



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:42 PM UTC

PDB ID : 7BAG / pdb_00007bag
Title : C3b in complex with CP40
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Deposited on : 2020-12-15
Resolution : 2.00 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

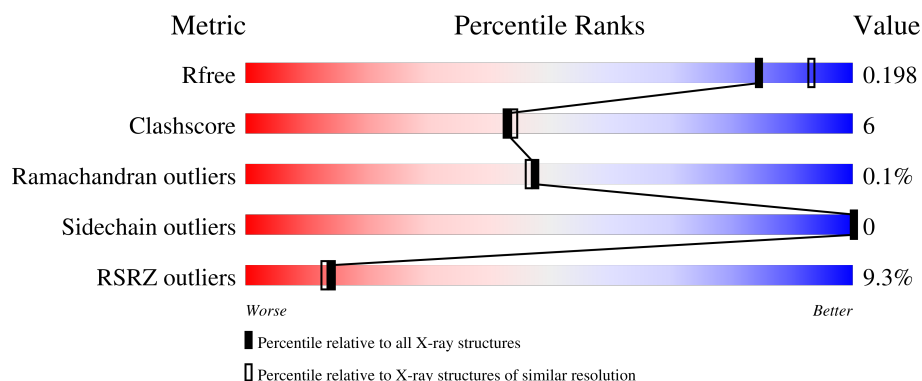
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	8% 87% 12%
2	B	915	9% 88% 11%
3	C	14	21% 71% 21% 7%
4	D	2	50% 50%

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
6	PEG	B	1703	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13417 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.

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 C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	915	Total	C	N	O	S	851	0	0
			7307	4626	1231	1412	38			

- Molecule 3 is a protein called Compstatin CP40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	S	0	0	0
			125	83	22	18	2			

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

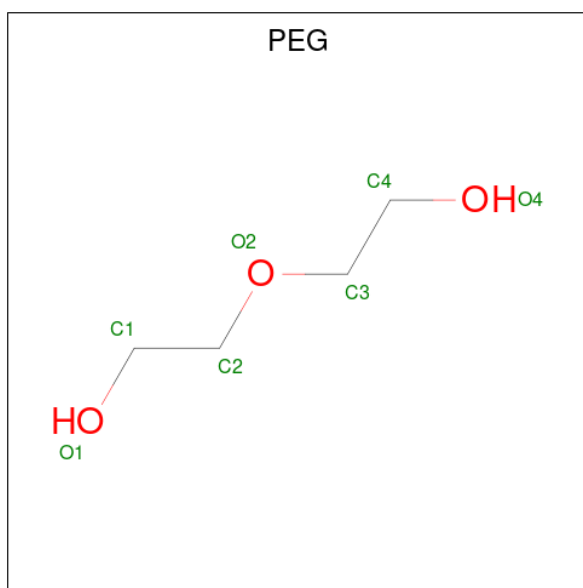


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			27	16	2	9			

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

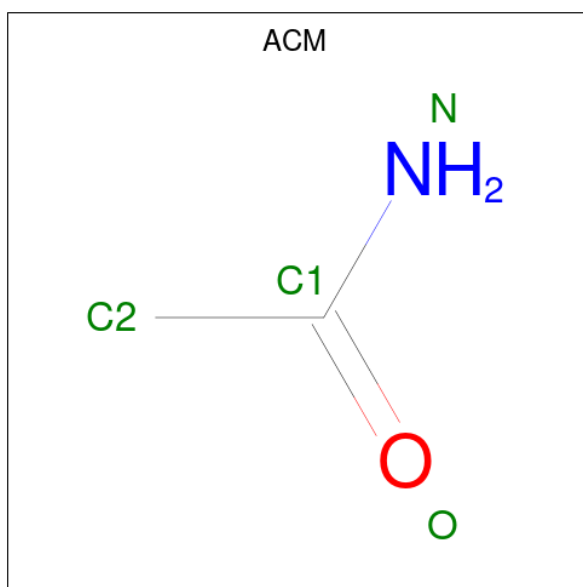
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



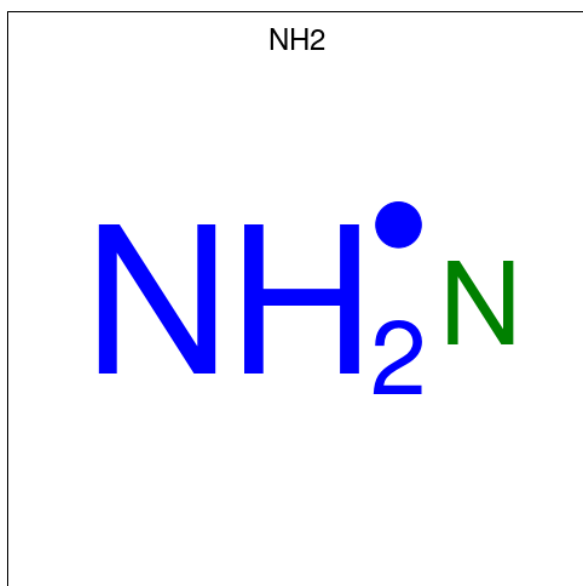
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is ACETAMIDE (CCD ID: ACM) (formula: C_2H_5NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 8 is AMINO GROUP (CCD ID: NH2) (formula: H₂N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	N	0	0
			1	1		

