0.63
2:B:1391:ARG:NH1	2:B:1453:HIS:O	2.32	0.62
1:A:225:LYS:HG3	7:A:1669:GOL:H2	1.82	0.62
2:B:996:ASP:HB3	2:B:999:ARG:HG3	1.82	0.62
3:C:149:GLN:HG2	3:C:150:LEU:H	1.65	0.61
2:B:1528:THR:HG23	2:B:1531:GLU:H	1.66	0.61
2:B:1499:ASP:OD1	2:B:1499:ASP:N	2.31	0.60
4:D:1:NAG:H62	4:D:2:NAG:N2	2.17	0.60
1:A:569:GLN:HG3	1:A:582:THR:H	1.68	0.59
3:C:230:VAL:HG23	3:C:246:SER:HB2	1.84	0.59
1:A:475:PHE:HE1	1:A:517:LEU:HB3	1.67	0.59
2:B:1152:GLN:OE1	7:B:2666:GOL:O3	2.20	0.59
1:A:427:LYS:HG3	7:A:1667:GOL:H32	1.85	0.59
3:C:22:THR:OG1	3:C:23:ILE:N	2.35	0.59
1:A:388:PRO:HB2	1:A:427:LYS:HB3	1.85	0.58
2:B:1091:ASN:OD1	2:B:1091:ASN:N	2.34	0.58
3:C:227:ASN:O	3:C:227:ASN:ND2	2.36	0.58
1:A:120:VAL:HG11	2:B:1039:LEU:HD12	1.86	0.58
2:B:758:GLU:OE1	2:B:881:ARG:NH2	2.36	0.58
2:B:1505:LEU:HD12	7:B:2674:GOL:H31	1.86	0.58
2:B:1533:LEU:HD12	2:B:1656:MET:HE2	1.86	0.58
2:B:1127:GLN:O	2:B:1130:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:OE2	1:A:212:ASN:ND2	2.27	0.57
1:A:233:GLU:OE2	1:A:258:ARG:NH1	2.38	0.57
2:B:934:GLU:CD	2:B:934:GLU:H	2.11	0.57
1:A:25:MET:SD	1:A:544:ARG:HG2	2.44	0.57
2:B:971:VAL:O	2:B:974:THR:OG1	2.18	0.57
2:B:1566:GLU:OE2	2:B:1601:HIS:NE2	2.38	0.57
2:B:1574:ASP:OD2	2:B:1620:TYR:OH	2.23	0.57
3:C:71:THR:HG23	3:C:73:THR:H	1.68	0.57
3:C:84:ARG:HB2	3:C:134:MET:HE2	1.86	0.57
3:C:206:CYS:HB3	3:C:254:TRP:HZ2	1.69	0.56
2:B:1641:GLU:N	2:B:1642:ASN:HA	2.19	0.56
3:C:77:LEU:HB2	7:C:1260:GOL:H32	1.87	0.56
2:B:1414:ASP:HB3	2:B:1417:ASP:HB2	1.87	0.56
1:A:32:ASN:HA	1:A:645:THR:HG23	1.88	0.56
1:A:45:GLU:OE1	1:A:534:TYR:OH	2.15	0.56
2:B:989:GLN:H	2:B:1289:HIS:HA	1.72	0.55
2:B:1515:GLU:H	7:B:2674:GOL:H2	1.71	0.55
1:A:496:ASN:OD1	1:A:497:LYS:HE2	2.06	0.55
2:B:1633:GLU:O	2:B:1637:CYS:N	2.35	0.55
2:B:1587:PRO:HG2	7:B:2674:GOL:H12	1.88	0.54
2:B:1128:GLU:HG2	2:B:1129:MET:N	2.21	0.54
9:B:2679:IOD:I	3:C:60:LYS:HE2	2.78	0.54
3:C:159:HIS:O	3:C:160:ASN:ND2	2.38	0.54
1:A:28:ILE:HG22	1:A:44:LEU:HD23	1.88	0.54
2:B:1113:LYS:NZ	2:B:1119:GLN:OE1	2.41	0.54
1:A:44:LEU:HD13	1:A:55:VAL:HG21	1.89	0.54
2:B:1597:GLU:HB2	2:B:1600:LYS:HG3	1.90	0.54
1:A:119:LYS:HD3	1:A:647:THR:OG1	2.09	0.53
3:C:152:PRO:O	3:C:174:TYR:OH	2.17	0.53
3:C:215:TYR:O	3:C:216:LEU:HB2	2.07	0.53
1:A:82:HIS:HE1	1:A:488:ARG:HH22	1.57	0.53
3:C:182:LEU:HD12	3:C:201:CYS:HB3	1.90	0.53
1:A:646:PHE:H	1:A:654:THR:HG23	1.75	0.52
3:C:154:ILE:HG13	3:C:199:PRO:O	2.10	0.52
2:B:1148:LEU:O	2:B:1152:GLN:HG2	2.09	0.52
2:B:1581:GLN:O	2:B:1582:ARG:NH1	2.40	0.52
2:B:978:THR:HB	2:B:1324:THR:HG23	1.92	0.52
2:B:1031:THR:HG22	2:B:1283:GLN:HG3	1.92	0.52
2:B:1399:THR:OG1	2:B:1400:MET:N	2.43	0.52
1:A:429:GLN:CD	1:A:429:GLN:H	2.16	0.52
2:B:754:ASP:OD2	2:B:918:HIS:ND1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:LEU:HD12	2:B:882:HIS:NE2	2.24	0.52
1:A:311:VAL:HG11	1:A:319:LEU:HD21	1.91	0.52
6:B:2676:CL:CL	10:B:2001:HOH:O	2.56	0.52
2:B:1032:GLU:HA	9:B:2678:IOD:I	2.79	0.51
3:C:159:HIS:HA	3:C:174:TYR:HA	1.91	0.51
3:C:45:ASN:N	3:C:48:ASP:OD2	2.37	0.51
1:A:503:ALA:HB3	4:D:4:FUC:H5	1.93	0.51
2:B:1442:ASN:OD1	2:B:1442:ASN:N	2.40	0.51
1:A:54:PRO:HA	1:A:75:VAL:HG22	1.93	0.51
1:A:433:GLU:OE2	7:A:1667:GOL:O3	2.28	0.51
1:A:528:SER:HA	1:A:555:VAL:HG23	1.93	0.51
3:C:253:THR:C	3:C:254:TRP:HD1	2.19	0.51
2:B:874:SER:HB2	2:B:900:ILE:HG22	1.92	0.51
2:B:918:HIS:C	2:B:919:HIS:HD1	2.18	0.51
3:C:244:SER:OG	3:C:245:SER:N	2.35	0.51
1:A:37:GLU:HG2	1:A:92:ALA:HA	1.93	0.51
2:B:1035:GLU:HA	2:B:1039:LEU:CD2	2.41	0.51
3:C:73:THR:O	3:C:73:THR:OG1	2.22	0.51
