



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 AM UTC

PDB ID : 7AD6 / pdb_00007ad6
Title : Crystal structure of human complement C5 in complex with the K92 bovine knob domain peptide.
Authors : Macpherson, A.; van den Elsen, J.M.H.; Schulze, M.E.; Birtley, J.R.
Deposited on : 2020-09-14
Resolution : 2.75 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

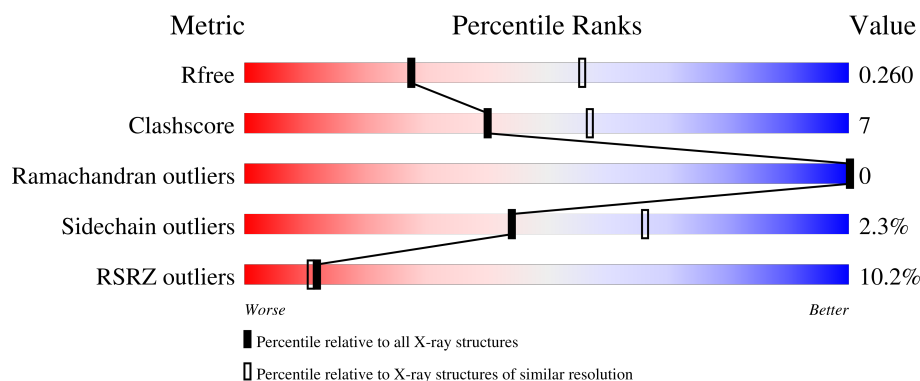
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	1676	5% 48% 9% 42%
1	B	1676	5% 31% 7% 61%
2	C	34	41% 74% 26%
3	D	3	67% 33%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13095 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.

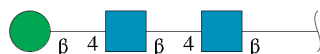
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	971	Total	C	N	O	S	0	0	0
			7664	4899	1274	1450	41			
1	B	646	Total	C	N	O	S	0	0	0
			5104	3272	817	1002	13			

- Molecule 2 is a protein called K92 knob domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	34	Total	C	N	O	S	0	0	0
			250	158	43	45	4			

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



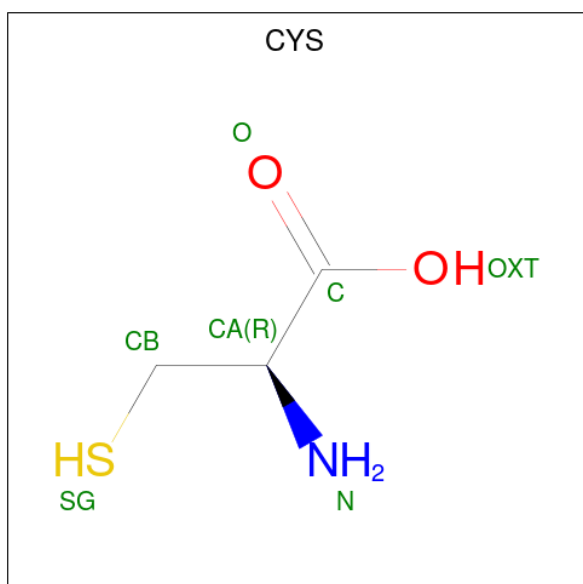
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



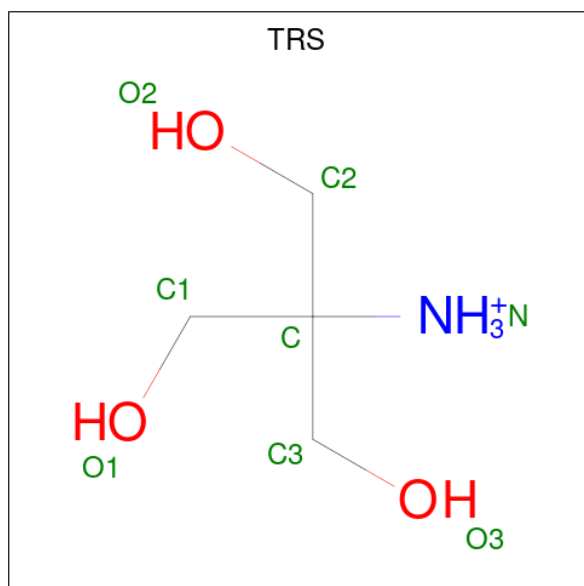
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			8	4	1	3		

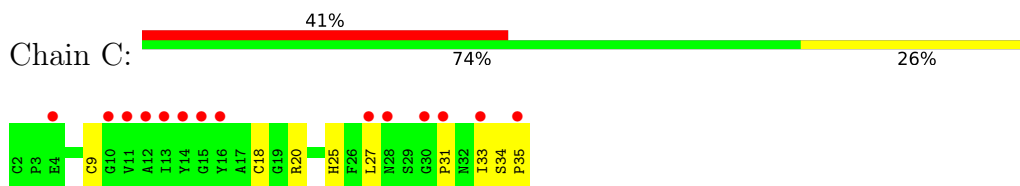
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	8	Total	O	0	0
			8	8		
7	B	4	Total	O	0	0
			4	4		

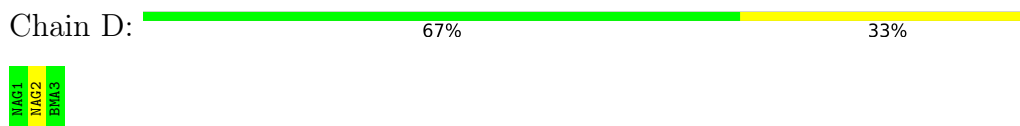


[illegible]

- Molecule 2: K92 knob domain



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.26Å 104.28Å 154.88Å 90.00° 124.90° 90.00°	Depositor
Resolution (Å)	83.77 – 2.75 83.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.77-2.75) 99.9 (83.77-2.75)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.5, PHENIX 1.18_3845	Depositor
R, R_{free}	0.219 , 0.254 0.231 , 0.260	Depositor DCC
R_{free} test set	3429 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtrriage
Anisotropy	0.309	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.3	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	0.94	EDS
Total number of atoms	13095	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, EDO, TRS, 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	0.10	0/7818	0.31	0/10591
1	B	0.10	0/5222	0.32	0/7104
2	C	0.12	0/260	0.40	0/354
All	All	0.10	0/13300	0.31	0/18049

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7664	0	7672	98	0
1	B	5104	0	5000	73	0
2	C	250	0	215	7	0
3	D	39	0	34	0	0
4	A	8	0	12	2	0
4	B	4	0	6	1	0
5	A	6	0	3	0	0
6	B	8	0	12	2	0
7	A	8	0	0	0	0
7	B	4	0	0	0	0
All	All	13095	0	12954	173	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 7.

