



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:22 PM UTC

PDB ID : 7OP0 / pdb_00007op0
Title : Crystal structure of complement C5 in complex with chemically synthesized K92 knob domain.
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Deposited on : 2021-05-28
Resolution : 2.57 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

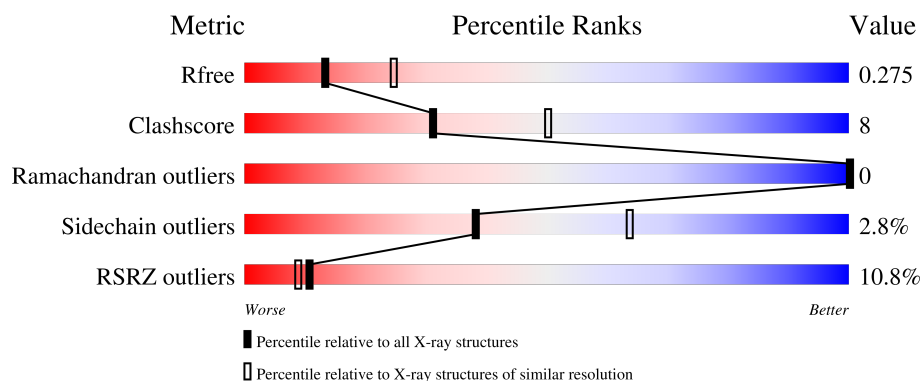
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	999	9% 78% 19% ..
2	B	657	11% 76% 21% ..
3	C	35	37% 66% 29% 6%
4	D	2	100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13067 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 C5 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	972	Total	C	N	O	S	0	0	0
			7665	4898	1275	1451	41			

- Molecule 2 is a protein called Complement C5 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	647	Total	C	N	O	S	0	0	0
			5080	3258	807	1003	12			

- Molecule 3 is a protein called K92chemFE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	S	0	0	0
			257	162	44	47	4			

- 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
			28	16	2	10				

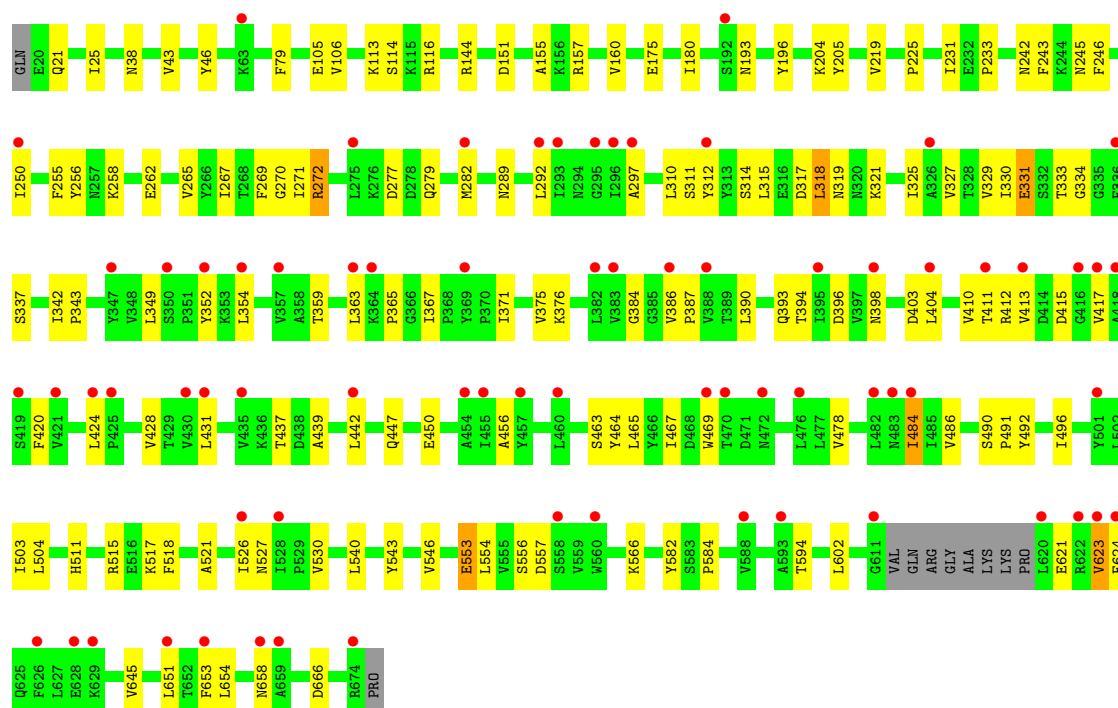
- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



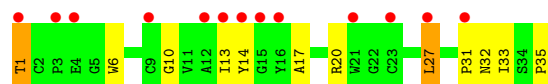
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	9	Total	O	0	0
			9	9		



• Molecule 3: K92chemFE



• 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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.84Å 104.82Å 155.06Å 90.00° 125.13° 90.00°	Depositor
Resolution (Å)	56.67 – 2.57 56.67 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (56.67-2.57) 99.8 (56.67-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5, PHENIX 1.18_3845	Depositor
R, R_{free}	0.231 , 0.264 0.243 , 0.275	Depositor DCC
R_{free} test set	4272 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.5	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13067	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: EDO, 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	0.14	0/7820	0.36	1/10597 (0.0%)
2	B	0.13	0/5198	0.36	0/7079
3	C	0.18	0/267	0.46	0/364
All	All	0.14	0/13285	0.37	1/18040 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1518	LYS	CB-CA-C	-9.65	105.44	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	7665	0	7656	122	0
2	B	5080	0	4940	88	0
3	C	257	0	225	9	0
4	D	28	0	25	0	0
5	A	8	0	12	1	0
6	A	20	0	0	1	0
6	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13067	0	12858	213	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 8.