2:B:1522:LYS:HB2	2:B:1523:SER:HB3	1.94	0.50
3:C:159:HIS:ND1	3:C:160:ASN:O	2.45	0.50
1:A:221:GLU:OE2	7:A:1673:GOL:O1	2.30	0.50
1:A:391:VAL:HG23	1:A:409:LEU:HD13	1.94	0.50
1:A:32:ASN:HB2	1:A:643:GLY:C	2.37	0.50
2:B:891:LYS:HB3	7:B:2664:GOL:H31	1.92	0.50
1:A:248:GLU:O	7:A:1668:GOL:O2	2.26	0.49
2:B:1199:MET:HE3	2:B:1201:ARG:HD3	1.93	0.49
1:A:355:ILE:HD13	1:A:424:VAL:HG12	1.94	0.49
1:A:580:GLN:HG2	7:A:1671:GOL:H2	1.95	0.49
1:A:102:ARG:HB3	1:A:103:ASN:CG	2.38	0.49
1:A:396:THR:OG1	1:A:397:VAL:N	2.45	0.49
2:B:1217:LYS:HE3	2:B:1248:PHE:CZ	2.46	0.49
1:A:46:ALA:O	1:A:82:HIS:HD2	1.95	0.48
1:A:43:VAL:HG22	4:D:4:FUC:H62	1.94	0.48
1:A:261:TYR:HB2	2:B:826:MET:HG2	1.95	0.48
2:B:766:GLU:OE2	3:C:90:ARG:HG2	2.13	0.48
1:A:104:LYS:HD3	1:A:104:LYS:HA	1.59	0.48
1:A:500:LEU:HD21	1:A:644:LEU:HD21	1.96	0.48
2:B:874:SER:OG	2:B:875:LEU:N	2.46	0.48
1:A:221:GLU:HG3	7:A:1673:GOL:H32	1.96	0.48
2:B:1237:LEU:HD23	2:B:1278:ALA:HB1	1.95	0.48
2:B:948:ASP:OD2	2:B:951:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:HB	1:A:397:VAL:HG11	1.95	0.48
3:C:121:GLU:HG3	3:C:138:PRO:HB2	1.94	0.48
1:A:36:LEU:HG	1:A:125:LEU:HA	1.95	0.48
2:B:800:THR:OG1	2:B:801:THR:N	2.46	0.48
3:C:149:GLN:HG2	3:C:150:LEU:N	2.26	0.47
3:C:33:LYS:HA	3:C:53:LEU:HD22	1.97	0.47
1:A:357:PHE:O	1:A:362:LYS:NZ	2.47	0.47
2:B:971:VAL:HB	2:B:974:THR:HG21	1.95	0.47
1:A:481:ARG:HA	1:A:484:GLU:HB2	1.95	0.47
2:B:1507:ARG:NE	2:B:1560:GLU:OE2	2.42	0.47
2:B:1111:LYS:NZ	2:B:1121:ASP:OD2	2.37	0.47
2:B:949:PRO:HA	2:B:958:GLN:HB2	1.97	0.47
2:B:1194:TYR:CE1	2:B:1238:LEU:HB3	2.50	0.47
2:B:1308:THR:HG22	2:B:1310:ARG:HD3	1.97	0.47
2:B:846:GLU:OE2	2:B:1406:SER:OG	2.24	0.46
2:B:1246:PHE:O	2:B:1250:PRO:HD3	2.14	0.46
2:B:784:ASN:HB2	2:B:785:GLY:H	1.48	0.46
2:B:974:THR:HA	7:B:2667:GOL:H11	1.98	0.46
2:B:1217:LYS:HE3	2:B:1248:PHE:HZ	1.79	0.46
1:A:334:SER:N	7:A:1674:GOL:O1	2.48	0.46
1:A:402:GLN:OE1	1:A:463:THR:HA	2.16	0.46
2:B:967:LEU:HB3	2:B:970:GLN:HB2	1.98	0.46
1:A:131:PHE:CZ	1:A:616:ILE:HG23	2.50	0.46
1:A:159:VAL:HG13	1:A:161:ARG:HG3	1.97	0.46
3:C:103:ASP:OD1	3:C:106:SER:OG	2.31	0.46
1:A:281:ARG:NH1	1:A:342:GLU:OE2	2.40	0.45
1:A:481:ARG:NH1	1:A:484:GLU:HG3	2.31	0.45
1:A:113:GLY:O	1:A:114:THR:HG22	2.17	0.45
1:A:292:PRO:HD2	7:A:1675:GOL:H12	1.98	0.45
2:B:1310:ARG:HG3	3:C:162:TYR:CD1	2.51	0.45
2:B:1196:LEU:HA	2:B:1199:MET:HE2	1.98	0.45
1:A:385:TYR:CD1	1:A:403:GLY:HA2	2.52	0.45
1:A:81:ASN:OD1	1:A:81:ASN:N	2.47	0.45
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.46	0.45
1:A:26:TYR:CD2	1:A:115:GLN:HG2	2.52	0.45
1:A:490:TYR:HE2	1:A:515:VAL:HG21	1.82	0.45
2:B:920:PHE:HB2	3:C:63[B]:MET:HE3	1.98	0.45
1:A:122:LEU:HD12	1:A:123:VAL:H	1.81	0.45
2:B:926:ARG:NH1	10:B:2009:HOH:O	2.49	0.45
1:A:496:ASN:ND2	1:A:525:PHE:HA	2.32	0.45
3:C:241:SER:HA	3:C:242:GLY:HA2	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1029:ASP:OD1	2:B:1034:TRP:NE1	2.43	0.45
1:A:198:LEU:O	2:B:979:ARG:NH2	2.50	0.45
2:B:1040:GLU:H	2:B:1040:GLU:HG3	1.43	0.44
1:A:102:ARG:HA	1:A:103:ASN:HA	1.67	0.44
1:A:66:LYS:HB2	1:A:67:LEU:HD23	1.99	0.44
2:B:1026:HIS:CG	2:B:1088:LEU:HD21	2.53	0.44
2:B:1238:LEU:HD11	2:B:1277:GLN:HG2	2.00	0.44
3:C:75:TRP:HB3	7:C:1260:GOL:H12	2.00	0.44
3:C:231:ASP:OD1	3:C:245:SER:OG	2.30	0.44
1:A:148:ARG:HG3	2:B:773:TRP:CZ2	2.52	0.44
1:A:484:GLU:CG	1:A:508:ARG:HH22	2.31	0.44
2:B:1577:GLN:HB3	2:B:1578:VAL:H	1.53	0.44
3:C:30:MET:HE1	3:C:77:LEU:HD21	1.99	0.44
2:B:841:ARG:HD3	2:B:905:THR:HG23	2.00	0.43