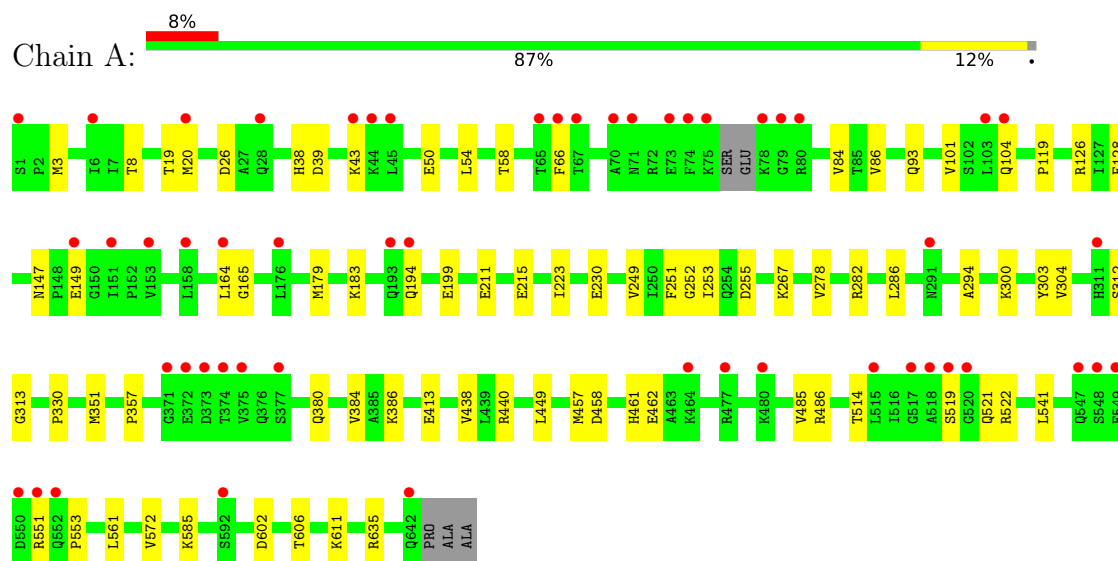
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	422	Total 422	O 422	0	0
9	B	499	Total 499	O 499	0	0
9	C	4	Total 4	O 4	0	0

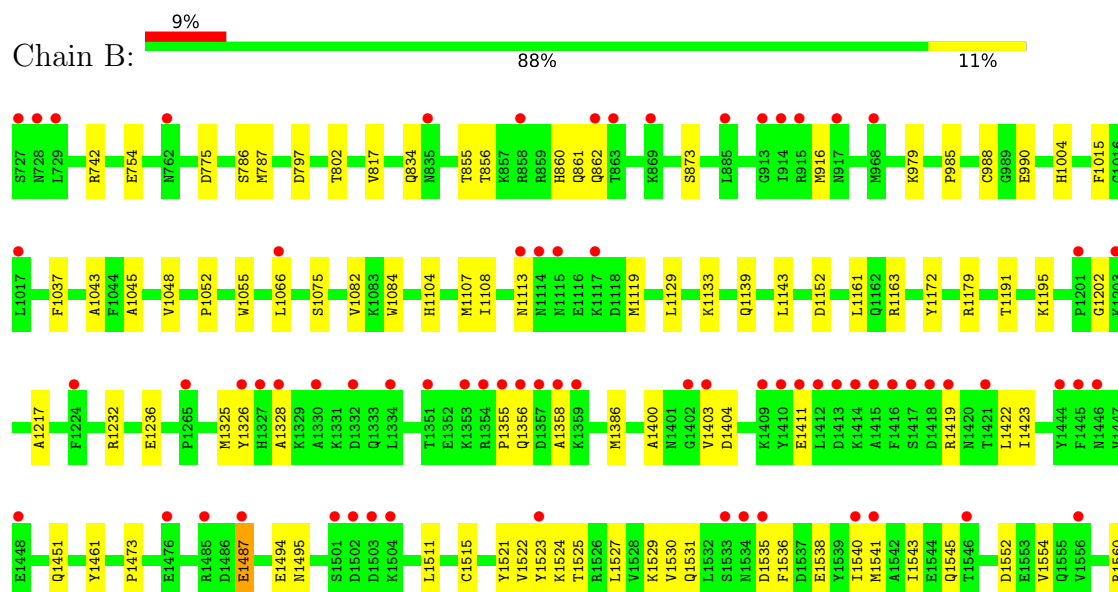
3 Residue-property plots

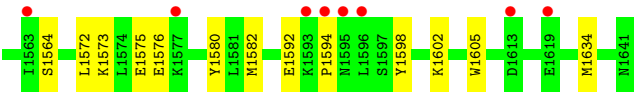
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

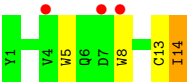


• Molecule 2: Complement C3





● Molecule 3: Compstatin CP40



● Molecule 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.51Å 90.53Å 140.09Å 90.00° 108.84° 90.00°	Depositor
Resolution (Å)	47.82 – 2.00 47.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.82-2.00) 98.1 (47.82-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.194 , 0.225 0.197 , 0.198	Depositor DCC
R_{free} test set	7878 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13417	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: EXL, SAR, PEG, NH2, ACM, CA, DTY, NAG, IML

