



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2022 – 07:11 pm BST

PDB ID : 7OP0
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

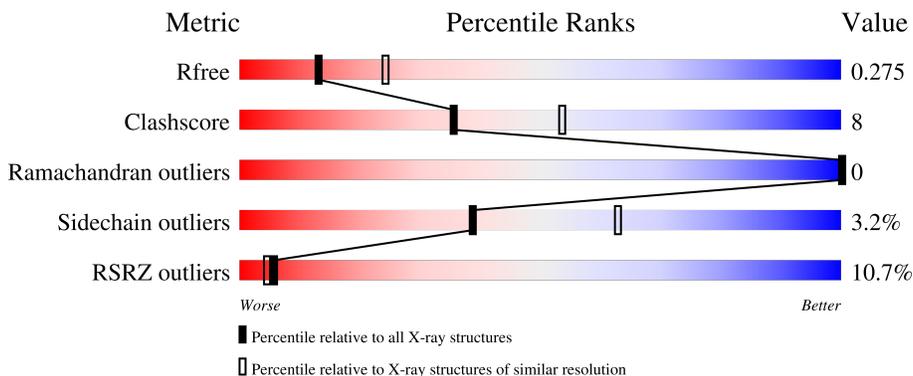
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

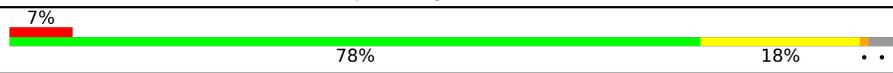
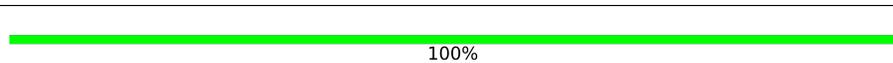
The reported resolution of this entry is 2.57 Å.

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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (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	
2	B	657	
3	C	35	
4	D	2	

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
			Total	C	N	O	S			
1	A	972	7665	4898	1275	1451	41	0	0	0

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

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

- Molecule 3 is a protein called K92chemFE.

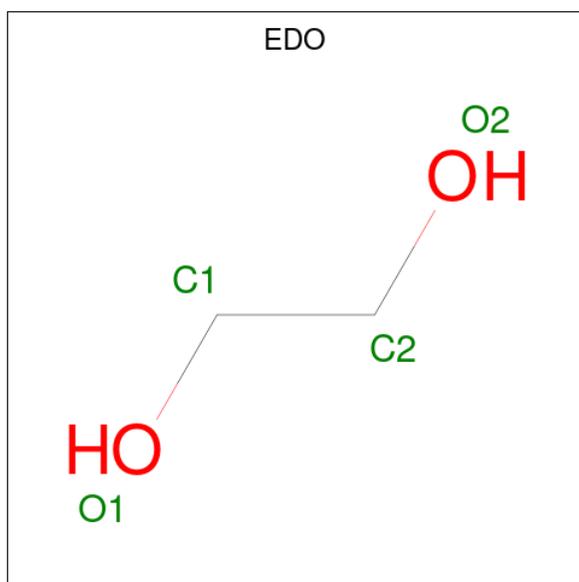
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	35	257	162	44	47	4	0	0	0

- 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
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