2:B:961:ASP:OD1	2:B:1331:THR:OG1	2.35	0.43
2:B:999:ARG:NH2	10:B:2044:HOH:O	2.50	0.43
2:B:1069:PHE:CD2	7:B:2668:GOL:H31	2.54	0.43
3:C:183:ILE:HD13	3:C:183:ILE:HA	1.73	0.43
1:A:484:GLU:CD	1:A:508:ARG:HH22	2.27	0.43
2:B:753:GLU:HB2	2:B:754:ASP:H	1.53	0.43
2:B:829:PHE:HA	2:B:852:TYR:O	2.18	0.43
2:B:1034:TRP:HB2	9:B:2678:IOD:I	2.88	0.43
2:B:1035:GLU:HA	2:B:1039:LEU:HD21	2.01	0.43
2:B:1152:GLN:OE1	7:B:2666:GOL:O2	2.31	0.43
2:B:1214:ALA:HB2	2:B:1220:TRP:CZ2	2.54	0.43
2:B:1441:ARG:HA	2:B:1441:ARG:HD2	1.77	0.43
3:C:59:ARG:HG2	3:C:84:ARG:HG2	1.99	0.43
1:A:94:ARG:HA	1:A:96:PHE:HE1	1.84	0.43
2:B:756:ILE:O	7:B:2665:GOL:O1	2.30	0.43
2:B:1436:LYS:HD2	2:B:1436:LYS:HA	1.80	0.43
1:A:55:VAL:HA	1:A:111:THR:O	2.19	0.43
1:A:431:LEU:HG	1:A:435:GLU:HB3	2.00	0.43
2:B:1199:MET:HG2	7:B:2666:GOL:O2	2.19	0.43
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.89	0.43
1:A:136:LYS:HE3	1:A:136:LYS:HB2	1.76	0.43
1:A:488:ARG:HG3	1:A:489:TYR:CD2	2.54	0.43
2:B:875:LEU:HA	2:B:875:LEU:HD23	1.65	0.43
1:A:459:SER:OG	1:A:474:ASN:HB2	2.19	0.42
1:A:26:TYR:H	1:A:649:SER:HG	1.67	0.42
3:C:190:CYS:HB2	3:C:195:TRP:CZ3	2.53	0.42
2:B:1111:LYS:HA	2:B:1111:LYS:HD3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HA	1:A:47:HIS:O	2.20	0.42
1:A:96:PHE:N	1:A:96:PHE:CD1	2.85	0.42
2:B:942:VAL:N	2:B:1344:VAL:O	2.51	0.42
1:A:299:GLU:H	7:A:1675:GOL:H31	1.84	0.42
3:C:218:SER:O	3:C:230:VAL:HG12	2.20	0.42
1:A:29:ILE:HA	1:A:645:THR:O	2.20	0.42
2:B:1219:ARG:HD2	2:B:1255:TRP:CE2	2.55	0.42
2:B:1565:ILE:HD13	2:B:1576:VAL:HG11	2.00	0.42
3:C:230:VAL:CG2	3:C:246:SER:HB2	2.49	0.42
1:A:135:ASP:OD2	2:B:770:SER:OG	2.37	0.42
2:B:891:LYS:HD2	7:B:2664:GOL:H31	2.00	0.42
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.55	0.42
1:A:55:VAL:HG22	1:A:74:THR:O	2.19	0.42
1:A:386:ARG:HH11	1:A:400:LEU:HD23	1.83	0.42
3:C:142:ILE:HD13	3:C:142:ILE:HA	1.85	0.42
2:B:1314:GLU:OE1	2:B:1315:SER:N	2.52	0.42
2:B:1618:LEU:HD12	2:B:1619:SER:N	2.35	0.42
3:C:154:ILE:HA	3:C:154:ILE:HD13	1.62	0.42
2:B:1065:ALA:HB2	2:B:1106:TRP:CD2	2.55	0.41
2:B:1519:PHE:HB2	2:B:1622:ILE:HG22	2.01	0.41
2:B:1298:LEU:HB3	2:B:1332:VAL:HG22	2.02	0.41
1:A:102:ARG:HB3	1:A:103:ASN:ND2	2.35	0.41
2:B:1044:GLY:O	2:B:1045:ALA:C	2.63	0.41
2:B:1326:GLU:OE1	2:B:1326:GLU:N	2.46	0.41
2:B:1615:LYS:HE2	2:B:1618:LEU:HB3	2.01	0.41
1:A:136:LYS:NZ	10:A:2013:HOH:O	2.52	0.41
1:A:456:LEU:HB2	1:A:535:TYR:HE2	1.85	0.41
2:B:1265:GLY:N	7:B:2675:GOL:O2	2.53	0.41
1:A:98:SER:O	1:A:99:GLU:HB2	2.19	0.41
2:B:780:GLU:HA	2:B:781:PRO:HD3	1.96	0.41
1:A:465:LEU:HD23	1:A:465:LEU:HA	1.88	0.41
2:B:879:LYS:H	2:B:879:LYS:HG2	1.66	0.41
2:B:1235:TYR:CE1	2:B:1274:MET:HE2	2.55	0.41
1:A:209:TYR:CD2	1:A:214:PRO:HA	2.55	0.41
2:B:1523:SER:HB2	2:B:1525:ASP:OD1	2.21	0.41
2:B:1535:LYS:O	2:B:1538:GLU:HB2	2.20	0.41
1:A:153:ASN:ND2	9:A:1677:IOD:I	3.24	0.41
2:B:1106:TRP:O	2:B:1110:GLU:HB2	2.21	0.41
7:A:1672:GOL:O3	7:A:1673:GOL:O3	2.38	0.40
2:B:831:ILE:HD13	2:B:912:VAL:HG12	2.03	0.40
3:C:21:CYS:HB2	3:C:22:THR:H	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:CD2	1:A:505:ARG:HH12	2.38	0.40
3:C:71:THR:HG23	3:C:73:THR:N	2.34	0.40
3:C:71:THR:HG22	3:C:74:GLY:O	2.21	0.40
1:A:398:GLN:HE22	1:A:400:LEU:HD13	1.86	0.40
2:B:1439:SER:HB2	2:B:1440:ASP:OD1	2.21	0.40
1:A:274:GLY:HA3	1:A:325:TYR:CZ	2.57	0.40
1:A:336:SER:HB2	2:B:834:ARG:HG3	2.04	0.40
1:A:387:VAL:HA	1:A:388:PRO:HD3	1.92	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)
2:B:1600:LYS:NZ	3:C:73:THR:O[1_545]	2.09	0.11

