



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 PM UTC

PDB ID : 2WII / pdb_00002wii
Title : Complement C3b in complex with factor H domains 1-4
Authors : Wu, J.; Janssen, B.J.C.; Gros, P.
Deposited on : 2009-05-12
Resolution : 2.70 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

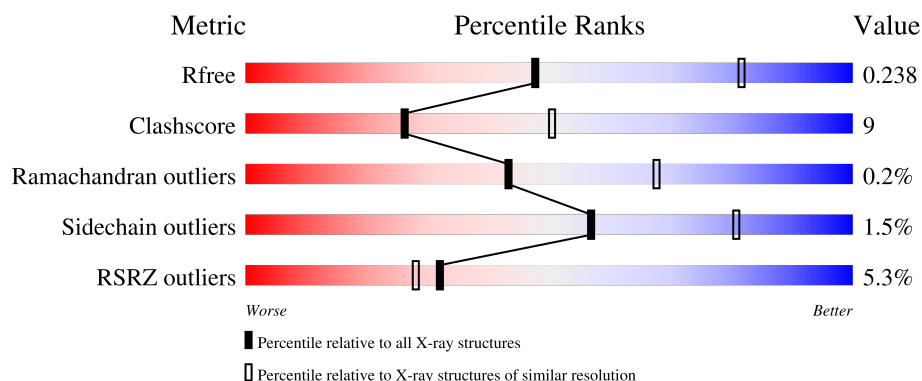
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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% 77% 21% ..
2	B	915	 4% 76% 22% ..
3	C	277	 14% 66% 22% 12%
4	D	6	 67% 33%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14442 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	640	Total	C	N	O	S	0	0	0
			4992	3179	846	952	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	896	Total	C	N	O	S	0	0	0
			7157	4536	1203	1380	38			

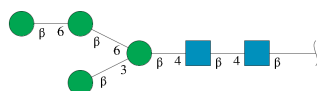
- Molecule 3 is a protein called COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	245	Total	C	N	O	S	0	0	0
			1932	1206	330	376	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	44	ILE	VAL	variant	UNP P08603

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

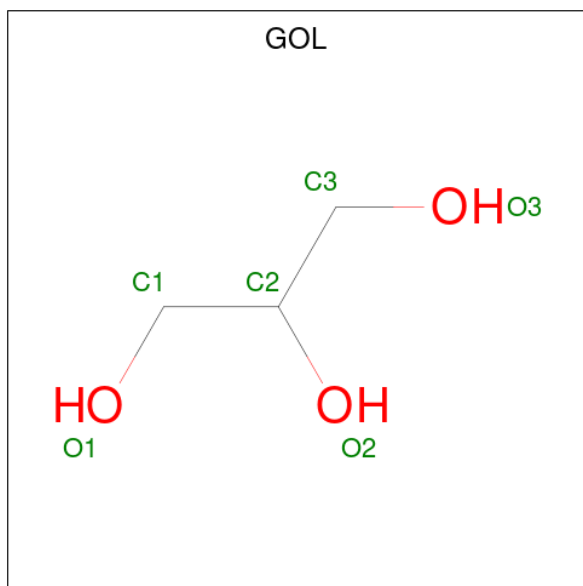


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



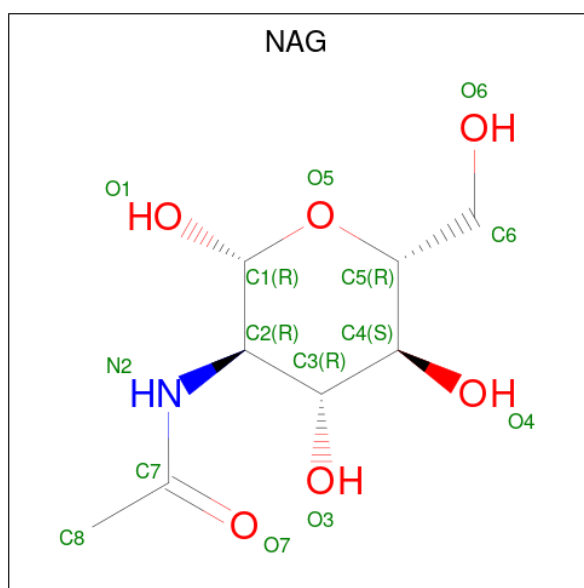
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

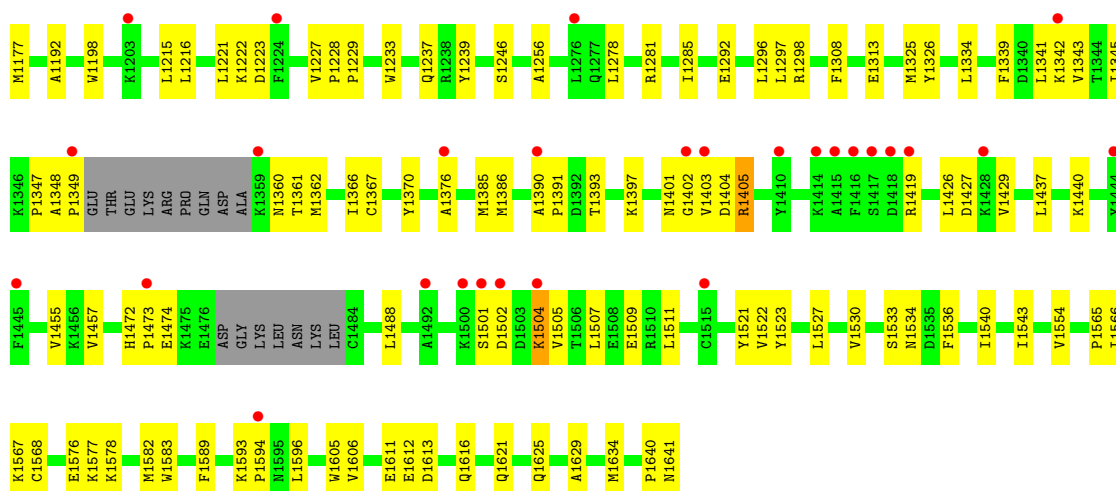
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	74	Total	O	0	0
			74	74		