All (213) 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:363:LEU:HB2	2:B:456:ALA:HA	1.54	0.89
1:A:701:ASP:OD2	1:A:1446:VAL:HG23	1.83	0.77
2:B:116:ARG:NH2	2:B:666:ASP:OD2	2.25	0.70
2:B:160:VAL:HG22	2:B:175:GLU:HG2	1.73	0.70
1:A:1013:MET:HE3	1:A:1287:THR:HB	1.74	0.70
3:C:33:ILE:HG12	3:C:35:PRO:HD2	1.75	0.67
1:A:718:ILE:HD13	1:A:1446:VAL:HG12	1.75	0.67
1:A:942:VAL:HB	1:A:957:LYS:HD3	1.76	0.66
3:C:20:ARG:HB3	3:C:31:PRO:HB3	1.77	0.66
1:A:1383:THR:HG21	1:A:1511:THR:HA	1.78	0.64
1:A:854:GLN:HB3	1:A:917:TRP:CD1	2.33	0.63
1:A:955:ARG:NH1	1:A:1350:THR:O	2.30	0.63
1:A:1316:SER:HB3	1:A:1322:ALA:HA	1.80	0.63
2:B:437:THR:HB	2:B:447:GLN:HB3	1.81	0.63
3:C:27:LEU:HB2	3:C:31:PRO:HB2	1.80	0.63
2:B:543:TYR:HB3	2:B:556:SER:HB3	1.82	0.62
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.83	0.61
1:A:858:LYS:HB2	1:A:881:SER:HB2	1.81	0.60
1:A:1401:ARG:HA	1:A:1478:ARG:HA	1.82	0.60
1:A:1577:TYR:OH	1:A:1602:LYS:NZ	2.33	0.60
2:B:272:ARG:NH1	2:B:343:PRO:O	2.34	0.60
1:A:1516:ILE:HG13	1:A:1518:LYS:H	1.68	0.59
2:B:546:VAL:HG22	2:B:553:GLU:HG2	1.85	0.58
2:B:113:LYS:HG2	2:B:654:LEU:HD23	1.85	0.58
1:A:1520:CYS:SG	6:A:1818:HOH:O	2.57	0.58
2:B:196:TYR:HA	2:B:219:VAL:HG23	1.86	0.58
1:A:718:ILE:HD11	1:A:720:LEU:HB2	1.84	0.58
2:B:504:LEU:HD21	2:B:651:LEU:HD11	1.84	0.58
1:A:1625:LEU:HD22	1:A:1636:ILE:HD11	1.84	0.58
1:A:1578:LYS:HG2	1:A:1599:THR:HG22	1.86	0.58
2:B:242:ASN:ND2	2:B:245:ASN:O	2.36	0.58
2:B:503:ILE:HB	2:B:511:HIS:HB3	1.84	0.58
2:B:354:LEU:HD23	2:B:375:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ILE:HD12	1:A:719:SER:H	1.70	0.57
2:B:393:GLN:HA	2:B:403:ASP:HA	1.86	0.57
1:A:1531:ASP:HA	1:A:1641:SER:HB3	1.87	0.56
1:A:823:VAL:HA	1:A:846:TYR:O	2.05	0.56
2:B:144:ARG:NH2	2:B:602:LEU:O	2.36	0.56
2:B:384:GLY:HA3	2:B:413:VAL:HA	1.89	0.55
2:B:225:PRO:HG2	2:B:255:PHE:HE2	1.71	0.55
1:A:721:GLY:O	1:A:725:ILE:HG13	2.07	0.55
2:B:325:ILE:HB	2:B:342:ILE:HG22	1.89	0.54
2:B:386:VAL:H	2:B:411:THR:HB	1.72	0.54
2:B:557:ASP:HA	2:B:645:VAL:HG21	1.90	0.54
1:A:739:ARG:HA	1:A:742:ILE:HG12	1.89	0.54
2:B:265:VAL:O	2:B:289:ASN:ND2	2.33	0.54
1:A:857:VAL:HA	1:A:913:SER:O	2.08	0.53
2:B:105:GLU:HG3	2:B:114:SER:HB3	1.90	0.53
1:A:1567:SER:HA	1:A:1613:LYS:HE2	1.90	0.53
2:B:25:ILE:HD13	2:B:106:VAL:HG11	1.90	0.53
1:A:718:ILE:HG21	1:A:725:ILE:HG12	1.91	0.53
1:A:1310:SER:HA	1:A:1328:MET:O	2.08	0.53
1:A:752:LEU:HA	1:A:755:LYS:HB2	1.91	0.53
1:A:708:ASP:OD2	1:A:1476:ARG:HD2	2.08	0.53
1:A:1288:GLN:O	1:A:1292:ASN:ND2	2.36	0.53
2:B:269:PHE:HD2	2:B:325:ILE:HG12	1.74	0.53
2:B:490:SER:OG	2:B:491:PRO:O	2.27	0.53
3:C:1:THR:HG23	3:C:35:PRO:HB3	1.91	0.52
2:B:231:ILE:HD11	2:B:327:VAL:HG12	1.91	0.52
2:B:478:VAL:HG11	2:B:566:LYS:HD2	1.92	0.52
1:A:1118:PHE:CG	1:A:1148:THR:HG21	2.45	0.52
1:A:1267:VAL:HA	1:A:1270:VAL:HG12	1.91	0.51
2:B:319:ASN:OD1	2:B:349:LEU:N	2.43	0.51
2:B:314:SER:OG	2:B:317:ASP:OD1	2.29	0.51
1:A:985:GLY:HA2	1:A:988:LEU:HB2	1.93	0.51
2:B:292:LEU:HD23	2:B:297:ALA:HB2	1.92	0.51
1:A:1386:ILE:HD11	1:A:1399:TYR:HB2	1.92	0.51
2:B:365:PRO:HG2	2:B:464:TYR:CZ	2.47	0.50
2:B:465:LEU:HD11	2:B:486:VAL:HG23	1.93	0.50
2:B:384:GLY:HA2	2:B:411:THR:HG22	1.92	0.50
3:C:6:TRP:HZ3	3:C:33:ILE:HB	1.75	0.50
2:B:21:GLN:HB3	2:B:46:TYR:CZ	2.47	0.50
2:B:250:ILE:HD11	2:B:265:VAL:HG11	1.94	0.49
1:A:1625:LEU:HB2	1:A:1636:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:GLN:OE1	1:A:917:TRP:NE1	2.39	0.49
1:A:1398:ASP:OD1	1:A:1398:ASP:N	2.45	0.49
2:B:439:ALA:HB3	2:B:442:LEU:HB2	1.94	0.49
1:A:946:PRO:HA	1:A:955:ARG:HG2	1.94	0.49
2:B:331:GLU:OE2	2:B:333:THR:N	2.44	0.49
2:B:155:ALA:HB1	2:B:157:ARG:HG3	1.93	0.49
2:B:484:ILE:HD13	2:B:540:LEU:HD21	1.94	0.49
1:A:1105:LEU:HA	1:A:1108:VAL:HG22	1.95	0.49
1:A:977:LEU:HD21	1:A:1315:VAL:HG21	1.94	0.49
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.47	0.49
1:A:818:LYS:O	2:B:582:TYR:N	2.44	0.49
1:A:1187:THR:HA	1:A:1190:ILE:HG22	1.94	0.49
2:B:225:PRO:HG2	2:B:255:PHE:CE2	2.47	0.49
1:A:1624:ALA:HB2	1:A:1637:TYR:CD2	2.47	0.48
1:A:1047:LYS:O	1:A:1051:GLU:HG2	2.13	0.48
1:A:861:ALA:HB1	1:A:865:ILE:HB	1.95	0.48
2:B:318:LEU:HA	2:B:321:LYS:HD3	1.96	0.48
1:A:1423:VAL:HG22	1:A:1463:GLN:HG2	1.95	0.48
2:B:393:GLN:HG2	2:B:403:ASP:HB3	1.96	0.48
1:A:840:GLN:HG3	1:A:897:THR:HG23	1.95	0.48
1:A:1053:MET:HG3	1:A:1089:VAL:HG11	1.96	0.48
1:A:1317:TYR:CE2	1:A:1342:LEU:HB2	2.49	0.48
1:A:1111:TYR:CE1	1:A:1121:ASN:HB3	2.49	0.47
2:B:262:GLU:HA	2:B:292:LEU:O	2.14	0.47
2:B:469:TRP:HB3	2:B:484:ILE:HG22	1.96	0.47
2:B:243:PHE:CD1	2:B:315:LEU:HD13	2.49	0.47
2:B:396:ASP:OD2	2:B:398:ASN:ND2	2.41	0.47
1:A:1119:LYS:HD3	1:A:1120:GLU:H	1.79	0.47
3:C:17:ALA:HB1	3:C:35:PRO:C	2.40	0.47
1:A:923:LEU:HD21	1:A:925:LYS:HE3	1.97	0.47
2:B:526:ILE:HD12	2:B:527:ASN:H	1.80	0.47
2:B:352:TYR:HA	2:B:376:LYS:O	2.15	0.47
1:A:1316:SER:HA	1:A:1323:LEU:H	1.80	0.46
1:A:715:ALA:O	1:A:718:ILE:HG22	2.14	0.46
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.50	0.46
2:B:271:ILE:HG21	2:B:318:LEU:HD22	1.97	0.46
1:A:780:VAL:HG13	1:A:784:LYS:HB2	1.97	0.46