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



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

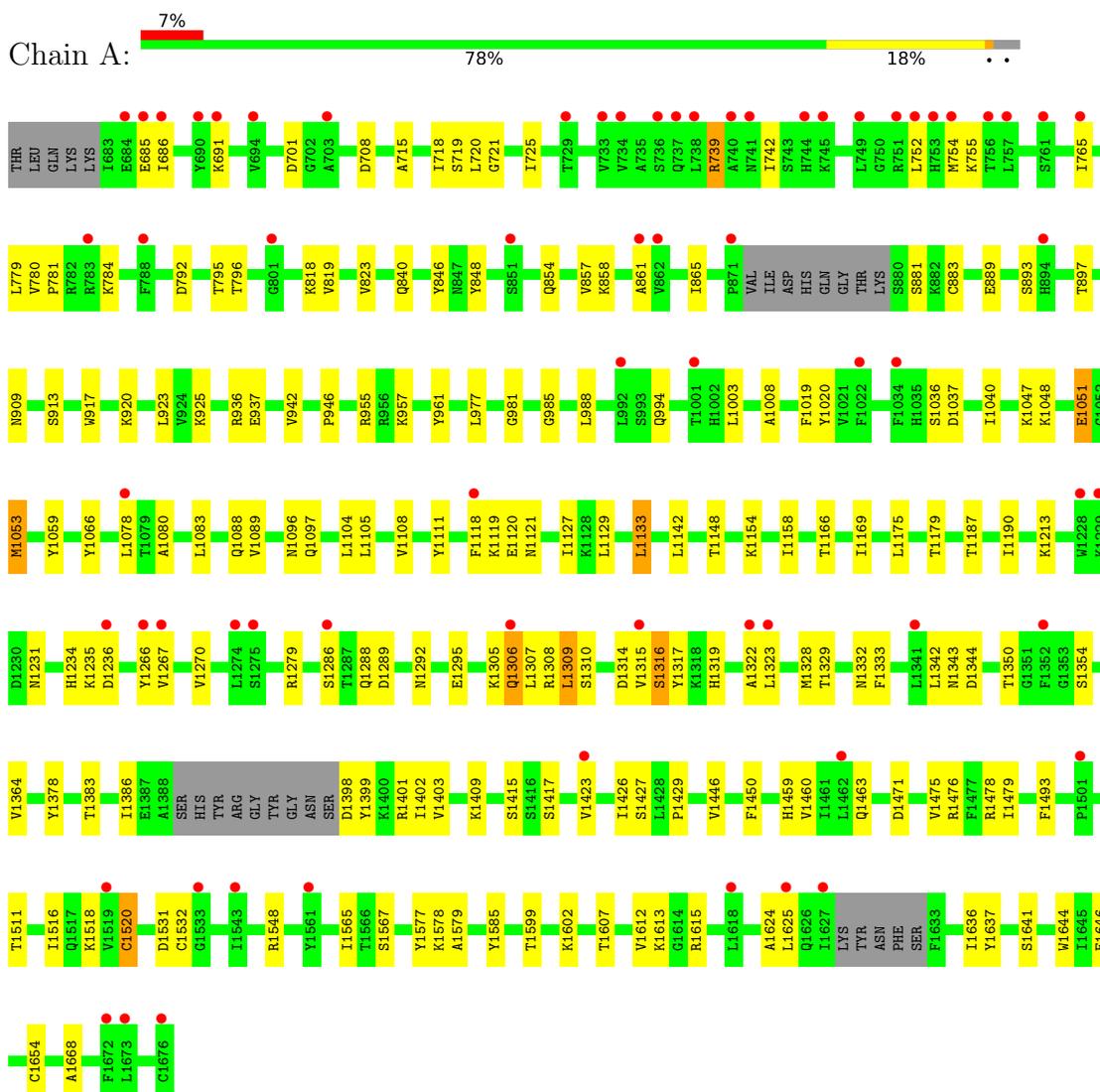
- Molecule 6 is water.

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

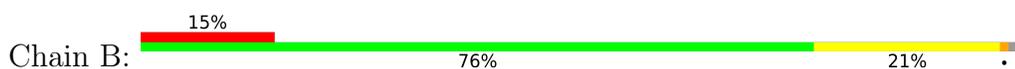
3 Residue-property plots [i](#)

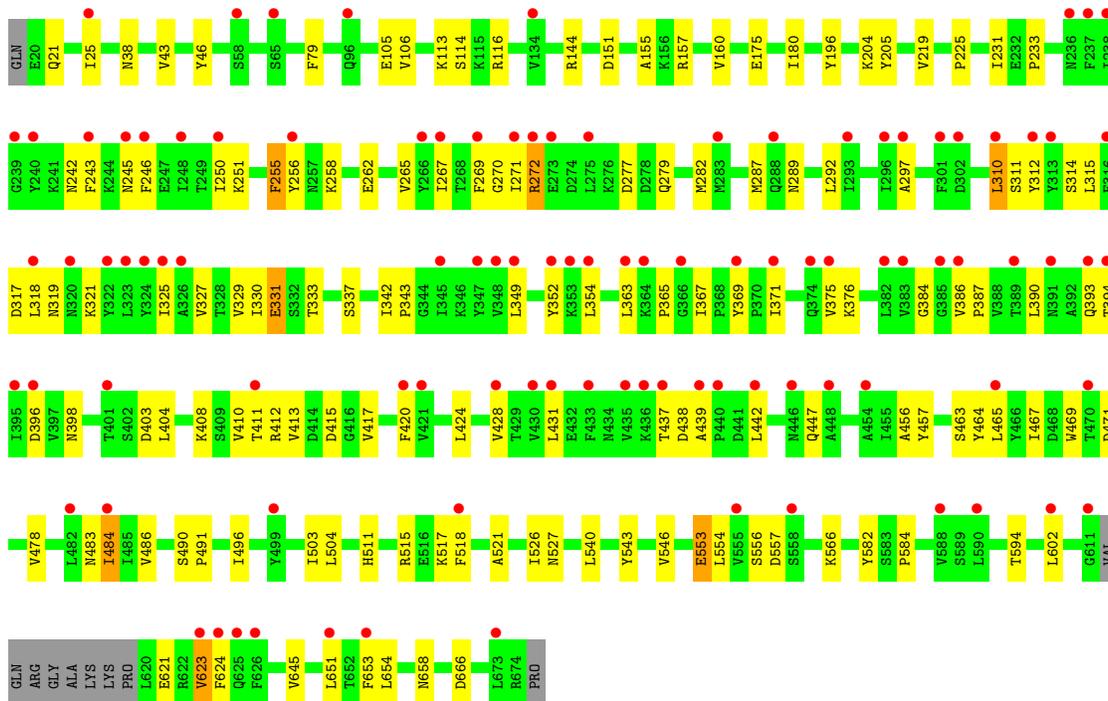
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 C5 alpha chain