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	A	643/645 (100%)	625 (97%)	15 (2%)	3 (0%)	24	46
2	B	898/915 (98%)	875 (97%)	22 (2%)	1 (0%)	48	70
3	C	240/245 (98%)	218 (91%)	14 (6%)	8 (3%)	3	5
All	All	1781/1805 (99%)	1718 (96%)	51 (3%)	12 (1%)	18	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	21	CYS
3	C	240	LEU
3	C	256	PRO
1	A	82	HIS

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Mol	Chain	Res	Type
3	C	22	THR
3	C	160	ASN
1	A	99	GLU
2	B	1010	CYS
3	C	257	GLU
3	C	216	LEU
3	C	255	GLN
1	A	102	ARG

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	566/567 (100%)	487 (86%)	79 (14%)	3	6
2	B	797/810 (98%)	710 (89%)	87 (11%)	6	13
3	C	205/215 (95%)	165 (80%)	40 (20%)	1	2
All	All	1568/1592 (98%)	1362 (87%)	206 (13%)	4	8

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	50	GLN
1	A	53	VAL
1	A	55	VAL
1	A	56	THR
1	A	65	LYS
1	A	67	LEU
1	A	71	SER
1	A	72	GLU
1	A	73	LYS
1	A	74	THR
1	A	77	THR
1	A	80	THR
1	A	81	ASN

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Mol	Chain	Res	Type
1	A	86	VAL
1	A	87	THR
1	A	90	ILE
1	A	96	PHE
1	A	111	THR
1	A	112	PHE
1	A	114	THR
1	A	117	VAL
1	A	126	GLN
1	A	155	LYS
1	A	159	VAL
1	A	161	ARG
1	A	176	LYS
1	A	186	LEU
1	A	189	LEU
1	A	205	LYS
1	A	213	SER
1	A	216	GLN
1	A	236	VAL
1	A	248	GLU
1	A	249	LYS
1	A	252	GLU
1	A	265	VAL
1	A	279	GLU
1	A	297	SER
1	A	326	VAL
1	A	340[A]	GLN
1	A	340[B]	GLN
1	A	360	THR
1	A	365	LYS
1	A	389	VAL
1	A	394	GLU
1	A	398	GLN
1	A	400	LEU
1	A	411	ILE
1	A	413	THR
1	A	420	LEU
1	A	427	LYS
1	A	431	LEU
1	A	433	GLU
1	A	435	GLU
1	A	449	VAL

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Mol	Chain	Res	Type
1	A	451	ASN
1	A	461	LEU
1	A	463	THR
1	A	465	LEU
1	A	470	THR
1	A	471	LEU
1	A	478	ARG
1	A	484	GLU
1	A	493	LEU
1	A	499	ARG
1	A	502	LYS
1	A	507	VAL
1	A	514	LEU
1	A	515	VAL
1	A	537	LEU
1	A	543	GLN
1	A	551	VAL
1	A	553	VAL
1	A	600	LYS
1	A	605	LEU
1	A	634	ASP
1	A	647	THR
1	A	649	SER
2	B	753	GLU
2	B	783	LYS
2	B	784	ASN
2	B	789	LYS
2	B	803	GLU
2	B	826	MET
2	B	845	VAL
2	B	867	LEU
2	B	874	SER
2	B	879	LYS
2	B	880	ARG
2	B	891	LYS
2	B	936	ILE
2	B	937	ARG
2	B	957	VAL
2	B	975	GLU
2	B	979	ARG
2	B	999	ARG
2	B	1006	THR

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Mol	Chain	Res	Type
2	B	1008	SER
2	B	1032	GLU
2	B	1039	LEU
2	B	1040	GLU
2	B	1041	LYS
2	B	1088	LEU
2	B	1090	VAL
2	B	1091	ASN
2	B	1133	LEU
2	B	1135	ASN
2	B	1136	ASN
2	B	1159	GLU
2	B	1171	LYS
2	B	1177	GLU
2	B	1206	LEU
2	B	1212	THR
2	B	1249	VAL
2	B	1259	GLN
2	B	1260	ARG
2	B	1275	VAL
2	B	1277	GLN
2	B	1284	LYS
2	B	1288	ASP
2	B	1293	ASN
2	B	1298	LEU
2	B	1300	LEU
2	B	1302	SER
2	B	1304	SER
2	B	1307	ILE
2	B	1310	ARG
2	B	1314	GLU
2	B	1324	THR
2	B	1331	THR
2	B	1347	MET
2	B	1348	TYR
2	B	1357	THR
2	B	1364	LYS
2	B	1366	THR
2	B	1383	THR
2	B	1415	THR
2	B	1436	LYS
2	B	1450	LYS

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Mol	Chain	Res	Type
2	B	1455	GLU
2	B	1468	ASN
2	B	1497	LYS
2	B	1510	LEU
2	B	1522	LYS
2	B	1526	LYS
2	B	1527	VAL
2	B	1531	GLU
2	B	1533	LEU
2	B	1537	CYS
2	B	1548	ARG
2	B	1554	LEU
2	B	1566	GLU
2	B	1576	VAL
2	B	1577	GLN
2	B	1592	GLU
2	B	1596	LEU
2	B	1614	GLU
2	B	1619	SER
2	B	1624	LYS
2	B	1634	GLU
2	B	1637	CYS
2	B	1638	GLN
2	B	1639	ASP
2	B	1644	LYS
2	B	1657	VAL
3	C	23	ILE
3	C	28	ILE
3	C	38	THR
3	C	53	LEU
3	C	59	ARG
3	C	60	LYS
3	C	66	ILE
3	C	71	THR
3	C	73	THR
3	C	88	SER
3	C	97	LEU
3	C	107	SER
3	C	108	ILE
3	C	109	THR
3	C	111	SER
3	C	119	ILE