1:A:1427:SER:HB3	1:A:1459:HIS:CE1	2.50	0.46
1:A:792:ASP:HA	2:B:584:PRO:HB3	1.98	0.46
1:A:936:ARG:HA	1:A:936:ARG:HD3	1.59	0.46
1:A:1314:ASP:OD2	1:A:1316:SER:OG	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1548:ARG:NH1	1:A:1646:GLU:OE1	2.48	0.46
2:B:371:ILE:O	2:B:420:PHE:HB2	2.15	0.46
2:B:415:ASP:HB3	2:B:417:VAL:HG23	1.98	0.46
2:B:359:THR:O	2:B:359:THR:OG1	2.31	0.46
2:B:387:PRO:HB3	2:B:410:VAL:HA	1.98	0.46
1:A:718:ILE:CD1	1:A:1446:VAL:HG12	2.46	0.46
1:A:752:LEU:HD12	1:A:755:LYS:HB3	1.98	0.45
2:B:484:ILE:H	2:B:484:ILE:HG13	1.69	0.45
1:A:846:TYR:HE1	2:B:256:TYR:HA	1.81	0.45
1:A:1008:ALA:HB2	1:A:1059:TYR:CD2	2.51	0.45
1:A:1058:SER:OG	2:B:193:ASN:O	2.24	0.45
1:A:1080:ALA:HB1	1:A:1148:THR:HA	1.99	0.45
1:A:1166:THR:O	1:A:1169:ILE:HG13	2.16	0.45
2:B:43:VAL:HG23	2:B:79:PHE:HB3	1.97	0.45
1:A:1329:THR:HG23	1:A:1332:ASN:H	1.79	0.45
2:B:25:ILE:O	2:B:653:PHE:HA	2.16	0.45
1:A:1415:SER:HG	1:A:1417:SER:HG	1.64	0.45
2:B:424:LEU:HD12	2:B:428:VAL:HG21	1.98	0.45
1:A:961:TYR:CZ	1:A:1343:ASN:HB3	2.51	0.45
1:A:1612:VAL:HB	1:A:1615:ARG:HD2	1.99	0.45
2:B:412:ARG:HB2	2:B:417:VAL:HB	1.98	0.45
1:A:1097:GLN:NE2	1:A:1158:ILE:O	2.46	0.45
1:A:1083:LEU:HD13	1:A:1104:LEU:HD23	1.99	0.44
1:A:1548:ARG:HD3	1:A:1644:TRP:CH2	2.53	0.44
2:B:267:ILE:HG22	2:B:327:VAL:HB	1.98	0.44
1:A:796:THR:HG22	1:A:818:LYS:HG3	2.00	0.44
1:A:853:MET:HE2	1:A:853:MET:HB3	1.76	0.44
1:A:1051:GLU:HG2	1:A:1051:GLU:H	1.57	0.44
2:B:311:SER:OG	2:B:312:TYR:N	2.50	0.44
1:A:1047:LYS:HA	1:A:1047:LYS:HD3	1.76	0.44
2:B:621:GLU:OE2	2:B:623:VAL:HG13	2.16	0.44
1:A:1133:LEU:HD22	1:A:1415:SER:HB2	1.98	0.44
2:B:363:LEU:HD21	2:B:431:LEU:HB2	1.99	0.44
2:B:386:VAL:O	2:B:411:THR:OG1	2.32	0.44
2:B:233:PRO:HB2	2:B:246:PHE:CZ	2.53	0.44
2:B:442:LEU:O	2:B:447:GLN:NE2	2.51	0.44
1:A:779:LEU:HG	1:A:781:PRO:HD3	1.99	0.44
1:A:1037:ASP:HB3	1:A:1040:ILE:HG12	2.01	0.43
1:A:1402:ILE:HG13	1:A:1479:ILE:HD13	1.99	0.43
2:B:543:TYR:CD1	2:B:554:LEU:HD23	2.53	0.43
1:A:1317:TYR:CE1	1:A:1342:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:GLU:OE1	1:A:685:GLU:N	2.47	0.43
1:A:1142:LEU:HD11	1:A:1179:THR:HG22	1.99	0.43
2:B:515:ARG:HE	2:B:526:ILE:HD13	1.83	0.43
1:A:1565:ILE:HD13	1:A:1579:ALA:HB2	2.00	0.43
1:A:1426:ILE:HG12	1:A:1493:PHE:CD1	2.54	0.43
1:A:1426:ILE:HB	1:A:1460:VAL:HG13	2.01	0.42
2:B:518:PHE:HB2	2:B:521:ALA:HB3	2.00	0.42
1:A:893:SER:H	2:B:258:LYS:NZ	2.17	0.42
1:A:937:GLU:HG2	1:A:1364:VAL:HG22	2.01	0.42
1:A:718:ILE:HD12	1:A:719:SER:N	2.34	0.42
3:C:10:GLY:O	3:C:14:TYR:HB2	2.19	0.42
1:A:795:THR:O	1:A:819:VAL:HG22	2.19	0.42
1:A:1234:HIS:CE1	1:A:1235:LYS:HE3	2.54	0.42
1:A:1317:TYR:CZ	1:A:1342:LEU:HB2	2.54	0.42
1:A:1213:LYS:HE3	1:A:1266:TYR:CZ	2.54	0.42
2:B:277:ASP:OD2	2:B:279:GLN:HG2	2.19	0.42
1:A:854:GLN:HB3	1:A:917:TRP:NE1	2.34	0.42
1:A:1231:ASN:ND2	1:A:1236:ASP:HB3	2.34	0.42
1:A:1020:TYR:OH	1:A:1295:GLU:OE1	2.38	0.42
1:A:1518:LYS:O	1:A:1607:THR:HG21	2.19	0.42
1:A:1066:TYR:HB3	1:A:1078:LEU:HD23	2.02	0.41
1:A:1096:ASN:H	5:A:1701:EDO:H21	1.85	0.41
1:A:1585:TYR:CE1	1:A:1668:ALA:HB1	2.55	0.41
1:A:1175:LEU:O	1:A:1179:THR:HG23	2.20	0.41
1:A:1305:LYS:HB3	1:A:1305:LYS:HE2	1.84	0.41
1:A:1309:LEU:H	1:A:1309:LEU:HD23	1.86	0.41
2:B:330:ILE:HG22	2:B:337:SER:HA	2.01	0.41
1:A:1003:LEU:HD11	1:A:1286:SER:HA	2.01	0.41
1:A:1544:SER:C	1:A:1546:GLU:H	2.28	0.41
2:B:267:ILE:HD12	2:B:269:PHE:HZ	1.85	0.41
2:B:394:THR:HG23	2:B:404:LEU:HD23	2.02	0.41
1:A:1036:SER:OG	1:A:1037:ASP:N	2.54	0.41
1:A:1048:LYS:HA	1:A:1051:GLU:HG3	2.02	0.41
1:A:1127:ILE:HD13	1:A:1129:LEU:HG	2.03	0.41
2:B:331:GLU:CD	2:B:334:GLY:H	2.26	0.41
2:B:463:SER:HA	2:B:490:SER:HB2	2.02	0.41
1:A:1139:GLU:OE2	1:A:1184:SER:OG	2.29	0.41
1:A:1307:LEU:H	1:A:1307:LEU:HD23	1.85	0.41
1:A:1319:HIS:N	1:A:1344:ASP:OD2	2.51	0.41
2:B:270:GLY:HA3	2:B:282:MET:HA	2.02	0.41
2:B:325:ILE:HB	2:B:342:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:504:LEU:HD11	2:B:651:LEU:HG	2.02	0.41
1:A:1289:ASP:OD1	1:A:1289:ASP:N	2.54	0.41
2:B:204:LYS:HG2	2:B:205:TYR:N	2.36	0.41
2:B:265:VAL:HG13	2:B:329:VAL:HG12	2.01	0.41
2:B:396:ASP:HA	2:B:428:VAL:HA	2.02	0.41
2:B:496:ILE:HG13	2:B:517:LYS:HE2	2.02	0.41
1:A:1142:LEU:HD21	1:A:1179:THR:HG22	2.03	0.41
1:A:1308:ARG:O	1:A:1354:SER:OG	2.38	0.41
2:B:38:ASN:HB2	3:C:14:TYR:OH	2.22	0.40
2:B:621:GLU:H	2:B:621:GLU:HG3	1.72	0.40
1:A:1306:GLN:HE21	1:A:1306:GLN:HB2	1.54	0.40
1:A:1429:PRO:HG2	1:A:1511:THR:HG23	2.03	0.40
1:A:765:ILE:HD12	1:A:765:ILE:HA	1.88	0.40
3:C:6:TRP:CZ3	3:C:33:ILE:HB	2.55	0.40
1:A:1133:LEU:CD2	1:A:1415:SER:HB2	2.51	0.40
1:A:1378:TYR:CZ	1:A:1409:LYS:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	964/999 (96%)	912 (95%)	52 (5%)	0	100	100
2	B	643/657 (98%)	610 (95%)	33 (5%)	0	100	100
3	C	33/35 (94%)	26 (79%)	7 (21%)	0	100	100
All	All	1640/1691 (97%)	1548 (94%)	92 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	856/886 (97%)	837 (98%)	19 (2%)	45	70
2	B	566/582 (97%)	548 (97%)	18 (3%)	34	59
3	C	26/26 (100%)	22 (85%)	4 (15%)	2	4
All	All	1448/1494 (97%)	1407 (97%)	41 (3%)	38	64

