



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:25 PM UTC

PDB ID : 6ZFA / pdb_00006zfa
Title : Structure of the catalytic domain of human endo-alpha-mannosidase MANEA in complex with GlcIFG, alpha-1,2-mannobiose and hexatungstotellurate(VI) TEW
Authors : Sobala, L.F.; Fernandes, P.Z.; Hakki, Z.; Thompson, A.J.; Howe, J.D.; Hill, M.; Zitzmann, N.; Davies, S.; Stamatakis, Z.; Butters, T.D.; Alonzi, D.S.; Williams, S.J.; Davies, G.J.
Deposited on : 2020-06-16
Resolution : 1.80 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)

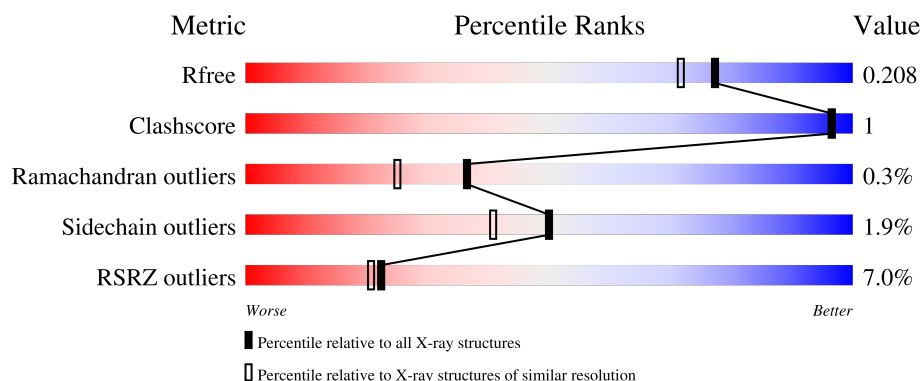
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	AAA	382	7% 91% • 6%
2	A	2	50% 50%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3275 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 Glycoprotein endo-alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	358	Total	C	N	O	S	0	7	0
			2974	1922	498	549	5			

There are 17 discrepancies between the modelled and reference sequences:

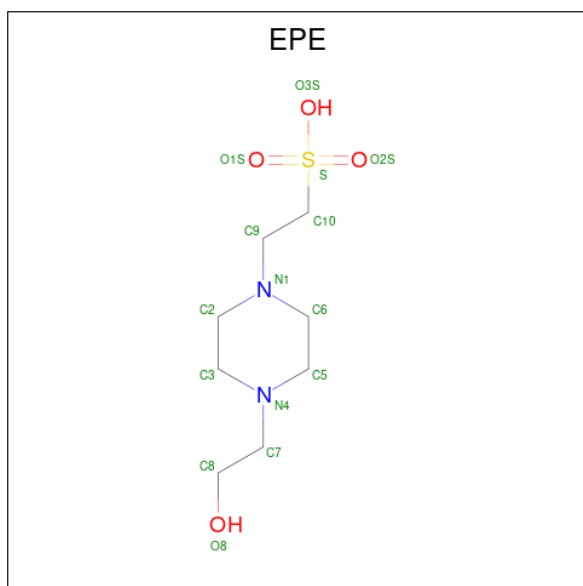
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	81	MET	-	initiating methionine	UNP Q5SRI9
AAA	82	ASN	-	expression tag	UNP Q5SRI9
AAA	83	HIS	-	expression tag	UNP Q5SRI9
AAA	84	LYS	-	expression tag	UNP Q5SRI9
AAA	85	VAL	-	expression tag	UNP Q5SRI9
AAA	86	HIS	-	expression tag	UNP Q5SRI9
AAA	87	HIS	-	expression tag	UNP Q5SRI9
AAA	88	HIS	-	expression tag	UNP Q5SRI9
AAA	89	HIS	-	expression tag	UNP Q5SRI9
AAA	90	HIS	-	expression tag	UNP Q5SRI9
AAA	91	HIS	-	expression tag	UNP Q5SRI9
AAA	92	ILE	-	expression tag	UNP Q5SRI9
AAA	93	GLU	-	expression tag	UNP Q5SRI9
AAA	94	GLY	-	expression tag	UNP Q5SRI9
AAA	95	ARG	-	expression tag	UNP Q5SRI9
AAA	96	HIS	-	expression tag	UNP Q5SRI9
AAA	97	MET	-	expression tag	UNP Q5SRI9

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	A	2	Total	C	O	0	1	0
			34	18	16			

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

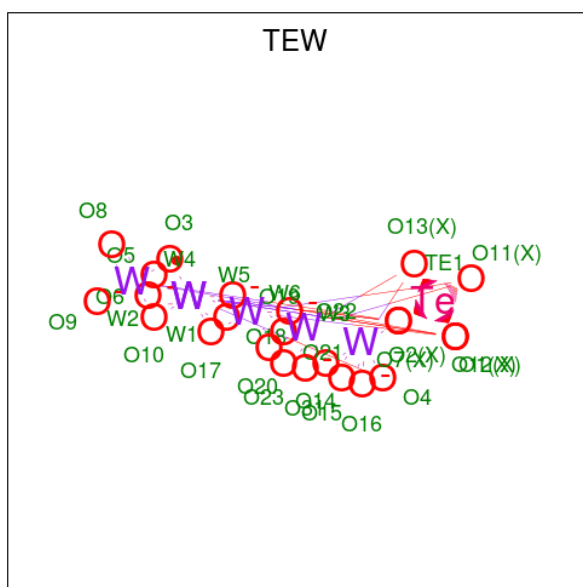


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

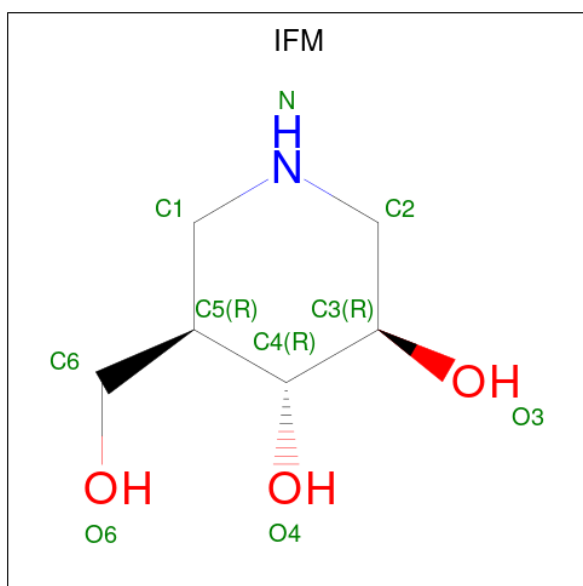
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 6-tungstotellurate(VI) (CCD ID: TEW) (formula: $O_{24}TeW_6$).