- Molecule 2: Complement C5 beta chain





● 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) 99.9 (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)	Xtrriage
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	Xtrriage
Anisotropy	0.276	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.26	0/7820	0.45	0/10597
2	B	0.26	0/5198	0.49	1/7079 (0.0%)
3	C	0.29	0/267	0.49	0/364
All	All	0.26	0/13285	0.47	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($^{\circ}$)	Ideal($^{\circ}$)
2	B	310	LEU	CA-CB-CG	5.52	128.00	115.30

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	119	0
2	B	5080	0	4940	86	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	209	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 (209) 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
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
1:A:718:ILE:HD12	1:A:719:SER:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:314:SER:OG	2:B:317:ASP:OD1	2.29	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
1:A:854:GLN:OE1	1:A:917:TRP:NE1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:ASP:N	1:A:1398:ASP:OD1	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
1:A:719:SER:O	1:A:719:SER:OG	2.31	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
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:HD3	1:A:936:ARG:HA	1.59	0.46
1:A:1314:ASP:OD2	1:A:1316:SER:OG	2.32	0.46
1:A:1415:SER:HG	1:A:1417:SER:HG	1.63	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
1:A:1154:LYS:NZ	1:A:1295:GLU:OE2	2.48	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: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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:A:1309:LEU:H	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
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:463:SER:HA	2:B:490:SER:HB2	2.02	0.41
3:C:17:ALA:HB1	3:C:35:PRO:C	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:483:ASN:N	2:B:483:ASN:OD1	2.53	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	856/886 (97%)	834 (97%)	22 (3%)	46	69
2	B	566/582 (97%)	544 (96%)	22 (4%)	32	56
3	C	26/26 (100%)	24 (92%)	2 (8%)	13	24
All	All	1448/1494 (97%)	1402 (97%)	46 (3%)	39	63

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	686	ILE
1	A	691	LYS
1	A	739	ARG
1	A	754	MET
1	A	848	TYR
1	A	883	CYS
1	A	889	GLU
1	A	909	ASN
1	A	920	LYS
1	A	994	GLN
1	A	1051	GLU
1	A	1053	MET
1	A	1133	LEU
1	A	1279	ARG
1	A	1306	GLN
1	A	1309	LEU
1	A	1316	SER
1	A	1403	VAL
1	A	1471	ASP
1	A	1520	CYS
1	A	1532	CYS
1	A	1654	CYS
2	B	151	ASP
2	B	180	ILE
2	B	251	LYS
2	B	255	PHE
2	B	272	ARG
2	B	287	MET
2	B	310	LEU
2	B	331	GLU
2	B	367	ILE

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Mol	Chain	Res	Type
2	B	369	TYR
2	B	390	LEU
2	B	408	LYS
2	B	438	ASP
2	B	457	TYR
2	B	467	ILE
2	B	471	ASP
2	B	484	ILE
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	27	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	193	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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	0.36	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.26	0	17,19,21	0.45	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	-	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.