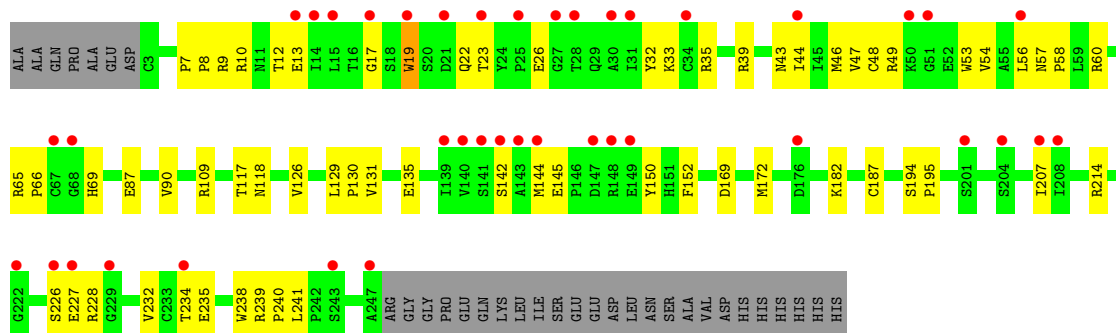
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	81	Total	O	0	0
			81	81		
8	C	17	Total	O	0	0
			17	17		



• Molecule 3: COMPLEMENT FACTOR H



• Molecule 4: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-3)]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 2	Depositor
Cell constants a, b, c, α , β , γ	223.49Å 84.95Å 128.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.48 – 2.70 64.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (64.48-2.70) 99.6 (64.48-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.252 0.206 , 0.238	Depositor DCC
R_{free} test set	3436 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14442	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 2.68% 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: GOL, CA, BMA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/5092	0.70	3/6917 (0.0%)
2	B	0.25	0/7300	0.67	2/9884 (0.0%)
3	C	0.23	0/1981	0.69	0/2683
All	All	0.25	0/14373	0.68	5/19484 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LEU	CA-C-N	6.65	126.16	119.24
1	A	207	LEU	C-N-CA	6.65	126.16	119.24
2	B	926	ASP	CA-C-N	5.49	124.95	119.24
2	B	926	ASP	C-N-CA	5.49	124.95	119.24
1	A	518	ALA	CB-CA-C	-5.24	110.55	116.63

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	A	4992	0	5055	84	0
2	B	7157	0	7076	145	0
3	C	1932	0	1820	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	72	0	61	4	0
5	A	1	0	0	0	0
6	A	18	0	24	1	0
6	B	78	0	104	8	0
6	C	6	0	8	0	0
7	B	14	0	13	0	0
8	A	74	0	0	0	0
8	B	81	0	0	0	0
8	C	17	0	0	0	0
All	All	14442	0	14161	266	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 9.

