



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:25 PM UTC

PDB ID : 6YU7 / pdb_00006yu7
Title : Crystal structure of MhsT in complex with L-tyrosine
Authors : Focht, D.; Neumann, C.; Lyons, J.; Eguskiza Bilbao, A.; Blunck, R.; Malinauskaitė, L.; Schwarz, I.O.; Javitch, J.A.; Quick, M.; Nissen, P.
Deposited on : 2020-04-25
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

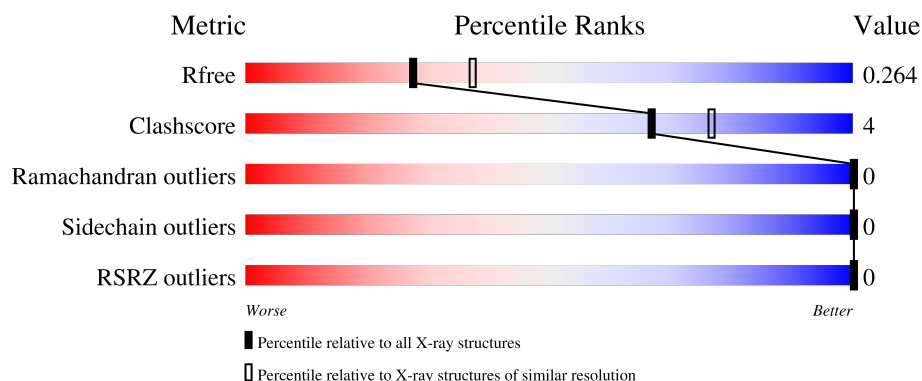
1 Overall quality at a glance

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	455	 87% 11% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3505 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.

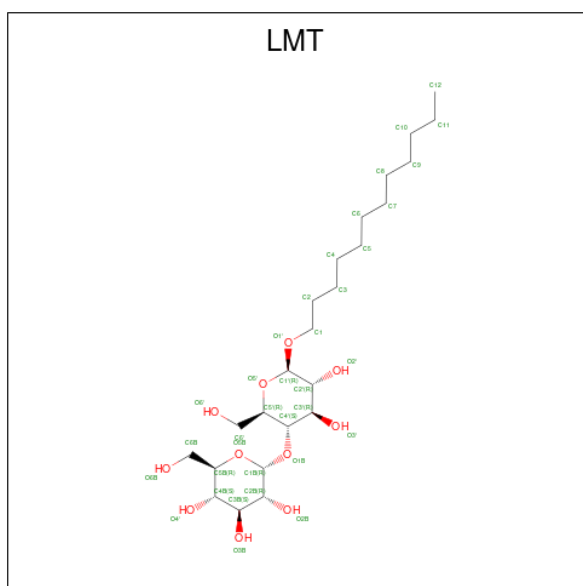
- Molecule 1 is a protein called Sodium-dependent transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3324	2240	514	562	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0A4Y7X244
A	0	MET	-	expression tag	UNP A0A4Y7X244
A	1	ALA	-	expression tag	UNP A0A4Y7X244

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	A	1	Total	C	O	0	0
			13	12	1		

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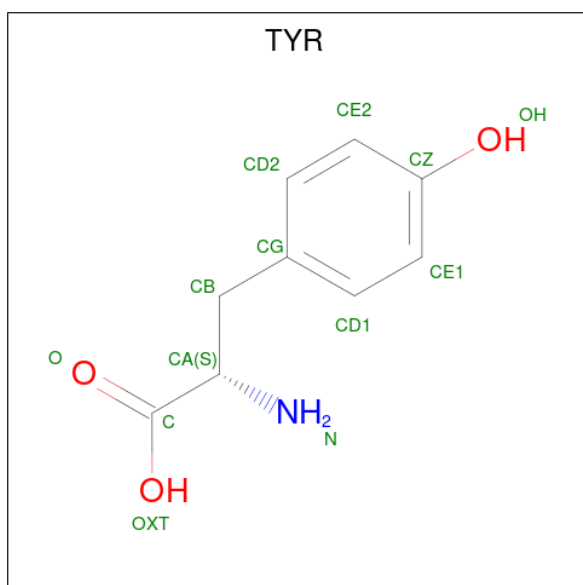
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	12	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