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	ILE
1	A	848	TYR
1	A	889	GLU
1	A	909	ASN
1	A	973	ILE
1	A	1051	GLU
1	A	1053	MET
1	A	1078	LEU
1	A	1127	ILE
1	A	1133	LEU
1	A	1279	ARG
1	A	1306	GLN
1	A	1316	SER
1	A	1403	VAL
1	A	1476	ARG
1	A	1532	CYS
1	A	1570	VAL
1	A	1654	CYS
1	A	1671	ILE
2	B	151	ASP
2	B	180	ILE
2	B	272	ARG
2	B	310	LEU
2	B	318	LEU
2	B	331	GLU
2	B	367	ILE

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Mol	Chain	Res	Type
2	B	390	LEU
2	B	450	GLU
2	B	467	ILE
2	B	484	ILE
2	B	492	TYR
2	B	530	VAL
2	B	553	GLU
2	B	594	THR
2	B	623	VAL
2	B	624	PHE
2	B	658	ASN
3	C	1	THR
3	C	13	ILE
3	C	27	LEU
3	C	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	707	ASN
1	A	744	HIS
1	A	838	GLN
1	A	994	GLN
1	A	1233	GLN
1	A	1278	GLN
1	A	1366	HIS
2	B	77	ASN
2	B	193	ASN
2	B	320	ASN
2	B	447	GLN
2	B	462	GLN
2	B	562	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