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	0.19	0/5092	0.46	0/6917
2	B	0.19	0/7453	0.44	2/10092 (0.0%)
3	C	0.22	0/84	0.77	0/110
All	All	0.19	0/12629	0.45	2/17119 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1487	GLU	CA-CB-CG	-6.21	101.68	114.10
2	B	1325	MET	CG-SD-CE	-6.12	87.43	100.90

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	65	0
2	B	7307	0	7228	79	0
3	C	125	0	103	2	0
4	D	27	0	23	1	0
5	A	1	0	0	0	0
6	A	14	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	21	0	30	10	0
7	B	4	0	3	0	0
8	C	1	0	0	0	0
9	A	422	0	0	18	2
9	B	499	0	0	22	2
9	C	4	0	0	0	0
All	All	13417	0	12462	143	2

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 6.

All (143) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ASP:OD1	9:A:801:HOH:O	1.84	0.95
2:B:1461:TYR:OH	9:B:1801:HOH:O	1.81	0.95
6:B:1703:PEG:O4	9:B:1802:HOH:O	1.93	0.86
1:A:215:GLU:OE2	9:A:802:HOH:O	1.96	0.81
1:A:58:THR:OG1	9:A:803:HOH:O	1.98	0.81
2:B:1048:VAL:O	9:B:1803:HOH:O	1.97	0.81
1:A:282:ARG:HH11	6:A:702:PEG:H21	1.47	0.80
1:A:20:MET:HE3	1:A:66:PHE:HZ	1.47	0.78
2:B:754:GLU:OE2	9:B:1805:HOH:O	2.01	0.76
1:A:300:LYS:NZ	9:A:807:HOH:O	2.06	0.76
2:B:861:GLN:NE2	9:B:1814:HOH:O	2.19	0.75
1:A:635:ARG:O	9:A:805:HOH:O	2.05	0.75
1:A:26:ASP:O	9:A:806:HOH:O	2.06	0.74
1:A:458:ASP:OD1	1:A:461:HIS:ND1	2.20	0.74
2:B:797:ASP:OD1	9:B:1806:HOH:O	2.07	0.72
1:A:19:THR:HG21	4:D:1:NAG:H82	1.73	0.71
1:A:249:VAL:HG11	1:A:278:VAL:HG11	1.73	0.70
1:A:20:MET:HE3	1:A:66:PHE:CZ	2.26	0.69
1:A:119:PRO:HG3	1:A:179:MET:HE1	1.75	0.69
2:B:1403:VAL:HA	9:B:1804:HOH:O	1.92	0.68
2:B:1529:LYS:HD3	2:B:1540:ILE:HD12	1.74	0.68
2:B:1202:GLY:O	9:B:1807:HOH:O	2.10	0.67
2:B:1564:SER:OG	9:B:1808:HOH:O	2.13	0.67
1:A:458:ASP:CG	1:A:461:HIS:HD1	2.03	0.66
2:B:1404:ASP:N	9:B:1804:HOH:O	2.00	0.66
2:B:1400:ALA:O	9:B:1809:HOH:O	2.15	0.64
1:A:611:LYS:NZ	9:A:820:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:HG3	1:A:199:GLU:HG2	1.79	0.64
2:B:1511:LEU:HD22	2:B:1634:MET:HE2	1.80	0.64
2:B:1521:TYR:HB2	2:B:1523:TYR:CE2	2.32	0.64
1:A:438:VAL:HG13	1:A:449:LEU:HD11	1.78	0.63
2:B:1523:TYR:CD1	2:B:1543:ILE:HD12	2.33	0.63
1:A:521:GLN:OE1	1:A:521:GLN:N	2.27	0.62
2:B:1515:CYS:SG	2:B:1634:MET:HE1	2.40	0.62
2:B:1602:LYS:HD3	6:B:1703:PEG:H21	1.81	0.61
2:B:1163:ARG:NH2	9:B:1812:HOH:O	2.33	0.61
2:B:1525:THR:HB	2:B:1541:MET:HG3	1.83	0.60
2:B:1356:GLN:HG2	2:B:1358:ALA:H	1.67	0.60
2:B:1494:GLU:HB2	6:B:1703:PEG:H12	1.83	0.60
2:B:1560:ARG:HG2	2:B:1598:TYR:HE1	1.67	0.60
1:A:351:MET:HE3	1:A:440:ARG:HD2	1.84	0.59
2:B:1522:VAL:C	2:B:1523:TYR:HD2	2.10	0.59
2:B:1552:ASP:O	9:B:1811:HOH:O	2.17	0.59
2:B:1530:VAL:HG23	2:B:1576:GLU:HG3	1.84	0.58
1:A:8:THR:HG22	1:A:20:MET:HG2	1.86	0.58
1:A:211:GLU:OE2	9:A:809:HOH:O	2.17	0.57
2:B:1580:TYR:OH	9:B:1810:HOH:O	2.16	0.57
2:B:817:VAL:HB	9:B:2028:HOH:O	2.03	0.57
2:B:856:THR:OG1	6:B:1703:PEG:H22	2.07	0.55
2:B:1531:GLN:HB2	2:B:1538:GLU:HB2	1.88	0.55
1:A:3:MET:SD	1:A:522:ARG:HG2	2.48	0.54
2:B:1113:ASN:O	9:B:1812:HOH:O	2.18	0.54
1:A:313:GLY:HA3	2:B:1423:ILE:HD11	1.89	0.53
1:A:585:LYS:NZ	9:A:813:HOH:O	2.24	0.53
2:B:1326:TYR:CE2	2:B:1328:ALA:HB2	2.43	0.53
1:A:485:VAL:HG22	9:A:804:HOH:O	2.07	0.53
2:B:1043:ALA:HB2	2:B:1084:TRP:CD2	2.43	0.53
2:B:1045:ALA:HB2	2:B:1052:PRO:HA	1.90	0.53
2:B:1004:HIS:HB2	2:B:1066:LEU:HD21	1.91	0.52
2:B:1104:HIS:O	2:B:1107:MET:HG2	2.09	0.52
1:A:54:LEU:HA	9:A:803:HOH:O	2.10	0.52
1:A:267:LYS:NZ	9:A:830:HOH:O	2.43	0.51
1:A:514:THR:OG1	1:A:522:ARG:HD2	2.11	0.51
2:B:1191:THR:OG1	9:B:1813:HOH:O	2.19	0.51