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Mol	Chain	Res	Type
3	C	122	TYR
3	C	128	LEU
3	C	130	SER
3	C	142	ILE
3	C	148	CYS
3	C	153	SER
3	C	154	ILE
3	C	158	ARG
3	C	159	HIS
3	C	162	TYR
3	C	165	PHE
3	C	173	THR
3	C	182	LEU
3	C	183	ILE
3	C	194	GLU
3	C	204	VAL
3	C	211	ILE
3	C	216	LEU
3	C	225	SER
3	C	229	ASN
3	C	240	LEU
3	C	243	SER
3	C	252	ASN
3	C	253	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	82	HIS
1	A	115	GLN
1	A	126	GLN
1	A	177	GLN
1	A	216	GLN
1	A	412	ASN
1	A	661	GLN
2	B	792	ASN
2	B	883	GLN
2	B	1135	ASN
2	B	1163	ASN
2	B	1277	GLN
2	B	1349	HIS

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Mol	Chain	Res	Type
2	B	1503	ASN
2	B	1553	GLN
3	C	41	ASN
3	C	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	4,1	14,14,15	0.54	0	17,19,21	0.91	0
4	NAG	D	2	4	14,14,15	0.60	0	17,19,21	0.87	0
4	BMA	D	3	4	11,11,12	0.71	0	15,15,17	0.84	1 (6%)
4	FUC	D	4	4	10,10,11	1.02	0	14,14,16	1.10	1 (7%)
5	NAG	E	1	2,5	14,14,15	0.71	0	17,19,21	0.81	0
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.62	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	D	1	4,1	1/1/5/7	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
5	NAG	E	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	O2-C2-C3	-2.23	105.53	110.15
4	D	4	FUC	O5-C5-C4	2.15	113.43	109.55

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1	NAG	C1

All (7) torsion outliers are listed below:

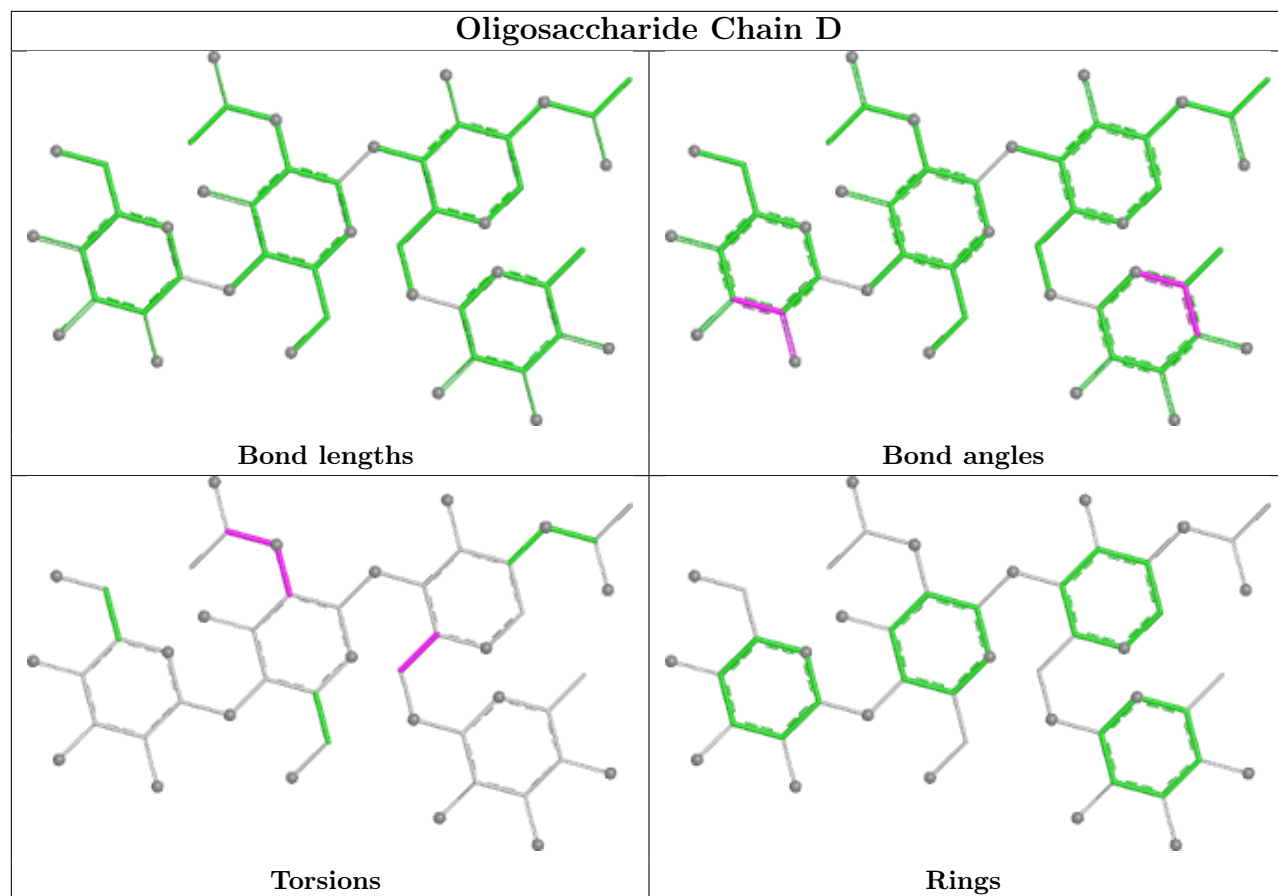
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2