All (173) 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:B:363:LEU:HB2	1:B:456:ALA:HA	1.70	0.74
1:B:160:VAL:HG22	1:B:175:GLU:HG2	1.72	0.70
2:C:27:LEU:HB2	2:C:31:PRO:HB2	1.73	0.69
1:A:1577:TYR:OH	1:A:1602:LYS:NZ	2.25	0.68
1:B:353:LYS:HZ1	1:B:378:SER:HA	1.57	0.68
1:B:384:GLY:HA3	1:B:413:VAL:HA	1.75	0.68
2:C:18:CYS:HB2	2:C:33:ILE:HG22	1.77	0.67
1:B:465:LEU:HD11	1:B:486:VAL:HG13	1.78	0.66
1:A:1013:MET:HE3	1:A:1287:THR:HB	1.79	0.65
1:B:265:VAL:HG23	1:B:292:LEU:HB2	1.79	0.63
1:B:411:THR:HG22	1:B:418:ALA:HB2	1.81	0.62
1:B:503:ILE:HB	1:B:511:HIS:HB3	1.80	0.62
1:B:387:PRO:HG3	1:B:410:VAL:HG23	1.83	0.60
1:A:823:VAL:HG21	1:A:916:THR:HG21	1.81	0.60
1:B:442:LEU:HD12	1:B:443:PRO:HD2	1.83	0.60
1:B:396:ASP:OD2	1:B:400:GLU:HB2	2.01	0.60
1:A:1383:THR:HG21	1:A:1511:THR:HA	1.83	0.60
1:A:1423:VAL:HG22	1:A:1463:GLN:HG2	1.83	0.60
1:A:1516:ILE:HG22	1:A:1518:LYS:H	1.67	0.59
1:A:905:ILE:HD13	1:A:931:PRO:HG3	1.85	0.59
1:A:1401:ARG:HA	1:A:1478:ARG:HA	1.84	0.58
1:A:695:VAL:HG11	1:A:724:CYS:HA	1.84	0.58
1:B:265:VAL:HG22	1:B:329:VAL:HG12	1.85	0.58
1:A:1229:LYS:NZ	1:A:1236:ASP:O	2.34	0.58
1:A:1142:LEU:HD21	1:A:1179:THR:HG22	1.85	0.57
1:B:573:VAL:HG12	1:B:592:MET:HG2	1.85	0.57
1:B:279:GLN:NE2	1:B:281:GLU:OE2	2.37	0.57
1:A:1129:LEU:HD13	1:A:1139:GLU:HB3	1.86	0.57
1:A:792:ASP:HA	1:B:584:PRO:HB3	1.87	0.56
1:B:487:THR:HG22	1:B:523:TYR:HB2	1.87	0.56
2:C:20:ARG:HB3	2:C:31:PRO:HB3	1.88	0.56
1:A:1426:ILE:HB	1:A:1460:VAL:HG13	1.88	0.56
1:A:696:LYS:HD2	1:A:697:LYS:H	1.71	0.55
1:B:39:ILE:HD12	1:B:85:LEU:HD12	1.89	0.55
1:A:849:ARG:O	1:A:891:SER:N	2.39	0.55
1:B:196:TYR:HA	1:B:219:VAL:HG23	1.89	0.55
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:LEU:HA	1:A:755:LYS:HB2	1.88	0.55
1:B:30:ILE:HG22	1:B:118:PRO:HG2	1.89	0.55
1:A:1130:GLN:HG2	1:A:1414:GLU:HG3	1.89	0.54
1:B:531:THR:OG1	1:B:532:GLN:N	2.41	0.54
1:B:303:SER:O	1:B:307:VAL:HB	2.08	0.54
1:B:259:VAL:HG13	1:B:295:GLY:HA3	1.91	0.53
1:A:1545:ALA:HB2	1:A:1663:ASN:HB3	1.90	0.53
1:B:225:PRO:HG2	1:B:255:PHE:CE2	2.44	0.53
1:A:1544:SER:C	1:A:1546:GLU:H	2.16	0.52
1:A:1590:ALA:HB3	1:A:1623:GLU:OE2	2.09	0.52
1:A:703:ALA:O	1:A:739:ARG:NH2	2.42	0.52
1:B:444:GLU:HA	1:B:447:GLN:HG3	1.91	0.52
1:A:715:ALA:HA	1:A:718:ILE:HG13	1.92	0.52
1:A:946:PRO:HA	1:A:955:ARG:HG2	1.91	0.51
1:A:1315:VAL:HG22	1:A:1348:VAL:HG12	1.92	0.51
1:A:1398:ASP:N	1:A:1398:ASP:OD1	2.42	0.51
1:B:224:LEU:HD22	1:B:225:PRO:HD2	1.91	0.51
1:B:21:GLN:HB3	1:B:46:TYR:CZ	2.46	0.51
1:A:705:VAL:HA	1:A:739:ARG:HH12	1.76	0.51
1:A:846:TYR:HE1	1:B:256:TYR:HA	1.75	0.51
1:A:1118:PHE:CG	1:A:1148:THR:HG21	2.46	0.51
1:A:1068:VAL:HA	1:A:1078:LEU:HD22	1.93	0.50
1:B:469:TRP:HZ3	1:B:559:VAL:HG21	1.76	0.50
1:A:1442:LEU:HD21	4:A:1702:EDO:H12	1.93	0.50
1:B:186:PRO:HG2	4:B:1701:EDO:H12	1.92	0.50
1:B:311:SER:OG	1:B:312:TYR:N	2.41	0.50
1:B:25:ILE:O	1:B:653:PHE:HA	2.11	0.50
1:A:1179:THR:HG21	1:A:1191:SER:OG	2.12	0.50
1:B:515:ARG:HG3	1:B:526:ILE:HG21	1.94	0.50
1:A:1624:ALA:HB2	1:A:1637:TYR:CD2	2.47	0.50
1:B:144:ARG:NH2	1:B:602:LEU:O	2.43	0.50
1:A:1105:LEU:HA	1:A:1108:VAL:HG22	1.94	0.49
1:A:1543:ILE:HG21	1:A:1548:ARG:HH12	1.77	0.49
1:B:43:VAL:HG23	1:B:79:PHE:HB3	1.93	0.49
2:C:25:HIS:HB3	2:C:27:LEU:HD23	1.94	0.49
1:A:708:ASP:OD2	1:A:1476:ARG:HD2	2.13	0.49
1:A:1323:LEU:HD11	1:A:1340:VAL:HG12	1.94	0.49
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.46	0.49
1:A:766:ARG:HB3	1:B:225:PRO:HG3	1.95	0.49
1:B:315:LEU:HD22	1:B:349:LEU:HD13	1.95	0.48
1:A:857:VAL:HA	1:A:913:SER:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1584:ILE:HG21	1:A:1587:THR:HG23	1.95	0.48
1:A:695:VAL:CG1	1:A:724:CYS:HA	2.44	0.48
1:A:735:ALA:O	1:A:739:ARG:HG3	2.12	0.48
1:B:24:VAL:HG11	1:B:554:LEU:HD21	1.96	0.48
1:A:975:ARG:HB2	1:A:1340:VAL:HG22	1.96	0.48
1:A:1154:LYS:NZ	1:A:1295:GLU:OE2	2.46	0.48
1:A:1187:THR:HA	1:A:1190:ILE:HG22	1.95	0.48
1:B:484:ILE:HG13	1:B:526:ILE:HG13	1.97	0.47
1:A:1543:ILE:HD13	1:A:1548:ARG:NH2	2.30	0.47
1:A:914:LEU:HB3	1:A:921:GLU:HG2	1.97	0.47
1:A:889:GLU:OE2	1:A:889:GLU:N	2.38	0.47
1:B:118:PRO:HB2	6:B:1702:TRS:H12	1.95	0.47
1:B:254:TYR:CE2	1:B:260:VAL:HA	2.49	0.47
1:B:373:VAL:HG11	1:B:435:VAL:HG21	1.96	0.47
1:B:397:VAL:HG23	1:B:427:GLY:O	2.15	0.47
1:B:667:GLU:OE2	6:B:1702:TRS:H32	2.14	0.47
1:B:349:LEU:HG	1:B:446:ASN:HA	1.96	0.47
1:A:1548:ARG:HH11	1:A:1644:TRP:HH2	1.61	0.46