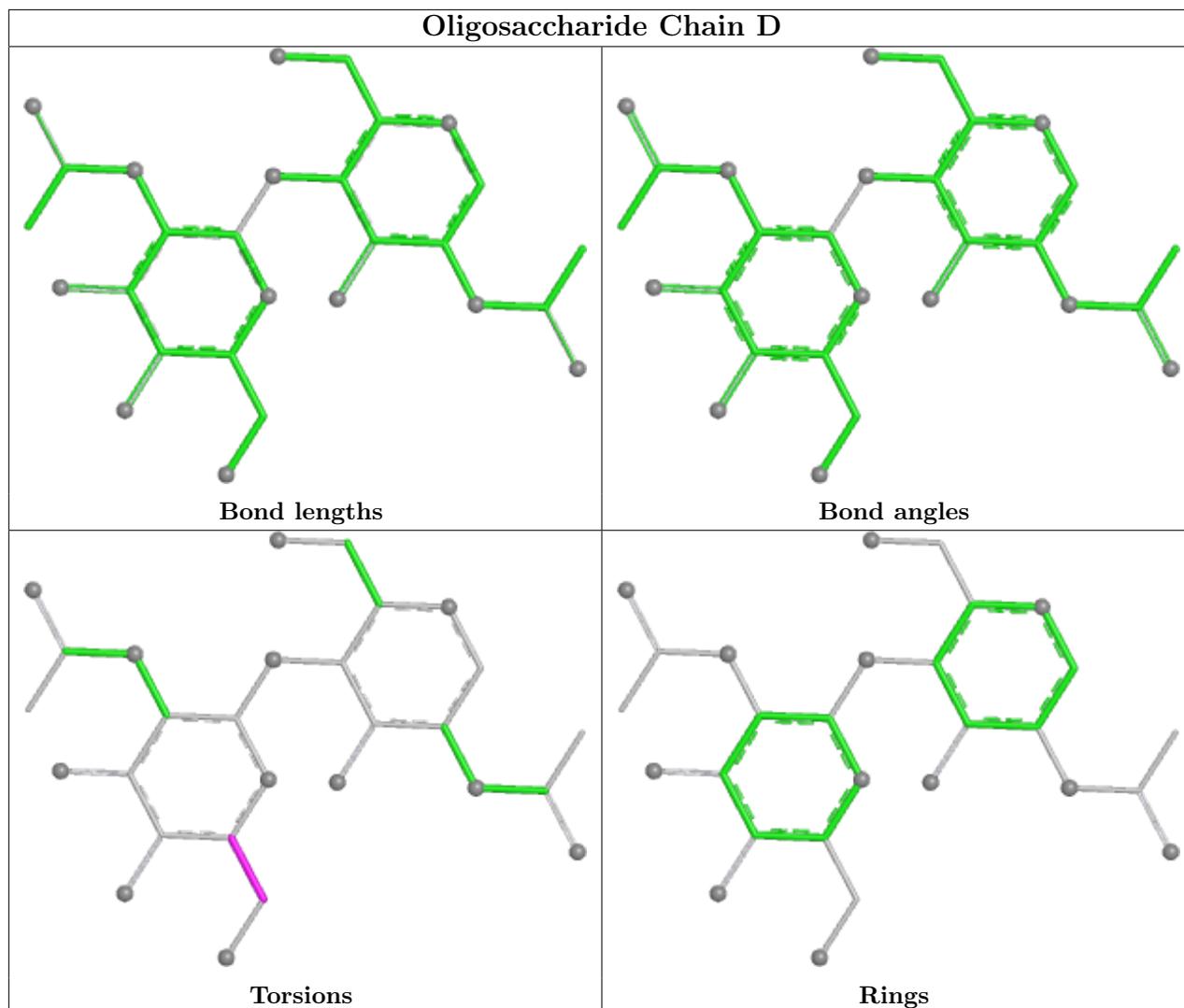
All (2) torsion outliers are listed below:

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	1701	-	3,3,3	0.48	0	2,2,2	0.35	0
5	EDO	A	1702	-	3,3,3	0.47	0	2,2,2	0.20	