All (266) 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:1405:ARG:HG3	2:B:1405:ARG:HH11	1.28	0.96
2:B:840:VAL:HG22	2:B:894:VAL:HG12	1.56	0.88
3:C:49:ARG:HE	3:C:54:VAL:HG21	1.40	0.86
2:B:1640:PRO:O	2:B:1641:ASN:HB2	1.80	0.82
1:A:452:ASN:HB3	1:A:492:LEU:HD11	1.65	0.77
2:B:753:VAL:HG23	6:B:2649:GOL:H2	1.67	0.76
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.67	0.75
2:B:850:PHE:HZ	2:B:907:LEU:HD11	1.51	0.75
2:B:1405:ARG:HG3	2:B:1405:ARG:NH1	1.97	0.73
2:B:1098:GLU:HG2	6:B:2653:GOL:H2	1.71	0.72
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.24	0.72
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.74	0.69
2:B:1126:LEU:HD21	2:B:1177:MET:CE	2.23	0.68
2:B:957:ARG:HG3	2:B:1325:MET:HE1	1.75	0.68
1:A:19:THR:HG21	4:D:1:NAG:H82	1.76	0.68
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.77	0.66
1:A:408:GLU:HG2	1:A:409:LEU:HD12	1.78	0.66
1:A:22:LEU:HD13	1:A:33:VAL:HG11	1.78	0.65
2:B:894:VAL:HG23	2:B:897:HIS:HB2	1.80	0.64
2:B:751:TRP:CD1	6:B:2649:GOL:HO2	2.16	0.64
2:B:1341:LEU:HD12	2:B:1457:VAL:HG22	1.80	0.64
1:A:330:PRO:HG2	1:A:409:LEU:HD21	1.80	0.63
1:A:443:LEU:HD21	1:A:499:ILE:HG13	1.81	0.62
1:A:176:LEU:HD21	6:B:2646:GOL:H32	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:22:GLN:HG3	3:C:23:THR:HG23	1.81	0.61
1:A:23:GLU:HG2	1:A:61:MET:HG3	1.83	0.61
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.83	0.61
3:C:194:SER:HB2	3:C:207:ILE:HA	1.82	0.61
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.83	0.60
2:B:959:LEU:HD22	2:B:1297:LEU:HD11	1.83	0.59
1:A:1:SER:HB3	1:A:2:PRO:HD3	1.84	0.59
2:B:852:SER:HA	2:B:1488:LEU:HD11	1.85	0.59
2:B:1376:ALA:HB3	2:B:1429:VAL:HG22	1.85	0.59
2:B:1403:VAL:HG13	2:B:1405:ARG:HG3	1.86	0.57
2:B:850:PHE:CZ	2:B:907:LEU:HD11	2.37	0.57
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.86	0.57
3:C:32:TYR:CE2	3:C:46:MET:HG3	2.40	0.57
1:A:208:PRO:O	1:A:209:SER:HB3	2.05	0.56
2:B:1511:LEU:HD23	2:B:1634:MET:HE2	1.85	0.56
1:A:45:LEU:HD21	1:A:73:GLU:HG3	1.88	0.56
1:A:426:THR:HG23	1:A:429:ASN:HA	1.88	0.56
2:B:932:ARG:HH12	2:B:937:LYS:HB2	1.70	0.55
2:B:1405:ARG:HD3	2:B:1426:LEU:HD22	1.87	0.55
2:B:1341:LEU:CD2	2:B:1343:VAL:HG23	2.36	0.55
2:B:1370:TYR:CD1	2:B:1376:ALA:HB2	2.42	0.55
2:B:1533:SER:HB3	2:B:1536:PHE:O	2.07	0.55
2:B:744:GLU:C	2:B:746:PRO:HD3	2.32	0.54
3:C:17:GLY:HA3	3:C:19:TRP:CZ3	2.42	0.54
3:C:10:ARG:HB2	3:C:13:GLU:HB2	1.90	0.54
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.88	0.54
3:C:57:ASN:HB3	3:C:60:ARG:HB3	1.90	0.54
3:C:131:VAL:HG11	3:C:172:MET:HE1	1.90	0.54
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.88	0.54
2:B:1385:MET:HE2	2:B:1385:MET:HA	1.89	0.54
1:A:181:GLN:O	1:A:183:LYS:HE3	2.08	0.54
2:B:1104:HIS:O	2:B:1107:MET:HG2	2.08	0.54
3:C:126:VAL:HG22	3:C:152:PHE:HB2	1.90	0.54
3:C:39:ARG:HG2	3:C:65:ARG:HA	1.90	0.53
3:C:47:VAL:HG21	3:C:56:LEU:HD12	1.89	0.53
3:C:169:ASP:OD1	3:C:182:LYS:HD2	2.08	0.53
2:B:1114:ASN:O	2:B:1115:ASN:O	2.25	0.53
2:B:1593:LYS:HB3	2:B:1594:PRO:HD3	1.90	0.53
4:D:3:BMA:H4	4:D:6:BMA:O2	2.08	0.53
1:A:13:ARG:HH11	1:A:132:HIS:CD2	2.26	0.53
2:B:1192:ALA:HB2	2:B:1198:TRP:CZ2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:HIS:CG	2:B:760:PRO:HG3	2.44	0.52
2:B:1119:MET:HG3	2:B:1161:LEU:HD21	1.91	0.52
1:A:227:LYS:HD3	1:A:230:GLU:OE2	2.09	0.52
2:B:1347:PRO:HA	2:B:1362:MET:HG2	1.90	0.52
2:B:1589:PHE:HB3	2:B:1596:LEU:HD11	1.90	0.52
2:B:913:GLY:HA3	2:B:949:VAL:HG21	1.90	0.52
1:A:472:ILE:HD12	1:A:480:LYS:HB3	1.92	0.52
1:A:561:LEU:HD21	2:B:782:ILE:HD13	1.92	0.52
2:B:1403:VAL:HG13	2:B:1405:ARG:CG	2.40	0.52
3:C:19:TRP:HE3	3:C:19:TRP:H	1.58	0.52
2:B:872:LEU:HD23	2:B:873:SER:N	2.25	0.51
2:B:997:THR:HB	2:B:998:PRO:HD3	1.90	0.51
2:B:1391:PRO:HD2	2:B:1419:ARG:HD3	1.91	0.51
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.93	0.51
2:B:1115:ASN:C	2:B:1116:GLU:HG2	2.35	0.51
1:A:510:VAL:HG11	1:A:622:LEU:HD12	1.91	0.51
1:A:544:LYS:HD2	1:A:562:LYS:HD2	1.93	0.51
2:B:1385:MET:HG3	2:B:1391:PRO:HD3	1.92	0.51
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.46	0.51
1:A:389:ILE:HD11	1:A:398:LEU:HD21	1.93	0.51
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.46	0.51
1:A:464:LYS:HE3	1:A:515:LEU:HA	1.93	0.51
3:C:234:THR:HG22	3:C:235:GLU:N	2.25	0.51
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.93	0.50