1:B:467:ILE:HD11	1:B:542:VAL:HB	1.96	0.46
1:A:942:VAL:HB	1:A:957:LYS:HD3	1.96	0.46
1:A:949:ILE:HG21	1:A:1307:LEU:HD11	1.97	0.46
1:A:1316:SER:HA	1:A:1323:LEU:H	1.80	0.46
1:A:1402:ILE:HG13	1:A:1479:ILE:HD13	1.97	0.46
1:B:489:LYS:HD3	1:B:489:LYS:HA	1.84	0.46
1:B:243:PHE:CE2	1:B:304:GLU:HB3	2.50	0.46
1:B:504:LEU:HD21	1:B:651:LEU:HG	1.97	0.46
1:A:1612:VAL:HB	1:A:1615:ARG:HD2	1.98	0.46
2:C:33:ILE:HG13	2:C:34:SER:H	1.80	0.46
1:B:320:ASN:HA	1:B:346:LYS:HE2	1.98	0.46
1:A:822:ASP:HB3	1:A:849:ARG:HD3	1.97	0.46
1:A:862:VAL:HG13	1:A:864:GLY:H	1.80	0.46
1:B:25:ILE:HD12	1:B:106:VAL:HG11	1.98	0.46
1:A:1429:PRO:HG2	1:A:1511:THR:HG23	1.98	0.45
2:C:33:ILE:HG23	2:C:35:PRO:HD2	1.99	0.45
1:B:105:GLU:HG3	1:B:114:SER:HB3	1.97	0.45
1:B:470:THR:OG1	1:B:471:ASP:N	2.50	0.45
1:A:821:LYS:HE3	1:B:584:PRO:HD2	1.98	0.45
1:B:469:TRP:HB3	1:B:484:ILE:HG22	1.97	0.45
1:A:1403:VAL:HG12	1:A:1476:ARG:HG2	1.98	0.44
1:A:693:SER:O	1:A:696:LYS:HG3	2.16	0.44
1:A:1008:ALA:HB2	1:A:1059:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ASP:HA	1:B:428:VAL:HA	1.98	0.44
1:B:90:LYS:HD2	1:B:90:LYS:HA	1.71	0.44
1:A:1080:ALA:HB1	1:A:1148:THR:HA	1.98	0.44
1:A:1213:LYS:HE3	1:A:1266:TYR:CZ	2.52	0.44
1:A:697:LYS:HE2	1:A:701:ASP:OD2	2.18	0.44
1:A:861:ALA:HB1	1:A:865:ILE:HB	1.98	0.44
1:A:1083:LEU:HD13	1:A:1104:LEU:HD23	1.99	0.44
1:B:265:VAL:CG2	1:B:292:LEU:HB2	2.46	0.44
1:B:355:ASN:N	1:B:355:ASN:OD1	2.50	0.44
1:A:726:LYS:HG3	1:A:727:ALA:N	2.33	0.44
1:A:780:VAL:HG22	1:A:784:LYS:HB3	1.99	0.44
1:A:823:VAL:HA	1:A:846:TYR:O	2.18	0.43
1:A:1008:ALA:HB2	1:A:1059:TYR:CD2	2.53	0.43
1:B:359:THR:HG21	1:B:372:LYS:H	1.84	0.43
1:A:1426:ILE:HG12	1:A:1493:PHE:CD1	2.53	0.43
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.53	0.43
1:A:998:ASN:O	1:A:1001:THR:HG23	2.18	0.43
1:A:963:ILE:HB	1:A:1627:ILE:HG22	2.01	0.43
1:B:267:ILE:HG13	1:B:327:VAL:HG23	2.00	0.43
2:C:20:ARG:N	2:C:31:PRO:O	2.48	0.43
1:A:755:LYS:O	1:A:759:PRO:HG2	2.19	0.43
1:A:1020:TYR:OH	1:A:1295:GLU:OE1	2.32	0.43
1:B:307:VAL:HG21	1:B:318:LEU:HD11	2.00	0.43
1:A:869:GLU:H	1:A:869:GLU:HG3	1.52	0.42
1:A:1012:LEU:HG	1:A:1056:ILE:HD13	2.01	0.42
1:A:745:LYS:NZ	1:B:291:MET:HE1	2.35	0.42
1:A:1226:ARG:HG2	1:A:1270:VAL:HG22	2.02	0.42
1:B:312:TYR:O	1:B:314:SER:N	2.44	0.42
1:B:304:GLU:HG3	1:B:305:THR:N	2.34	0.42
1:B:232:GLU:HG3	1:B:249:THR:OG1	2.20	0.42
1:A:1329:THR:HG23	1:A:1331:LYS:H	1.84	0.41
1:A:1577:TYR:CE1	1:A:1611:LEU:HB2	2.55	0.41
1:A:823:VAL:HG12	1:A:847:ASN:HA	2.02	0.41
1:A:1076:THR:HG23	1:A:1107:LEU:HD22	2.01	0.41
1:A:1135:VAL:HA	1:A:1138:ARG:HD3	2.01	0.41
1:A:712:GLU:OE1	1:A:712:GLU:N	2.50	0.41
1:A:751:ARG:HB3	1:A:755:LYS:HE3	2.02	0.41
1:B:128:ILE:HB	1:B:215:ALA:HB2	2.03	0.41
1:A:1559:TYR:O	1:A:1620:MET:HA	2.21	0.41
1:A:1585:TYR:CE1	1:A:1668:ALA:HB1	2.56	0.41
1:B:23:TYR:CE1	1:B:656:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ARG:HA	1:A:726:LYS:HG2	2.02	0.41
1:A:995:GLU:H	1:A:995:GLU:HG3	1.41	0.41
1:B:22:THR:HA	1:B:656:ASN:HD21	1.86	0.41
1:A:1551:THR:HG21	1:A:1644:TRP:CD1	2.56	0.41
1:B:469:TRP:CZ3	1:B:559:VAL:HG21	2.56	0.41
1:A:708:ASP:OD2	4:A:1702:EDO:O1	2.39	0.40
1:A:1008:ALA:HB3	1:A:1078:LEU:HD21	2.03	0.40
1:A:1034:PHE:CD2	1:A:1041:GLU:HG3	2.55	0.40
1:A:1564:SER:HB2	1:A:1582:LEU:HD11	2.04	0.40
1:B:166:PRO:HD3	1:B:199:TRP:CD1	2.56	0.40
1:B:518:PHE:HB3	1:B:521:ALA:HB3	2.03	0.40
1:A:765:ILE:HG13	1:A:767:SER:H	1.86	0.40
1:B:253:ARG:HG3	1:B:258:LYS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	963/1676 (58%)	914 (95%)	49 (5%)	0	100	100
1	B	642/1676 (38%)	617 (96%)	25 (4%)	0	100	100
2	C	32/34 (94%)	28 (88%)	4 (12%)	0	100	100
All	All	1637/3386 (48%)	1559 (95%)	78 (5%)	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	857/1484 (58%)	840 (98%)	17 (2%)	48	69
1	B	572/1484 (38%)	557 (97%)	15 (3%)	40	63
2	C	25/25 (100%)	24 (96%)	1 (4%)	28	50
All	All	1454/2993 (49%)	1421 (98%)	33 (2%)	44	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	694	VAL
1	A	696	LYS
1	A	742	ILE
1	A	760	VAL
1	A	761	SER
1	A	782	ARG
1	A	786	LEU
1	A	869	GLU
1	A	995	GLU
1	A	1139	GLU
1	A	1309	LEU
1	A	1323	LEU
1	A	1460	VAL
1	A	1587	THR
1	A	1654	CYS
1	A	1664	LEU
1	A	1669	GLU
1	B	115	LYS
1	B	307	VAL
1	B	367	ILE
1	B	447	GLN
1	B	471	ASP
1	B	530	VAL
1	B	531	THR
1	B	549	GLU
1	B	550	GLN
1	B	623	VAL
1	B	625	GLN
1	B	626	PHE
1	B	628	GLU
1	B	652	THR