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	1,4	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	D	2	4	14,14,15	0.27	0	17,19,21	0.47	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	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

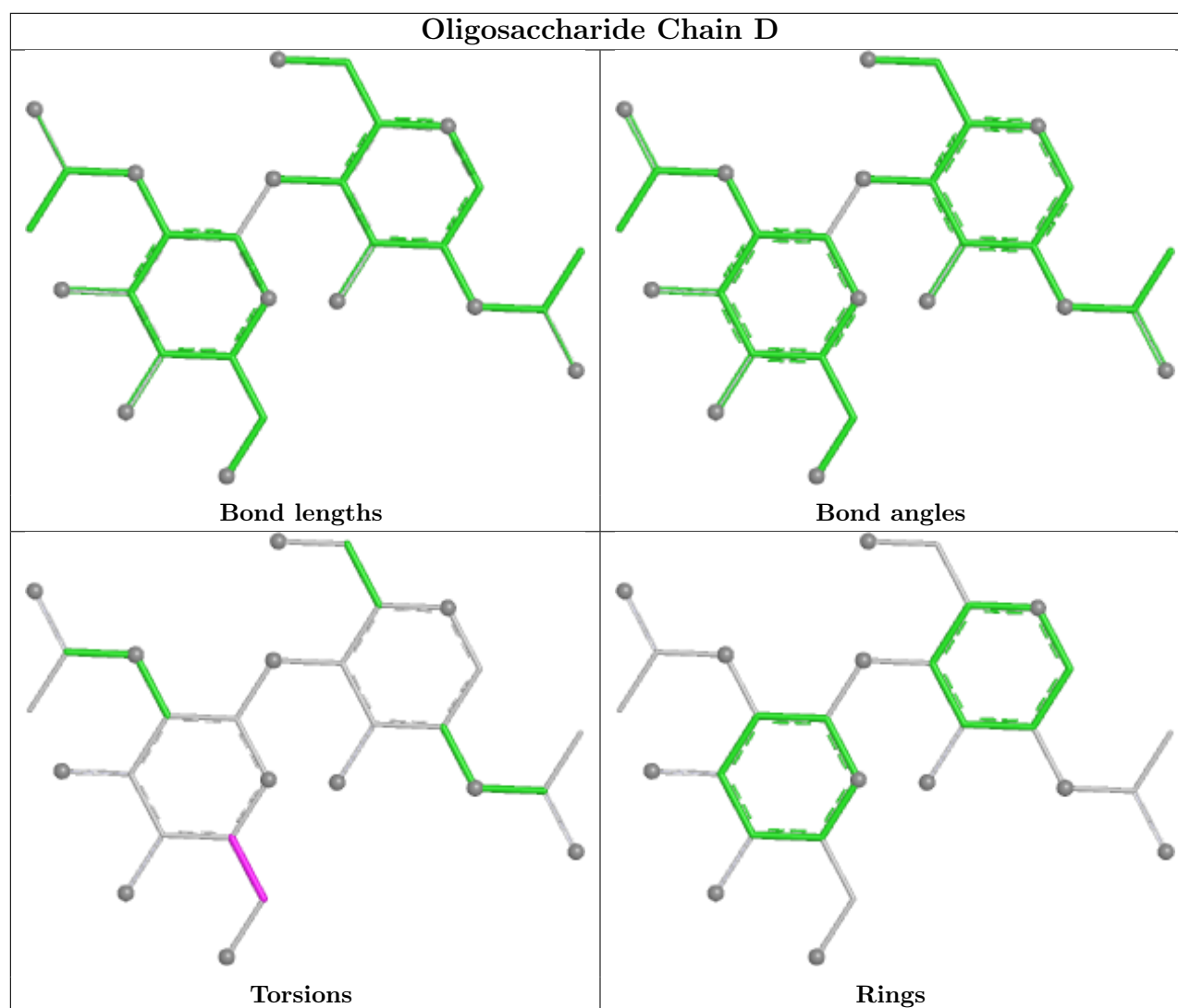
All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

2 ligands 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	$\# Z > 2$
5	EDO	A	1702	-	3,3,3	0.43	0	2,2,2	0.25	0
5	EDO	A	1701	-	3,3,3	0.45	0	2,2,2	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1702	-	-	1/1/1/1	-
5	EDO	A	1701	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