2:B:819:ARG:HE	2:B:883:THR:HG23	1.77	0.50
2:B:1501:SER:O	2:B:1505:VAL:HG23	2.11	0.50
3:C:32:TYR:HB2	3:C:44:ILE:O	2.10	0.50
2:B:1472:HIS:CD2	2:B:1473:PRO:HD2	2.47	0.50
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.47	0.50
2:B:1298:ARG:HH12	3:C:144:MET:HG3	1.76	0.50
2:B:1239:TYR:OH	2:B:1246:SER:HB2	2.12	0.50
2:B:1583:TRP:CD1	2:B:1583:TRP:C	2.90	0.50
2:B:1393:THR:O	2:B:1397:LYS:HG3	2.12	0.49
1:A:208:PRO:O	1:A:209:SER:CB	2.60	0.49
2:B:898:PHE:CZ	3:C:39:ARG:HD3	2.47	0.49
3:C:109:ARG:HG2	3:C:117:THR:O	2.12	0.49
2:B:894:VAL:CG2	2:B:897:HIS:HB2	2.42	0.49
1:A:349:ASP:HB3	1:A:386:LYS:HE3	1.93	0.49
2:B:1403:VAL:O	2:B:1405:ARG:HG2	2.13	0.49
4:D:3:BMA:H4	4:D:6:BMA:C2	2.43	0.48
1:A:249:VAL:HG11	1:A:278:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:CYS:HB2	3:C:53:TRP:CZ3	2.49	0.48
2:B:1113:ASN:O	2:B:1114:ASN:C	2.57	0.48
2:B:1345:ILE:HD11	2:B:1362:MET:HB3	1.96	0.48
1:A:241:LYS:HG3	2:B:832:TYR:CE2	2.49	0.48
2:B:745:PHE:N	2:B:746:PRO:HD3	2.28	0.48
2:B:822:GLN:OE1	2:B:1488:LEU:HD23	2.14	0.48
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.54	0.48
1:A:544:LYS:HG3	1:A:562:LYS:HB3	1.95	0.47
3:C:142:SER:HB2	3:C:150:TYR:OH	2.15	0.47
1:A:606:THR:OG1	1:A:619:ASP:HB3	2.14	0.47
3:C:19:TRP:HE3	3:C:19:TRP:N	2.12	0.47
1:A:155:GLN:HG3	2:B:1296:LEU:HD13	1.96	0.47
2:B:1068:VAL:O	3:C:228:ARG:HD2	2.14	0.47
2:B:1341:LEU:HD23	2:B:1342:LYS:N	2.30	0.47
1:A:10:ASN:HD21	1:A:618:SER:HA	1.80	0.47
2:B:907:LEU:H	2:B:907:LEU:HD12	1.79	0.47
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.14	0.47
2:B:1419:ARG:O	2:B:1419:ARG:HG2	2.15	0.47
3:C:195:PRO:HG3	3:C:238:TRP:NE1	2.30	0.47
1:A:464:LYS:HD3	1:A:515:LEU:HB2	1.97	0.46
2:B:988:CYS:HA	2:B:1037:PHE:CZ	2.50	0.46
1:A:323:GLY:O	1:A:325:PRO:HD3	2.15	0.46
2:B:1534:ASN:O	2:B:1566:ILE:HD13	2.16	0.46
1:A:187:TYR:CD1	1:A:192:PRO:HA	2.51	0.46
3:C:7:PRO:HA	3:C:8:PRO:HD3	1.79	0.46
1:A:426:THR:HG21	1:A:431:ASN:H	1.80	0.46
3:C:234:THR:HG22	3:C:235:GLU:H	1.80	0.46
1:A:437:SER:OG	1:A:452:ASN:HB2	2.15	0.46
1:A:163:GLN:HB3	1:A:166:VAL:O	2.16	0.46
2:B:1292:GLU:H	2:B:1292:GLU:CD	2.23	0.46
2:B:1611:GLU:HA	6:B:2652:GOL:H12	1.98	0.46
2:B:753:VAL:CG2	6:B:2649:GOL:H2	2.41	0.46
2:B:1522:VAL:HG22	2:B:1583:TRP:HB2	1.98	0.46
1:A:171:TRP:CZ3	1:A:173:ILE:HG12	2.52	0.45
3:C:238:TRP:HB2	3:C:241:LEU:HD23	1.97	0.45
3:C:226:SER:O	3:C:227:GLU:HB2	2.17	0.45
2:B:1341:LEU:HD11	2:B:1455:VAL:HG12	1.98	0.45
2:B:1341:LEU:HD21	2:B:1343:VAL:HG23	1.98	0.45
1:A:407:GLN:O	1:A:408:GLU:CB	2.64	0.45
2:B:1126:LEU:HD21	2:B:1177:MET:HE1	1.98	0.45
2:B:1521:TYR:O	2:B:1583:TRP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:THR:O	1:A:511:ALA:HA	2.17	0.45
2:B:1102:VAL:HG22	6:B:2653:GOL:O3	2.16	0.45
2:B:1105:GLN:O	2:B:1108:ILE:HG12	2.17	0.45
2:B:1339:PHE:HE2	2:B:1429:VAL:HG21	1.82	0.45
1:A:112:THR:HG22	1:A:125:TYR:HB3	1.99	0.45
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.52	0.45
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.52	0.45
1:A:329:SER:HA	1:A:330:PRO:HD3	1.81	0.45
2:B:918:LYS:HE2	2:B:1326:TYR:OH	2.17	0.45
2:B:979:LYS:HD3	2:B:1015:PHE:CE1	2.52	0.45
2:B:1576:GLU:O	2:B:1577:LYS:HB2	2.17	0.45
1:A:109:PHE:CZ	1:A:594:ILE:HG23	2.51	0.44
1:A:501:THR:HB	1:A:538:VAL:HG13	1.99	0.44
2:B:1154:LEU:O	2:B:1158:TYR:HB2	2.17	0.44
1:A:330:PRO:O	1:A:357:PRO:HD3	2.17	0.44
1:A:596:ASP:O	1:A:600:LYS:HG2	2.16	0.44
2:B:1041:SER:O	2:B:1042:SER:HB2	2.18	0.44
2:B:1582:MET:HA	2:B:1605:TRP:O	2.16	0.44
2:B:853:LEU:HD12	2:B:860:HIS:CE1	2.52	0.44
2:B:1278:LEU:HD23	2:B:1308:PHE:HB3	2.00	0.44
3:C:56:LEU:HD23	3:C:56:LEU:O	2.17	0.44
1:A:465:ILE:HB	1:A:486:ARG:HH11	1.83	0.44
2:B:1437:LEU:C	2:B:1437:LEU:HD12	2.43	0.44
3:C:117:THR:HG22	3:C:118:ASN:CG	2.42	0.44
2:B:1278:LEU:HD12	2:B:1281:ARG:HG3	2.00	0.44
2:B:1360:ASN:OD1	2:B:1361:THR:N	2.51	0.44
1:A:350:LEU:CD2	1:A:400:ILE:HG21	2.48	0.44
2:B:1401:ASN:O	2:B:1403:VAL:HG12	2.18	0.44
1:A:624:PHE:O	1:A:631:GLN:HA	2.18	0.43
2:B:779:THR:OG1	2:B:802:THR:HG22	2.17	0.43
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.48	0.43
1:A:110:ILE:HB	1:A:198:THR:OG1	2.19	0.43
1:A:456:ARG:HA	6:A:1646:GOL:O3	2.18	0.43
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.19	0.43
1:A:363:TYR:CZ	1:A:364:ARG:HG3	2.53	0.43
2:B:1051:ALA:HA	2:B:1052:PRO:HD3	1.92	0.43
2:B:1066:LEU:HD23	2:B:1066:LEU:O	2.18	0.43