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Mol	Chain	Res	Type
1	B	660	ASP
2	C	9	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1098	ASN
1	A	1102	ASN
1	A	1178	ASN
1	A	1204	GLN
1	A	1233	GLN
1	A	1454	GLN

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 ⓘ

3 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	$\# Z > 2$
3	NAG	D	1	3,1	14,14,15	0.44	0	17,19,21	0.48	0
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	0.82	1 (5%)
3	BMA	D	3	3	11,11,12	0.50	0	15,15,17	0.73	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
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	2.15	115.06	112.19

There are no chirality outliers.

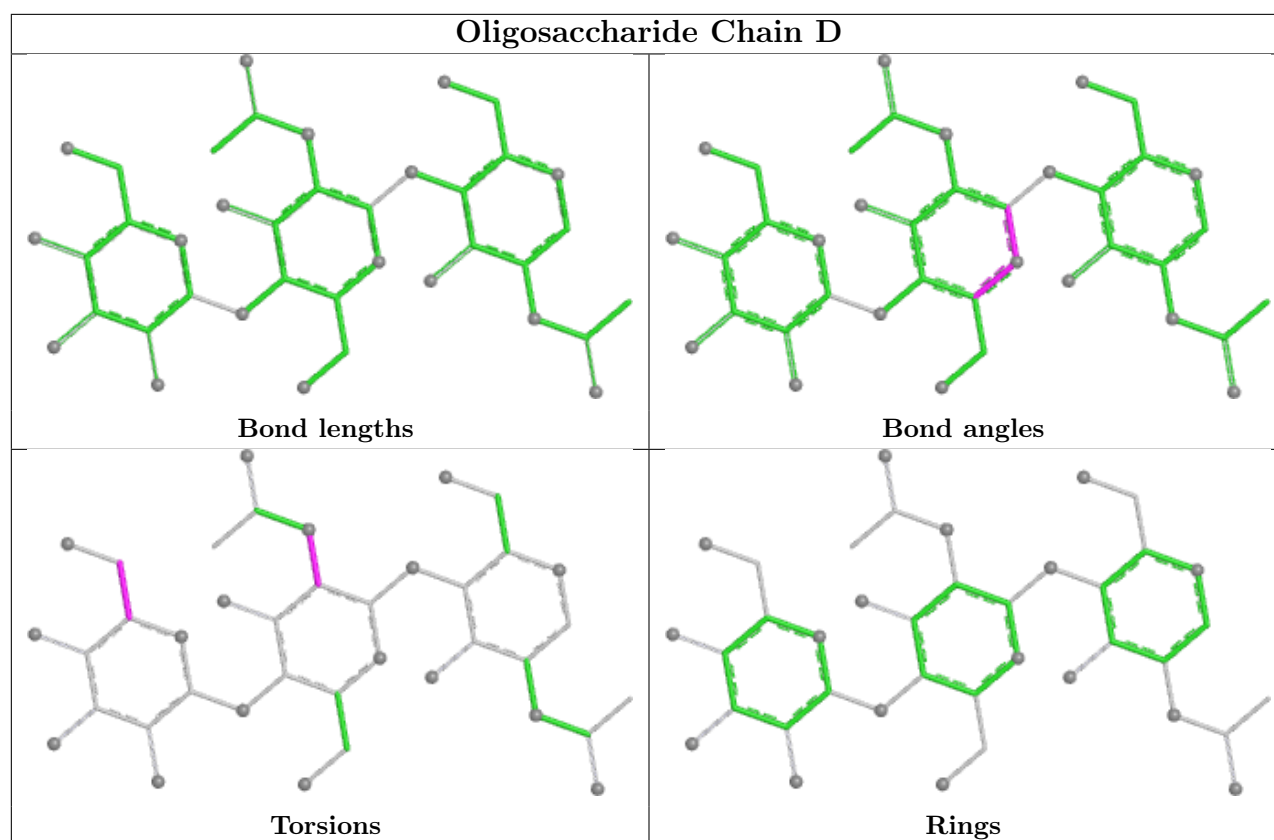
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	3	BMA	O5-C5-C6-O6
3	D	2	NAG	C3-C2-N2-C7
3	D	2	NAG	C1-C2-N2-C7

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](#)

5 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	$\# Z > 2$
4	EDO	B	1701	-	3,3,3	0.43	0	2,2,2	0.33	0
5	CYS	A	1703	1	4,5,6	0.59	0	1,5,7	0.08	0
4	EDO	A	1701	-	3,3,3	0.43	0	2,2,2	0.35	0
6	TRS	B	1702	-	7,7,7	0.35	0	9,9,9	0.30	0
4	EDO	A	1702	-	3,3,3	0.43	0	2,2,2	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	1701	-	-	0/1/1/1	-
5	CYS	A	1703	1	-	0/1/4/6	-
4	EDO	A	1701	-	-	0/1/1/1	-
6	TRS	B	1702	-	-	6/9/9/9	-
4	EDO	A	1702	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

