



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:27 PM UTC

PDB ID : 7AD7 / pdb_00007ad7
Title : Crystal structure of human complement C5 in complex with the K8 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 : 2.30 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

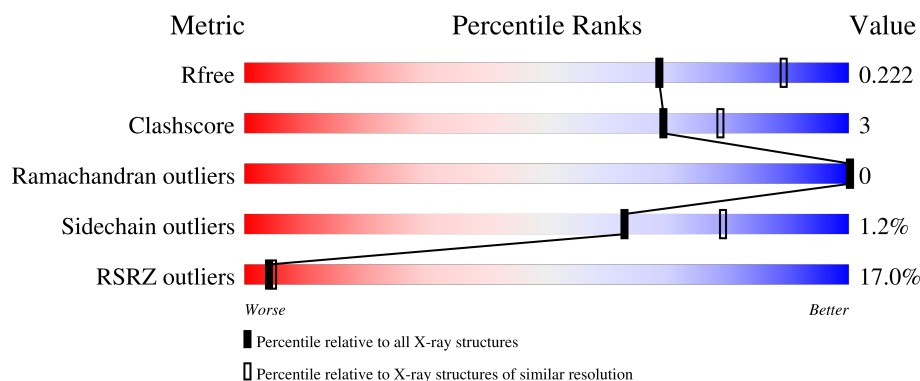
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

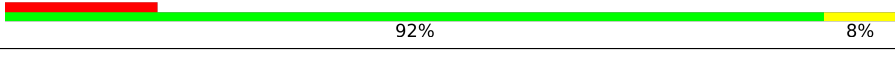
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	
1	B	1676	
2	C	52	
3	D	2	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12100 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	B	635	Total	C	N	O	S	0	1	0
			4998	3211	794	980	13			
1	A	782	Total	C	N	O	S	0	2	0
			6177	3958	1032	1159	28			

- Molecule 2 is a protein called K8 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	52	Total	C	N	O	S	0	2	0
			437	269	80	82	6			

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



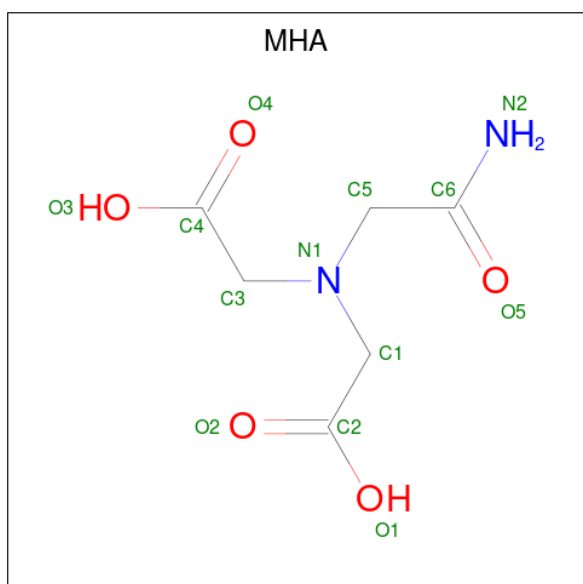
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O) (labeled as "Ligand of Interest" by depositor).



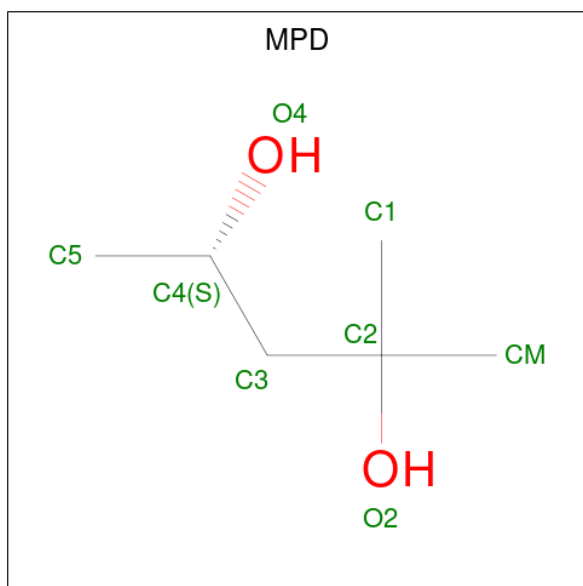
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	2	1		
4	B	1	Total	C	O	0	0
			3	2	1		
4	A	1	Total	C	O	0	0
			3	2	1		
4	C	1	Total	C	O	0	0
			3	2	1		

- Molecule 5 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (CCD ID: MHA) (formula: $C_6H_{10}N_2O_5$) (labeled as "Ligand of Interest" by depositor).



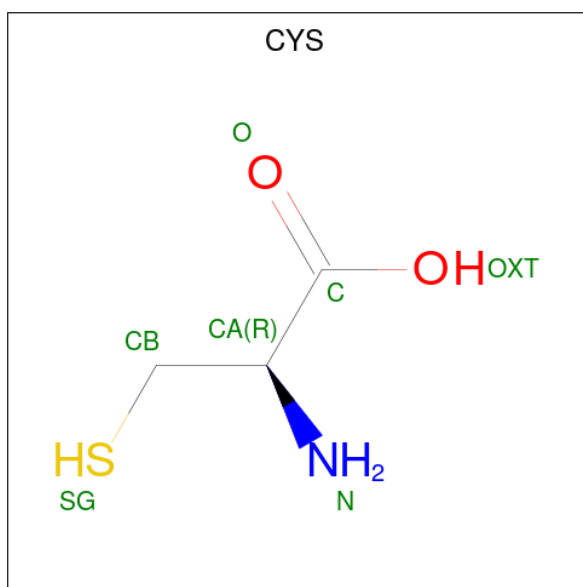
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			13	6	2	5		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$) (labeled as "Ligand of Interest" by depositor).



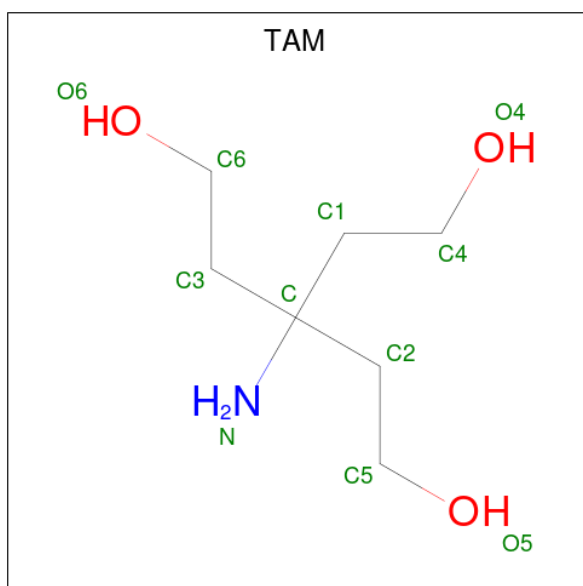
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is CYSTEINE (CCD ID: CYS) (formula: $C_3H_7NO_2S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	7	1	3		

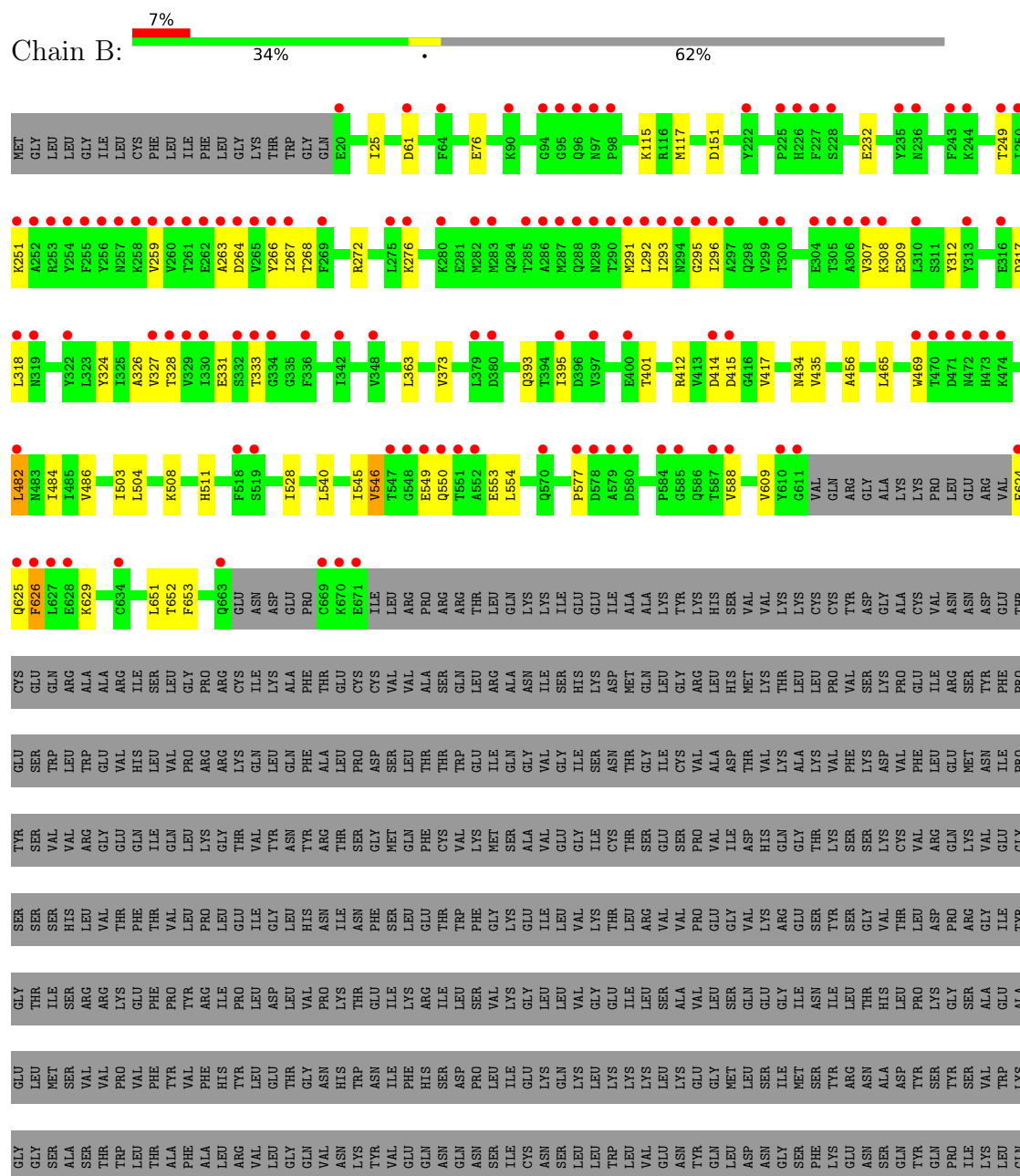
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	160	Total 160	O 160	0	0
9	A	223	Total 223	O 223	0	0
9	C	19	Total 19	O 19	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Complement C5



[illegible]