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	1701	-	-	1/1/1/1	-
5	EDO	A	1702	-	-	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:

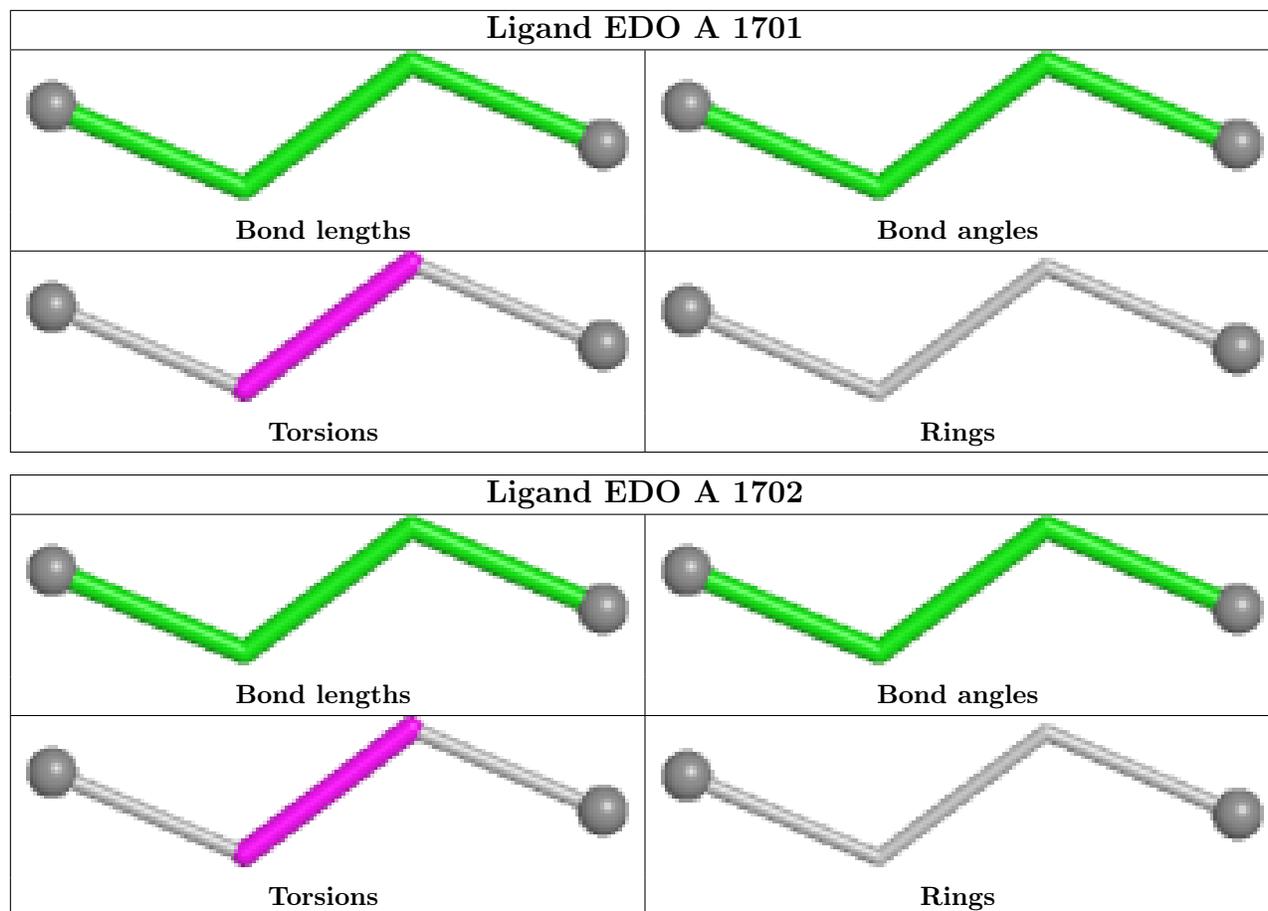
Mol	Chain	Res	Type	Atoms
5	A	1702	EDO	O1-C1-C2-O2
5	A	1701	EDO	O1-C1-C2-O2