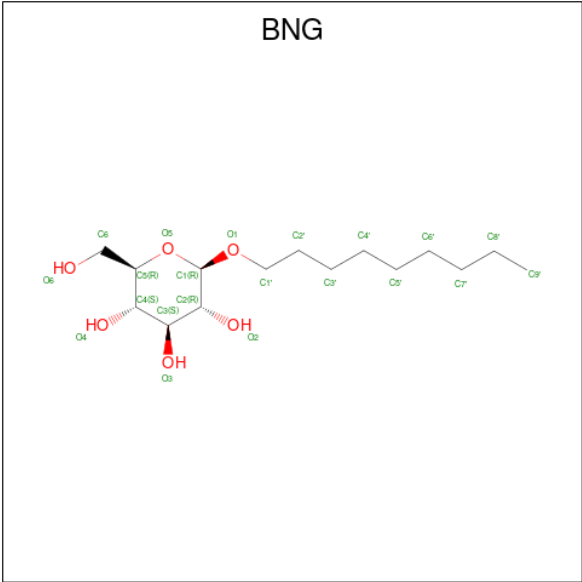
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

- Molecule 4 is TYROSINE (CCD ID: TYR) (formula: C₉H₁₁NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 5 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O	0	0
			63	63		

i

- Molecule 1: Sodium-dependent transporter

L234	L266	L298	L330	L362	L394	L426	L458	L490	L522	L554	L586	L618	L650	L682	L714	L746	L778	L810	L842	L874	L906	L938	L970	L1002	L1034	L1066	L1098	L1130	L1162	L1194	L1226	L1258	L1290	L1322	L1354	L1386	L1418	L1450	L1482	L1514	L1546	L1578	L1610	L1642	L1674	L1706	L1738	L1770	L1802	L1834	L1866	L1898	L1930	L1962	L1994	L2026	L2058	L2090	L2122	L2154	L2186	L2218	L2250	L2282	L2314	L2346	L2378	L2410	L2442	L2474	L2506	L2538	L2570	L2602	L2634	L2666	L2698	L2730	L2762	L2794	L2826	L2858	L2890	L2922	L2954	L2986	L3018	L3050	L3082	L3114	L3146	L3178	L3210	L3242	L3274	L3306	L3338	L3370	L3402	L3434	L3466	L3498	L3530	L3562	L3594	L3626	L3658	L3690	L3722	L3754	L3786	L3818	L3850	L3882	L3914	L3946	L3978	L4010	L4042	L4074	L4106	L4138	L4170	L4202	L4234	L4266	L4298	L4330	L4362	L4394	L4426	L4458	L4490	L4522	L4554	L4586	L4618	L4650	L4682	L4714	L4746	L4778	L4810	L4842	L4874	L4906	L4938	L4970	L5002	L5034	L5066	L5098	L5130	L5162	L5194	L5226	L5258	L5290	L5322	L5354	L5386	L5418	L5450	L5482	L5514	L5546	L5578	L5610	L5642	L5674	L5706	L5738	L5770	L5802	L5834	L5866	L5898	L5930	L5962	L5994	L6026	L6058	L6090	L6122	L6154	L6186	L6218	L6250	L6282	L6314	L6346	L6378	L6410	L6442	L6474	L6506	L6538	L6570	L6602	L6634	L6666	L6698	L6730	L6762	L6794	L6826	L6858	L6890	L6922	L6954	L6986	L7018	L7050	L7082	L7114	L7146	L7178	L7210	L7242	L7274	L7306	L7338	L7370	L7402	L7434	L7466	L7498	L7530	L7562	L7594	L7626	L7658	L7690	L7722	L7754	L7786	L7818	L7850	L7882	L7914	L7946	L7978	L8010	L8042	L8074	L8106	L8138	L8170	L8202	L8234	L8266	L8298	L8330	L8362	L8394	L8426	L8458	L8490	L8522	L8554	L8586	L8618	L8650	L8682	L8714	L8746	L8778	L8810	L8842	L8874	L8906	L8938	L8970	L9002	L9034	L9066	L9098	L9130	L9162	L9194	L9226	L9258	L9290	L9322	L9354	L9386	L9418	L9450	L9482	L9514	L9546	L9578	L9610	L9642	L9674	L9706	L9738	L9770	L9802	L9834	L9866	L9898	L9930	L9962	L9994	L10026	L10058	L10090	L10122	L10154	L10186	L10218	L10250	L10282	L10314	L10346	L10378	L10410	L10442	L10474	L10506	L10538	L10570	L10602	L10634	L10666	L10698	L10730	L10762	L10794	L10826	L10858	L10890	L10922	L10954	L10986	L11018	L11050	L11082	L11114	L11146	L11178	L11210	L11242	L11274	L11306	L11338	L11370	L11402	L11434	L11466	L11498	L11530	L11562	L11594	L11626	L11658	L11690	L11722	L11754	L11786	L11818	L11850	L11882	L11914	L11946	L11978	L12010	L12042	L12074	L12106	L12138	L12170	L12202	L12234	L12266	L12298	L12330	L12362	L12394	L12426	L12458	L12490	L12522	L12554	L12586	L12618	L12650	L12682	L12714	L12746	L12778	L12810	L12842	L12874	L12906	L12938	L12970	L13002	L13034	L13066	L13098	L13130	L13162	L13194	L13226	L13258	L13290	L13322	L13354	L13386	L13418	L13450	L13482	L13514	L13546	L13578	L13610	L13642	L13674	L13706	L13738	L13770	L13802	L13834	L13866	L13898	L13930	L13962	L13994	L14026	L14058	L14090	L14122	L14154	L14186	L14218	L14250	L14282	L14314	L14346	L
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	44.10Å 49.90Å 110.30Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	29.83 – 2.30 29.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.83-2.30) 97.2 (29.83-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.223 , 0.263 0.224 , 0.264	Depositor DCC
R_{free} test set	750 reflections (2.66%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3505	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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: LMT, NA, BNG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/3416	0.31	0/4654