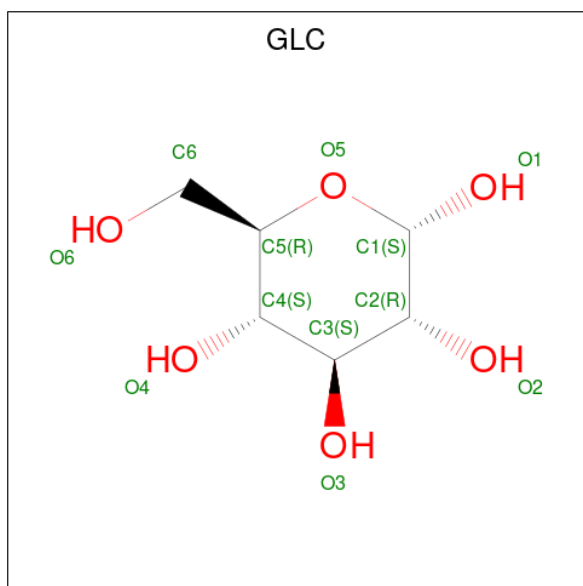
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	O	Te	W	0	0
			31	24	1	6		
5	AAA	1	Total	O	Te	W	0	0
			31	24	1	6		
5	AAA	1	Total	O	Te	W	0	0
			31	24	1	6		

- Molecule 6 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (CCD ID: IFM) (formula: $C_6H_{13}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 7 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	136	Total	O	0	3
			137	137		

- Molecule 1: Glycoprotein endo-alpha-1,2-mannosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	127.89Å 127.89Å 48.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	110.76 – 1.80 110.76 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (110.76-1.80) 100.0 (110.76-1.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.185 , 0.217 (Not available) , 0.208	Depositor DCC
R_{free} test set	2094 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3275	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: EPE, TEW, MG, MAN, GLC, IFM

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	AAA	0.77	0/3093	0.91	0/4212

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	AAA	2974	0	2858	4	0
2	A	34	0	31	1	0
3	AAA	15	0	17	0	0
4	AAA	1	0	0	0	0
5	AAA	93	0	0	3	0
6	AAA	10	0	12	0	0
7	AAA	11	0	10	0	0
8	AAA	137	0	0	2	0
All	All	3275	0	2928	6	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 1.

All (6) 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:AAA:256[B]:THR:OG1	5:AAA:503:TEW:O6	2.05	0.73
1:AAA:343[B]:LEU:HD23	5:AAA:504:TEW:O18	1.94	0.67
5:AAA:504:TEW:O6	5:AAA:504:TEW:O8	2.24	0.54
1:AAA:450:ARG:NH2	8:AAA:601:HOH:O	2.41	0.52
1:AAA:170:GLU:HG2	1:AAA:211:LYS:HD2	1.95	0.47
8:AAA:678[A]:HOH:O	2:A:2[A]:MAN:H2	2.18	0.43

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	AAA	363/382 (95%)	354 (98%)	8 (2%)	1 (0%)	36 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	323	TYR

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	AAA	323/345 (94%)	317 (98%)	6 (2%)	50 41

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	110	TRP
1	AAA	184	LEU
1	AAA	194	ASN
1	AAA	195	ASP
1	AAA	404	GLU
1	AAA	456	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	$\# Z > 2$
2	MAN	A	1	2	12,12,12	0.43	0	17,17,17	0.71	0
2	MAN	A	2[A]	2	11,11,12	0.41	0	15,15,17	1.64	2 (13%)
2	MAN	A	2[B]	2	11,11,12	0.49	0	15,15,17	0.67	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
2	MAN	A	1	2	-	0/2/22/22	0/1/1/1
2	MAN	A	2[A]	2	-	0/2/19/22	0/1/1/1
2	MAN	A	2[B]	2	-	0/2/19/22	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(°)	Ideal(°)
2	A	2[A]	MAN	C1-O5-C5	5.03	118.93	112.19
2	A	2[A]	MAN	C1-C2-C3	2.08	112.67	109.64

There are no chirality outliers.

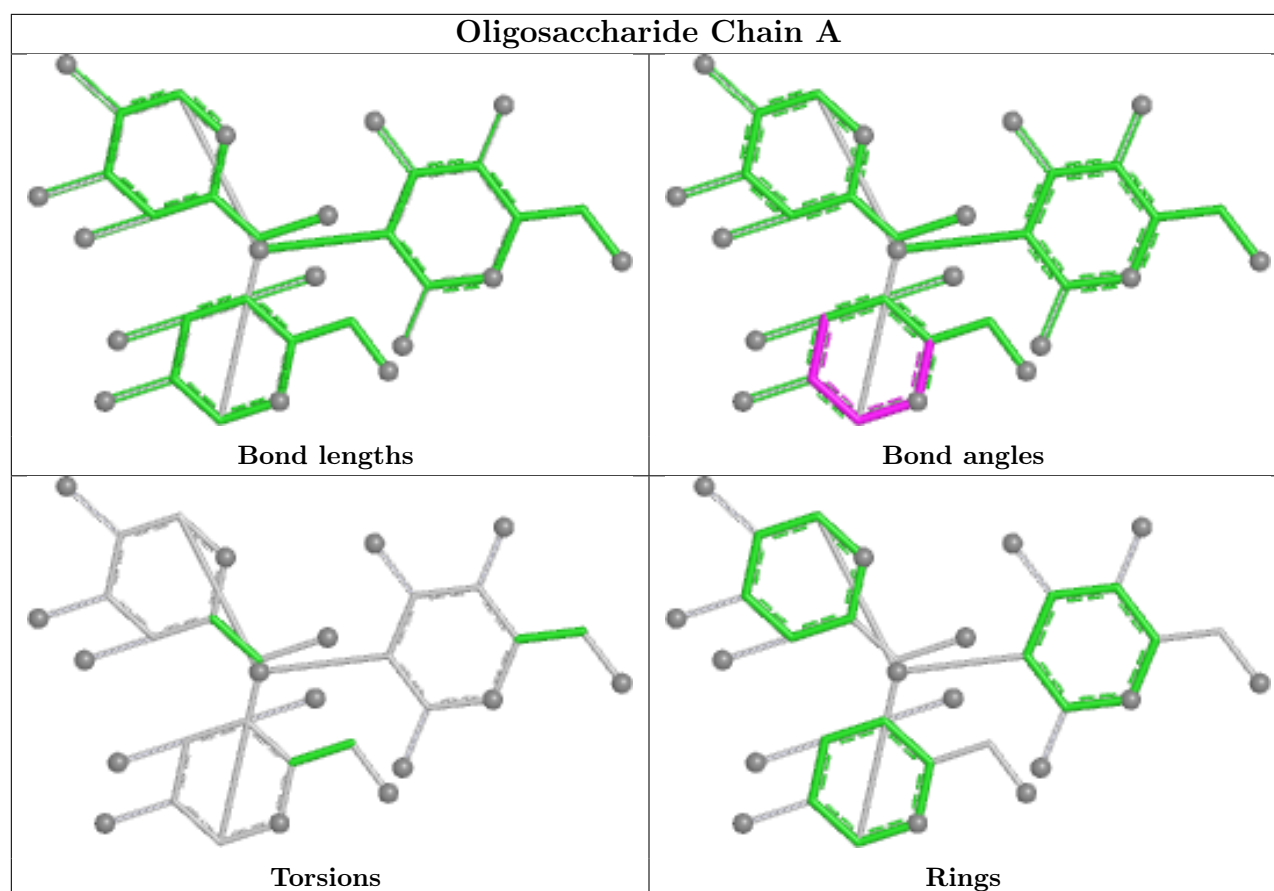
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2[A]	MAN	1	0