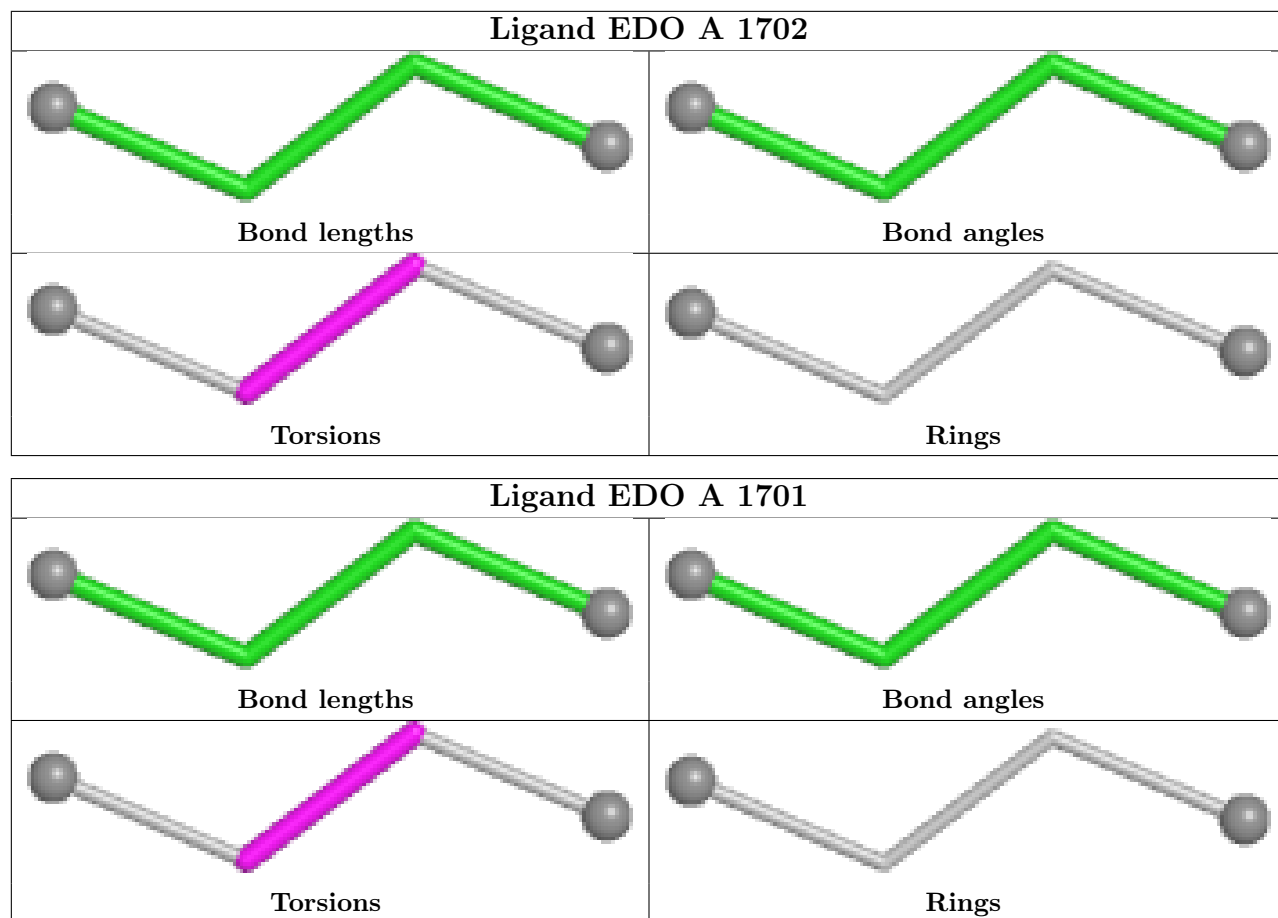
Mol	Chain	Res	Type	Atoms
5	A	1702	EDO	O1-C1-C2-O2
5	A	1701	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1701	EDO	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	972/999 (97%)	0.80	93 (9%) 13 11	71, 108, 186, 239	0
2	B	647/657 (98%)	0.92	72 (11%) 10 8	67, 128, 191, 275	0
3	C	35/35 (100%)	1.73	13 (37%) 1 0	127, 181, 210, 224	0
All	All	1654/1691 (97%)	0.87	178 (10%) 11 9	67, 114, 191, 275	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1673	LEU	6.7
1	A	1335	GLY	5.2
1	A	686	ILE	5.1
1	A	1388	ALA	4.9
1	A	694	VAL	4.8
2	B	623	VAL	4.6
1	A	729	THR	4.6
2	B	382	LEU	4.5
2	B	558	SER	4.2
1	A	683	ILE	3.9
1	A	690	TYR	3.8
1	A	756	THR	3.8
2	B	293	ILE	3.8
2	B	659	ALA	3.8
3	C	12	ALA	3.7
1	A	734	VAL	3.6
2	B	460	LEU	3.6
2	B	482	LEU	3.5
2	B	476	LEU	3.5
2	B	653	PHE	3.5
2	B	295	GLY	3.5
2	B	483	ASN	3.4
1	A	1239	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	920	LYS	3.4
3	C	14	TYR	3.4
1	A	1672	PHE	3.4
1	A	782	ARG	3.3
1	A	1387	GLU	3.3
3	C	15	GLY	3.3
2	B	624	PHE	3.2
2	B	386	VAL	3.2
3	C	13	ILE	3.2
1	A	1352	PHE	3.1
1	A	763	PRO	3.1
2	B	363	LEU	3.1
1	A	1627	ILE	3.1
2	B	626	PHE	3.1
1	A	738	LEU	3.1
1	A	1034	PHE	3.1
1	A	1674	ASN	3.1
1	A	1280	TYR	3.0
1	A	744	HIS	3.0
2	B	658	ASN	3.0
2	B	417	VAL	3.0
1	A	1533	GLY	3.0
2	B	296	ILE	3.0
1	A	754	MET	2.9
1	A	759	PRO	2.9
1	A	1056	ILE	2.9
2	B	404	LEU	2.9
2	B	352	TYR	2.8
1	A	1519	VAL	2.8
1	A	1062	ALA	2.8
2	B	620	LEU	2.8
2	B	336	PHE	2.8
2	B	347	TYR	2.7
1	A	952	THR	2.7
2	B	628	GLU	2.7
1	A	997	ILE	2.7
2	B	424	LEU	2.7
2	B	629	LYS	2.7
1	A	760	VAL	2.7
1	A	854	GLN	2.7
1	A	1230	ASP	2.6
1	A	781	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1541	LEU	2.6
3	C	21	TRP	2.6
3	C	31	PRO	2.6
2	B	484	ILE	2.6
3	C	27	LEU	2.6
1	A	731	CYS	2.6
1	A	1664	LEU	2.5
2	B	326	ALA	2.5
3	C	3	PRO	2.5
1	A	733	VAL	2.5
1	A	1656	SER	2.5
2	B	622	ARG	2.5
1	A	889	GLU	2.5
1	A	1011	GLU	2.5
1	A	728	PHE	2.5
1	A	1539	LEU	2.5
2	B	297	ALA	2.5
1	A	965	LEU	2.5
2	B	292	LEU	2.5
2	B	593	ALA	2.5
2	B	350	SER	2.5
2	B	457	TYR	2.4
1	A	1307	LEU	2.4
1	A	753	HIS	2.4
1	A	924	VAL	2.4
2	B	472	ASN	2.4
1	A	1638	PRO	2.4
2	B	395	ILE	2.4
2	B	651	LEU	2.4
2	B	383	VAL	2.4
1	A	715	ALA	2.4
1	A	722	PRO	2.4
2	B	354	LEU	2.4
2	B	674	ARG	2.4
1	A	1633	PHE	2.4
1	A	1162	VAL	2.4
2	B	588	VAL	2.4
2	B	419	SER	2.4
1	A	718	ILE	2.4
1	A	758	LEU	2.4
2	B	413	VAL	2.4
1	A	755	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	560	TRP	2.4
1	A	700	TYR	2.3
1	A	1514	ILE	2.3
3	C	23	CYS	2.3
2	B	398	ASN	2.3
1	A	1240	PRO	2.3
1	A	880	SER	2.3
1	A	1544	SER	2.3
2	B	442	LEU	2.3
2	B	455	ILE	2.3
2	B	425	PRO	2.3
1	A	917	TRP	2.3
1	A	983	LEU	2.3
1	A	1671	ILE	2.3
2	B	469	TRP	2.3
1	A	1229	LYS	2.3
2	B	63	LYS	2.3
3	C	4	GLU	2.3
2	B	421	VAL	2.3
1	A	1676	CYS	2.3
2	B	611	GLY	2.2
1	A	1642	LEU	2.2
2	B	528	ILE	2.2
3	C	9	CYS	2.2
1	A	691	LYS	2.2
1	A	1279	ARG	2.2
1	A	1119	LYS	2.2
1	A	1536	GLN	2.2
2	B	369	TYR	2.2
1	A	1351	GLY	2.2
2	B	416	GLY	2.2
2	B	431	LEU	2.2
1	A	918	PHE	2.2
2	B	357	VAL	2.2
1	A	1178	ASN	2.2
2	B	418	ALA	2.2
1	A	1547	THR	2.2
1	A	1133	LEU	2.2
1	A	993	SER	2.2
1	A	689	LYS	2.2
1	A	1186	PHE	2.2
2	B	388	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	703	ALA	2.1
3	C	1	THR	2.1
1	A	950	TYR	2.1
1	A	1531	ASP	2.1
1	A	1278	GLN	2.1
1	A	757	LEU	2.1
2	B	275	LEU	2.1
2	B	526	ILE	2.1
2	B	501	TYR	2.1
1	A	761	SER	2.1
2	B	282	MET	2.1
2	B	454	ALA	2.1
1	A	1323	LEU	2.1
2	B	470	THR	2.1
3	C	16	TYR	2.1
1	A	1019	PHE	2.1
2	B	430	VAL	2.1
2	B	435	VAL	2.1
1	A	784	LYS	2.1
2	B	364	LYS	2.1
1	A	1238	SER	2.1
1	A	1545	ALA	2.0
1	A	1054	LEU	2.0
1	A	765	ILE	2.0
2	B	250	ILE	2.0
2	B	312	TYR	2.0
2	B	411	THR	2.0
1	A	1134	PRO	2.0
2	B	192	SER	2.0