1:A:147:ASN:ND2	1:A:149:GLU:OE1	2.44	0.50
1:A:351:MET:HE2	1:A:384:VAL:HG11	1.93	0.50
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	1.94	0.49
2:B:990:GLU:OE1	2:B:1104:HIS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1386:MET:SD	2:B:1473:PRO:HD3	2.53	0.49
1:A:351:MET:HE1	9:A:931:HOH:O	2.13	0.49
1:A:462:GLU:OE2	1:A:486:ARG:NH2	2.33	0.49
1:A:255:ASP:HB2	1:A:300:LYS:HD3	1.95	0.48
1:A:286:LEU:HD12	6:A:702:PEG:H32	1.95	0.48
1:A:457:MET:O	3:C:8:TRP:NE1	2.38	0.48
2:B:1411:GLU:OE2	2:B:1422:LEU:HA	2.13	0.48
1:A:413:GLU:OE2	9:A:810:HOH:O	2.20	0.48
2:B:856:THR:HG23	6:B:1703:PEG:H11	1.94	0.48
2:B:1523:TYR:HD1	2:B:1543:ILE:HD12	1.76	0.48
2:B:834:GLN:NE2	9:B:1815:HOH:O	2.20	0.48
2:B:1560:ARG:HG2	2:B:1598:TYR:CE1	2.47	0.48
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.95	0.47
6:A:702:PEG:C1	9:A:812:HOH:O	2.62	0.47
1:A:215:GLU:HG2	9:A:802:HOH:O	2.14	0.47
1:A:50:GLU:HG3	1:A:66:PHE:HB3	1.96	0.47
1:A:252:GLY:HA3	1:A:303:TYR:CZ	2.50	0.47
2:B:1524:LYS:HB3	2:B:1545:GLN:HB3	1.97	0.47
1:A:253:ILE:HD11	1:A:300:LYS:HD2	1.96	0.47
2:B:862:GLN:HB2	9:B:1840:HOH:O	2.15	0.47
1:A:330:PRO:O	1:A:357:PRO:HD3	2.14	0.46
1:A:104:GLN:CD	1:A:194:GLN:NE2	2.74	0.46
2:B:1133:LYS:HA	2:B:1143:LEU:HD21	1.98	0.46
2:B:1487:GLU:H	2:B:1487:GLU:HG3	1.31	0.46
2:B:1133:LYS:HE2	9:B:2218:HOH:O	2.16	0.45
2:B:1592:GLU:HG3	2:B:1594:PRO:HD2	1.97	0.45
1:A:553:PRO:HD2	2:B:802:THR:O	2.17	0.45
1:A:380:GLN:HG2	1:A:384:VAL:O	2.17	0.45
1:A:606:THR:C	6:A:703:PEG:H31	2.43	0.44
2:B:1573:LYS:HG2	6:B:1702:PEG:H41	1.99	0.44
2:B:742:ARG:HB3	2:B:775:ASP:HB3	2.00	0.44
1:A:38:HIS:HB3	1:A:43:LYS:HA	2.00	0.44
1:A:164:LEU:O	2:B:787:MET:HG2	2.18	0.44
2:B:1419:ARG:HA	2:B:1419:ARG:HD2	1.80	0.43
2:B:1495:ASN:H	6:B:1703:PEG:H31	1.83	0.43
2:B:1163:ARG:CZ	9:B:1812:HOH:O	2.66	0.43
2:B:1195:LYS:HE2	2:B:1195:LYS:HB3	1.87	0.43
2:B:1055:TRP:CE2	2:B:1108:ILE:HG22	2.54	0.43
1:A:128:PHE:HA	1:A:165:GLY:O	2.18	0.43
2:B:1535:ASP:HB3	2:B:1536:PHE:CD1	2.53	0.43
2:B:1075:SER:HB3	2:B:1139:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1704:PEG:H31	6:B:1704:PEG:H12	1.55	0.43
1:A:126:ARG:CZ	1:A:572:VAL:HB	2.48	0.43
2:B:1572:LEU:O	2:B:1573:LYS:HE2	2.18	0.43
2:B:1582:MET:HA	2:B:1605:TRP:O	2.20	0.42
1:A:551:ARG:NH1	1:A:553:PRO:HA	2.34	0.42
2:B:916:MET:HG3	2:B:1328:ALA:HB3	2.02	0.42
2:B:1232:ARG:O	2:B:1236:GLU:OE1	2.37	0.42
3:C:13:CYS:HA	3:C:14:IML:HN1	1.57	0.42
2:B:985:PRO:HG3	9:B:2086:HOH:O	2.20	0.42
1:A:93:GLN:CD	9:A:834:HOH:O	2.63	0.42
2:B:1543:ILE:HG13	2:B:1554:VAL:HG21	2.02	0.42
1:A:20:MET:HE1	1:A:86:VAL:CG2	2.50	0.41
1:A:255:ASP:CG	1:A:300:LYS:HE2	2.44	0.41
1:A:351:MET:HE3	1:A:440:ARG:CD	2.49	0.41
2:B:979:LYS:HD3	2:B:1015:PHE:CZ	2.54	0.41
2:B:1152:ASP:OD1	2:B:1179:ARG:NH2	2.31	0.41
1:A:312:SER:HB2	2:B:873:SER:HB2	2.01	0.41
2:B:1119:MET:HG3	2:B:1161:LEU:HD21	2.01	0.41
2:B:1172:TYR:HA	2:B:1217:ALA:HB2	2.01	0.41
2:B:855:THR:HB	6:B:1703:PEG:H42	2.02	0.41
1:A:20:MET:HG3	1:A:66:PHE:HE1	1.85	0.41
1:A:561:LEU:HD23	1:A:561:LEU:HA	1.97	0.41
2:B:1541:MET:HE3	2:B:1582:MET:SD	2.61	0.41
2:B:1495:ASN:N	6:B:1703:PEG:H31	2.36	0.41
1:A:39:ASP:OD2	1:A:39:ASP:N	2.52	0.41
1:A:230:GLU:OE2	9:A:811:HOH:O	2.22	0.41
1:A:386:LYS:HD2	1:A:440:ARG:HG2	2.03	0.41
2:B:1527:LEU:HD23	2:B:1575:GLU:C	2.46	0.41
1:A:438:VAL:CG1	1:A:449:LEU:HD11	2.46	0.40
2:B:860:HIS:HE1	2:B:1451:GLN:OE1	2.04	0.40
1:A:84:VAL:HG13	1:A:101:VAL:HG21	2.03	0.40
1:A:223:ILE:HG13	1:A:294:ALA:HB1	2.03	0.40
1:A:251:PHE:CD2	1:A:304:VAL:HG22	2.57	0.40
2:B:988:CYS:HA	2:B:1037:PHE:CZ	2.57	0.40