2:B:1540:ILE:HD12	2:B:1540:ILE:N	2.33	0.43
3:C:12:THR:C	3:C:35:ARG:HD3	2.44	0.43
1:A:84:VAL:HG13	1:A:101:VAL:HG21	2.00	0.43
2:B:1390:ALA:HA	2:B:1391:PRO:HD3	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1507:LEU:HD11	2:B:1629:ALA:HB3	2.00	0.43
1:A:422:LEU:HA	1:A:423:PRO:HD3	1.90	0.43
2:B:910:VAL:HG13	2:B:911:PRO:HD2	2.01	0.43
2:B:1543:ILE:HG13	2:B:1554:VAL:HG21	1.99	0.43
2:B:1565:PRO:HB2	2:B:1567:LYS:HG2	2.00	0.43
3:C:56:LEU:C	3:C:58:PRO:HD3	2.44	0.43
1:A:10:ASN:HB3	1:A:635:ARG:HD3	2.01	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.80	0.42
2:B:1342:LYS:HB2	2:B:1367:CYS:HB2	2.01	0.42
3:C:19:TRP:N	3:C:19:TRP:CE3	2.87	0.42
2:B:1404:ASP:HB3	2:B:1427:ASP:HB2	2.00	0.42
2:B:1565:PRO:HG2	2:B:1568:CYS:SG	2.59	0.42
2:B:1021:GLN:O	2:B:1025:GLU:HG2	2.19	0.42
2:B:1472:HIS:CG	2:B:1473:PRO:HD2	2.55	0.42
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.54	0.42
1:A:119:PRO:HG2	1:A:179:MET:HE1	2.00	0.42
1:A:220:PHE:HB3	1:A:357:PRO:HG2	2.00	0.42
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.84	0.42
1:A:453:PHE:HB2	1:A:493:VAL:CG2	2.49	0.42
2:B:1281:ARG:HH11	2:B:1285:ILE:HD11	1.85	0.42
2:B:1348:ALA:HA	2:B:1349:PRO:HD3	1.92	0.42
1:A:248:PHE:HB2	1:A:307:THR:HB	2.02	0.42
2:B:1391:PRO:HD2	2:B:1419:ARG:CD	2.50	0.42
3:C:135:GLU:O	3:C:187:CYS:HB2	2.19	0.42
1:A:166:VAL:O	1:A:168:PRO:HD3	2.19	0.42
1:A:553:PRO:HB3	2:B:773:LEU:CD1	2.50	0.42
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.55	0.42
2:B:804:MET:HG2	2:B:805:GLN:N	2.35	0.42
3:C:65:ARG:HA	3:C:66:PRO:HD3	1.79	0.42
3:C:126:VAL:CG2	3:C:152:PHE:HB2	2.50	0.42
2:B:984:THR:HA	2:B:985:PRO:HD3	1.92	0.42
1:A:333:ILE:HG23	1:A:352:VAL:HG13	2.01	0.41
1:A:372:GLU:HB3	1:A:375:VAL:HG23	2.02	0.41
2:B:1612:GLU:O	2:B:1616:GLN:HG2	2.20	0.41
1:A:547:GLN:NE2	1:A:559:MET:HG3	2.35	0.41
1:A:408:GLU:CG	1:A:409:LEU:HD12	2.49	0.41
2:B:1405:ARG:NH1	2:B:1405:ARG:CG	2.73	0.41
2:B:829:LEU:N	2:B:829:LEU:HD12	2.36	0.41
2:B:836:GLN:C	2:B:868:PRO:HG3	2.45	0.41
2:B:1401:ASN:O	2:B:1402:GLY:C	2.62	0.41
2:B:894:VAL:HG22	2:B:899:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:MET:HG2	1:A:456:ARG:HD3	2.02	0.41
2:B:975:ALA:HB2	2:B:1011:GLN:HB3	2.03	0.41
3:C:9:ARG:O	3:C:9:ARG:HG2	2.20	0.41
1:A:210:PHE:O	1:A:317:VAL:HG21	2.20	0.41
1:A:541:LEU:HG	2:B:796:ALA:HB2	2.03	0.41
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.20	0.41
3:C:129:LEU:HA	3:C:130:PRO:HD3	1.97	0.41
1:A:21:VAL:HG21	1:A:471:LEU:HD23	2.02	0.41
1:A:295:GLU:CD	1:A:295:GLU:H	2.29	0.41
2:B:1065:SER:O	2:B:1068:VAL:HG22	2.21	0.41
2:B:1582:MET:HE3	2:B:1606:VAL:HG22	2.02	0.41
3:C:87:GLU:O	3:C:90:VAL:HG22	2.20	0.41
3:C:195:PRO:HG3	3:C:238:TRP:CD1	2.56	0.41
3:C:238:TRP:O	3:C:239:ARG:HD2	2.21	0.41
2:B:1504:LYS:HB3	2:B:1504:LYS:NZ	2.36	0.41
2:B:1621:GLN:O	2:B:1625:GLN:HG2	2.20	0.41
1:A:110:ILE:HD13	1:A:184:ILE:HG22	2.03	0.40
1:A:510:VAL:HG11	1:A:622:LEU:CD1	2.51	0.40
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	2.04	0.40
2:B:1343:VAL:HG22	2:B:1366:ILE:HG12	2.03	0.40
3:C:56:LEU:HD23	3:C:56:LEU:C	2.45	0.40
3:C:214:ARG:HG2	3:C:232:VAL:HG22	2.03	0.40
1:A:473:MET:SD	1:A:622:LEU:HD21	2.62	0.40
2:B:1278:LEU:HD23	2:B:1308:PHE:CB	2.52	0.40
4:D:3:BMA:O3	4:D:6:BMA:H61	2.22	0.40
1:A:581:PHE:HA	1:A:584:ASN:O	2.21	0.40
2:B:752:ASN:HD21	6:B:2643:GOL:H31	1.86	0.40
2:B:927:PRO:HB3	2:B:1313:GLU:HA	2.02	0.40
2:B:1505:VAL:HA	2:B:1509:GLU:OE1	2.20	0.40
2:B:1527:LEU:HD21	2:B:1530:VAL:HG22	2.04	0.40
2:B:1221:LEU:O	2:B:1222:LYS:HB2	2.22	0.40
1:A:427:VAL:HB	1:A:523:GLU:HG3	2.03	0.40
2:B:744:GLU:HG3	3:C:69:HIS:HB3	2.03	0.40
2:B:852:SER:HB3	2:B:878:ILE:HG22	2.02	0.40
2:B:1473:PRO:O	2:B:1474:GLU:HB2	2.21	0.40
3:C:33:LYS:HA	3:C:43:ASN:OD1	2.22	0.40
3:C:239:ARG:HA	3:C:240:PRO:HA	1.85	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	A	636/645 (99%)	617 (97%)	18 (3%)	1 (0%)	43	68
2	B	890/915 (97%)	866 (97%)	22 (2%)	2 (0%)	43	68
3	C	243/277 (88%)	227 (93%)	15 (6%)	1 (0%)	30	54
All	All	1769/1837 (96%)	1710 (97%)	55 (3%)	4 (0%)	43	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1115	ASN
1	A	209	SER
2	B	1114	ASN
3	C	145	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/567 (100%)	554 (98%)	10 (2%)	51	78
2	B	793/810 (98%)	782 (99%)	11 (1%)	59	82
3	C	214/240 (89%)	212 (99%)	2 (1%)	70	87
All	All	1571/1617 (97%)	1548 (98%)	23 (2%)	57	81