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

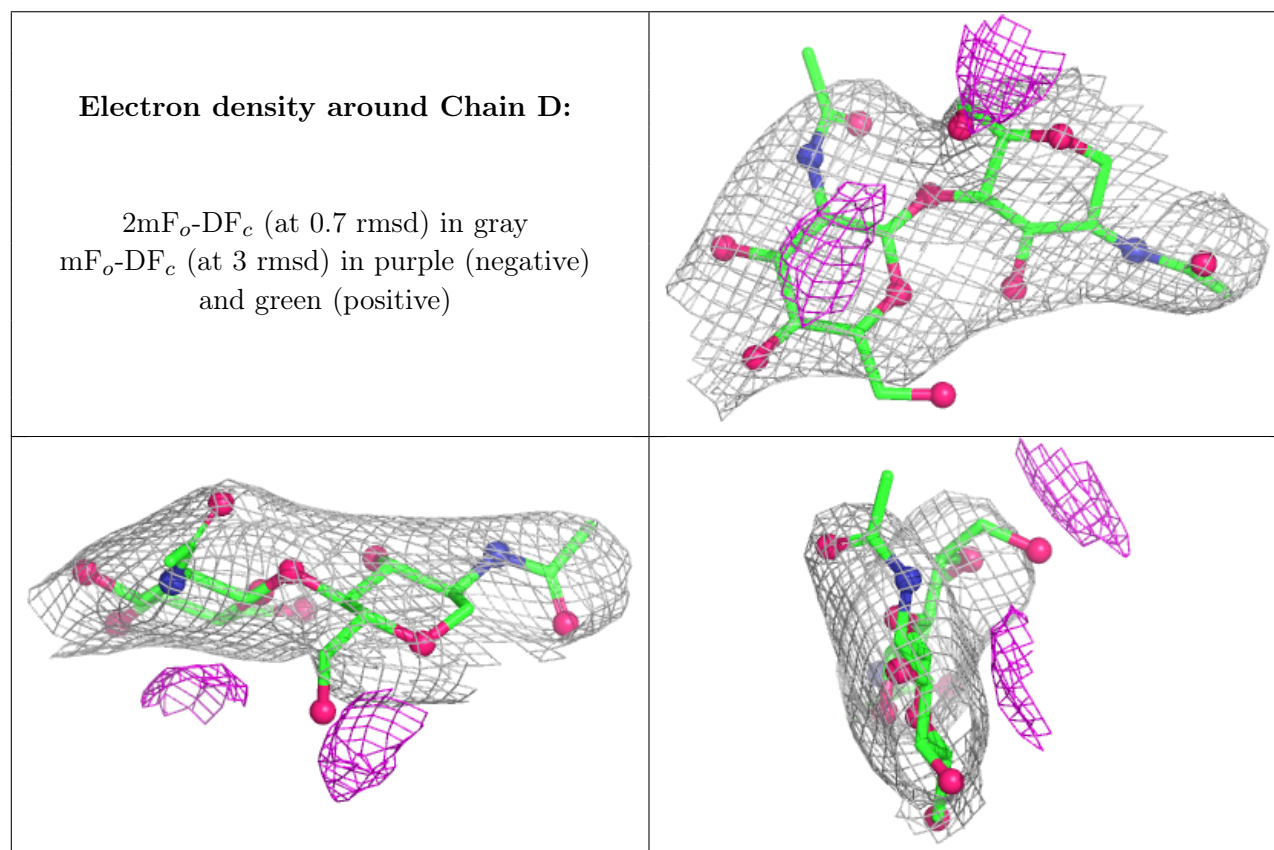
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	D	2	14/15	0.65	0.13	139,145,155,183	0
4	NAG	D	1	14/15	0.80	0.13	111,125,133,159	0