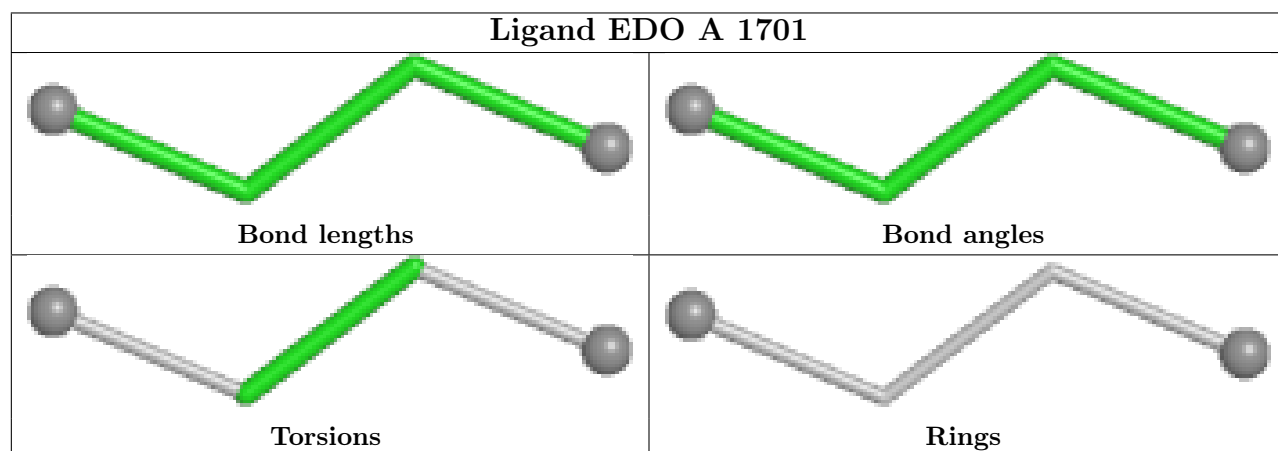
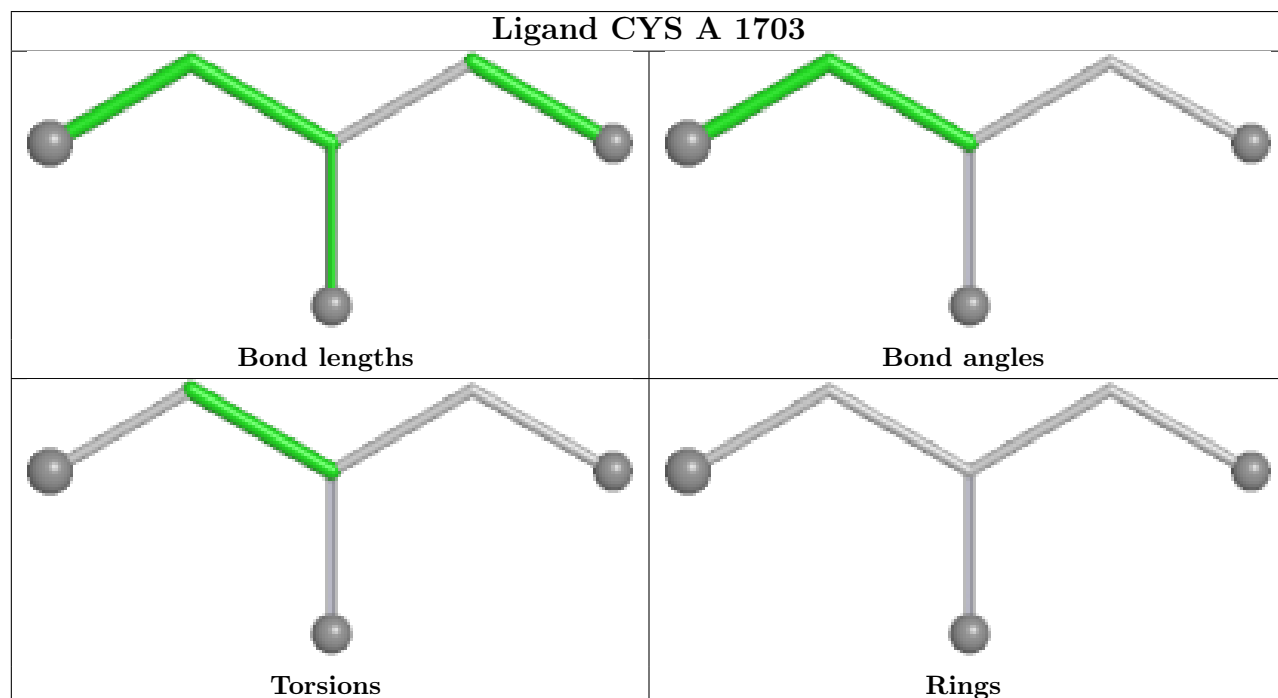
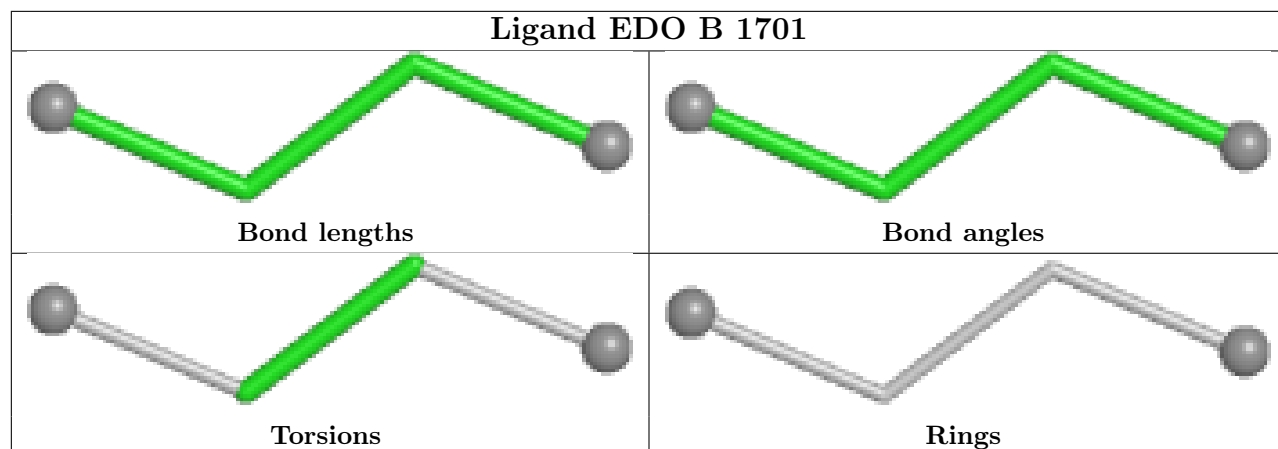
Mol	Chain	Res	Type	Atoms
6	B	1702	TRS	C2-C-C1-O1
6	B	1702	TRS	N-C-C1-O1
6	B	1702	TRS	C3-C-C1-O1
6	B	1702	TRS	N-C-C3-O3
6	B	1702	TRS	C1-C-C3-O3
6	B	1702	TRS	C2-C-C3-O3