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	46	VAL
1	A	94	VAL
1	A	193	GLN
1	A	243	VAL
1	A	408	GLU
1	A	439	LEU
1	A	510	VAL
1	A	564	GLU
1	A	583	LEU
2	B	907	LEU
2	B	935	VAL
2	B	1149	LYS
2	B	1163	ARG
2	B	1334	LEU
2	B	1405	ARG
2	B	1440	LYS
2	B	1502	ASP
2	B	1504	LYS
2	B	1578	LYS
2	B	1613	ASP
3	C	19	TRP
3	C	26	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	GLN
1	A	547	GLN
2	B	834	GLN
2	B	836	GLN
2	B	967	GLN
2	B	1076	GLN
2	B	1186	ASN
2	B	1204	GLN
2	B	1237	GLN
2	B	1472	HIS
3	C	151	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 ⓘ

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	0.52	0	17,19,21	0.86	0
4	NAG	D	2	4	14,14,15	0.75	0	17,19,21	1.26	3 (17%)
4	BMA	D	3	4	11,11,12	0.80	0	15,15,17	1.48	1 (6%)
4	BMA	D	4	4	11,11,12	0.63	0	15,15,17	1.14	2 (13%)
4	BMA	D	5	4	11,11,12	0.62	0	15,15,17	1.01	1 (6%)
4	BMA	D	6	4	11,11,12	0.55	0	15,15,17	0.91	1 (6%)