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



5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TEW	AAA	503	1	24,42,42	1.71	4 (16%)	12,129,129	1.84	5 (41%)
3	EPE	AAA	501	-	15,15,15	1.53	1 (6%)	19,20,20	1.60	5 (26%)
5	TEW	AAA	505	-	24,42,42	1.08	0	12,129,129	1.17	2 (16%)
6	IFM	AAA	506	7	10,10,10	0.94	0	9,13,13	2.46	1 (11%)
7	GLC	AAA	507	6	11,11,12	0.43	0	15,15,17	1.10	2 (13%)
5	TEW	AAA	504	-	24,42,42	1.33	3 (12%)	12,129,129	2.61	5 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IFM	AAA	506	7	-	0/2/16/16	0/1/1/1
7	GLC	AAA	507	6	-	0/2/19/22	0/1/1/1
3	EPE	AAA	501	-	-	3/9/19/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	501	EPE	C10-S	-5.41	1.70	1.77
5	AAA	503	TEW	W2-O8	-4.10	1.64	1.72
5	AAA	503	TEW	W4-O18	3.84	1.80	1.72
5	AAA	503	TEW	W5-O21	2.40	1.77	1.72
5	AAA	504	TEW	W2-O8	-2.32	1.67	1.72
5	AAA	504	TEW	W4-O18	-2.28	1.68	1.72
5	AAA	504	TEW	W1-O5	-2.07	1.70	2.09
5	AAA	503	TEW	W5-O22	-2.05	1.70	2.09

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AAA	506	IFM	C1-N-C2	6.83	119.70	111.78
5	AAA	504	TEW	O13-TE1-O1	-5.83	89.41	94.65
5	AAA	504	TEW	O13-TE1-O11	3.50	89.34	85.21
3	AAA	501	EPE	C7-N4-C5	3.47	120.49	111.24
5	AAA	504	TEW	O11-TE1-O2	-3.39	91.60	94.65
5	AAA	504	TEW	O7-TE1-O1	3.26	89.06	85.21
5	AAA	503	TEW	O11-TE1-O2	3.20	97.54	94.65
5	AAA	504	TEW	O11-TE1-O7	-2.75	92.17	94.65
5	AAA	505	TEW	O1-TE1-O12	2.72	97.10	94.65
5	AAA	503	TEW	O13-TE1-O1	-2.59	92.32	94.65
3	AAA	501	EPE	C9-N1-C6	2.51	117.93	111.24
5	AAA	503	TEW	O13-TE1-O12	-2.50	92.40	94.65
3	AAA	501	EPE	O1S-S-C10	2.50	110.50	106.73
7	AAA	507	GLC	O3-C3-C2	-2.43	105.09	110.05
7	AAA	507	GLC	C1-O5-C5	2.29	115.25	112.19
3	AAA	501	EPE	C8-C7-N4	2.18	121.10	113.44
5	AAA	505	TEW	O12-TE1-O11	-2.06	82.78	85.21
5	AAA	503	TEW	O11-TE1-O7	-2.04	92.81	94.65
3	AAA	501	EPE	C3-C2-N1	-2.04	106.54	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AAA	503	TEW	O13-TE1-O11	2.04	87.61	85.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	501	EPE	C10-C9-N1-C6
3	AAA	501	EPE	C8-C7-N4-C5
3	AAA	501	EPE	C10-C9-N1-C2

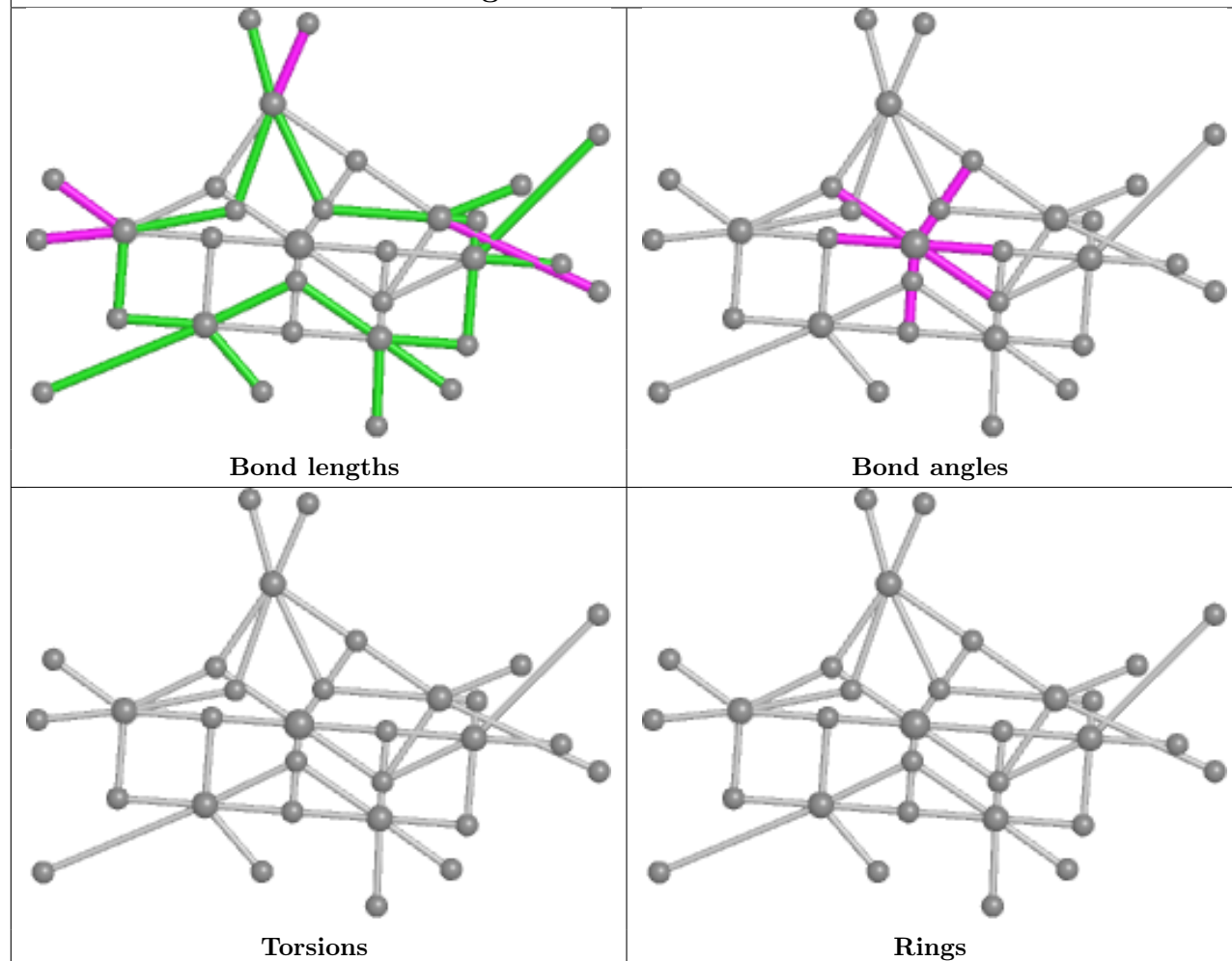
There are no ring outliers.