- Molecule 1: Complement C5

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.56Å 161.69Å 187.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.69 – 2.30 93.69 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (93.69-2.30) 99.9 (93.69-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5, PHENIX 1.18_3845	Depositor
R, R_{free}	0.202 , 0.234 (Not available) , 0.222	Depositor DCC
R_{free} test set	5596 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12100	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: EOH, TAM, MPD, NAG, MHA

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	0.16	0/6309	0.37	0/8554
1	B	0.15	0/5117	0.38	0/6962
2	C	0.16	0/452	0.40	0/611
All	All	0.16	0/11878	0.37	0/16127

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 [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	6177	0	6167	33	1
1	B	4998	0	4888	43	1
2	C	437	0	364	2	0
3	D	28	0	25	1	0
4	A	3	0	6	0	0
4	B	6	0	12	0	0
4	C	3	0	6	0	0
5	B	13	0	8	1	0
6	A	16	0	28	1	0
7	A	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	11	0	17	3	0
9	A	223	0	0	2	0
9	B	160	0	0	1	0
9	C	19	0	0	0	0
All	All	12100	0	11524	81	1

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 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:CYS:SG	9:A:2012:HOH:O	2.42	0.78
1:B:307:VAL:HB	1:B:312:TYR:HB2	1.70	0.72
1:A:833:VAL:HG11	1:A:839:ILE:HD13	1.75	0.68
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.76	0.67
1:A:799:ILE:HB	1:A:815:VAL:HG23	1.76	0.67
1:B:484:ILE:HD13	1:B:540:LEU:HD21	1.78	0.64
1:A:1094:GLU:HB2	6:A:1703:MPD:H51	1.82	0.62
1:B:412:ARG:HB2	1:B:415:ASP:HB2	1.81	0.61
1:A:683:ILE:HA	1:A:686:ILE:HD12	1.87	0.57
1:B:545:ILE:HG12	1:B:554:LEU:HD23	1.87	0.56
1:A:1230:ASP:HB3	1:A:1246:ARG:HG3	1.87	0.56
1:A:858:LYS:NZ	9:A:1804:HOH:O	2.38	0.55
1:B:465:LEU:HD11	1:B:486:VAL:HG13	1.90	0.53
1:B:577:PRO:HD2	1:B:588:VAL:HG23	1.90	0.53
1:B:307:VAL:HG11	1:B:318:LEU:HD11	1.89	0.53
1:A:1047:LYS:HG2	1:A:1051:GLU:OE2	2.09	0.52
1:A:1378:TYR:CZ	1:A:1409:LYS:HD2	2.44	0.52
1:B:115:LYS:HE2	1:B:652:THR:OG1	2.10	0.51
1:B:503:ILE:HB	1:B:511:HIS:HB2	1.93	0.51
1:B:373:VAL:HG21	1:B:435:VAL:HG11	1.93	0.51
1:A:1187:THR:HA	1:A:1190:ILE:HG22	1.93	0.50
1:B:469:TRP:HB3	1:B:484:ILE:HG22	1.93	0.49
1:B:415:ASP:HB3	1:B:417:VAL:HB	1.93	0.49
1:A:1000:LEU:HD11	1:A:1017:PRO:HG3	1.94	0.49
1:B:25:ILE:O	1:B:653:PHE:HA	2.12	0.48
1:B:151:ASP:OD1	1:B:508:LYS:HE3	2.13	0.48
1:A:937:GLU:HG2	1:A:1364:VAL:HG22	1.95	0.48
5:B:1703:MHA:O1	5:B:1703:MHA:HC31	2.13	0.48
1:A:923:LEU:HD21	1:A:925:LYS:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1:NAG:H62	3:D:2:NAG:H82	1.96	0.47
1:A:765:ILE:HG12	1:A:767:SER:H	1.79	0.47
1:B:363:LEU:HB2	1:B:456:ALA:HA	1.97	0.47
1:B:504:LEU:HD11	1:B:651:LEU:HD11	1.96	0.47
2:C:26:TRP:CZ3	8:C:102:TAM:H22	2.50	0.47
2:C:20:PHE:CE2	2:C:22:THR:HG22	2.51	0.46
1:B:549:GLU:H	1:B:549:GLU:CD	2.23	0.46
1:B:264:ASP:OD2	1:B:266:TYR:HE1	1.99	0.46
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.50	0.46
1:A:1412:ARG:O	1:A:1413[A]:GLU:HB2	2.16	0.46
1:B:626:PHE:HD1	1:B:629:LYS:HD3	1.81	0.46
1:B:263:ALA:O	1:B:291:MET:HG2	2.16	0.46
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.51	0.46
1:B:267:ILE:HG12	1:B:327:VAL:HG22	1.98	0.45
1:A:840:GLN:HG2	1:A:1484:GLU:HG2	1.98	0.45
1:B:609:VAL:HG12	1:A:769:PHE:CG	2.52	0.45
1:A:858:LYS:HE3	1:A:883:CYS:HB2	1.98	0.45
1:A:701:ASP:HA	1:A:704:CYS:SG	2.58	0.44
1:A:1111:TYR:CZ	1:A:1121:ASN:HB2	2.52	0.44
1:A:1036:SER:OG	1:A:1037:ASP:N	2.50	0.44
1:A:1129:LEU:HD13	1:A:1139:GLU:HB3	2.00	0.44
1:B:117:MET:HE3	1:B:117:MET:HB3	1.86	0.43
1:A:1320:LYS:HG2	1:A:1342:LEU:HD13	2.00	0.43
1:B:76:GLU:N	1:B:76:GLU:OE1	2.51	0.43
1:A:950:TYR:HE1	1:A:1356:LEU:HD11	1.83	0.43
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.54	0.43
1:B:469:TRP:CD1	1:B:469:TRP:H	2.37	0.43
1:A:781:PRO:C	1:A:783:ARG:H	2.26	0.43
1:B:276:LYS:HA	1:B:276:LYS:HD3	1.84	0.43
1:B:292:LEU:HD21	1:B:295:GLY:HA2	1.99	0.43
1:B:546:VAL:HG23	1:B:553:GLU:HB3	2.01	0.43
1:B:263:ALA:HB3	1:B:292:LEU:HD22	2.01	0.43
1:B:272:ARG:HG3	1:B:324:TYR:HB2	2.01	0.43
8:C:102:TAM:O5	8:C:102:TAM:N	2.52	0.43
1:B:414:ASP:OD1	1:B:415:ASP:N	2.52	0.42
1:B:503:ILE:HD11	1:B:528:ILE:HG21	2.01	0.42
1:B:308:LYS:HE2	1:B:309:GLU:N	2.34	0.42
1:B:251:LYS:HG2	1:B:296:ILE:HD13	2.01	0.42
1:A:837:GLU:O	1:A:902:PRO:HD2	2.20	0.42
1:B:259:VAL:HB	1:B:295:GLY:HA3	2.00	0.42
1:B:232:GLU:HB2	1:B:249:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:GLN:NE2	9:B:1811:HOH:O	2.52	0.41
1:B:395:ILE:HG12	1:B:401:THR:HG22	2.03	0.41
1:B:268:THR:OG1	1:B:326:ALA:HB3	2.21	0.41
1:A:1180:LEU:HA	1:A:1181:PRO:C	2.46	0.41
1:B:266:TYR:HB2	1:B:328:THR:OG1	2.21	0.40
1:A:961:TYR:CZ	1:A:1343:ASN:HB3	2.56	0.40
8:C:102:TAM:H21	8:C:102:TAM:H61	1.50	0.40
1:B:312:TYR:HD1	1:B:317:ASP:HB3	1.87	0.40
1:B:482:LEU:HD21	1:B:484:ILE:HG23	2.03	0.40
1:A:1127:ILE:HD13	1:A:1129:LEU:HG	2.03	0.40
1:B:331:GLU:OE2	1:B:333:THR:OG1	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ASN:OD1	1:A:955:ARG:NH2[3_655]	2.04	0.16

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	774/1676 (46%)	753 (97%)	21 (3%)	0	100	100
1	B	630/1676 (38%)	612 (97%)	18 (3%)	0	100	100
2	C	52/52 (100%)	52 (100%)	0	0	100	100
All	All	1456/3404 (43%)	1417 (97%)	39 (3%)	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	689/1484 (46%)	683 (99%)	6 (1%)	70	84
1	B	558/1484 (38%)	550 (99%)	8 (1%)	59	76
2	C	45/43 (105%)	44 (98%)	1 (2%)	45	65
All	All	1292/3011 (43%)	1277 (99%)	15 (1%)	63	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	ASP
1	B	293	ILE
1	B	482	LEU
1	B	546	VAL
1	B	550	GLN
1	B	624	PHE
1	B	625	GLN
1	B	626	PHE
1	A	694	VAL
1	A	738	LEU
1	A	807	THR
1	A	862	VAL
1	A	1078	LEU
1	A	1127	ILE
2	C	52	GLN

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

Mol	Chain	Res	Type
1	B	21	GLN
1	B	320	ASN
1	B	381	GLN
1	B	391	ASN
1	B	393	GLN
1	B	574	HIS

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Mol	Chain	Res	Type
1	A	854	GLN
1	A	886	GLN
1	A	1102	ASN
1	A	1110	ASN
1	A	1130	GLN
1	A	1343	ASN
1	A	1366	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	$\# Z > 2$
3	NAG	D	1	3,1	14,14,15	0.26	0	17,19,21	0.59	0
3	NAG	D	2	3	14,14,15	0.32	0	17,19,21	1.15	2 (11%)

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	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	2	NAG	C1-O5-C5	3.35	116.68	112.19
3	D	2	NAG	C3-C4-C5	2.59	114.93	110.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