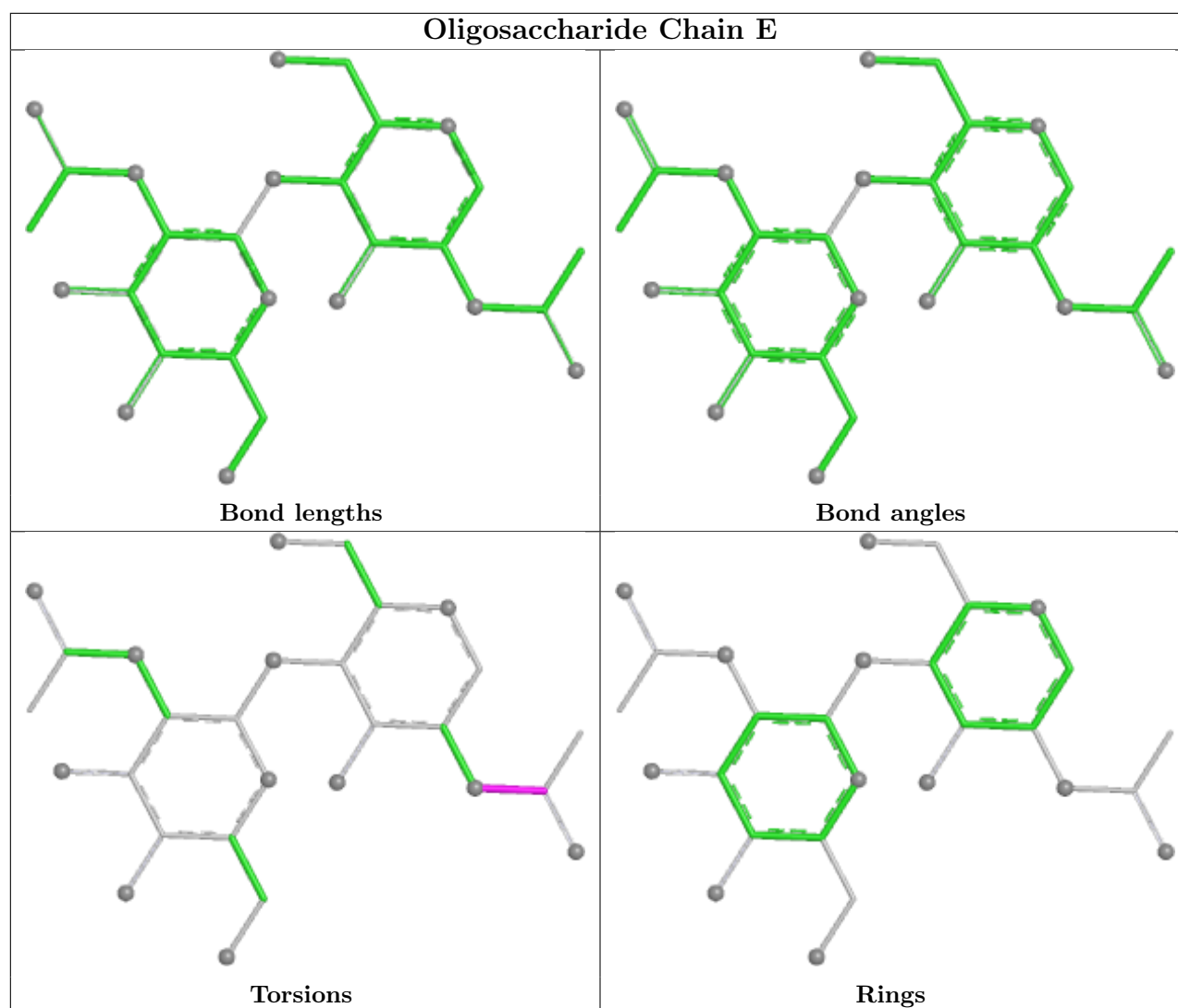
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0
4	D	2	NAG	1	0
4	D	4	FUC	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 38 ligands modelled in this entry, 14 are monoatomic - leaving 24 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	$\# Z > 2$
7	GOL	B	2667	-	5,5,5	0.36	0	5,5,5	0.35	0
7	GOL	B	2670	-	5,5,5	0.37	0	5,5,5	0.28	0
7	GOL	A	1671	-	5,5,5	0.38	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	1668	-	5,5,5	0.37	0	5,5,5	0.32	0
7	GOL	A	1672	-	5,5,5	0.36	0	5,5,5	0.33	0
7	GOL	B	2668	-	5,5,5	0.35	0	5,5,5	0.33	0
7	GOL	B	2665	-	5,5,5	0.36	0	5,5,5	0.38	0
7	GOL	B	2666	-	5,5,5	0.37	0	5,5,5	0.42	0
7	GOL	A	1669	-	5,5,5	0.36	0	5,5,5	0.26	0
7	GOL	A	1666	-	5,5,5	0.38	0	5,5,5	0.29	0
7	GOL	B	2674	-	5,5,5	0.39	0	5,5,5	0.30	0
7	GOL	A	1674	-	5,5,5	0.37	0	5,5,5	0.33	0
7	GOL	B	2671	-	5,5,5	0.36	0	5,5,5	0.37	0
7	GOL	A	1675	-	5,5,5	0.36	0	5,5,5	0.41	0
7	GOL	B	2675	-	5,5,5	0.40	0	5,5,5	0.35	0
7	GOL	C	1260	-	5,5,5	0.38	0	5,5,5	0.33	0
7	GOL	C	1259	-	5,5,5	0.37	0	5,5,5	0.32	0
7	GOL	A	1667	-	5,5,5	0.35	0	5,5,5	0.37	0
7	GOL	B	2664	-	5,5,5	0.38	0	5,5,5	0.34	0
7	GOL	B	2669	-	5,5,5	0.39	0	5,5,5	0.37	0
7	GOL	B	2673	-	5,5,5	0.37	0	5,5,5	0.31	0
7	GOL	A	1670	-	5,5,5	0.35	0	5,5,5	0.36	0
7	GOL	A	1673	-	5,5,5	0.38	0	5,5,5	0.29	0
7	GOL	B	2672	-	5,5,5	0.38	0	5,5,5	0.33	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
7	GOL	B	2667	-	-	2/4/4/4	-
7	GOL	B	2670	-	-	2/4/4/4	-
7	GOL	A	1671	-	-	2/4/4/4	-
7	GOL	A	1668	-	-	2/4/4/4	-
7	GOL	A	1672	-	-	2/4/4/4	-
7	GOL	B	2668	-	-	2/4/4/4	-
7	GOL	B	2665	-	-	2/4/4/4	-
7	GOL	B	2666	-	-	3/4/4/4	-
7	GOL	A	1669	-	-	2/4/4/4	-
7	GOL	A	1666	-	-	2/4/4/4	-
7	GOL	B	2674	-	-	2/4/4/4	-
7	GOL	A	1674	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	2671	-	-	2/4/4/4	-
7	GOL	A	1675	-	-	2/4/4/4	-
7	GOL	B	2675	-	-	2/4/4/4	-
7	GOL	C	1260	-	-	0/4/4/4	-
7	GOL	C	1259	-	-	2/4/4/4	-
7	GOL	A	1667	-	-	2/4/4/4	-
7	GOL	B	2664	-	-	4/4/4/4	-
7	GOL	B	2669	-	-	2/4/4/4	-
7	GOL	B	2673	-	-	2/4/4/4	-
7	GOL	A	1670	-	-	2/4/4/4	-
7	GOL	A	1673	-	-	2/4/4/4	-
7	GOL	B	2672	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1666	GOL	C1-C2-C3-O3
7	A	1667	GOL	C1-C2-C3-O3
7	A	1668	GOL	C1-C2-C3-O3
7	A	1669	GOL	O2-C2-C3-O3
7	A	1670	GOL	C1-C2-C3-O3
7	A	1671	GOL	C1-C2-C3-O3
7	A	1672	GOL	C1-C2-C3-O3
7	A	1675	GOL	C1-C2-C3-O3
7	B	2664	GOL	C1-C2-C3-O3
7	B	2665	GOL	O1-C1-C2-C3
7	B	2666	GOL	C1-C2-C3-O3
7	B	2667	GOL	C1-C2-C3-O3
7	B	2668	GOL	C1-C2-C3-O3
7	B	2669	GOL	C1-C2-C3-O3
7	B	2670	GOL	C1-C2-C3-O3
7	B	2671	GOL	C1-C2-C3-O3
7	B	2671	GOL	O2-C2-C3-O3
7	B	2672	GOL	C1-C2-C3-O3
7	B	2673	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	B	2674	GOL	C1-C2-C3-O3
7	B	2675	GOL	C1-C2-C3-O3
7	C	1259	GOL	C1-C2-C3-O3
7	A	1670	GOL	O2-C2-C3-O3
7	A	1675	GOL	O2-C2-C3-O3
7	B	2664	GOL	O2-C2-C3-O3
7	B	2665	GOL	O1-C1-C2-O2
7	B	2670	GOL	O2-C2-C3-O3
7	B	2674	GOL	O2-C2-C3-O3
7	A	1669	GOL	C1-C2-C3-O3
7	B	2664	GOL	O1-C1-C2-C3
7	A	1666	GOL	O2-C2-C3-O3
7	A	1667	GOL	O2-C2-C3-O3
7	A	1668	GOL	O2-C2-C3-O3
7	A	1671	GOL	O2-C2-C3-O3
7	A	1672	GOL	O2-C2-C3-O3
7	B	2666	GOL	O2-C2-C3-O3
7	B	2667	GOL	O2-C2-C3-O3
7	B	2669	GOL	O2-C2-C3-O3
7	B	2672	GOL	O2-C2-C3-O3
7	B	2675	GOL	O2-C2-C3-O3
7	B	2668	GOL	O2-C2-C3-O3
7	B	2673	GOL	O2-C2-C3-O3
7	C	1259	GOL	O2-C2-C3-O3
7	A	1673	GOL	O2-C2-C3-O3
7	B	2664	GOL	O1-C1-C2-O2
7	B	2666	GOL	O1-C1-C2-O2
7	A	1674	GOL	O2-C2-C3-O3
7	A	1673	GOL	C1-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2667	GOL	1	0
7	A	1671	GOL	1	0
7	A	1668	GOL	2	0
7	A	1672	GOL	1	0
7	B	2668	GOL	2	0
7	B	2665	GOL	1	0
7	B	2666	GOL	3	0
7	A	1669	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2674	GOL	3	0
7	A	1674	GOL	1	0
7	A	1675	GOL	2	0
7	B	2675	GOL	1	0
7	C	1260	GOL	2	0
7	A	1667	GOL	2	0
7	B	2664	GOL	2	0
7	A	1673	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	642/645 (99%)	0.11	20 (3%)	51 45	28, 73, 140, 195	3 (0%)
2	B	902/915 (98%)	-0.03	8 (0%)	81 78	28, 74, 121, 174	0
3	C	240/245 (97%)	0.42	14 (5%)	29 23	35, 91, 171, 207	2 (0%)
All	All	1784/1805 (98%)	0.08	42 (2%)	59 54	28, 75, 142, 207	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ALA	4.7
2	B	1298	LEU	4.2
2	B	1307	ILE	3.8
1	A	93	ASN	3.8
3	C	165	PHE	3.3
1	A	98	SER	3.2
1	A	533	ALA	3.0
1	A	503	ALA	3.0
2	B	1291	GLU	2.8
1	A	94	ARG	2.8
1	A	97	LYS	2.8
3	C	217	SER	2.8
3	C	223	SER	2.7
3	C	209	PRO	2.7
3	C	21	CYS	2.7
1	A	532	VAL	2.6
3	C	246	SER	2.5
1	A	430	GLU	2.4
3	C	150	LEU	2.4
3	C	258	LEU	2.4
2	B	1109	LEU	2.3
3	C	82	ILE	2.3
1	A	538	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	2.3
1	A	65	LYS	2.2
2	B	1578	VAL	2.2
3	C	23	ILE	2.2
3	C	236	TYR	2.2
2	B	1438	PHE	2.2
1	A	83	MET	2.1
3	C	220	PHE	2.1
1	A	90	ILE	2.1
1	A	481	ARG	2.1
1	A	114	THR	2.1
2	B	1287	PRO	2.1
1	A	534	TYR	2.1
2	B	1319	LEU	2.0
3	C	96[A]	HIS	2.0
1	A	79	ALA	2.0
1	A	36	LEU	2.0
1	A	493	LEU	2.0
3	C	216	LEU	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](#)