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	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	BMA	D	4	4	-	1/2/19/22	0/1/1/1
4	BMA	D	5	4	-	0/2/19/22	0/1/1/1
4	BMA	D	6	4	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	BMA	C1-C2-C3	4.49	116.18	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C4-C3-C2	2.90	115.27	111.02
4	D	4	BMA	C1-C2-C3	-2.68	105.74	109.64
4	D	5	BMA	C1-O5-C5	-2.59	108.71	112.19
4	D	6	BMA	C1-O5-C5	2.36	115.35	112.19
4	D	2	NAG	C2-N2-C7	-2.32	119.79	122.90
4	D	2	NAG	O5-C5-C4	-2.20	105.47	110.83
4	D	4	BMA	C3-C4-C5	2.08	114.00	110.23

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	4	BMA	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

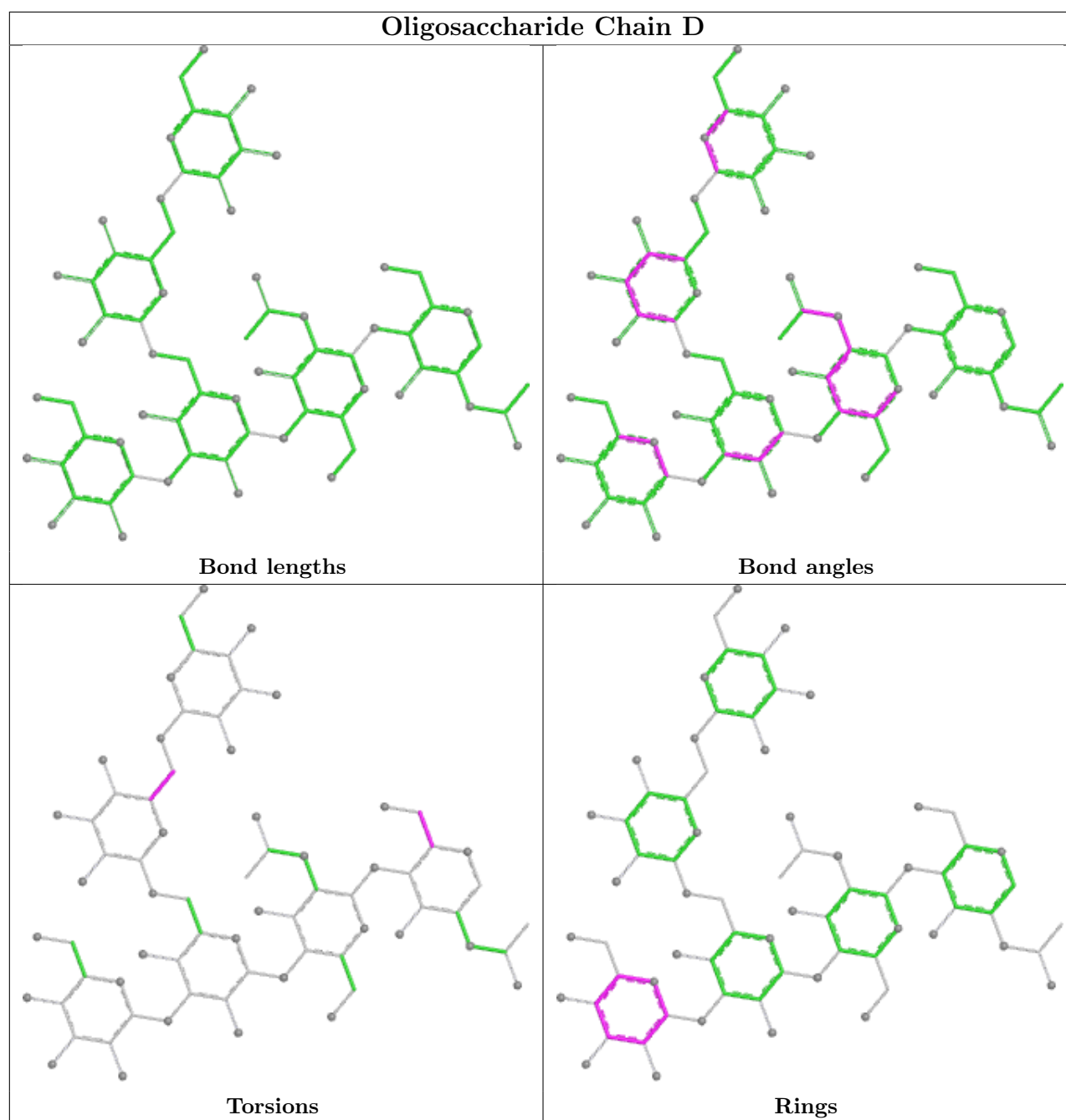
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	6	BMA	3	0
4	D	1	NAG	1	0
4	D	3	BMA	3	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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
6	GOL	A	1646	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	B	2644	-	5,5,5	0.38	0	5,5,5	0.31	0
6	GOL	B	2645	-	5,5,5	0.39	0	5,5,5	0.33	0
6	GOL	A	1645	-	5,5,5	0.38	0	5,5,5	0.33	0
6	GOL	B	2649	-	5,5,5	0.37	0	5,5,5	0.29	0
6	GOL	B	2643	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	B	2646	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	C	1248	-	5,5,5	0.38	0	5,5,5	0.29	0
6	GOL	B	2642	-	5,5,5	0.38	0	5,5,5	0.32	0
6	GOL	B	2653	-	5,5,5	0.37	0	5,5,5	0.32	0
6	GOL	B	2648	-	5,5,5	0.38	0	5,5,5	0.34	0
6	GOL	B	2647	-	5,5,5	0.37	0	5,5,5	0.32	0
6	GOL	B	2650	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	B	2652	-	5,5,5	0.37	0	5,5,5	0.31	0
7	NAG	B	2655	2	14,14,15	0.52	0	17,19,21	0.73	1 (5%)
6	GOL	B	2651	-	5,5,5	0.37	0	5,5,5	0.31	0
6	GOL	B	2654	-	5,5,5	0.38	0	5,5,5	0.31	0
6	GOL	A	1644	-	5,5,5	0.38	0	5,5,5	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	1646	-	-	2/4/4/4	-
6	GOL	B	2644	-	-	2/4/4/4	-
6	GOL	B	2645	-	-	2/4/4/4	-
6	GOL	A	1645	-	-	2/4/4/4	-
6	GOL	B	2649	-	-	2/4/4/4	-
6	GOL	B	2643	-	-	2/4/4/4	-
6	GOL	B	2646	-	-	2/4/4/4	-
6	GOL	C	1248	-	-	2/4/4/4	-
6	GOL	B	2642	-	-	2/4/4/4	-
6	GOL	B	2653	-	-	2/4/4/4	-
6	GOL	B	2648	-	-	2/4/4/4	-
6	GOL	B	2647	-	-	2/4/4/4	-
6	GOL	B	2650	-	-	2/4/4/4	-
6	GOL	B	2652	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	2655	2	-	3/6/23/26	0/1/1/1
6	GOL	B	2651	-	-	2/4/4/4	-
6	GOL	B	2654	-	-	2/4/4/4	-
6	GOL	A	1644	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2655	NAG	C1-O5-C5	2.33	115.31	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1644	GOL	C1-C2-C3-O3
6	A	1645	GOL	C1-C2-C3-O3
6	A	1646	GOL	C1-C2-C3-O3
6	B	2642	GOL	C1-C2-C3-O3
6	B	2643	GOL	C1-C2-C3-O3
6	B	2646	GOL	C1-C2-C3-O3
6	B	2647	GOL	C1-C2-C3-O3
6	B	2651	GOL	C1-C2-C3-O3
6	B	2651	GOL	O2-C2-C3-O3
6	B	2652	GOL	C1-C2-C3-O3
6	B	2653	GOL	C1-C2-C3-O3
6	B	2654	GOL	C1-C2-C3-O3
6	C	1248	GOL	C1-C2-C3-O3
7	B	2655	NAG	C1-C2-N2-C7
7	B	2655	NAG	C8-C7-N2-C2
7	B	2655	NAG	O7-C7-N2-C2
6	B	2643	GOL	O2-C2-C3-O3
6	B	2644	GOL	C1-C2-C3-O3
6	B	2645	GOL	C1-C2-C3-O3
6	B	2648	GOL	C1-C2-C3-O3
6	B	2649	GOL	C1-C2-C3-O3
6	B	2650	GOL	C1-C2-C3-O3
6	A	1645	GOL	O2-C2-C3-O3
6	A	1646	GOL	O2-C2-C3-O3
6	B	2646	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	B	2647	GOL	O2-C2-C3-O3
6	B	2649	GOL	O2-C2-C3-O3
6	B	2654	GOL	O2-C2-C3-O3
6	C	1248	GOL	O2-C2-C3-O3
6	A	1644	GOL	O2-C2-C3-O3
6	B	2642	GOL	O2-C2-C3-O3
6	B	2644	GOL	O2-C2-C3-O3
6	B	2645	GOL	O2-C2-C3-O3
6	B	2648	GOL	O2-C2-C3-O3
6	B	2650	GOL	O2-C2-C3-O3
6	B	2652	GOL	O2-C2-C3-O3
6	B	2653	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1646	GOL	1	0
6	B	2649	GOL	3	0
6	B	2643	GOL	1	0
6	B	2646	GOL	1	0
6	B	2653	GOL	2	0
6	B	2652	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	640/645 (99%)	0.21	17 (2%) 56 53	29, 55, 98, 146	0
2	B	896/915 (97%)	0.30	37 (4%) 41 37	29, 62, 115, 161	0
3	C	245/277 (88%)	1.17	40 (16%) 4 4	45, 79, 175, 204	0
All	All	1781/1837 (96%)	0.39	94 (5%) 32 28	29, 61, 121, 204	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	140	VAL	5.9
3	C	247	ALA	5.4
3	C	141	SER	4.8
3	C	207	ILE	4.3
3	C	67	CYS	4.3
2	B	1416	PHE	4.2
3	C	14	ILE	4.1
2	B	1349	PRO	3.9
3	C	226	SER	3.8
2	B	1113	ASN	3.7
3	C	142	SER	3.4
3	C	44	ILE	3.3
2	B	1502	ASP	3.3
2	B	1419	ARG	3.3
3	C	149	GLU	3.2
3	C	204	SER	3.2
1	A	312	SER	3.1
3	C	143	ALA	3.1
3	C	31	ILE	3.1
3	C	19	TRP	3.1
3	C	50	LYS	3.0
2	B	1415	ALA	3.0
2	B	913	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	1403	VAL	3.0
3	C	15	LEU	3.0
3	C	227	GLU	2.9
1	A	103	LEU	2.9
3	C	243	SER	2.9
2	B	1594	PRO	2.8
3	C	34	CYS	2.8
1	A	73	GLU	2.8
3	C	68	GLY	2.8
3	C	21	ASP	2.8
2	B	1224	PHE	2.8
2	B	851	CYS	2.7
1	A	407	GLN	2.7
1	A	70	ALA	2.7
3	C	208	ILE	2.6
3	C	144	MET	2.6
3	C	229	GLY	2.6
1	A	464	LYS	2.6
2	B	1473	PRO	2.6
1	A	290	GLN	2.6
3	C	234	THR	2.6
2	B	1276	LEU	2.6
1	A	289	VAL	2.5
1	A	78	LYS	2.5
2	B	1515	CYS	2.5
2	B	1410	TYR	2.5
2	B	1504	LYS	2.4
1	A	72	ARG	2.4
2	B	1428	LYS	2.4
3	C	222	GLY	2.4
2	B	1501	SER	2.4
3	C	176	ASP	2.4
3	C	23	THR	2.4
2	B	1402	GLY	2.4
1	A	439	LEU	2.3
2	B	737	GLU	2.3
1	A	91	GLY	2.3
3	C	51	GLY	2.3
1	A	374	THR	2.3
3	C	201	SER	2.3
3	C	27	GLY	2.3
3	C	139	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	1342	LYS	2.3
2	B	1203	LYS	2.2
2	B	1359	LYS	2.2
3	C	25	PRO	2.2
3	C	147	ASP	2.2
2	B	850	PHE	2.2
2	B	802	THR	2.2
3	C	148	ARG	2.2
2	B	1418	ASP	2.2
3	C	17	GLY	2.2
3	C	28	THR	2.2
3	C	56	LEU	2.2
2	B	1417	SER	2.2
2	B	1445	PHE	2.1
3	C	13	GLU	2.1
1	A	521	GLN	2.1
1	A	473	MET	2.1
2	B	1376	ALA	2.1
2	B	1390	ALA	2.1
1	A	605	CYS	2.1
1	A	485	VAL	2.1
2	B	1138	GLU	2.1
2	B	1492	ALA	2.1
2	B	1500	LYS	2.0
2	B	945	LEU	2.0
2	B	1444	TYR	2.0
2	B	1414	LYS	2.0
3	C	30	ALA	2.0
2	B	910	VAL	2.0