2 monomers are involved in 3 short contacts:

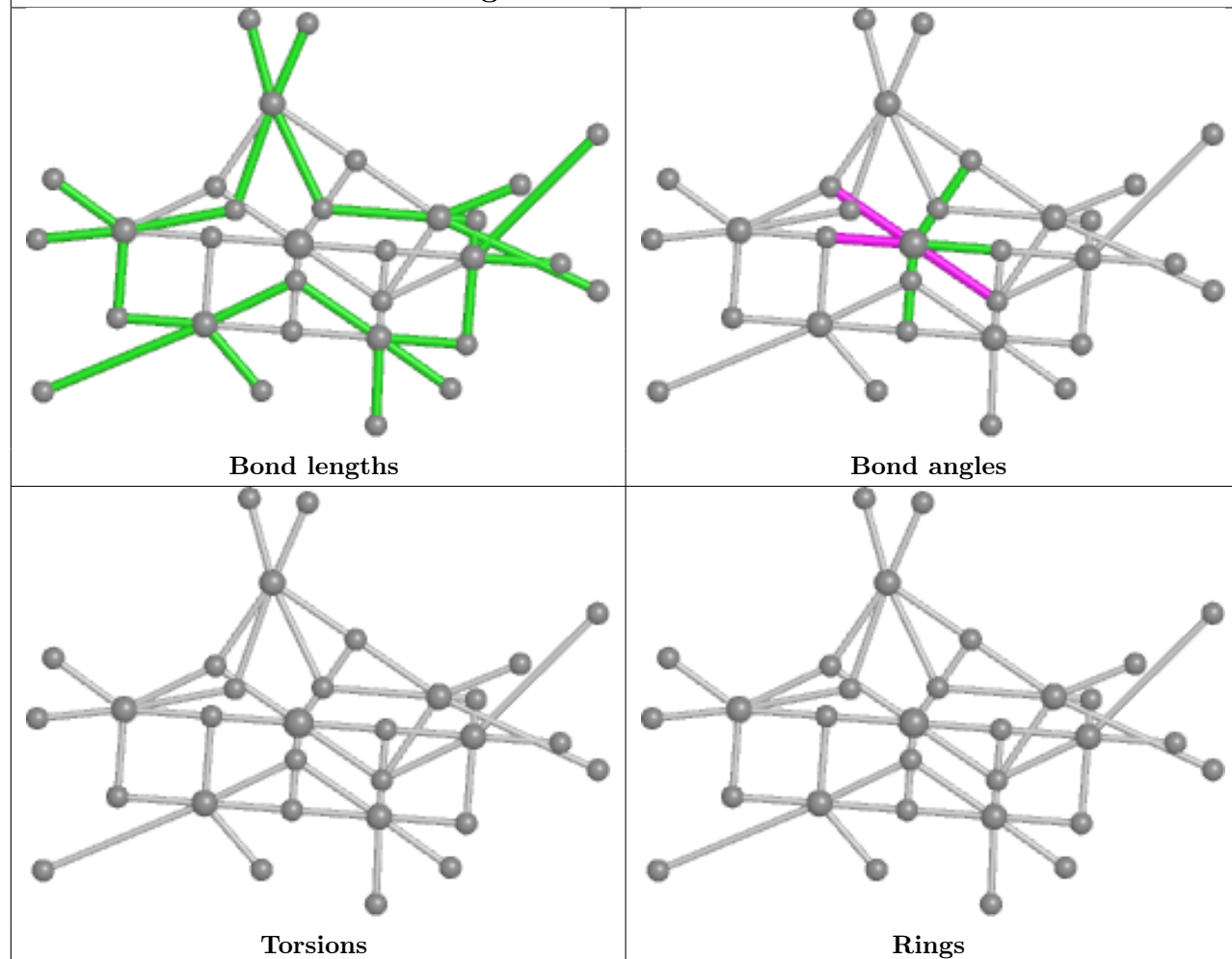
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	503	TEW	1	0
5	AAA	504	TEW	2	0

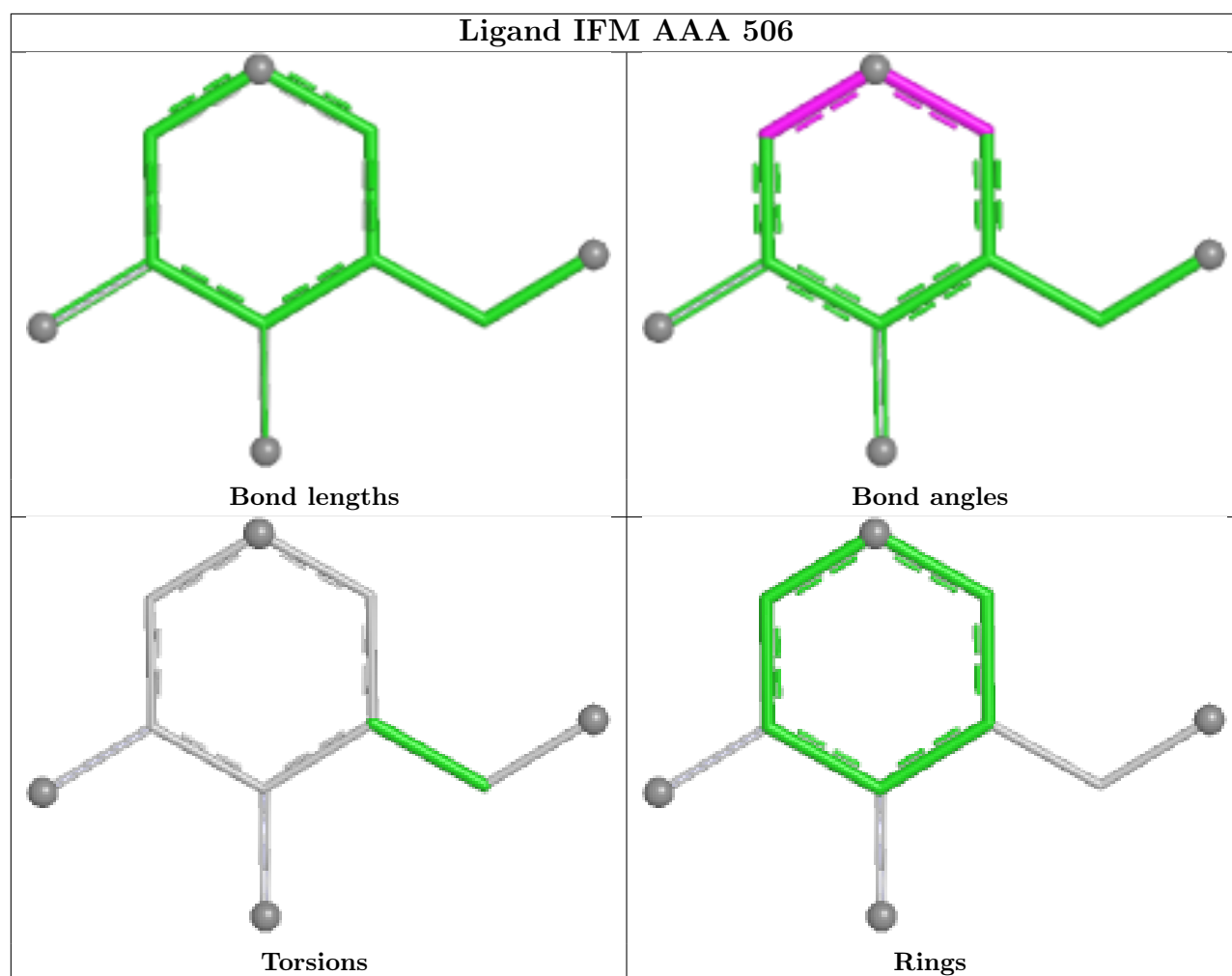
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