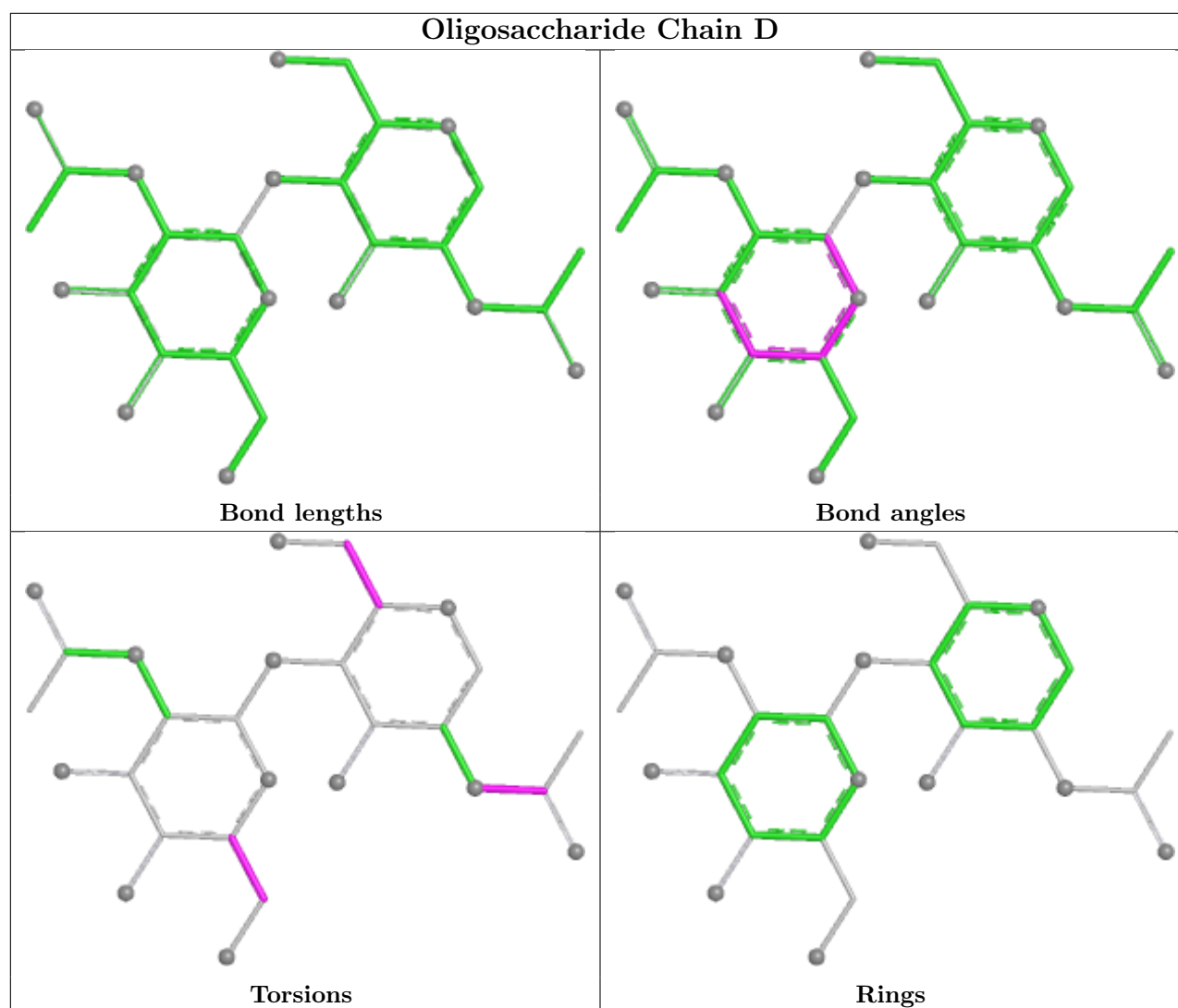
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	NAG	1	0
3	D	1	NAG	1	0

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



5.6 Ligand geometry [i](#)

9 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	EOH	A	1701	-	2,2,2	0.47	0	1,1,1	0.17	0
4	EOH	C	101	-	2,2,2	0.47	0	1,1,1	0.20	0
5	MHA	B	1703	-	12,12,12	1.56	1 (8%)	15,15,15	1.55	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CYS	A	1704	1	4,5,6	0.59	0	1,5,7	0.05	0
6	MPD	A	1703	-	7,7,7	0.28	0	9,10,10	0.42	0
4	EOH	B	1701	-	2,2,2	0.49	0	1,1,1	0.14	0
8	TAM	C	102	-	10,10,10	1.06	1 (10%)	12,12,12	2.10	3 (25%)
4	EOH	B	1702	-	2,2,2	0.46	0	1,1,1	0.18	0
6	MPD	A	1702	-	7,7,7	0.36	0	9,10,10	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MHA	B	1703	-	-	4/12/12/12	-
7	CYS	A	1704	1	-	0/1/4/6	-
8	TAM	C	102	-	-	9/12/12/12	-
6	MPD	A	1703	-	-	5/5/5/5	-
6	MPD	A	1702	-	-	5/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1703	MHA	C6-N2	3.91	1.45	1.32
8	C	102	TAM	C1-C	2.22	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	102	TAM	C4-C1-C	-4.71	110.41	115.97
8	C	102	TAM	C6-C3-C	-3.74	111.56	115.97
8	C	102	TAM	C5-C2-C	-3.69	111.61	115.97
5	B	1703	MHA	O1-C2-C1	2.75	124.24	113.38
5	B	1703	MHA	O1-C2-O2	-2.19	117.69	123.33

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1703	MHA	N1-C3-C4-O3
5	B	1703	MHA	N1-C3-C4-O4

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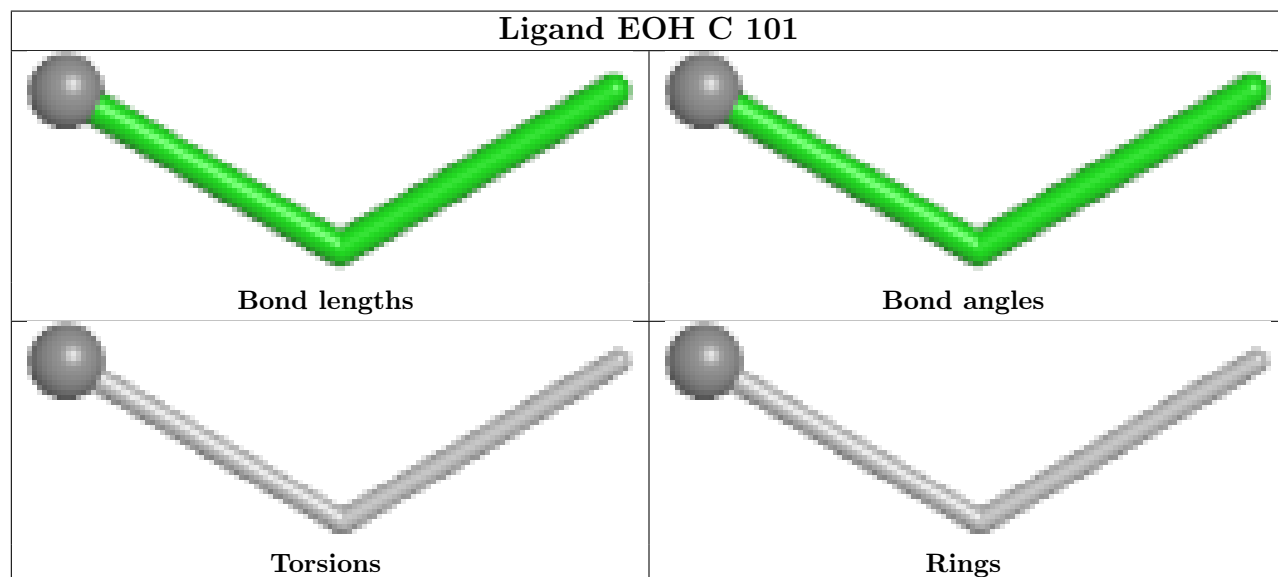
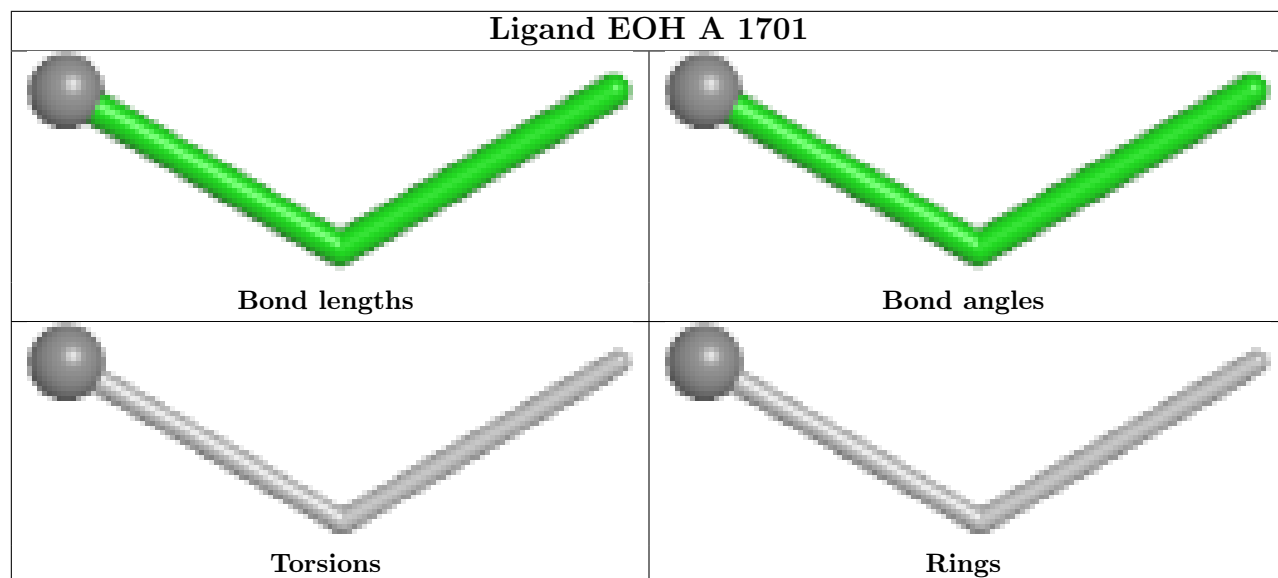
Mol	Chain	Res	Type	Atoms
6	A	1702	MPD	C2-C3-C4-O4
6	A	1702	MPD	C2-C3-C4-C5
6	A	1703	MPD	C1-C2-C3-C4
6	A	1703	MPD	C2-C3-C4-O4
6	A	1703	MPD	C2-C3-C4-C5
8	C	102	TAM	C3-C-C1-C4
8	C	102	TAM	N-C-C1-C4
8	C	102	TAM	C1-C-C2-C5
8	C	102	TAM	C3-C-C2-C5
8	C	102	TAM	N-C-C2-C5
8	C	102	TAM	C1-C-C3-C6
8	C	102	TAM	C2-C-C3-C6
8	C	102	TAM	N-C-C3-C6
8	C	102	TAM	C2-C-C1-C4
5	B	1703	MHA	C4-C3-N1-C5
5	B	1703	MHA	C2-C1-N1-C3
6	A	1702	MPD	C1-C2-C3-C4
6	A	1702	MPD	CM-C2-C3-C4
6	A	1703	MPD	CM-C2-C3-C4
6	A	1702	MPD	O2-C2-C3-C4
6	A	1703	MPD	O2-C2-C3-C4