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%)	0.61	67 (6%) 16 14	71, 108, 186, 239	0
2	B	647/657 (98%)	0.90	101 (15%) 2 1	67, 128, 191, 275	0
3	C	35/35 (100%)	1.48	9 (25%) 0 0	127, 181, 210, 224	0
All	All	1654/1691 (97%)	0.74	177 (10%) 6 4	67, 114, 191, 275	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	312	TYR	7.3
1	A	738	LEU	6.9
2	B	352	TYR	6.6
2	B	347	TYR	6.6
2	B	623	VAL	6.3
2	B	442	LEU	6.2
2	B	354	LEU	6.1
2	B	323	LEU	6.1
2	B	318	LEU	6.0
2	B	386	VAL	5.9
1	A	1673	LEU	5.8
1	A	754	MET	5.4
1	A	703	ALA	5.1
2	B	238	ILE	5.1
3	C	4	GLU	5.0
2	B	266	TYR	5.0
2	B	435	VAL	4.7
1	A	757	LEU	4.6
1	A	734	VAL	4.5
1	A	1323	LEU	4.5
2	B	248	ILE	4.4
2	B	293	ILE	4.3
2	B	237	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	783	ARG	4.3
1	A	685	GLU	4.2
1	A	753	HIS	4.1
2	B	301	PHE	4.1
2	B	345	ILE	4.0
2	B	246	PHE	4.0
2	B	624	PHE	4.0
2	B	446	ASN	3.9
1	A	749	LEU	3.9
3	C	15	GLY	3.9
2	B	420	PHE	3.8
2	B	310	LEU	3.8
2	B	349	LEU	3.8
2	B	256	TYR	3.8
2	B	673	LEU	3.8
2	B	395	ILE	3.8
2	B	482	LEU	3.8
1	A	756	THR	3.7
1	A	686	ILE	3.7
2	B	326	ALA	3.7
3	C	5	GLY	3.7
2	B	267	ILE	3.6
3	C	2	CYS	3.6
2	B	239	GLY	3.5
2	B	272	ARG	3.4
2	B	439	ALA	3.4
2	B	297	ALA	3.4
2	B	499	TYR	3.4
1	A	1519	VAL	3.4
2	B	518	PHE	3.4
1	A	1627	ILE	3.3
2	B	325	ILE	3.3
1	A	1676	CYS	3.2
2	B	430	VAL	3.2
1	A	733	VAL	3.2
1	A	740	ALA	3.1
2	B	271	ILE	3.1
2	B	363	LEU	3.1
2	B	375	VAL	3.1
2	B	382	LEU	3.1
1	A	744	HIS	3.1
2	B	245	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	729	THR	3.0
1	A	761	SER	3.0
2	B	250	ILE	3.0
2	B	625	GLN	3.0
2	B	383	VAL	3.0
2	B	369	TYR	3.0
2	B	558	SER	3.0
2	B	401	THR	3.0
2	B	611	GLY	2.9
3	C	30	GLY	2.9
1	A	745	LYS	2.9
2	B	590	LEU	2.9
2	B	313	TYR	2.9
3	C	14	TYR	2.9
1	A	1533	GLY	2.9
1	A	741	ASN	2.9
2	B	283	MET	2.8
1	A	1306	GLN	2.8
2	B	393	GLN	2.8
1	A	1672	PHE	2.8
2	B	302	ASP	2.8
2	B	316	GLU	2.7
2	B	324	TYR	2.7
2	B	320	ASN	2.7
1	A	1034	PHE	2.7
2	B	243	PHE	2.7
1	A	690	TYR	2.6
2	B	275	LEU	2.6
2	B	385	GLY	2.6
1	A	1315	VAL	2.6
2	B	433	PHE	2.6
1	A	751	ARG	2.6
1	A	871	PRO	2.6
2	B	454	ALA	2.6
2	B	58	SER	2.6
2	B	322	TYR	2.6
1	A	1352	PHE	2.6
1	A	1561	TYR	2.6
2	B	428	VAL	2.5
2	B	269	PHE	2.5
2	B	240	TYR	2.5
2	B	394	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	371	ILE	2.5
2	B	653	PHE	2.5
2	B	296	ILE	2.5
3	C	18	CYS	2.5
1	A	752	LEU	2.5
1	A	1022	PHE	2.5
2	B	440	PRO	2.5
2	B	651	LEU	2.4
2	B	421	VAL	2.4
2	B	484	ILE	2.4
2	B	348	VAL	2.4
2	B	273	GLU	2.4
2	B	353	LYS	2.4
2	B	236	ASN	2.4
1	A	765	ILE	2.4
1	A	1341	LEU	2.4
1	A	694	VAL	2.4
2	B	411	THR	2.4
2	B	431	LEU	2.3
2	B	555	VAL	2.3
1	A	1229	LYS	2.3
2	B	389	THR	2.3
1	A	862	VAL	2.3
1	A	861	ALA	2.3
3	C	34	SER	2.3
2	B	396	ASP	2.3
2	B	448	ALA	2.3
2	B	588	VAL	2.2
1	A	788	PHE	2.2
2	B	366	GLY	2.2
1	A	851	SER	2.2
2	B	65	SER	2.2
1	A	1322	ALA	2.2
2	B	626	PHE	2.2
1	A	1274	LEU	2.2
1	A	1423	VAL	2.2
1	A	737	GLN	2.2
1	A	1501	PRO	2.2
2	B	465	LEU	2.2
2	B	25	ILE	2.2
2	B	602	LEU	2.2
1	A	684	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	134	VAL	2.2
2	B	436	LYS	2.2
1	A	1625	LEU	2.2
1	A	1266	TYR	2.1
2	B	391	ASN	2.1
2	B	470	THR	2.1
1	A	736	SER	2.1
1	A	1267	VAL	2.1
1	A	1001	THR	2.1
1	A	691	LYS	2.1
2	B	437	THR	2.1
1	A	1462	LEU	2.1
1	A	1286	SER	2.1
2	B	364	LYS	2.1
2	B	288	GLN	2.1
1	A	1543	ILE	2.1
1	A	992	LEU	2.1
1	A	1078	LEU	2.1
1	A	1118	PHE	2.1
2	B	374	GLN	2.1
1	A	1275	SER	2.0
2	B	96	GLN	2.0
1	A	1228	TRP	2.0
1	A	894	HIS	2.0
3	C	28	ASN	2.0
1	A	801	GLY	2.0
1	A	1618	LEU	2.0
1	A	1236	ASP	2.0