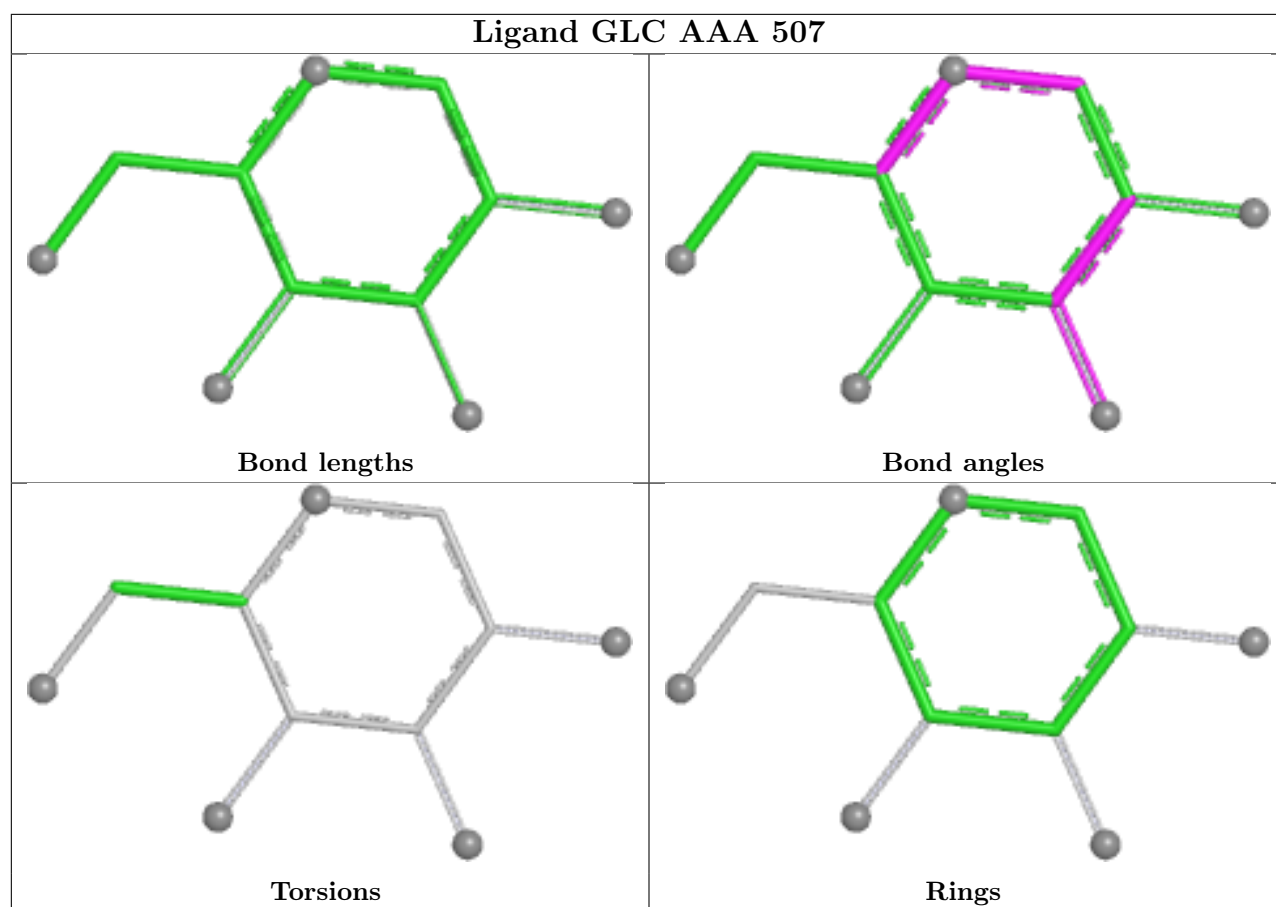
Ligand TEW AAA 503

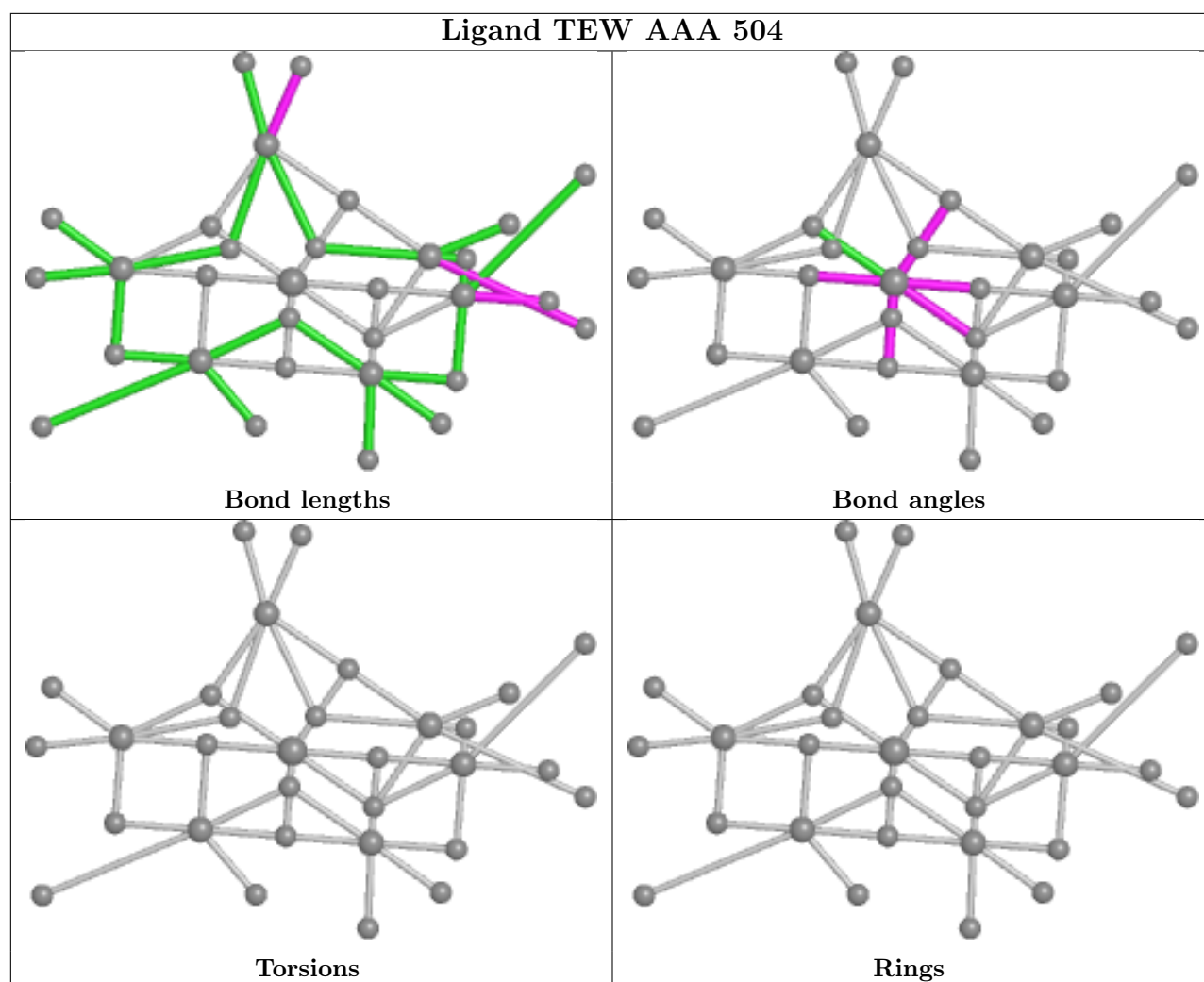


Ligand TEW AAA 505









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	AAA	358/382 (93%)	0.36	25 (6%) 22 21	10, 24, 41, 63	7 (1%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	259	GLY	5.6
1	AAA	456	ASP	4.6
1	AAA	453	TYR	4.5
1	AAA	131	TRP	4.2
1	AAA	260	ASN	4.1
1	AAA	455	LEU	4.0
1	AAA	451	ALA	3.7
1	AAA	99	LEU	3.6
1	AAA	448[A]	LYS	3.1
1	AAA	247	ASN	3.1
1	AAA	180	SER	3.0