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



6.4 Ligands ⓘ

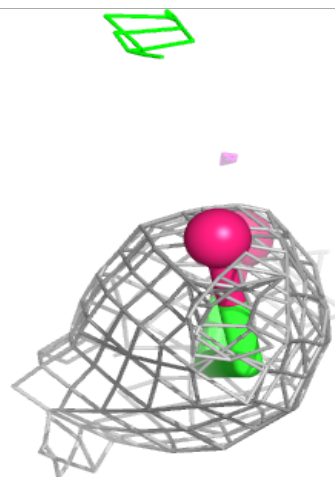
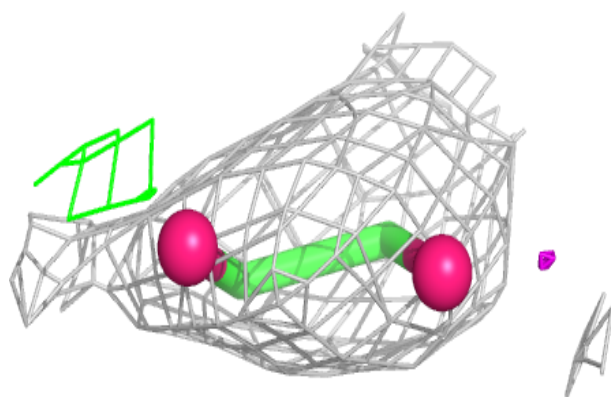
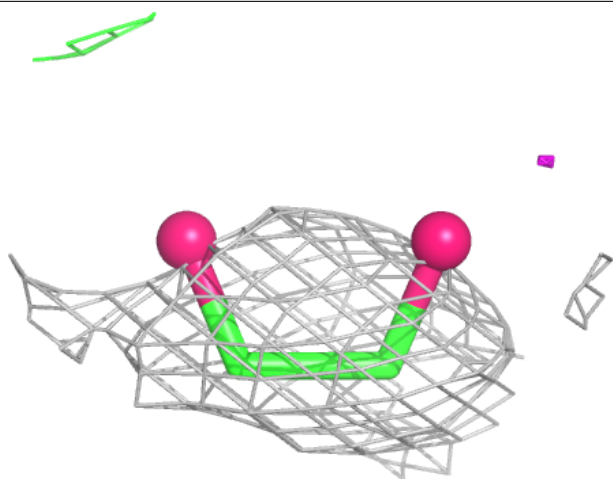
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

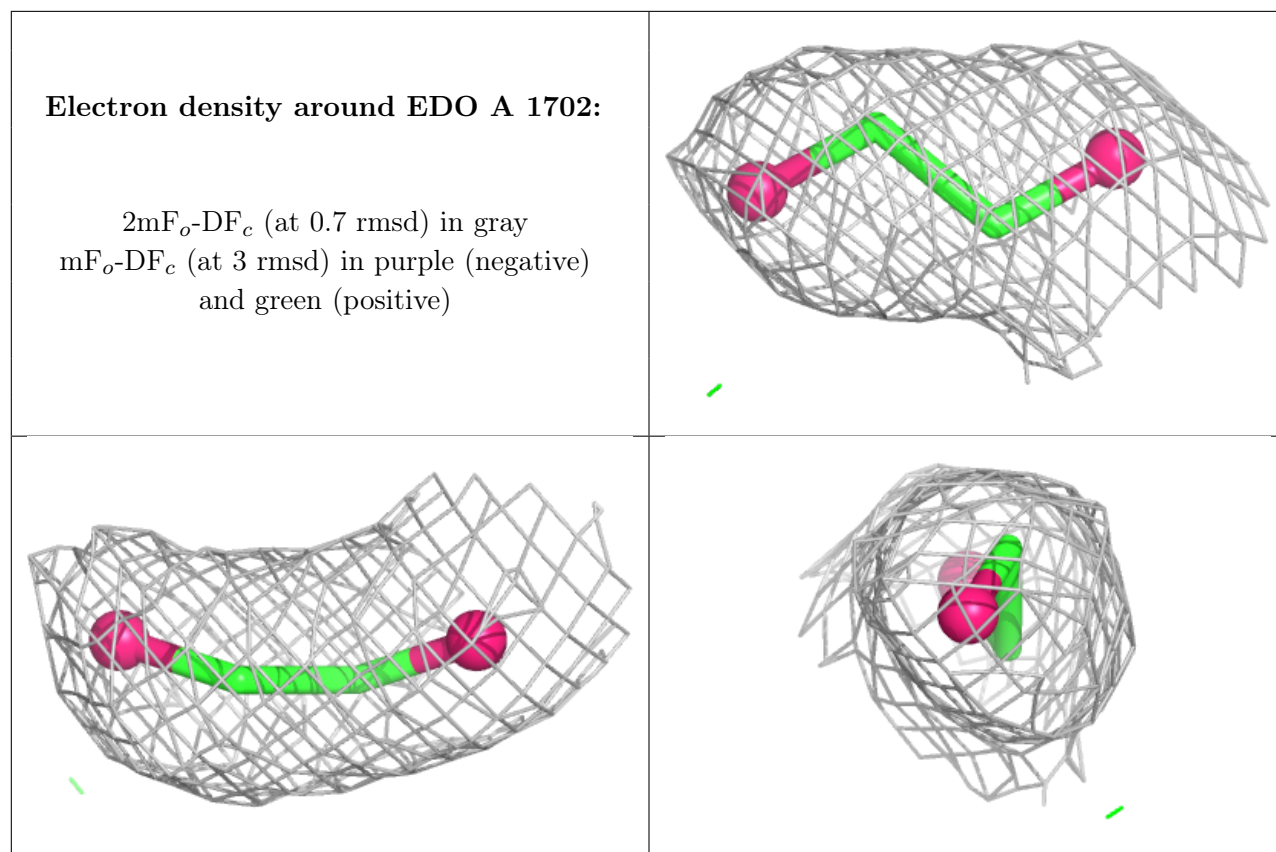
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	1701	4/4	0.86	0.30	105,116,150,156	0
5	EDO	A	1702	4/4	0.91	0.20	100,105,122,132	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EDO A 1701:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.