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

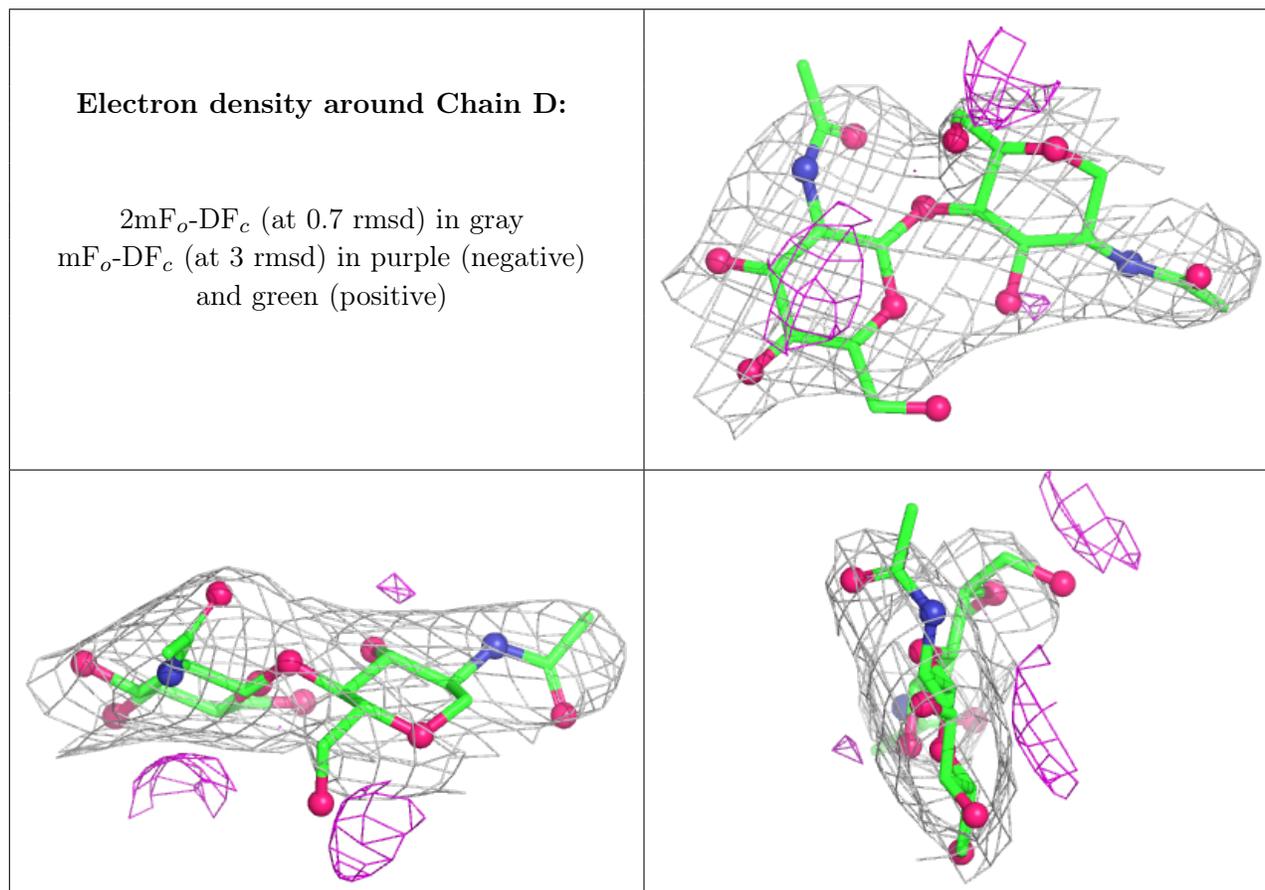
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	2	14/15	0.85	0.26	139,145,155,183	0
4	NAG	D	1	14/15	0.93	0.24	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.



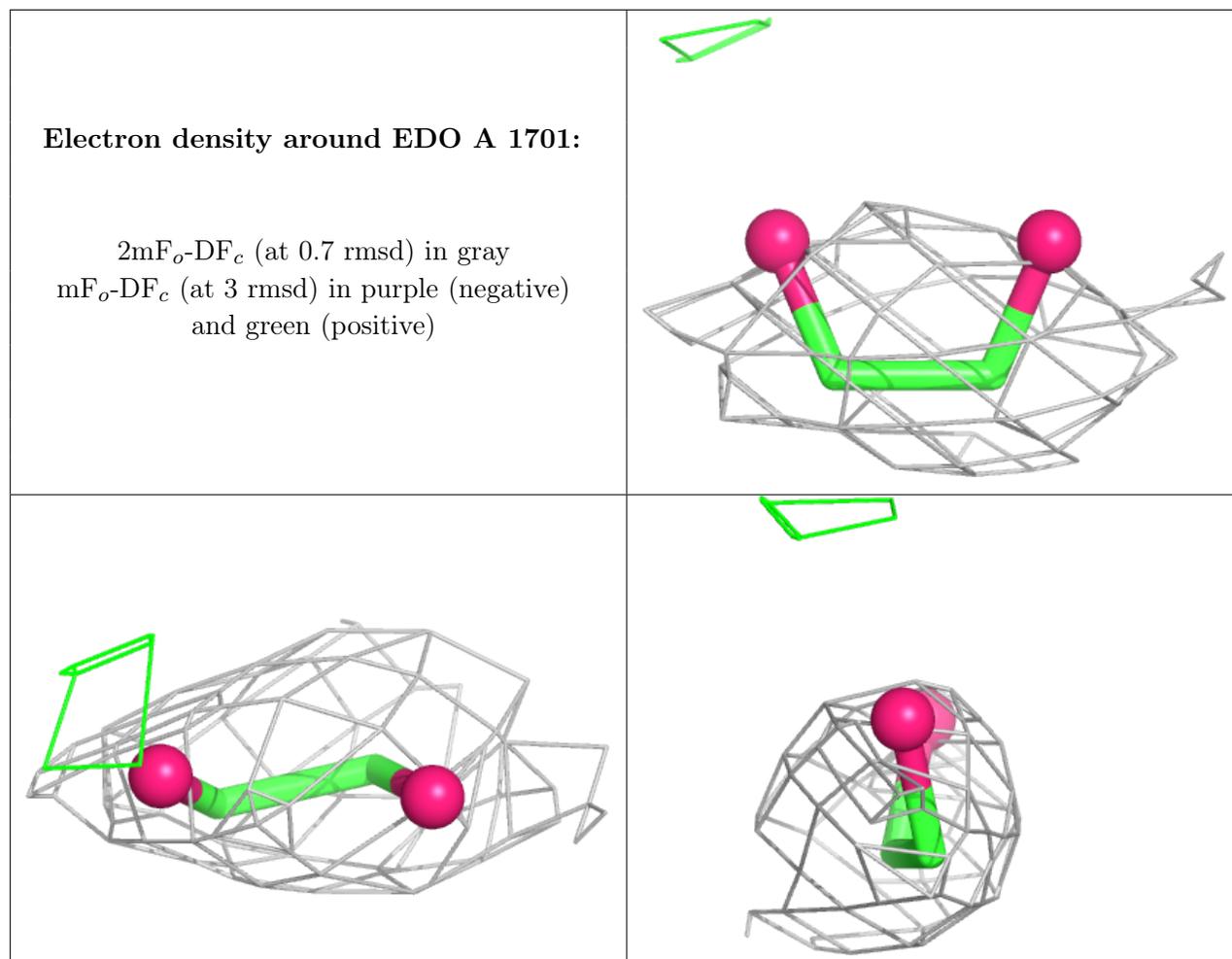
6.4 Ligands [i](#)