1	AAA	447	SER	2.9
1	AAA	258	THR	2.9
1	AAA	454	ALA	2.8
1	AAA	391	GLN	2.6
1	AAA	452	THR	2.6
1	AAA	167	SER	2.6
1	AAA	236	LYS	2.5
1	AAA	287	SER	2.4
1	AAA	145	ASN	2.3
1	AAA	336	GLN	2.3
1	AAA	192	ASP	2.2
1	AAA	449	GLU	2.1
1	AAA	288	ARG	2.1
1	AAA	450	ARG	2.1

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

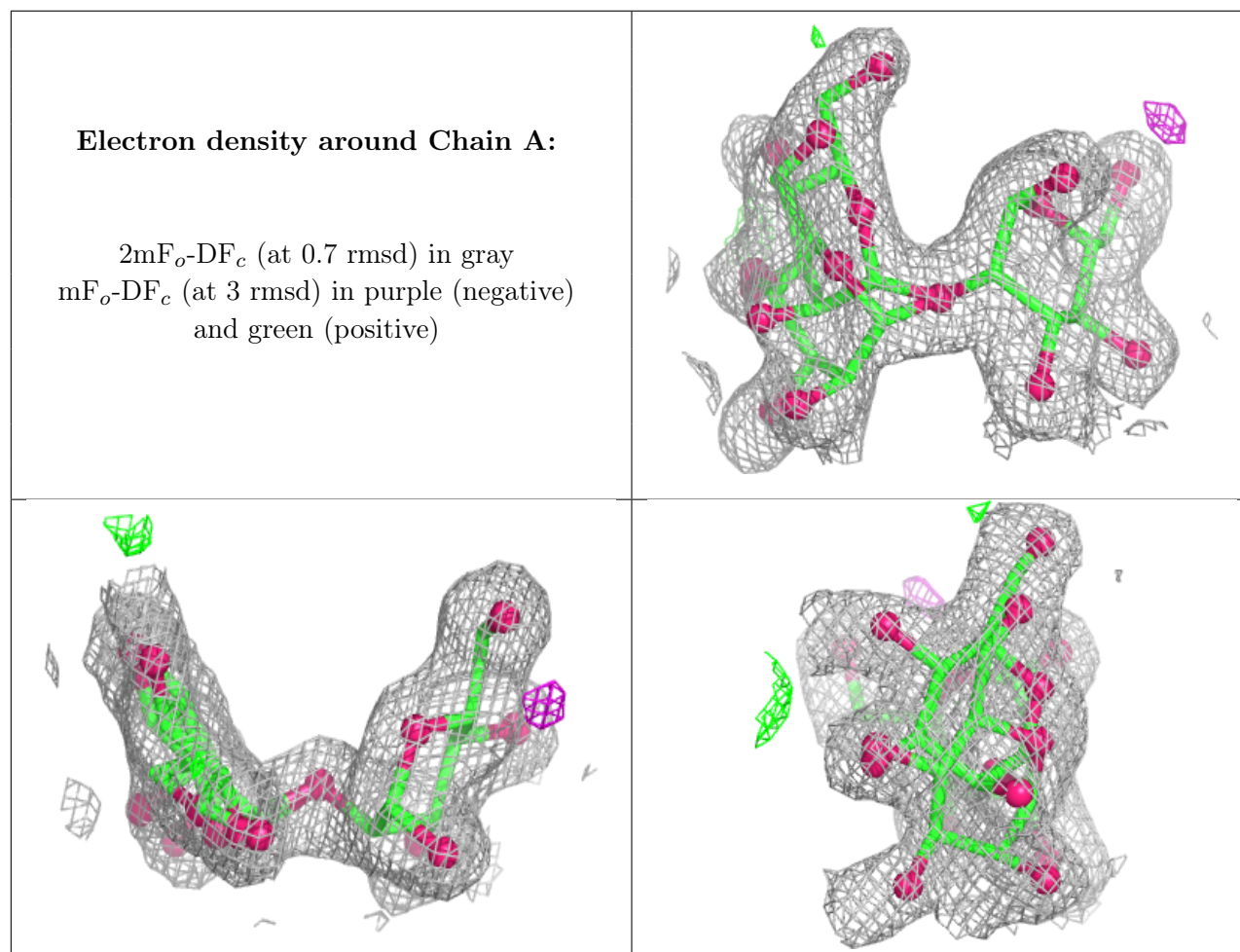
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	A	1	12/12	-	-	21,23,25,25	0
2	MAN	A	2[A]	11/12	-	-	22,24,25,25	11
2	MAN	A	2[B]	11/12	-	-	23,24,25,25	11