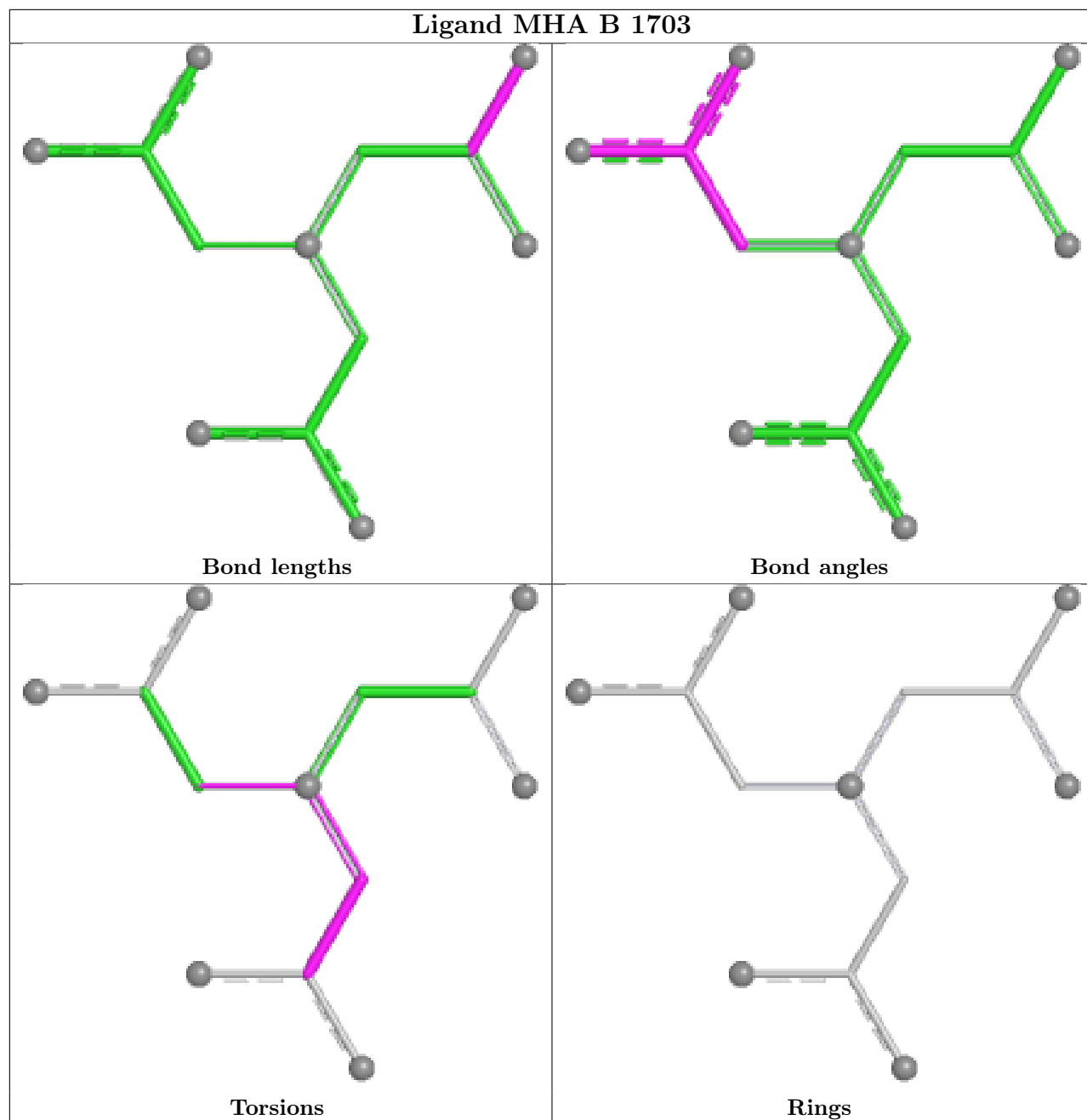
There are no ring outliers.

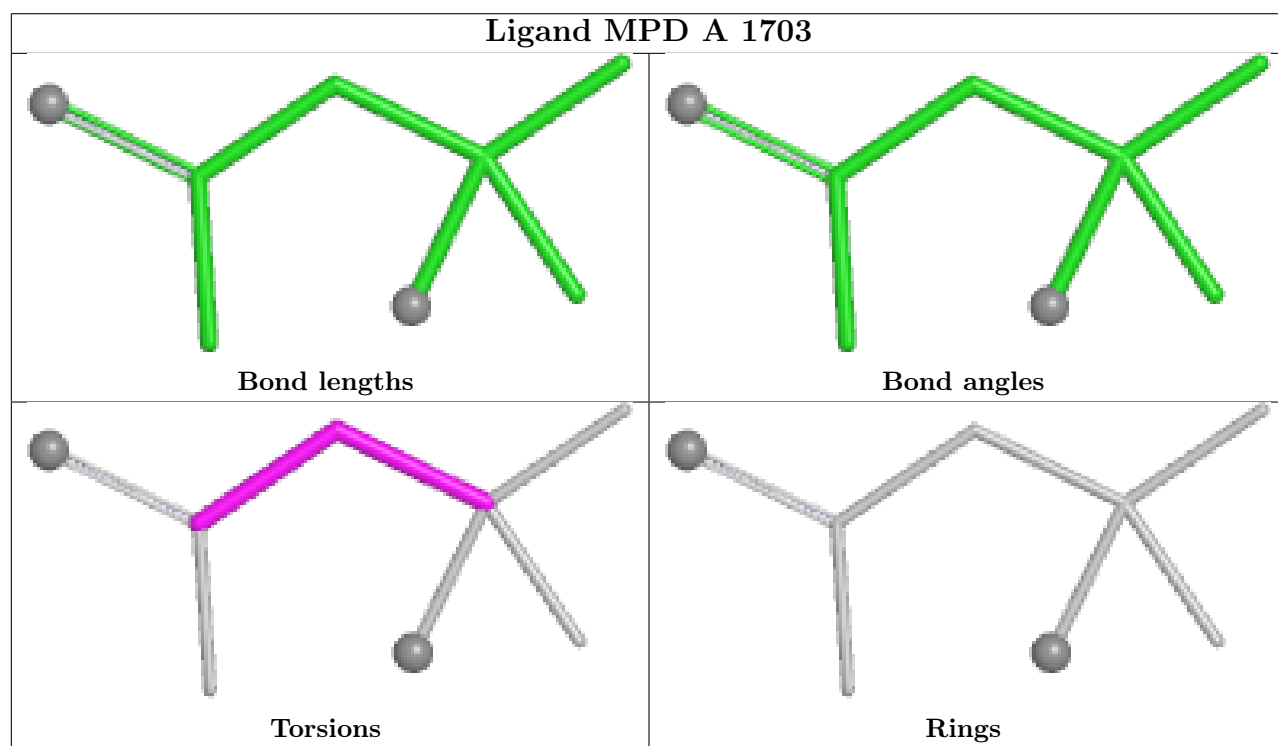
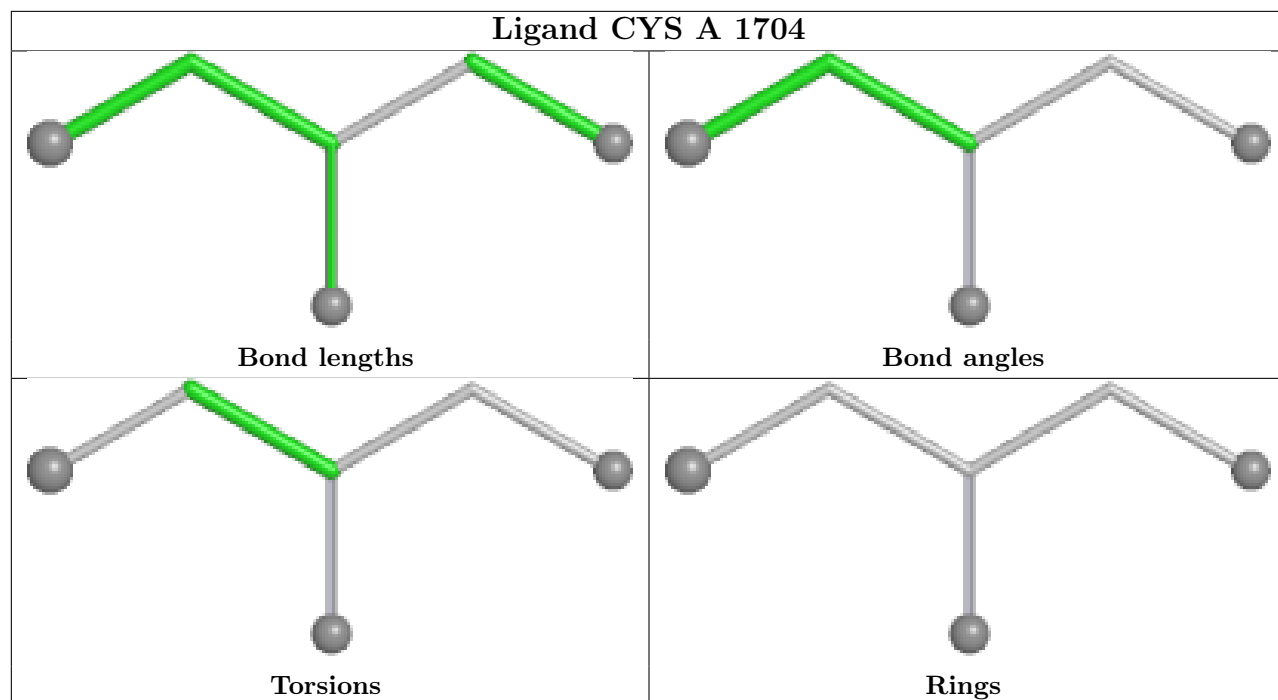
3 monomers are involved in 5 short contacts:

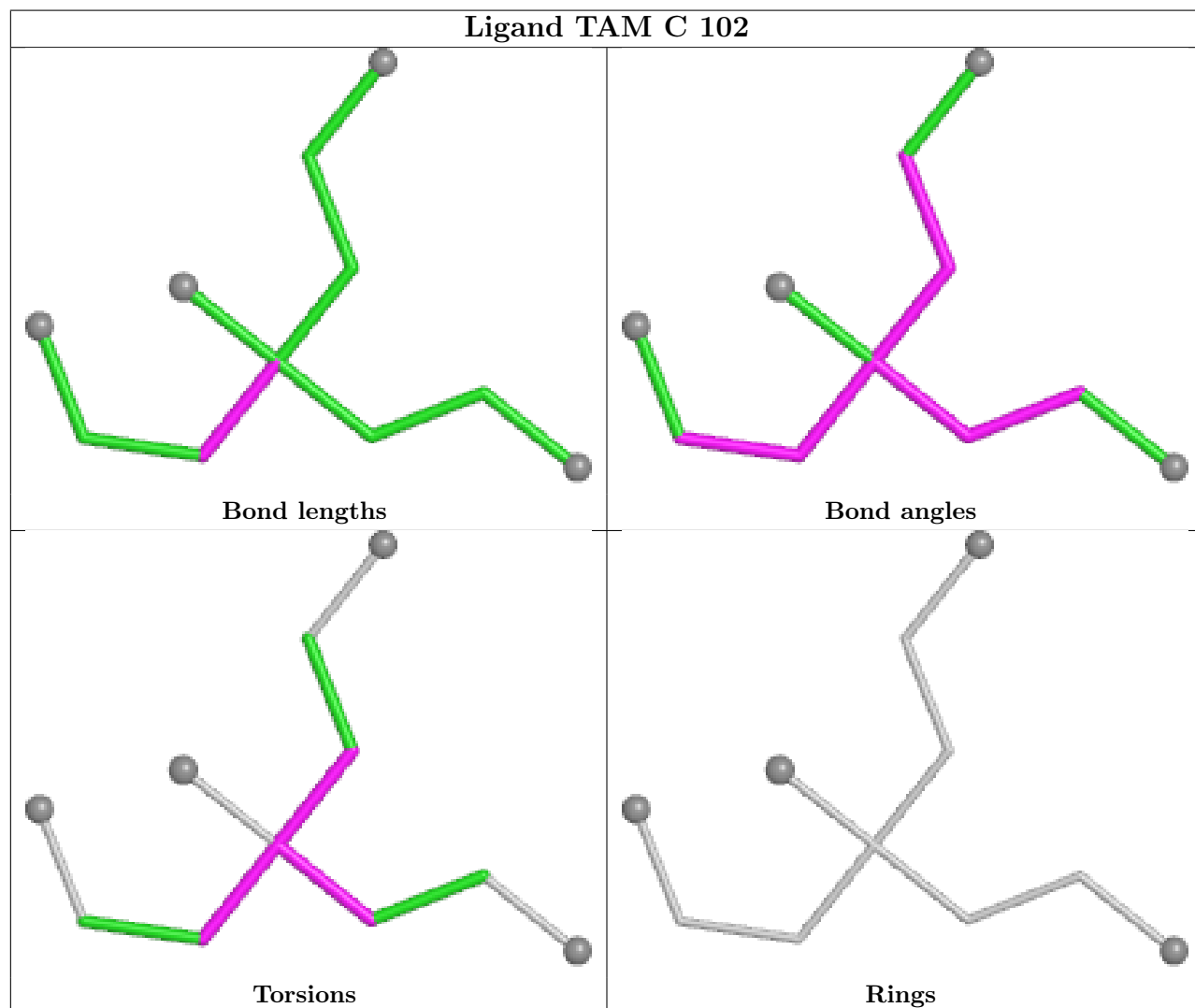
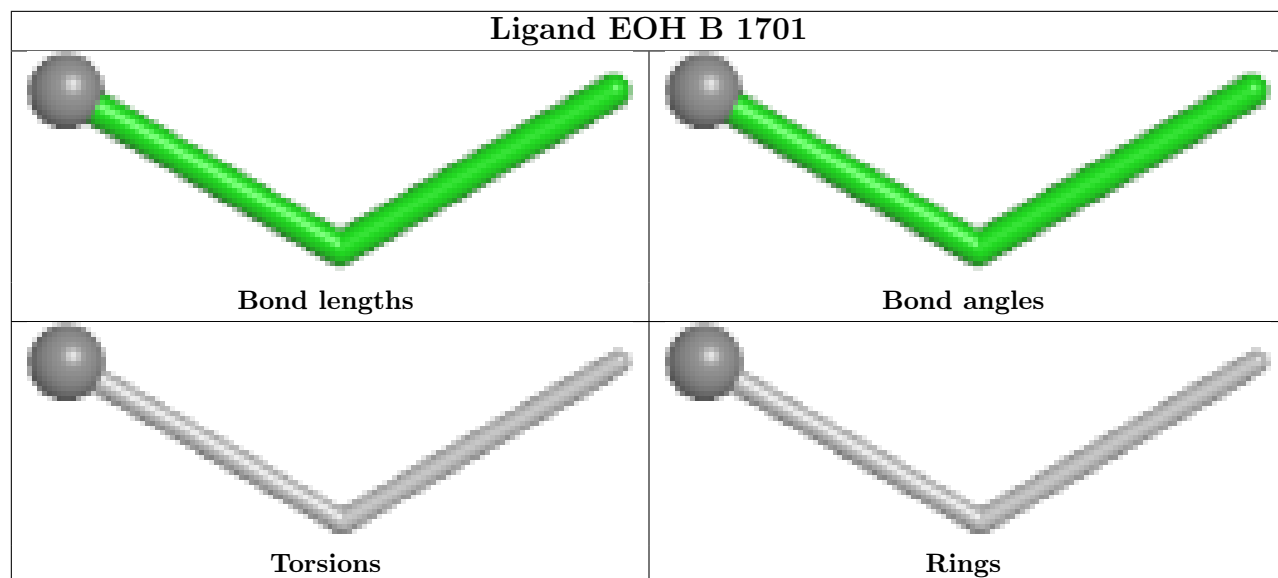
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1703	MHA	1	0
6	A	1703	MPD	1	0
8	C	102	TAM	3	0

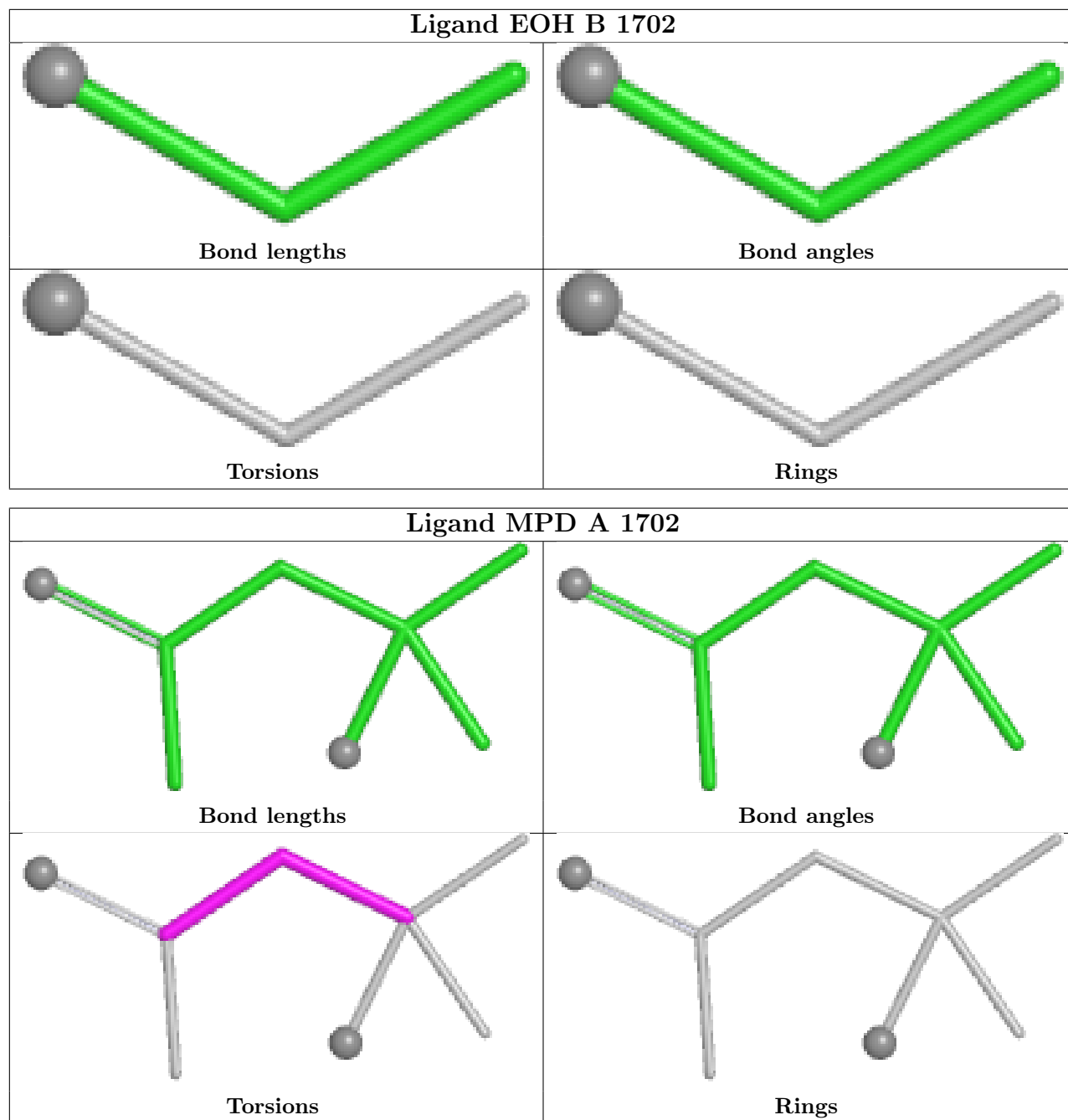
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	782/1676 (46%)	0.72	118 (15%) 5 6	30, 57, 108, 171	2 (0%)
1	B	635/1676 (37%)	0.95	122 (19%) 3 3	31, 59, 131, 153	1 (0%)
2	C	52/52 (100%)	0.53	9 (17%) 4 4	29, 46, 80, 108	2 (3%)
All	All	1469/3404 (43%)	0.81	249 (16%) 4 5	29, 58, 120, 171	5 (0%)