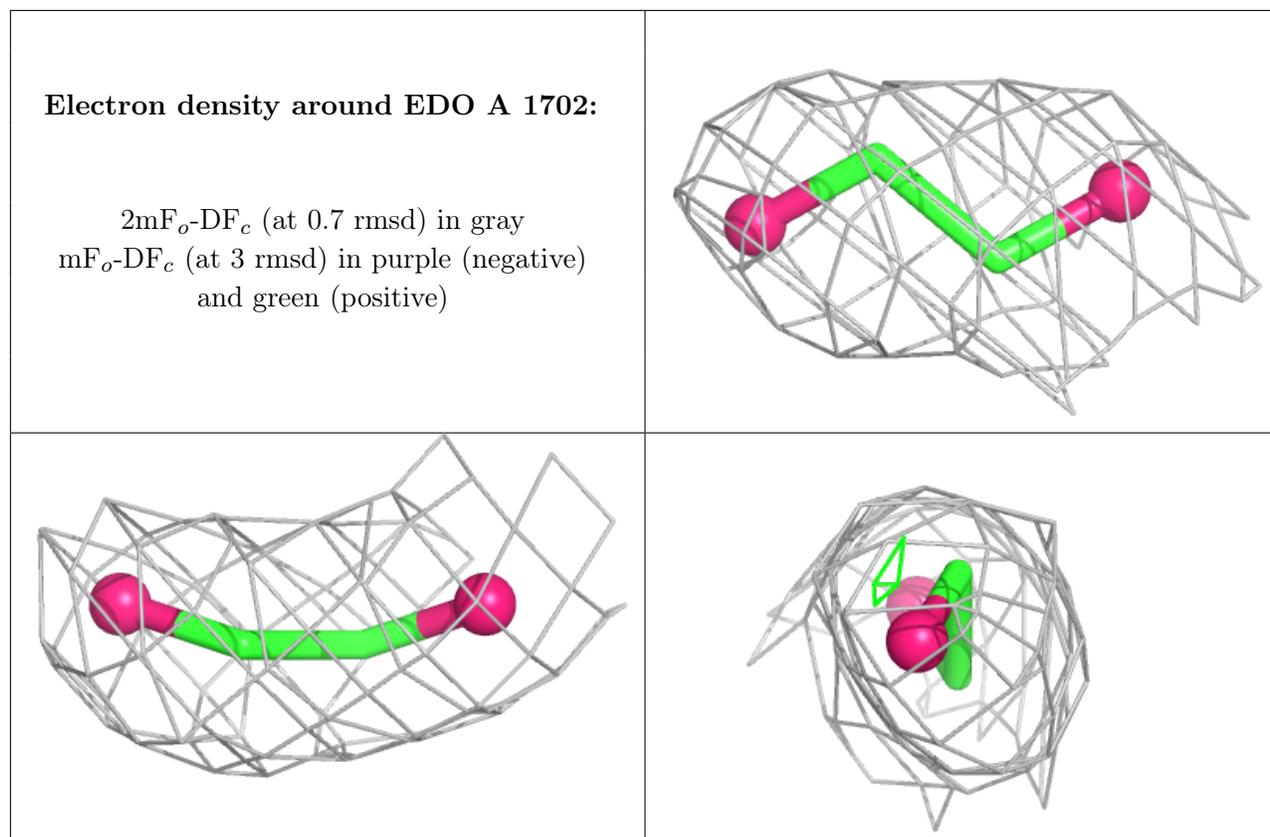
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	1701	4/4	0.88	0.45	105,116,150,156	0
5	EDO	A	1702	4/4	0.89	0.32	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.