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

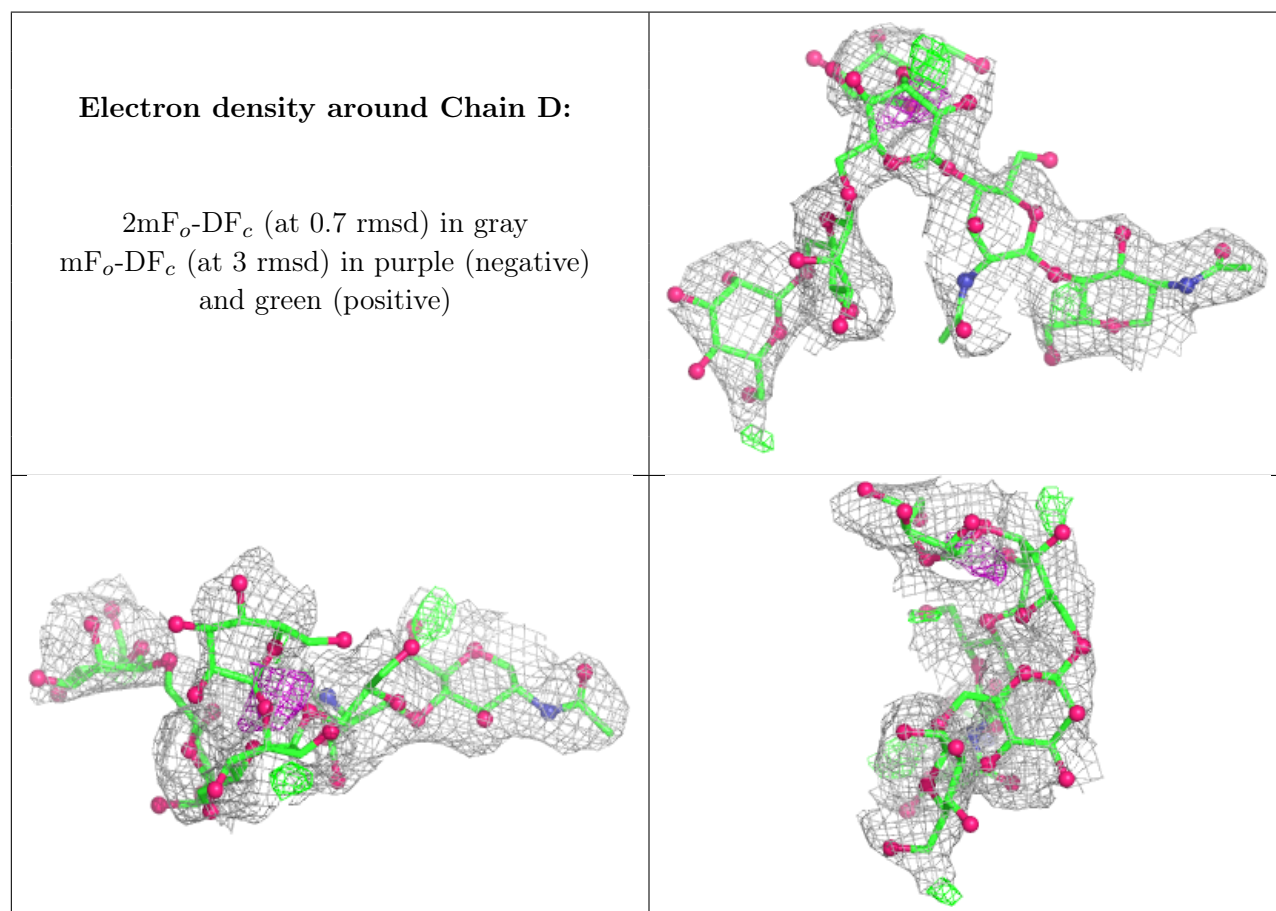
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	D	3	11/12	0.30	0.16	157,162,165,166	0
4	BMA	D	5	11/12	0.38	0.11	134,143,148,150	0
4	BMA	D	4	11/12	0.39	0.13	144,155,158,160	0
4	BMA	D	6	11/12	0.43	0.14	140,151,162,164	0
4	NAG	D	2	14/15	0.70	0.14	109,119,136,148	0
4	NAG	D	1	14/15	0.89	0.12	48,65,90,94	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
6	GOL	B	2651	6/6	0.64	0.14	105,114,116,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	2655	14/15	0.68	0.15	106,124,140,140	0
6	GOL	B	2649	6/6	0.77	0.24	77,85,92,93	0
6	GOL	C	1248	6/6	0.79	0.20	69,84,85,91	0
6	GOL	B	2650	6/6	0.79	0.16	88,106,110,110	0
6	GOL	B	2647	6/6	0.80	0.22	63,74,80,80	0
6	GOL	B	2652	6/6	0.80	0.18	80,94,101,103	0
6	GOL	A	1646	6/6	0.83	0.17	61,74,76,78	0
6	GOL	A	1644	6/6	0.83	0.20	73,81,86,90	0
5	CA	A	1643	1/1	0.85	0.11	63,63,63,63	0
6	GOL	A	1645	6/6	0.85	0.20	116,119,123,125	0
6	GOL	B	2645	6/6	0.86	0.20	72,88,92,94	0
6	GOL	B	2648	6/6	0.86	0.18	72,89,100,104	0
6	GOL	B	2643	6/6	0.88	0.17	44,74,77,77	0
6	GOL	B	2646	6/6	0.89	0.21	91,99,101,110	0
6	GOL	B	2654	6/6	0.89	0.17	79,84,88,98	0
6	GOL	B	2644	6/6	0.91	0.15	61,73,79,81	0
6	GOL	B	2642	6/6	0.92	0.16	68,77,79,82	0
6	GOL	B	2653	6/6	0.93	0.15	63,72,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.