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	TYR	9.5
1	B	255	PHE	8.2
1	A	683	ILE	8.1
1	A	1399	TYR	8.0
1	B	624	PHE	7.4
1	A	994	GLN	7.1
1	A	1398	ASP	7.0
1	A	999	ILE	6.9
1	A	740	ALA	6.8
1	A	1480	PHE	6.8
1	B	669	CYS	6.5
1	B	254	TYR	6.5
1	A	694	VAL	5.9
1	B	627	LEU	5.7
1	B	286	ALA	5.7
1	B	257	ASN	5.6
1	B	261	THR	5.6
1	A	896	VAL	5.6
1	A	686	ILE	5.5
1	A	1484	GLU	5.1
1	B	469	TRP	5.0
1	A	862	VAL	4.8
1	A	897	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	738	LEU	4.7
1	A	861	ALA	4.6
1	B	550	GLN	4.6
1	B	259	VAL	4.5
1	A	1413[A]	GLU	4.5
1	B	253	ARG	4.5
1	A	762	LYS	4.3
1	B	379	LEU	4.3
1	B	95	GLY	4.3
1	A	722	PRO	4.3
1	B	313	TYR	4.2
2	C	51	PHE	4.2
1	A	1324	HIS	4.2
1	A	895	LEU	4.2
1	B	260	VAL	4.2
1	B	578	ASP	4.2
1	B	328	THR	4.2
1	A	965	LEU	4.1
1	B	548	GLY	4.1
1	B	577	PRO	4.1
1	B	551	THR	4.1
1	B	625	GLN	4.1
1	A	695	VAL	4.1
1	B	258	LYS	4.0
1	B	549	GLU	4.0
1	B	587	THR	4.0
1	A	882	LYS	4.0
1	B	626	PHE	4.0
2	C	20	PHE	4.0
1	B	94	GLY	3.9
1	B	266	TYR	3.9
1	B	588	VAL	3.9
1	A	687	ALA	3.9
1	B	470	THR	3.9
1	B	64	PHE	3.9
1	A	688	ALA	3.9
1	B	262	GLU	3.9
1	A	918	PHE	3.8
1	B	296	ILE	3.8
1	B	336	PHE	3.8
1	B	473	HIS	3.8
1	B	611	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	720	LEU	3.8
1	A	1239	VAL	3.8
1	A	1482	LEU	3.8
1	B	319	ASN	3.7
1	B	265	VAL	3.7
1	A	820	PHE	3.7
1	B	628	GLU	3.7
1	A	1199	ASP	3.7
1	A	723	ARG	3.7
1	A	735	ALA	3.7
1	B	330	ILE	3.6
1	B	264	ASP	3.6
1	B	333	THR	3.6
1	B	293	ILE	3.6
1	B	285	THR	3.6
1	B	332	SER	3.5
1	A	789	ALA	3.5
1	B	580	ASP	3.5
1	A	721	GLY	3.5
1	B	90	LYS	3.5
1	B	97	ASN	3.5
1	B	244	LYS	3.4
1	A	1237	SER	3.4
1	B	471	ASP	3.4
1	B	96	GLN	3.4
1	B	305	THR	3.4
1	A	920	LYS	3.4
1	A	1412	ARG	3.4
1	B	299	VAL	3.4
1	A	692	HIS	3.4
1	B	472	ASN	3.4
1	A	1173	ASN	3.4
1	A	1387	GLU	3.3
1	B	395	ILE	3.3
2	C	19[A]	ARG	3.3
1	A	700	TYR	3.3
1	B	663	GLN	3.3
1	A	843	GLY	3.3
1	A	840	GLN	3.3
2	C	52	GLN	3.3
1	B	287	MET	3.2
1	A	1400	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	36[A]	HIS	3.2
1	A	791	PRO	3.2
1	A	690	TYR	3.2
1	B	282	MET	3.2
1	A	966	ASP	3.1
1	A	1513	ASN	3.1
1	A	739	ARG	3.1
1	A	1386	ILE	3.1
1	B	547	THR	3.1
1	A	924	VAL	3.1
1	B	98	PRO	3.1
1	B	482	LEU	3.1
1	A	898	PHE	3.1
1	B	397	VAL	3.1
1	A	705	VAL	3.1
1	B	579	ALA	3.0
1	A	1206	ARG	3.0
1	B	227	PHE	3.0
1	B	297	ALA	3.0
1	B	671	GLU	3.0
1	B	275	LEU	3.0
1	B	307	VAL	3.0
1	B	283	MET	3.0
1	A	1039	LEU	2.9
1	B	290	THR	2.9
1	A	1238	SER	2.9
1	A	1481	GLU	2.9
1	A	919	GLY	2.9
1	A	1487	PHE	2.9
1	A	922	ILE	2.9
1	A	972	GLU	2.9
1	B	294	ASN	2.9
1	A	885	ARG	2.8
1	B	225	PRO	2.8
1	A	768	TYR	2.8
2	C	49	LEU	2.8
1	B	263	ALA	2.8
1	B	318	LEU	2.7
1	A	794	LEU	2.7
1	A	831	TYR	2.7
1	B	518	PHE	2.7
1	B	61	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	2.7
1	B	415	ASP	2.7
1	A	697	LYS	2.7
1	B	228	SER	2.7
1	B	291	MET	2.7
1	B	308	LYS	2.6
1	A	787	GLN	2.6
1	A	970	LYS	2.6
1	A	1385	ASP	2.6
1	B	249	THR	2.6
1	A	793	SER	2.6
1	B	276	LYS	2.6
1	A	893	SER	2.6
1	B	288	GLN	2.5
2	C	48	ASN	2.5
1	A	1512	SER	2.5
1	A	1326	TYR	2.5
1	B	295	GLY	2.5
1	A	1335	GLY	2.5
1	A	1001	THR	2.5
1	B	380	ASP	2.5
1	B	334	GLY	2.5
1	B	519	SER	2.5
1	A	917	TRP	2.5
1	B	235	TYR	2.5
1	B	236	ASN	2.5
1	A	864	GLY	2.5
1	B	243	PHE	2.4
1	B	250	ILE	2.4
1	A	1000	LEU	2.4
1	A	1035	HIS	2.4
1	B	306	ALA	2.4
1	B	269	PHE	2.4
1	B	329	VAL	2.4
1	B	342	ILE	2.4
1	A	790	LEU	2.4
1	A	1341	LEU	2.4
1	A	909	ASN	2.4
1	A	1322	ALA	2.4
1	A	1044	LYS	2.4
1	B	327	VAL	2.4
1	A	733	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1321	GLY	2.4
1	B	280	LYS	2.4
1	B	585	GLY	2.3
1	A	736	SER	2.3
1	A	765	ILE	2.3
1	A	907	LEU	2.3
1	B	20	GLU	2.3
1	B	226	HIS	2.3
1	A	883	CYS	2.3
1	A	1265	ASN	2.3
1	A	703	ALA	2.3
2	C	1	SER	2.3
1	A	684	GLU	2.3
1	A	1331	LYS	2.3
1	B	634	CYS	2.3
1	A	1202	HIS	2.3
1	B	570[A]	GLN	2.3
1	A	734	VAL	2.3
1	A	792	ASP	2.2
1	B	300	THR	2.2
1	A	848	TYR	2.2
1	A	865	ILE	2.2
1	A	1483	PHE	2.2
1	B	252	ALA	2.2
1	B	610	TYR	2.2
1	B	414	ASP	2.2
1	B	552	ALA	2.2
1	A	867	THR	2.2
1	A	993	SER	2.2
1	B	222	TYR	2.2
1	A	846	TYR	2.2
1	A	982	LEU	2.1
1	B	289	ASN	2.1
1	A	1235	LYS	2.1
1	A	969	PRO	2.1
1	A	1036	SER	2.1
1	B	292	LEU	2.1
1	B	310	LEU	2.1
1	B	670	LYS	2.1
1	A	828	ASN	2.1
1	A	863	GLU	2.1
1	A	1325	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	729	THR	2.1
1	B	304	GLU	2.1
1	B	316	GLU	2.1
2	C	50	TYR	2.1
1	A	685	GLU	2.1
1	B	322	TYR	2.1
1	A	763	PRO	2.1
1	A	962	ARG	2.1
1	B	251	LYS	2.0
1	A	691	LYS	2.0
1	B	400	GLU	2.0
1	A	718	ILE	2.0
1	B	584	PRO	2.0
1	B	474	LYS	2.0
1	A	726	LYS	2.0
1	B	267	ILE	2.0

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

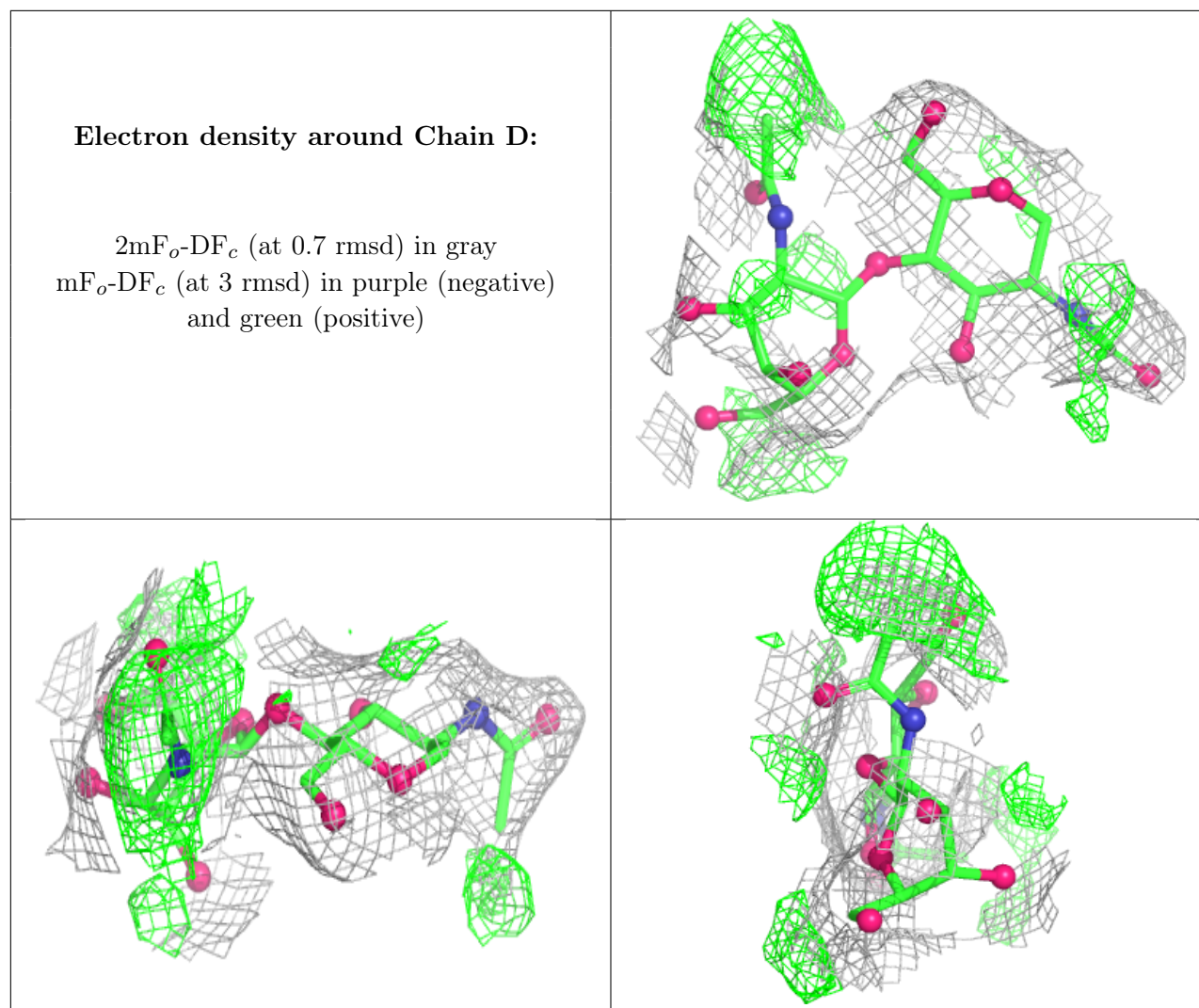
There are no non-standard protein/DNA/RNA residues in this entry.

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	NAG	D	2	14/15	0.20	0.20	96,123,129,130	0
3	NAG	D	1	14/15	0.68	0.18	96,104,116,122	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.