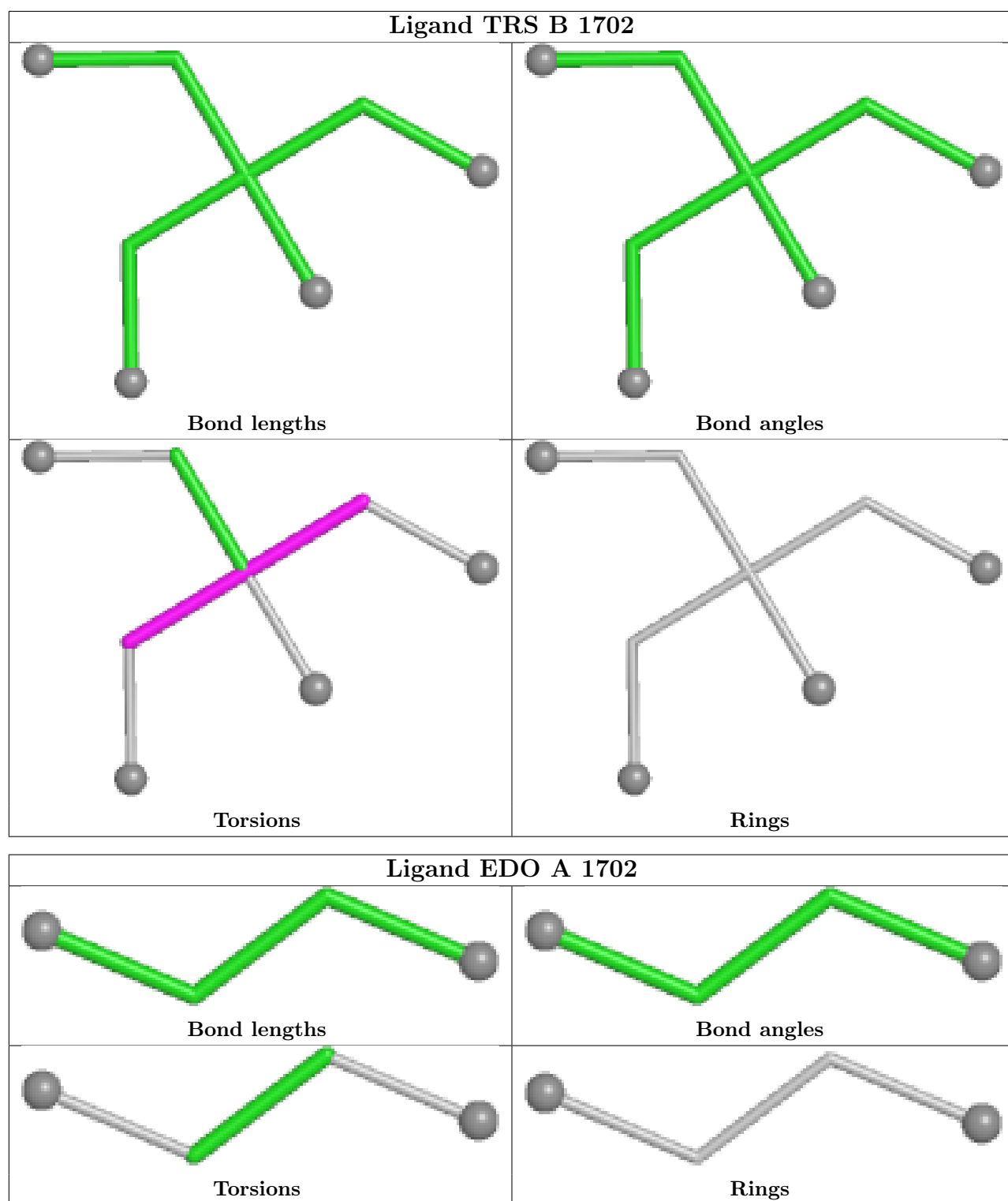
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1701	EDO	1	0
6	B	1702	TRS	2	0
4	A	1702	EDO	2	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	971/1676 (57%)	0.61	78 (8%)	18 18	53, 86, 158, 220	0
1	B	646/1676 (38%)	0.75	76 (11%)	9 7	52, 108, 164, 213	0
2	C	34/34 (100%)	2.19	14 (41%)	0 0	144, 189, 210, 223	0
All	All	1651/3386 (48%)	0.70	168 (10%)	12 11	52, 92, 166, 223	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1388	ALA	6.0
1	B	475	ALA	5.6
1	B	611	GLY	5.4
2	C	15	GLY	5.2
2	C	14	TYR	5.1
1	A	686	ILE	4.8
2	C	13	ILE	4.7
1	A	1519	VAL	4.5
1	B	623	VAL	4.5
1	B	256	TYR	4.3
1	A	920	LYS	4.3
1	A	919	GLY	4.2
1	B	621	GLU	4.1
1	B	474	LYS	4.1
1	A	690	TYR	4.0
1	A	1514	ILE	4.0
1	A	753	HIS	3.9
1	A	1656	SER	3.9
1	A	744	HIS	3.7
1	B	527	ASN	3.6
2	C	12	ALA	3.6
1	A	1307	LEU	3.5
1	A	1335	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	35	PRO	3.5
1	A	950	TYR	3.5
1	A	1131	GLY	3.4
1	A	694	VAL	3.4
1	A	997	ILE	3.4
2	C	28	ASN	3.4
1	B	310	LEU	3.3
1	B	293	ILE	3.3
1	A	754	MET	3.3
1	A	756	THR	3.3
1	A	1133	LEU	3.3
1	A	1676	CYS	3.2
1	B	592	MET	3.2
1	B	336	PHE	3.2
1	B	672	ILE	3.2
1	A	1398	ASP	3.2
1	B	363	LEU	3.1
1	B	557	ASP	3.1
2	C	33	ILE	3.1
1	A	1127	ILE	3.1
1	A	1352	PHE	3.1
1	A	1280	TYR	3.0
1	A	889	GLU	3.0
1	A	1512	SER	3.0
1	A	1062	ALA	3.0
1	A	1515	LYS	2.9
1	A	1543	ILE	2.9
1	B	223	VAL	2.8
2	C	10	GLY	2.8
1	A	1523	ALA	2.8
1	A	1524	ALA	2.8
2	C	11	VAL	2.8
2	C	30	GLY	2.8
1	B	222	TYR	2.8
1	B	425	PRO	2.8
1	B	526	ILE	2.8
1	A	1654	CYS	2.7
1	B	673	LEU	2.7
1	A	890	GLY	2.7
1	A	783	ARG	2.7
1	A	757	LEU	2.7
1	B	261	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	755	LYS	2.7
1	A	1306	GLN	2.7
1	A	1657	CYS	2.7
1	B	61	ASP	2.7
1	A	692	HIS	2.7
1	A	880	SER	2.7
1	B	485	ILE	2.6
1	A	760	VAL	2.6
1	B	465	LEU	2.6
2	C	4	GLU	2.6
1	B	518	PHE	2.6
1	B	626	PHE	2.6
1	A	1386	ILE	2.6
1	A	738	LEU	2.6
1	A	1387	GLU	2.6
1	B	20	GLU	2.6
1	B	383	VAL	2.6
1	A	1516	ILE	2.5
1	A	752	LEU	2.5
1	B	315	LEU	2.5
1	A	850	THR	2.5
1	B	627	LEU	2.5
1	B	674	ARG	2.5
1	B	523	TYR	2.5
2	C	16	TYR	2.5
1	B	624	PHE	2.5
1	B	457	TYR	2.5
1	A	695	VAL	2.5
1	A	1239	VAL	2.5
1	A	1518	LYS	2.5
1	B	423	ASN	2.5
1	B	273	GLU	2.5
1	A	820	PHE	2.5
1	B	470	THR	2.4
1	B	472	ASN	2.4
1	B	287	MET	2.4
1	A	765	ILE	2.4
1	B	382	LEU	2.4
1	B	591	ASN	2.4
1	B	364	LYS	2.4
1	A	1662	ALA	2.4
1	A	851	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	410	VAL	2.4
1	A	848	TYR	2.3
1	B	240	TYR	2.3
1	B	352	TYR	2.3
1	A	741	ASN	2.3
1	A	1513	ASN	2.3
1	B	303	SER	2.3
1	B	588	VAL	2.3
1	A	1545	ALA	2.3
1	A	1585	TYR	2.3
1	A	1240	PRO	2.3
1	B	427	GLY	2.3
1	B	421	VAL	2.3
1	B	404	LEU	2.3
1	B	456	ALA	2.3
1	A	952	THR	2.3
1	A	909	ASN	2.3
2	C	31	PRO	2.3
1	A	747	MET	2.2
1	A	1542	THR	2.2
1	B	312	TYR	2.2
1	A	1522	GLY	2.2
1	B	282	MET	2.2
1	A	763	PRO	2.2
1	B	278	ASP	2.2
1	B	386	VAL	2.2
1	B	484	ILE	2.2
1	B	294	ASN	2.2
1	B	94	GLY	2.2
1	A	1591	VAL	2.2
1	B	486	VAL	2.2
1	B	454	ALA	2.2
1	A	1544	SER	2.2
1	B	455	ILE	2.2
1	A	1134	PRO	2.1
2	C	27	LEU	2.1
1	B	335	GLY	2.1
1	B	511	HIS	2.1
1	B	239	GLY	2.1
1	B	481	HIS	2.1
1	B	573	VAL	2.1
1	A	1537	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1669	GLU	2.1
1	B	305	THR	2.1
1	A	779	LEU	2.1
1	A	1309	LEU	2.1
1	A	1356	LEU	2.1
1	B	424	LEU	2.1
1	B	607	SER	2.1
1	B	482	LEU	2.1
1	A	1110	ASN	2.1
1	A	1231	ASN	2.1
1	B	95	GLY	2.1
1	B	551	THR	2.0
1	A	895	LEU	2.0
1	B	476	LEU	2.0
1	B	416	GLY	2.0
1	A	945	ASP	2.0
1	B	224	LEU	2.0
1	B	467	ILE	2.0
1	B	313	TYR	2.0