All (2) 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)
9:A:835:HOH:O	9:B:2131:HOH:O[1_655]	2.13	0.07
9:A:1196:HOH:O	9:B:2264:HOH:O[2_455]	2.19	0.01

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%)	628 (99%)	7 (1%)	1 (0%)	43	42
2	B	913/915 (100%)	881 (96%)	31 (3%)	1 (0%)	48	46
3	C	10/14 (71%)	10 (100%)	0	0	100	100
All	All	1559/1574 (99%)	1519 (97%)	38 (2%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	519	SER
2	B	1355	PRO

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%)	564 (100%)	0	100	100
2	B	810/810 (100%)	810 (100%)	0	100	100
3	C	9/9 (100%)	9 (100%)	0	100	100
All	All	1383/1386 (100%)	1383 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	144	ASN
1	A	194	GLN
1	A	258	GLN
1	A	558	GLN
1	A	587	ASN
2	B	860	HIS
2	B	1104	HIS
2	B	1186	ASN
2	B	1237	GLN
2	B	1255	GLN
2	B	1555	GLN
2	B	1616	GLN
2	B	1621	GLN
2	B	1625	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	SAR	C	9	3	3,4,5	1.27	0	1,3,5	1.58	0
3	IML	C	14	3,8	7,8,9	0.59	0	6,9,11	2.25	1 (16%)
3	EXL	C	5	3	15,16,17	1.52	2 (13%)	17,22,24	1.07	1 (5%)

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
3	SAR	C	9	3	-	1/1/2/3	-
3	IML	C	14	3,8	-	4/8/10/12	-
3	EXL	C	5	3	-	1/5/6/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	EXL	C16-N02	-3.17	1.33	1.38
3	C	5	EXL	C11-C04	-3.06	1.39	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	IML	CB-CA-C	-5.12	105.75	112.77
3	C	5	EXL	C15-C16-N02	2.03	132.68	129.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5	EXL	O-C-CA-C05
3	C	9	SAR	C-CA-N-CN
3	C	14	IML	CA-CB-CG1-CD1
3	C	14	IML	CG2-CB-CG1-CD1
3	C	14	IML	N-CA-CB-CG1
3	C	14	IML	N-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	14	IML	1	0

5.5 Carbohydrates [i](#)

2 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	0.23	0	17,19,21	0.42	0
4	NAG	D	2	4	13,13,15	0.36	0	12,17,21	0.43	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	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/19/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