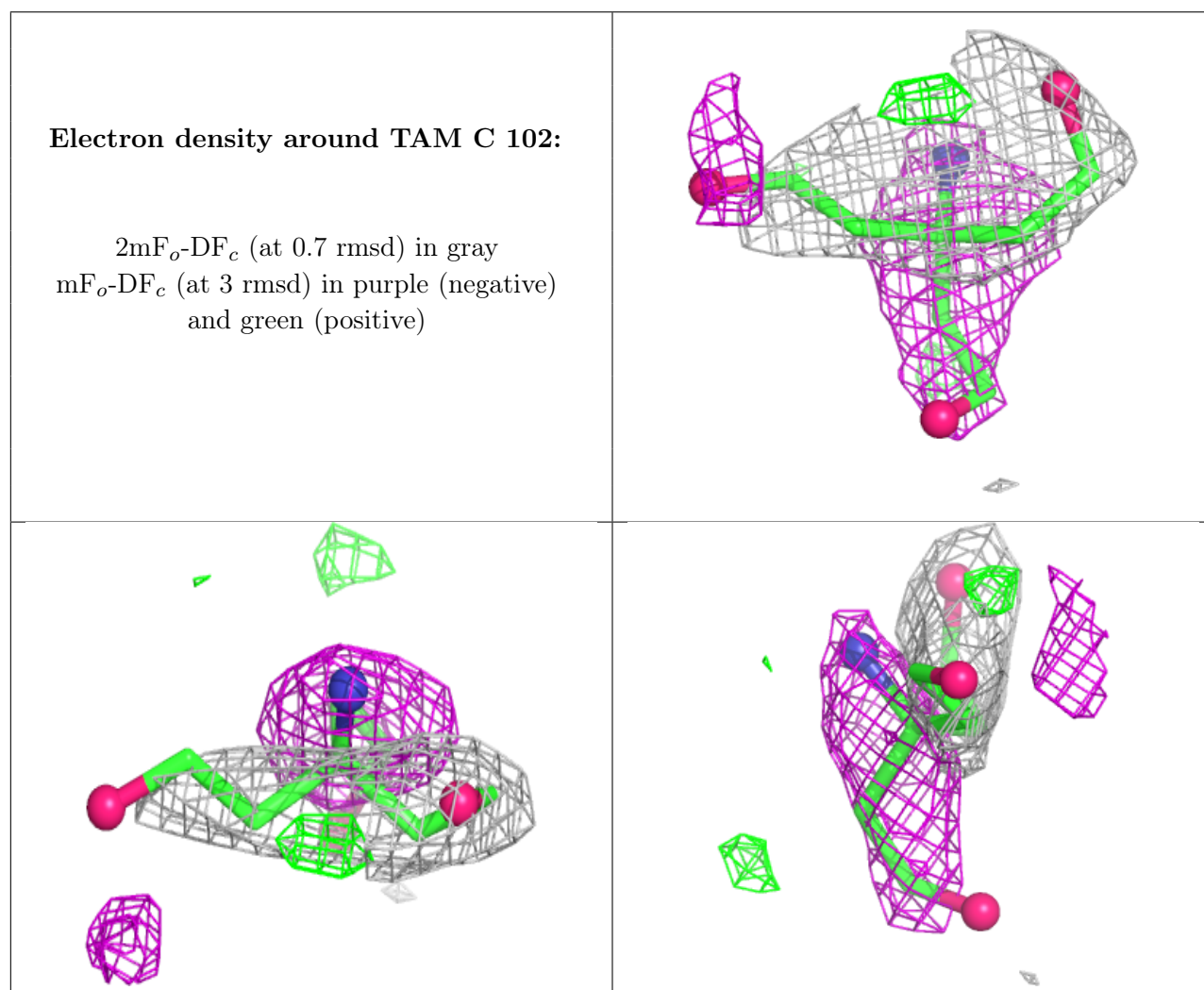
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	TAM	C	102	11/11	0.48	0.29	77,84,105,110	0
4	EOH	B	1701	3/3	0.60	0.31	55,55,66,68	0
7	CYS	A	1704	6/7	0.62	0.24	121,123,125,134	0
6	MPD	A	1703	8/8	0.67	0.29	74,82,91,91	0
4	EOH	C	101	3/3	0.78	0.20	49,49,60,74	0
4	EOH	A	1701	3/3	0.78	0.36	65,65,66,68	0
4	EOH	B	1702	3/3	0.79	0.28	69,69,70,74	0
6	MPD	A	1702	8/8	0.81	0.28	58,63,72,84	0

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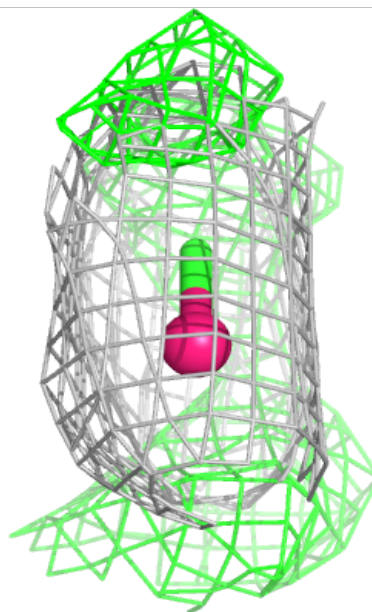
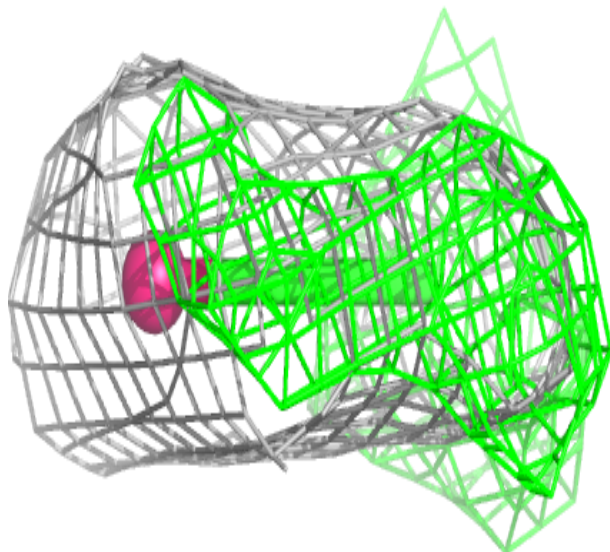
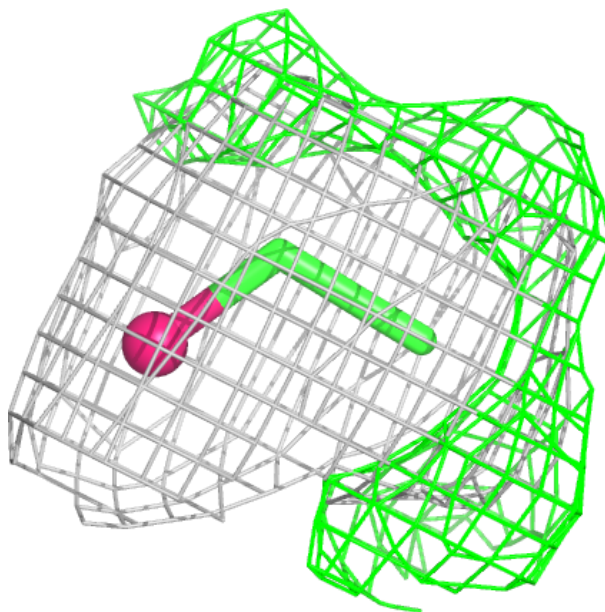
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MHA	B	1703	13/13	0.84	0.13	53,59,82,89	0

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.



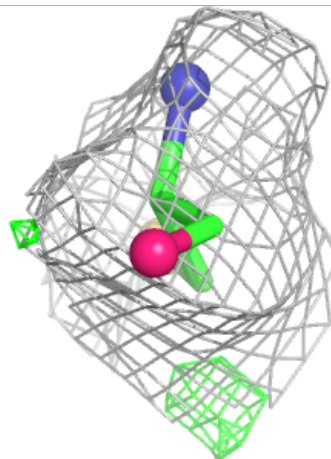
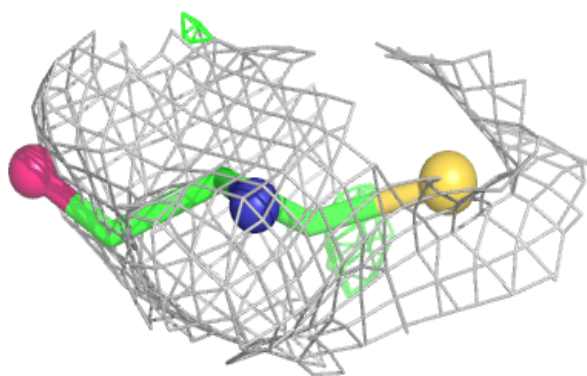
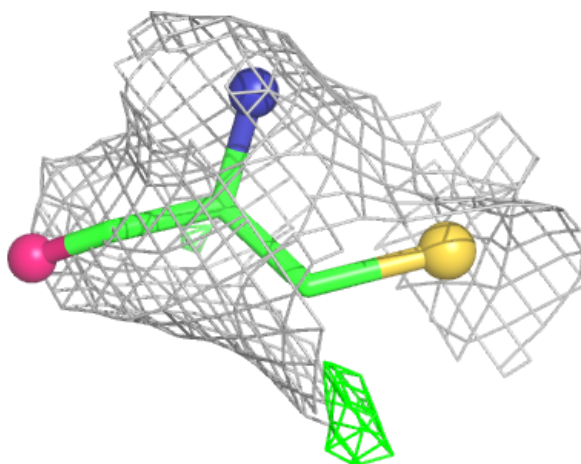
Electron density around EOH B 1701:

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



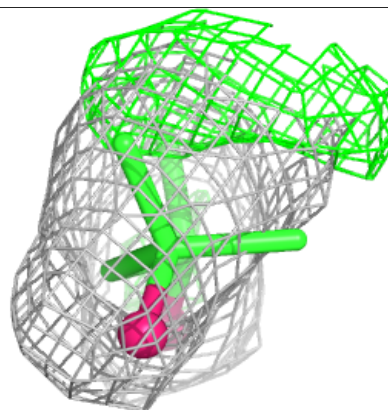
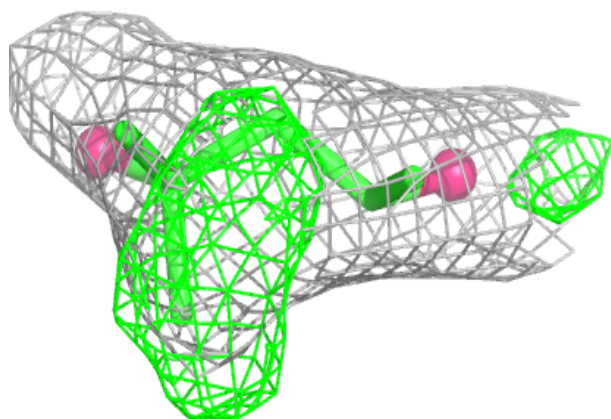
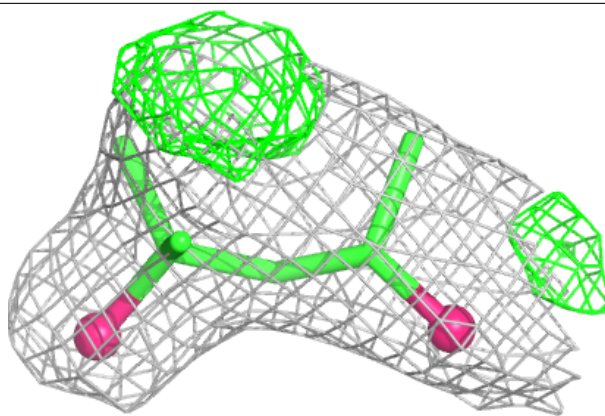
Electron density around CYS A 1704:

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



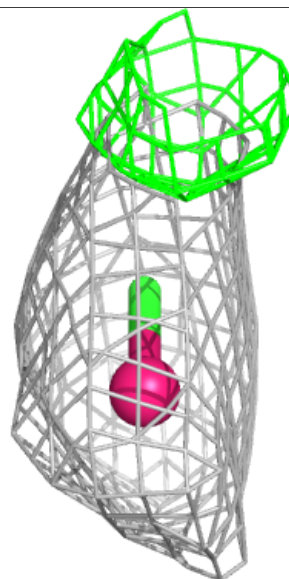
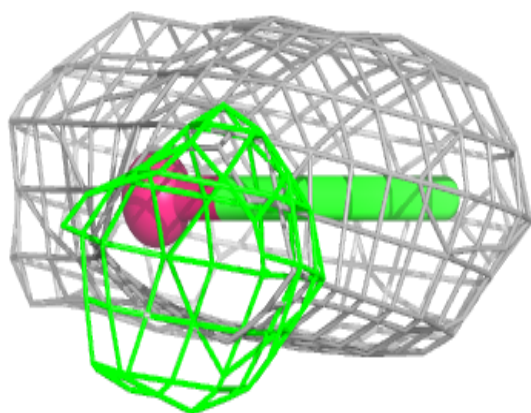
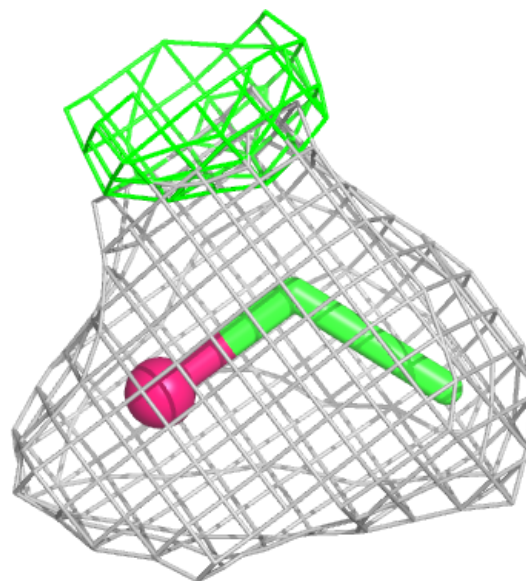
Electron density around MPD A 1703:

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



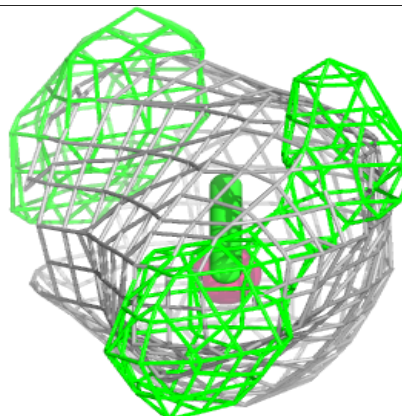
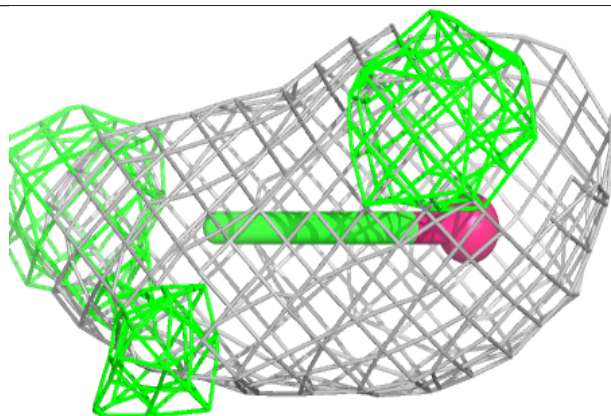
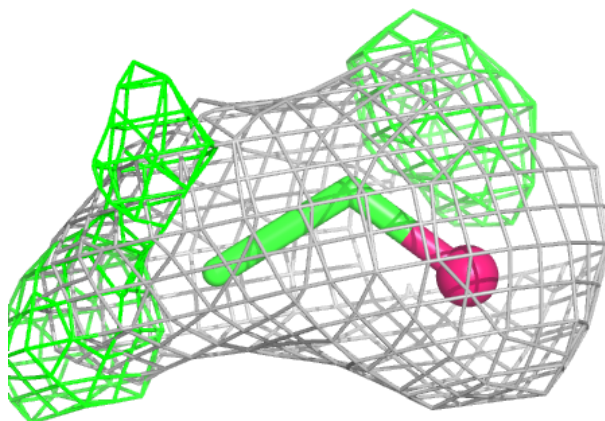
Electron density around EOH C 101:

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



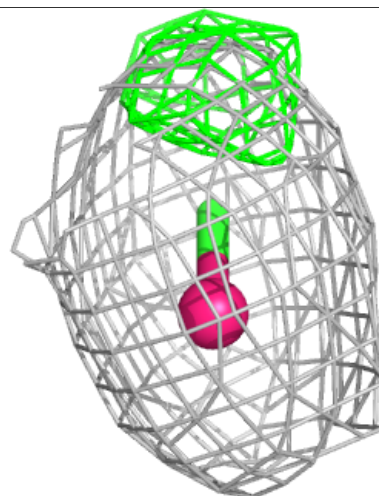
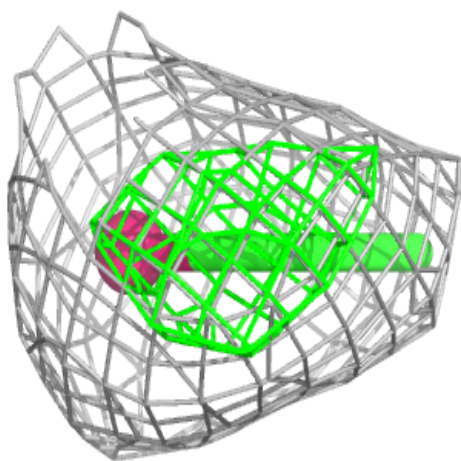
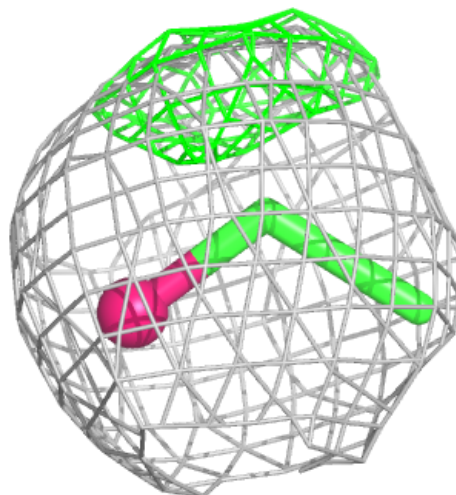
Electron density around EOH A 1701:

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



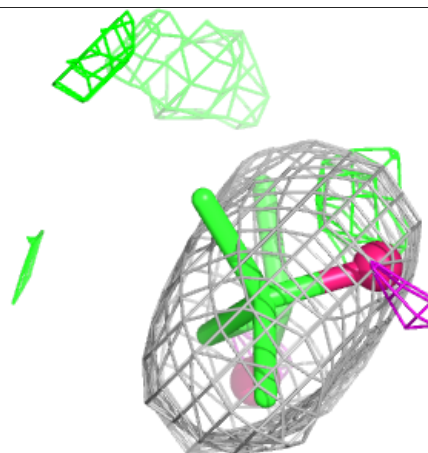
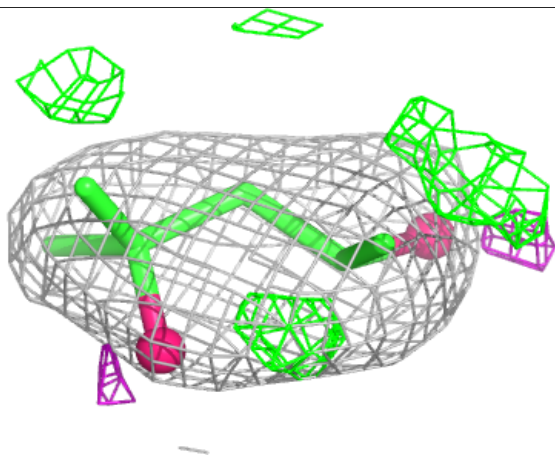
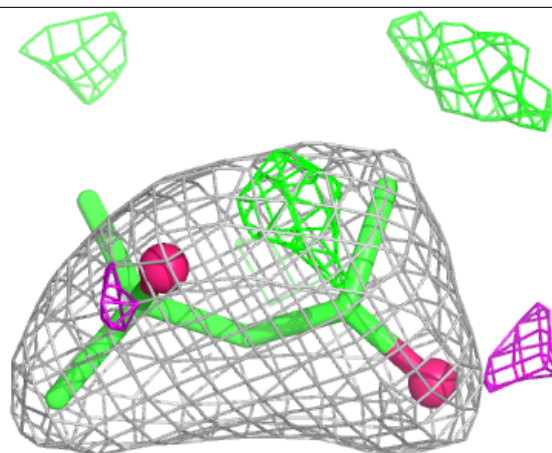
Electron density around EOH B 1702:

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



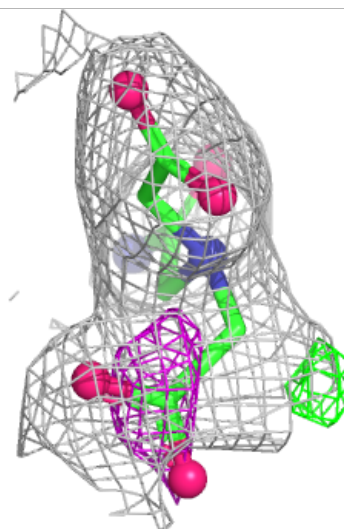
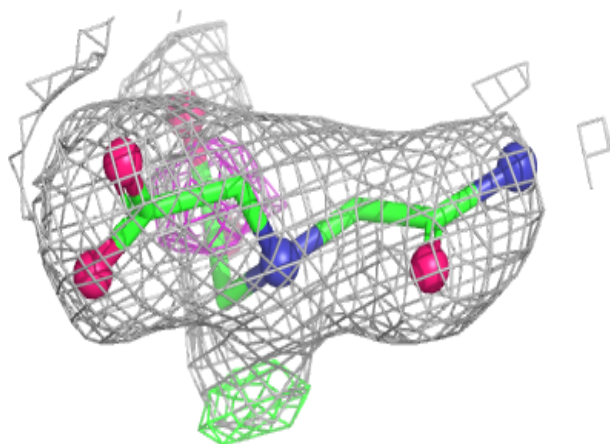
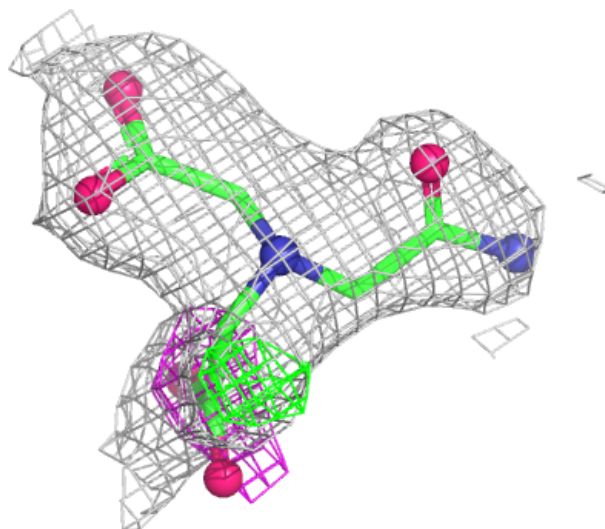
Electron density around MPD A 1702:

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



Electron density around MHA B 1703:

$2mF_o-DF_c$ (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.