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



6.4 Ligands

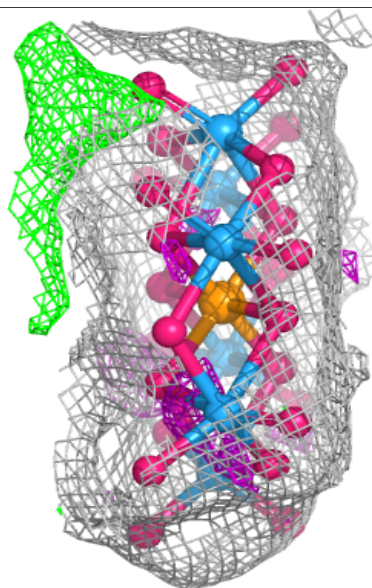
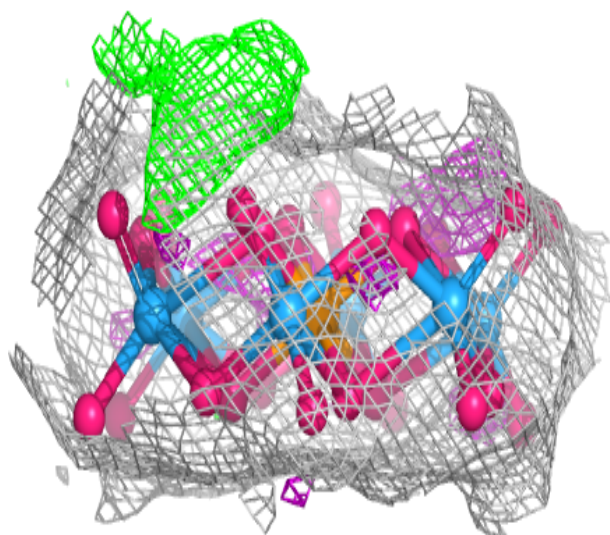
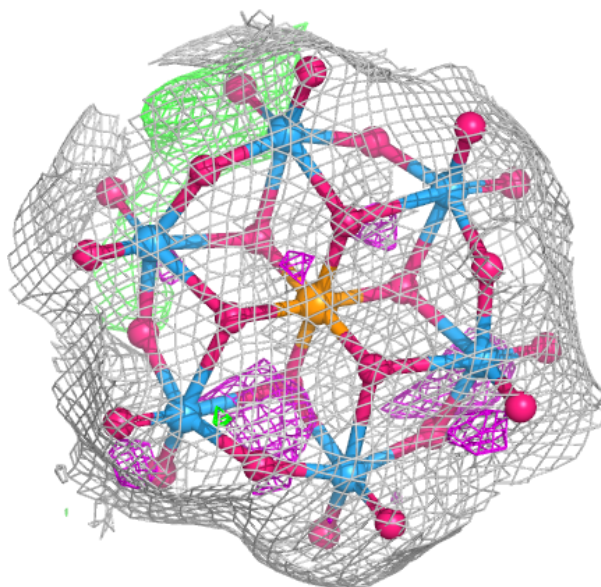
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	TEW	AAA	505	31/31	0.92	0.12	98,112,115,119	31
3	EPE	AAA	501	15/15	0.96	0.09	24,28,29,30	0
6	IFM	AAA	506	10/10	0.96	0.06	15,16,16,16	0
4	MG	AAA	502	1/1	0.97	0.08	28,28,28,28	0
5	TEW	AAA	504	31/31	0.97	0.11	21,50,61,64	0
7	GLC	AAA	507	11/12	0.97	0.05	16,16,17,18	0
5	TEW	AAA	503	31/31	0.99	0.08	20,32,40,42	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.

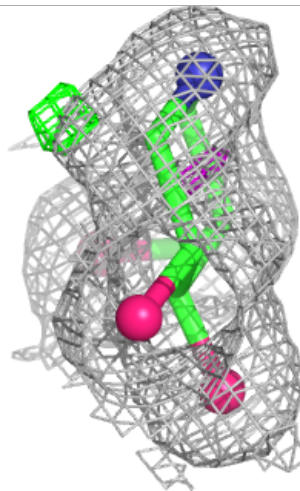
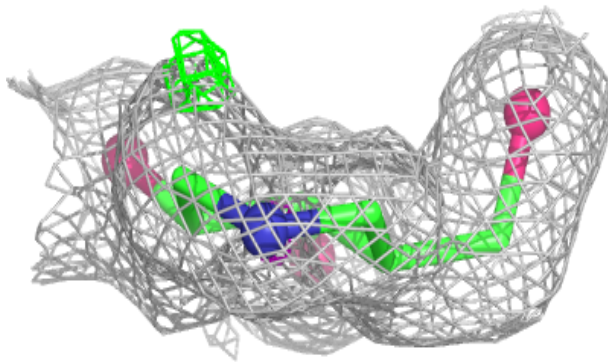
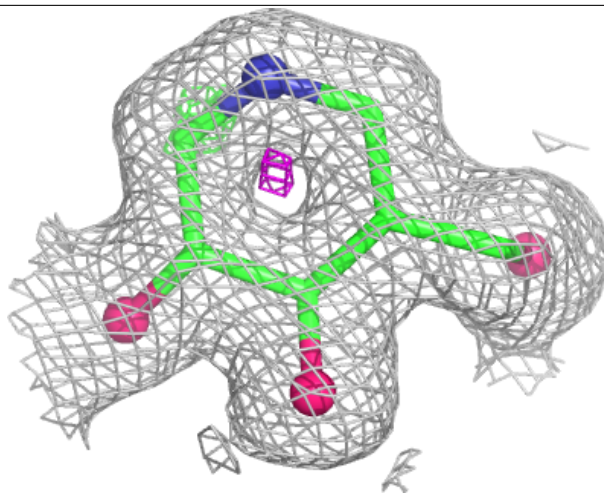
Electron density around TEW AAA 505:

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



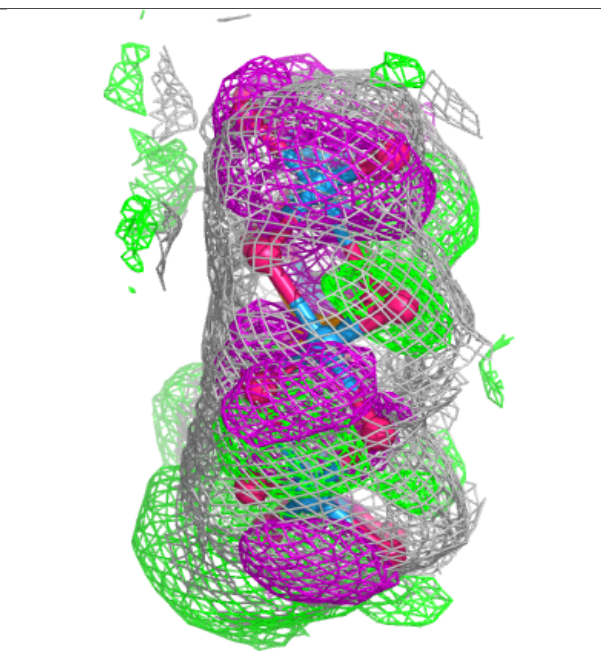
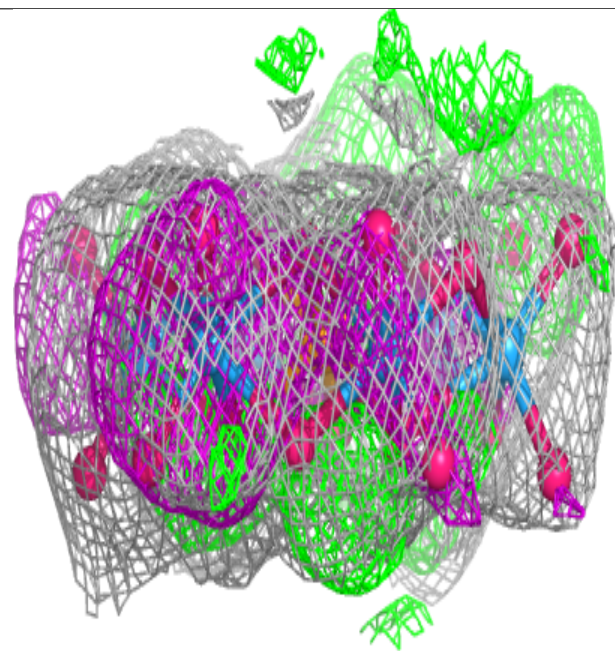
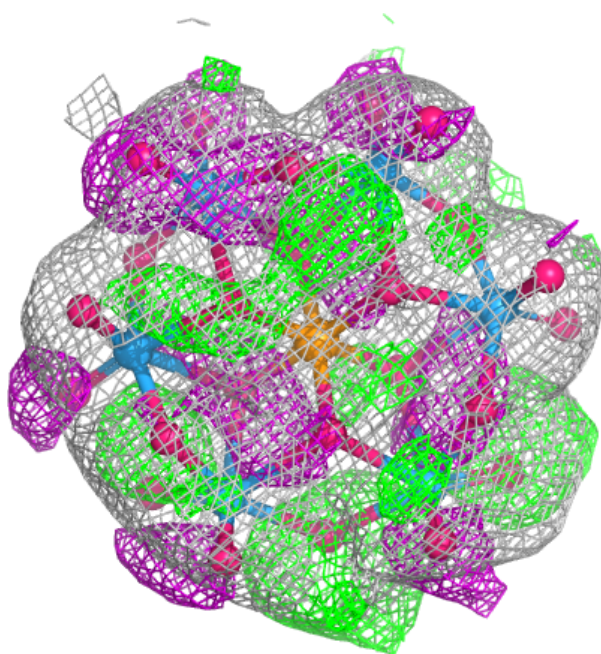
Electron density around IFM AAA 506:

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



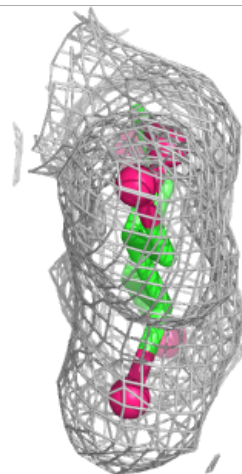
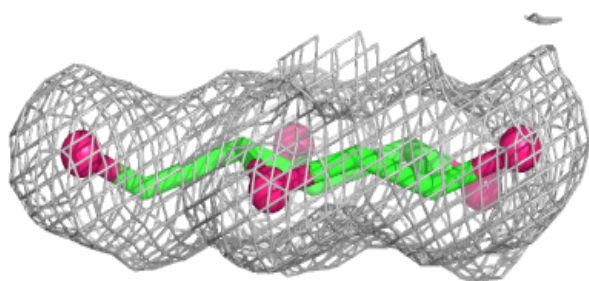
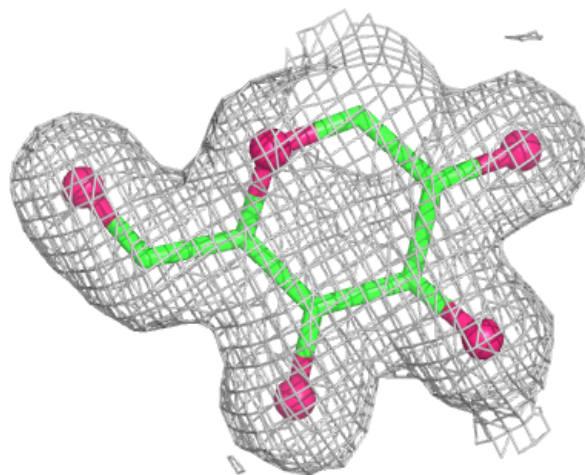
Electron density around TEW AAA 504:

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



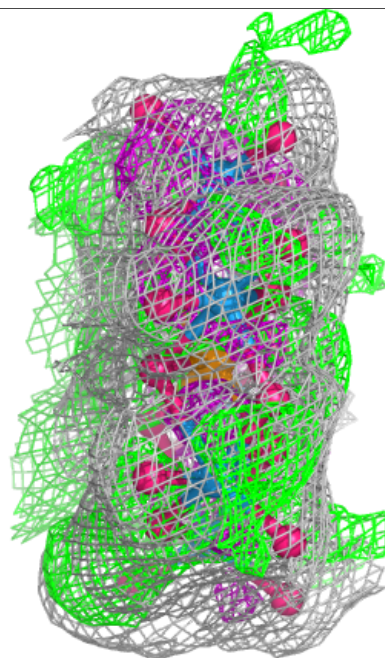
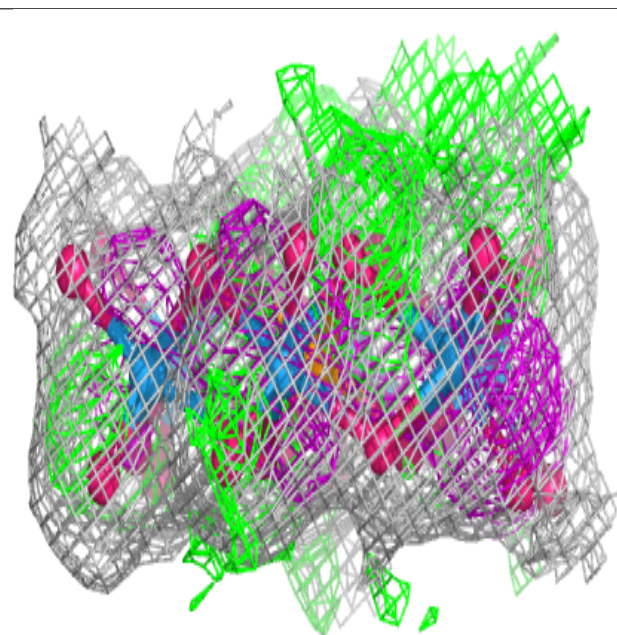
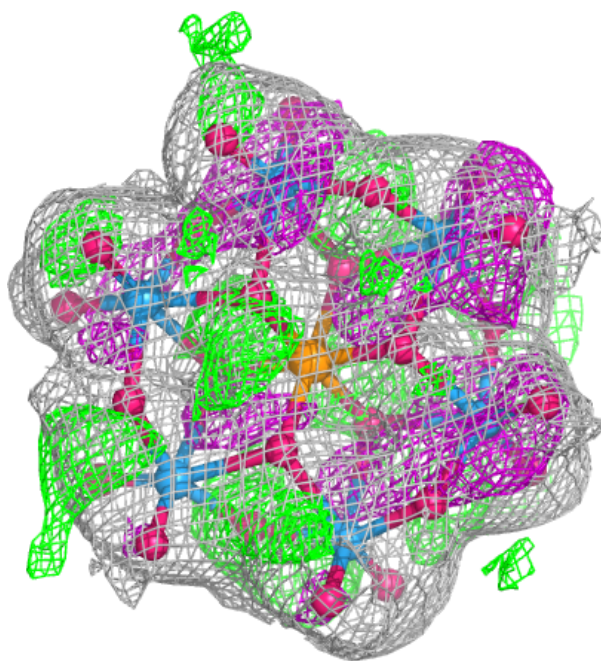
Electron density around GLC AAA 507:

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



Electron density around TEW AAA 503:

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.