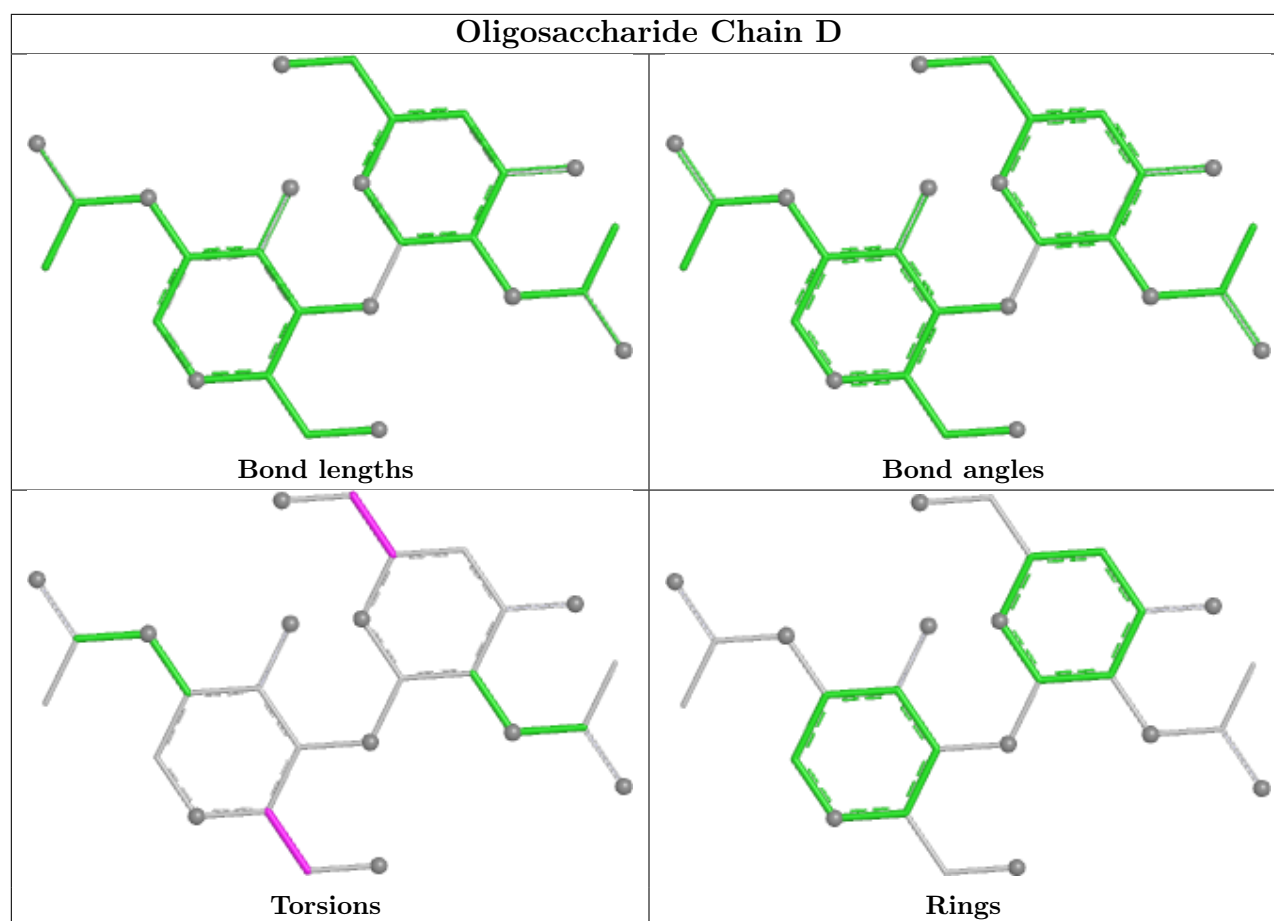
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic and 1 is modelled with single atom - leaving 6 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	ACM	B	1701	2	3,3,3	1.46	1 (33%)	3,3,3	0.81	0
6	PEG	A	703	-	6,6,6	0.49	0	5,5,5	0.35	0
6	PEG	B	1703	-	6,6,6	0.50	0	5,5,5	0.37	0
6	PEG	A	702	-	6,6,6	0.54	0	5,5,5	0.33	0
6	PEG	B	1704	-	6,6,6	0.51	0	5,5,5	0.30	0
6	PEG	B	1702	-	6,6,6	0.50	0	5,5,5	0.24	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	PEG	A	703	-	-	3/4/4/4	-
6	PEG	B	1703	-	-	3/4/4/4	-
6	PEG	A	702	-	-	2/4/4/4	-
6	PEG	B	1704	-	-	1/4/4/4	-
6	PEG	B	1702	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1701	ACM	C1-N	2.13	1.42	1.32