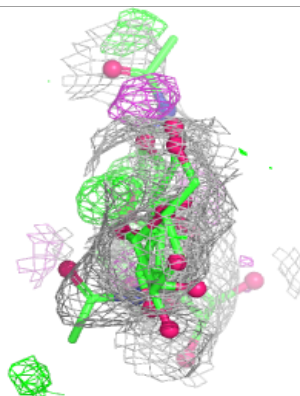
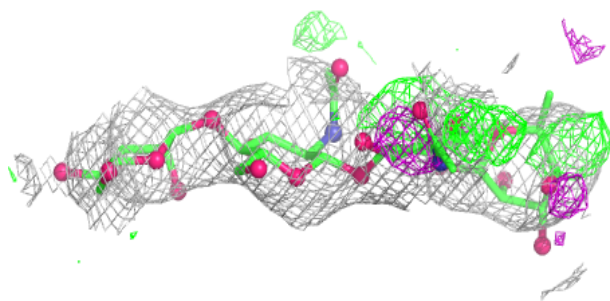
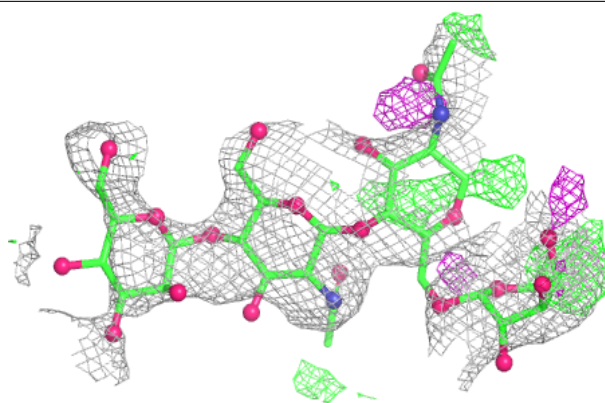
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BMA	D	3	11/12	0.15	0.15	148,156,159,161	0
5	NAG	E	2	14/15	0.39	0.12	153,160,164,164	0
5	NAG	E	1	14/15	0.52	0.13	103,130,146,146	0
4	NAG	D	1	14/15	0.55	0.18	98,124,145,149	0
4	NAG	D	2	14/15	0.64	0.12	137,141,147,152	0
4	FUC	D	4	10/11	0.79	0.19	67,116,142,148	0