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

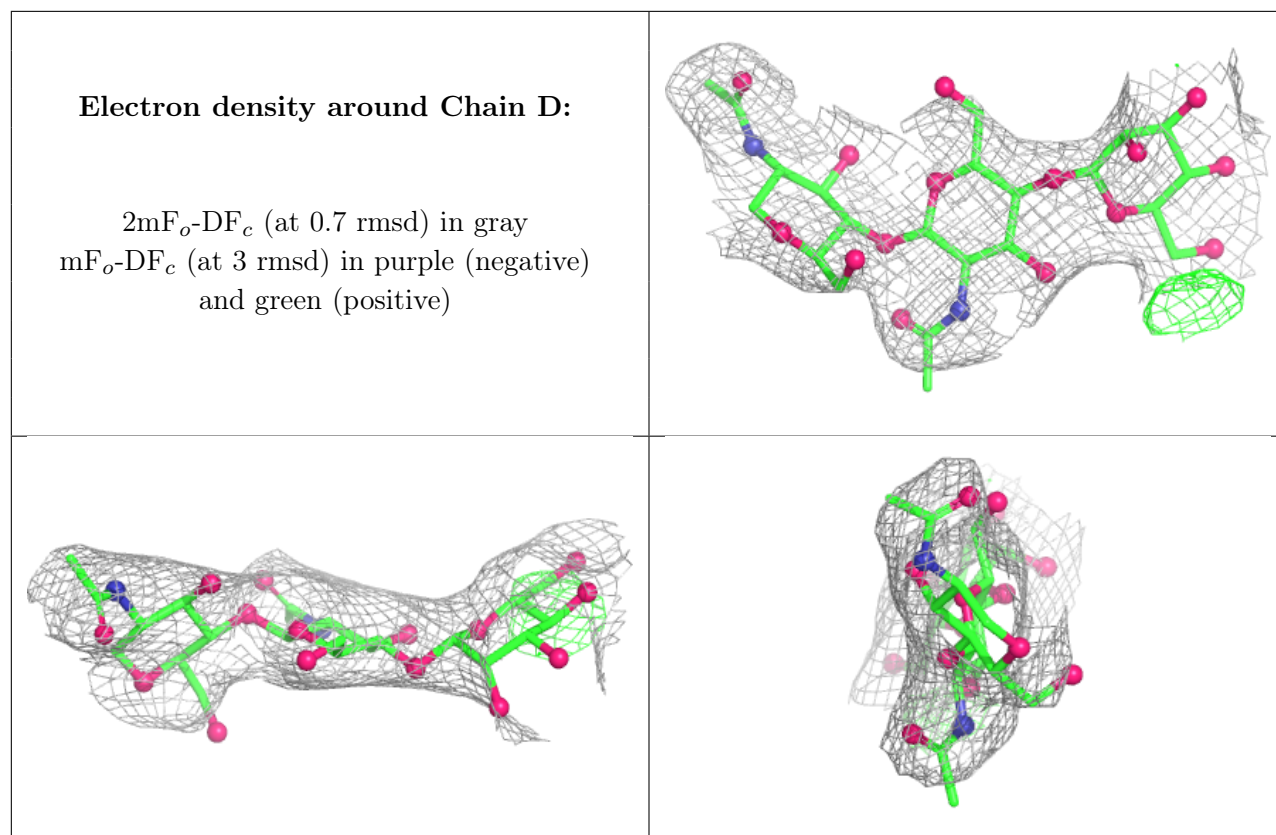
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
3	BMA	D	3	11/12	0.20	0.17	139,153,157,158	0
3	NAG	D	2	14/15	0.81	0.11	113,126,138,148	0
3	NAG	D	1	14/15	0.86	0.13	90,101,122,125	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](#)

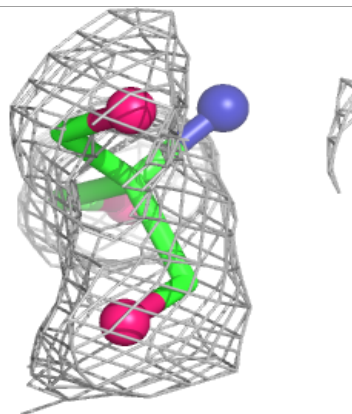
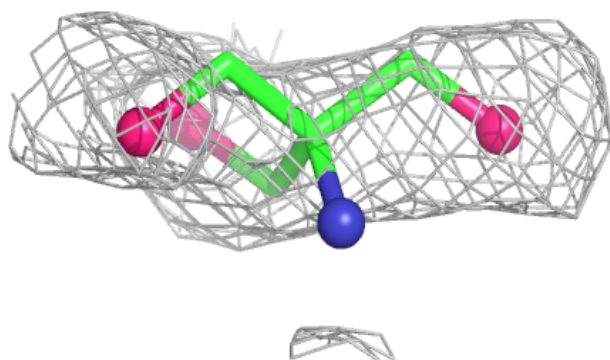
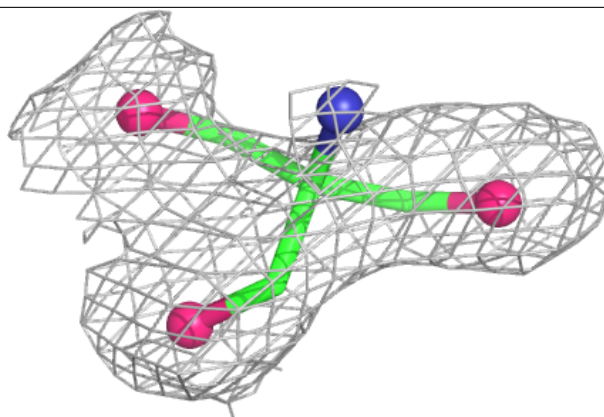
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TRS	B	1702	8/8	0.76	0.20	90,115,131,146	0
4	EDO	A	1701	4/4	0.86	0.28	96,124,137,155	0
5	CYS	A	1703	6/7	0.88	0.16	122,126,130,141	0
4	EDO	A	1702	4/4	0.91	0.21	101,104,121,151	0
4	EDO	B	1701	4/4	0.92	0.16	76,80,81,115	0

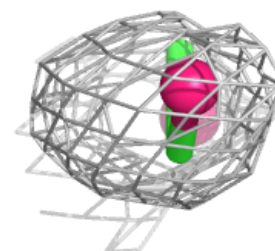
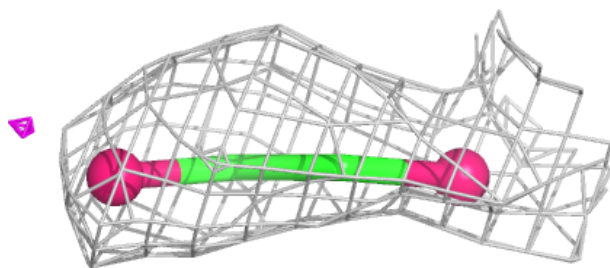
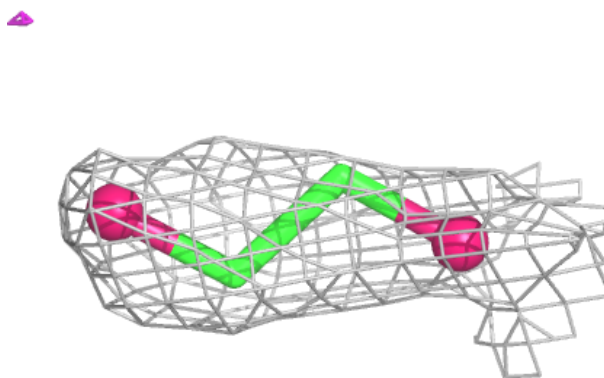
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRS B 1702:

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

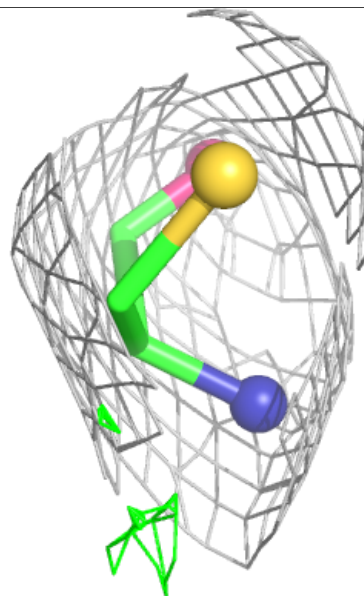
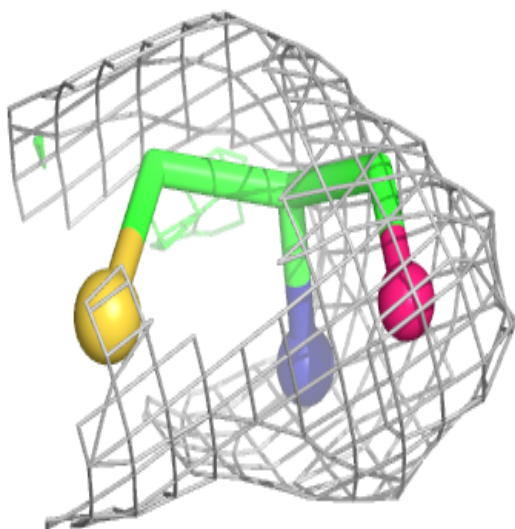
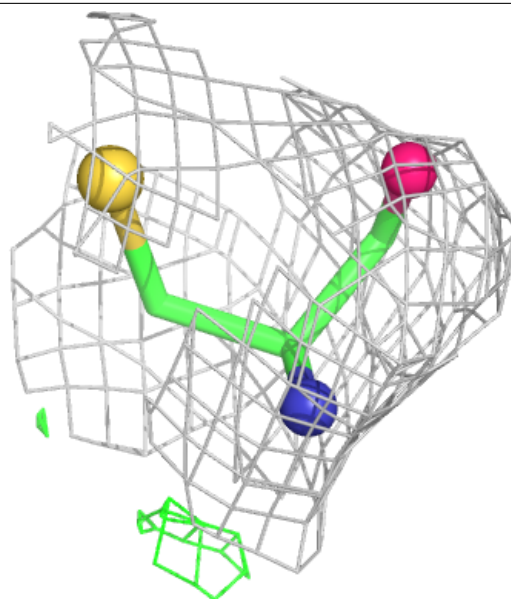
**Electron density around EDO A 1701:**

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



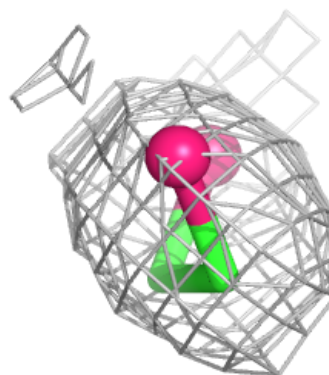
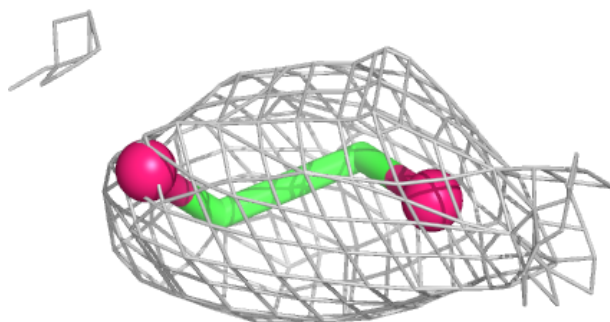
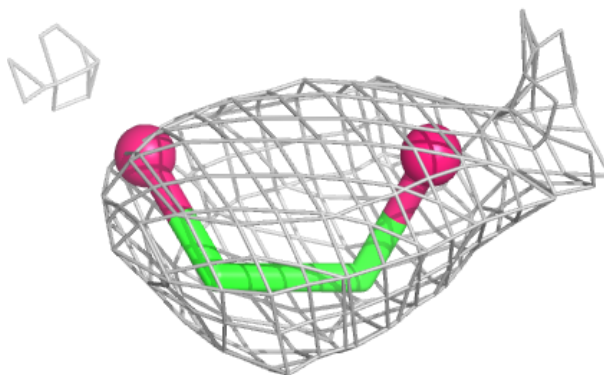
Electron density around CYS A 1703:

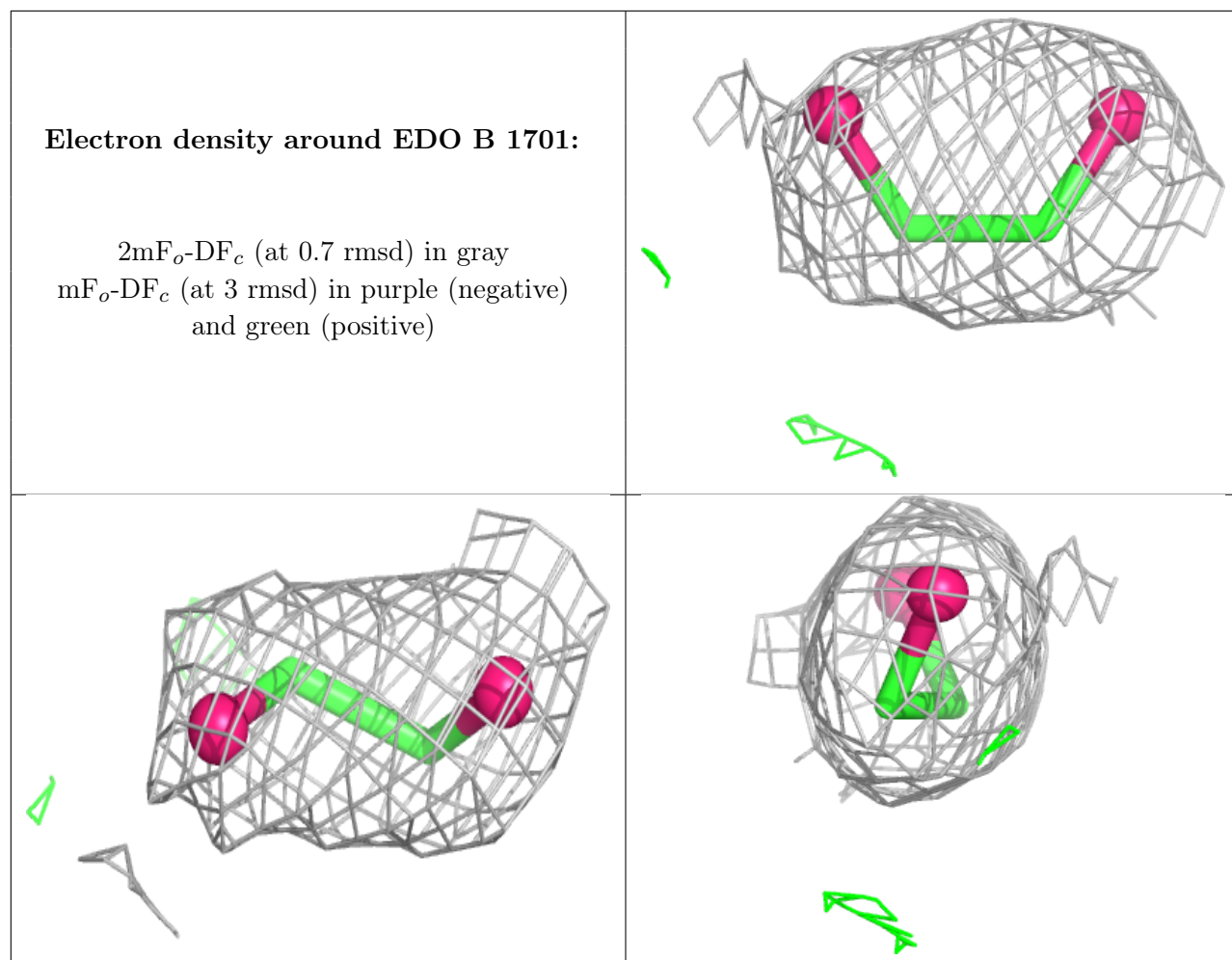
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EDO A 1702:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.