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1704	PEG	C1-C2-O2-C3
6	A	702	PEG	O1-C1-C2-O2
6	A	702	PEG	O2-C3-C4-O4
6	B	1703	PEG	O2-C3-C4-O4
6	A	703	PEG	O2-C3-C4-O4
6	B	1702	PEG	O2-C3-C4-O4
6	B	1703	PEG	C1-C2-O2-C3
6	A	703	PEG	C1-C2-O2-C3
6	B	1702	PEG	O1-C1-C2-O2
6	B	1702	PEG	C1-C2-O2-C3
6	A	703	PEG	O1-C1-C2-O2
6	B	1703	PEG	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	PEG	1	0
6	B	1703	PEG	8	0
6	A	702	PEG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1704	PEG	1	0
6	B	1702	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	640/645 (99%)	0.45	52 (8%)	18 17	27, 49, 88, 169	0
2	B	805/915 (87%)	0.46	80 (9%)	13 11	28, 50, 97, 185	0
3	C	10/14 (71%)	1.43	3 (30%)	1 1	69, 77, 91, 108	0
All	All	1455/1574 (92%)	0.46	135 (9%)	14 13	27, 50, 93, 185	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1417	SER	7.5
2	B	1358	ALA	7.1
2	B	913	GLY	6.9
1	A	374	THR	6.4
2	B	1416	PHE	6.3
1	A	550	ASP	6.1
1	A	103	LEU	5.7
1	A	519	SER	5.6
1	A	551	ARG	5.1
2	B	1265	PRO	5.0
1	A	75	LYS	4.9
2	B	1334	LEU	4.8
2	B	1403	VAL	4.8
2	B	1445	PHE	4.7
2	B	1357	ASP	4.7
2	B	1355	PRO	4.5
2	B	1410	TYR	4.4
2	B	1540	ILE	4.4
1	A	518	ALA	4.4
2	B	917	ASN	4.3
2	B	1448	GLU	4.3
1	A	371	GLY	4.1
2	B	1415	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	1351	THR	4.1
2	B	1419	ARG	4.0
1	A	104	GLN	4.0
1	A	548	SER	4.0
1	A	74	PHE	3.9
2	B	968	MET	3.8
1	A	66	PHE	3.7
1	A	1	SER	3.6
2	B	727	SER	3.6
2	B	1114	ASN	3.5
2	B	1359	LYS	3.5
2	B	1418	ASP	3.4
2	B	1353	LYS	3.4
1	A	70	ALA	3.3
1	A	158	LEU	3.3
1	A	78	LYS	3.3
2	B	1501	SER	3.3
2	B	1413	ASP	3.3
2	B	914	ILE	3.2
2	B	728	ASN	3.2
2	B	1113	ASN	3.2
1	A	20	MET	3.2
2	B	762	ASN	3.2
2	B	1523	TYR	3.1
1	A	43	LYS	3.1
1	A	547	GLN	3.1
1	A	28	GLN	3.1
1	A	642	GLN	3.1
1	A	153	VAL	3.1
1	A	45	LEU	3.1
2	B	1326	TYR	3.0
1	A	149	GLU	3.0
2	B	858	ARG	3.0
2	B	1595	ASN	3.0
1	A	372	GLU	2.9
1	A	176	LEU	2.9
2	B	1594	PRO	2.9
2	B	1414	LYS	2.9
2	B	1017	LEU	2.8
2	B	1354	ARG	2.8
2	B	729	LEU	2.8
2	B	1546	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	2.8
2	B	1356	GLN	2.8
2	B	1421	THR	2.8
2	B	1593	LYS	2.7
2	B	1066	LEU	2.7
2	B	1444	TYR	2.7
1	A	194	GLN	2.7
2	B	1115	ASN	2.7
2	B	1503	ASP	2.7
2	B	1596	LEU	2.7
2	B	835	ASN	2.7
2	B	862	GLN	2.7
2	B	1412	LEU	2.6
2	B	1556	VAL	2.6
2	B	869	LYS	2.6
3	C	4	VAL	2.6
2	B	1487	GLU	2.6
2	B	1203	LYS	2.6
2	B	1613	ASP	2.6
2	B	1541	MET	2.5
2	B	915	ARG	2.5
1	A	549	GLU	2.4
1	A	73	GLU	2.4
1	A	151	ILE	2.4
2	B	1502	ASP	2.4
2	B	1402	GLY	2.4
2	B	1224	PHE	2.4
2	B	1485	ARG	2.4
2	B	1327	HIS	2.4
1	A	377	SER	2.4
2	B	1577	LYS	2.3
2	B	1563	ILE	2.3
1	A	67	THR	2.3
2	B	1534	ASN	2.3
3	C	7	ASP	2.3
1	A	65	THR	2.3
1	A	373	ASP	2.3
1	A	515	LEU	2.3
1	A	6	ILE	2.2
2	B	1201	PRO	2.2
1	A	44	LYS	2.2
2	B	1535	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	ASN	2.2
2	B	1446	ASN	2.2
2	B	1332	ASP	2.2
1	A	79	GLY	2.2
2	B	1330	ALA	2.2
2	B	1476	GLU	2.2
1	A	464	LYS	2.2
2	B	1504	LYS	2.2
1	A	164	LEU	2.2
2	B	863	THR	2.2
1	A	520	GLY	2.1
3	C	8	TRP	2.1
2	B	1328	ALA	2.1
1	A	592	SER	2.1
1	A	291	ASN	2.1
2	B	1619	GLU	2.1
1	A	193	GLN	2.1
1	A	552	GLN	2.1
1	A	311	HIS	2.1
1	A	480	LYS	2.1
2	B	885	LEU	2.1
2	B	1411	GLU	2.1
1	A	477	ARG	2.1
1	A	517	GLY	2.1
1	A	80	ARG	2.0
2	B	1117	LYS	2.0
2	B	1533	SER	2.0
2	B	1409	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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.