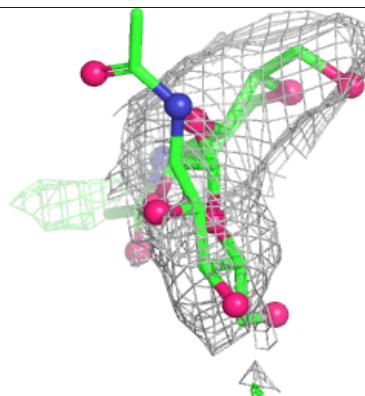
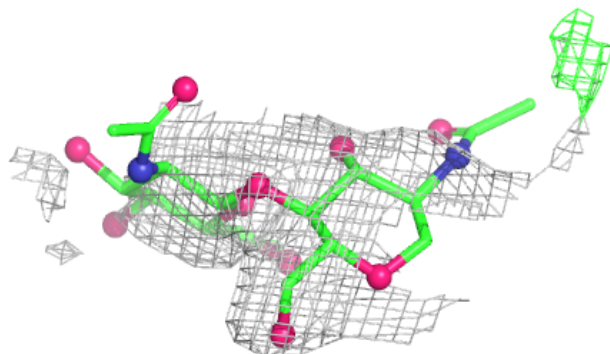
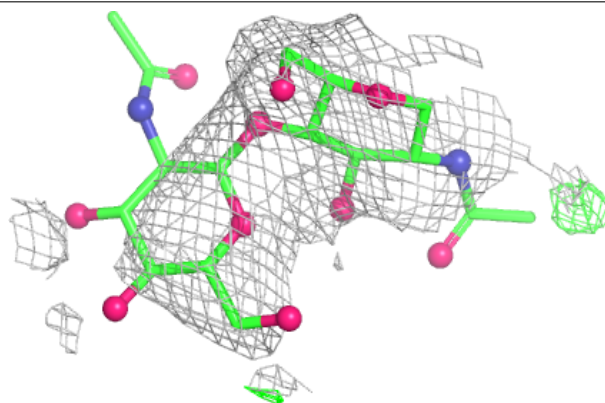
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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

**Electron density around Chain E:**

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



6.4 Ligands ⓘ

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
7	GOL	B	2669	6/6	0.40	0.16	116,118,119,119	0
7	GOL	B	2673	6/6	0.53	0.13	104,108,113,114	0
7	GOL	B	2672	6/6	0.70	0.10	105,110,115,116	0
6	CL	B	2682	1/1	0.76	0.19	66,66,66,66	0
7	GOL	A	1669	6/6	0.76	0.18	95,100,101,102	0
7	GOL	A	1675	6/6	0.76	0.17	121,124,125,128	0
7	GOL	B	2667	6/6	0.77	0.18	75,80,86,91	0
7	GOL	A	1666	6/6	0.77	0.14	76,92,95,99	0
7	GOL	A	1671	6/6	0.80	0.14	75,92,96,98	0
7	GOL	B	2668	6/6	0.81	0.12	56,77,84,88	0
7	GOL	B	2670	6/6	0.81	0.13	87,99,105,107	0
8	NA	A	1676	1/1	0.82	0.12	55,55,55,55	0
7	GOL	B	2671	6/6	0.83	0.10	77,79,80,82	0
7	GOL	A	1674	6/6	0.83	0.19	74,100,109,110	0
7	GOL	C	1259	6/6	0.84	0.13	77,94,98,101	0
7	GOL	B	2664	6/6	0.84	0.18	79,83,87,90	0
7	GOL	B	2674	6/6	0.86	0.17	72,77,85,87	0
7	GOL	A	1668	6/6	0.86	0.18	98,106,111,118	0
7	GOL	A	1672	6/6	0.86	0.15	81,86,89,94	0
8	NA	B	2677	1/1	0.86	0.10	85,85,85,85	0
7	GOL	A	1673	6/6	0.87	0.18	75,77,87,88	0
7	GOL	C	1260	6/6	0.89	0.13	54,83,89,90	0
7	GOL	A	1667	6/6	0.90	0.11	76,78,91,105	0
7	GOL	B	2665	6/6	0.90	0.12	59,64,71,77	0
6	CL	A	1665	1/1	0.92	0.09	87,87,87,87	0
7	GOL	B	2666	6/6	0.92	0.08	52,55,64,70	0
7	GOL	B	2675	6/6	0.93	0.08	76,84,85,88	0
7	GOL	A	1670	6/6	0.94	0.07	57,64,69,76	0
9	IOD	B	2680	1/1	0.94	0.08	68,68,68,68	1
6	CL	B	2676	1/1	0.96	0.08	72,72,72,72	0
9	IOD	A	1678	1/1	0.97	0.05	64,64,64,64	1
9	IOD	A	1677	1/1	0.98	0.04	55,55,55,55	1
6	CL	C	1261	1/1	0.98	0.09	49,49,49,49	0
9	IOD	B	2678	1/1	0.98	0.06	83,83,83,83	1
6	CL	C	1262	1/1	0.98	0.09	60,60,60,60	0
9	IOD	B	2679	1/1	0.99	0.04	67,67,67,67	1
9	IOD	A	1679	1/1	0.99	0.02	65,65,65,65	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	IOD	B	2681	1/1	0.99	0.03	75,75,75,75	1

6.5 Other polymers [i](#)

There are no such residues in this entry.