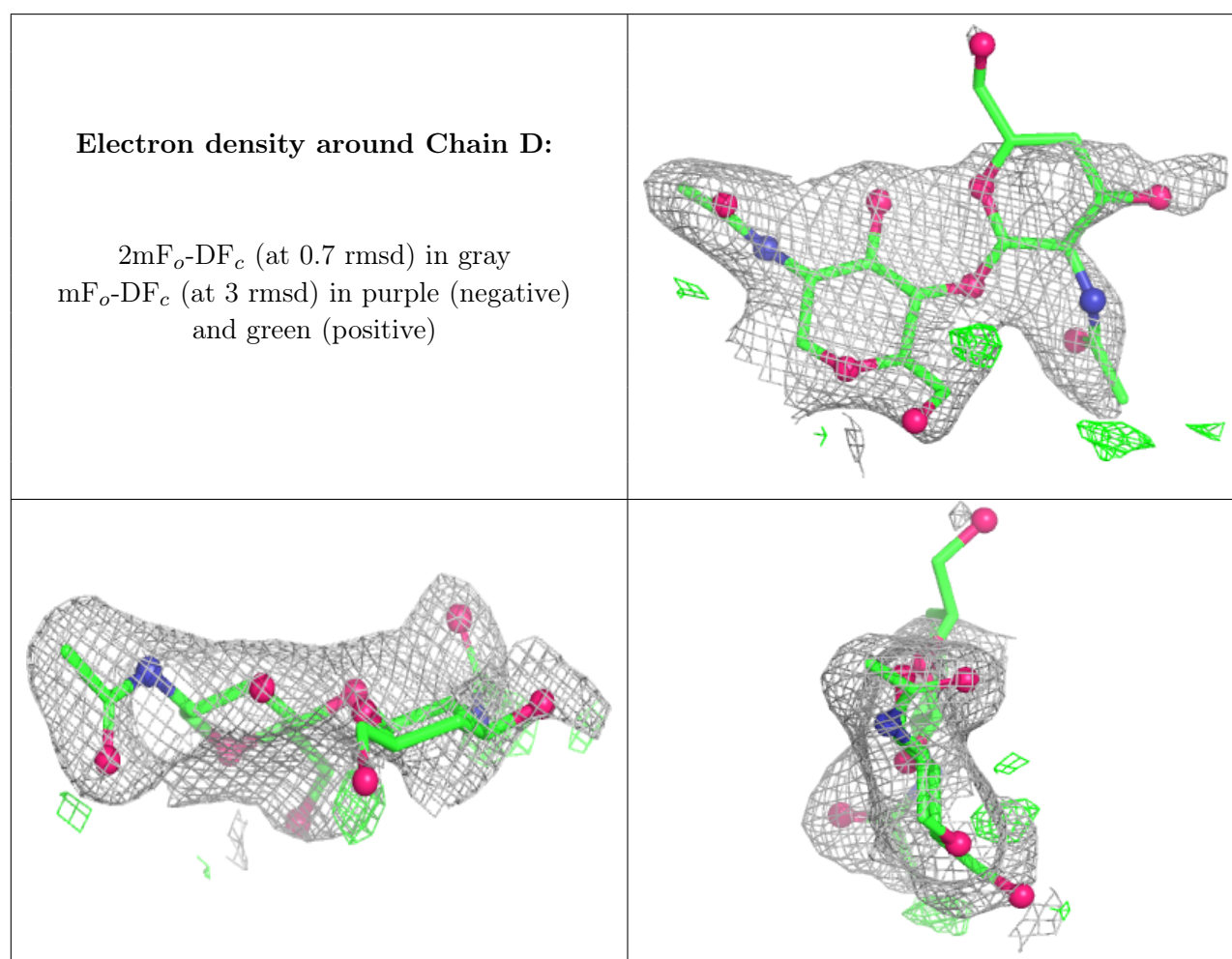
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IML	C	14	9/10	0.66	0.28	85,101,109,120	0
3	DTY	C	1	12/13	0.87	0.15	70,78,92,95	0
3	SAR	C	9	5/6	0.90	0.14	80,81,85,87	0
3	EXL	C	5	15/16	0.92	0.12	70,74,80,84	0

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	2	13/15	0.60	0.18	94,105,111,112	0
4	NAG	D	1	14/15	0.88	0.12	49,78,94,98	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	PEG	A	703	7/7	0.76	0.25	49,67,74,85	0
8	NH2	C	101	1/1	0.83	0.23	93,93,93,93	0
6	PEG	B	1704	7/7	0.86	0.23	36,43,66,83	0
6	PEG	B	1702	7/7	0.86	0.16	42,57,68,80	0
6	PEG	A	702	7/7	0.91	0.16	37,56,68,87	0
6	PEG	B	1703	7/7	0.94	0.12	38,57,61,64	0
7	ACM	B	1701	4/4	0.95	0.09	49,49,53,55	0
5	CA	A	701	1/1	0.98	0.13	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.