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	3324	0	3438	26	0
2	A	61	0	96	1	0
3	A	2	0	0	0	0
4	A	13	0	8	0	0
5	A	42	0	60	2	0
6	A	63	0	0	0	0
All	All	3505	0	3602	26	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 4.

The worst 5 of 26 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:85:ALA:HB1	1:A:88:LYS:HD2	1.77	0.65
1:A:107:PHE:HB2	1:A:381:PHE:CE2	2.38	0.59
1:A:209:SER:HB2	5:A:507:BNG:H1'2	1.87	0.56
1:A:192:ILE:HA	1:A:195:LEU:HD12	1.89	0.54
1:A:274:ILE:HD13	1:A:296:LEU:HD21	1.91	0.52

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	440/455 (97%)	430 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/348 (97%)	336 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are 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	BNG	A	508	-	21,21,21	1.31	3 (14%)	26,26,26	0.99	1 (3%)
2	LMT	A	501	-	36,36,36	1.15	2 (5%)	47,47,47	1.01	1 (2%)
4	TYR	A	506	3	12,13,13	0.79	0	13,17,17	0.80	0
2	LMT	A	503	-	12,12,36	0.68	0	11,11,47	0.87	0
5	BNG	A	507	-	21,21,21	1.24	2 (9%)	26,26,26	0.79	0
2	LMT	A	502	-	12,12,36	0.68	0	11,11,47	0.81	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	BNG	A	508	-	-	3/12/32/32	0/1/1/1
2	LMT	A	501	-	-	12/21/61/61	0/2/2/2
4	TYR	A	506	3	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	503	-	-	5/10/10/61	-
5	BNG	A	507	-	-	4/12/32/32	0/1/1/1
2	LMT	A	502	-	-	5/10/10/61	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	508	BNG	O5-C1	3.71	1.51	1.41
2	A	501	LMT	O5B-C1B	3.45	1.50	1.41
5	A	507	BNG	O5-C1	3.26	1.50	1.41
2	A	501	LMT	O5'-C1'	3.18	1.50	1.41
5	A	507	BNG	O1-C1	-2.42	1.36	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	LMT	C1B-O1B-C4'	-2.91	111.08	117.98
5	A	508	BNG	O5-C5-C4	2.06	113.41	109.70

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LMT	C4B-C5B-C6B-O6B
2	A	501	LMT	O5B-C5B-C6B-O6B
5	A	507	BNG	O1-C1'-C2'-C3'
2	A	502	LMT	C5-C6-C7-C8
2	A	503	LMT	C6-C7-C8-C9

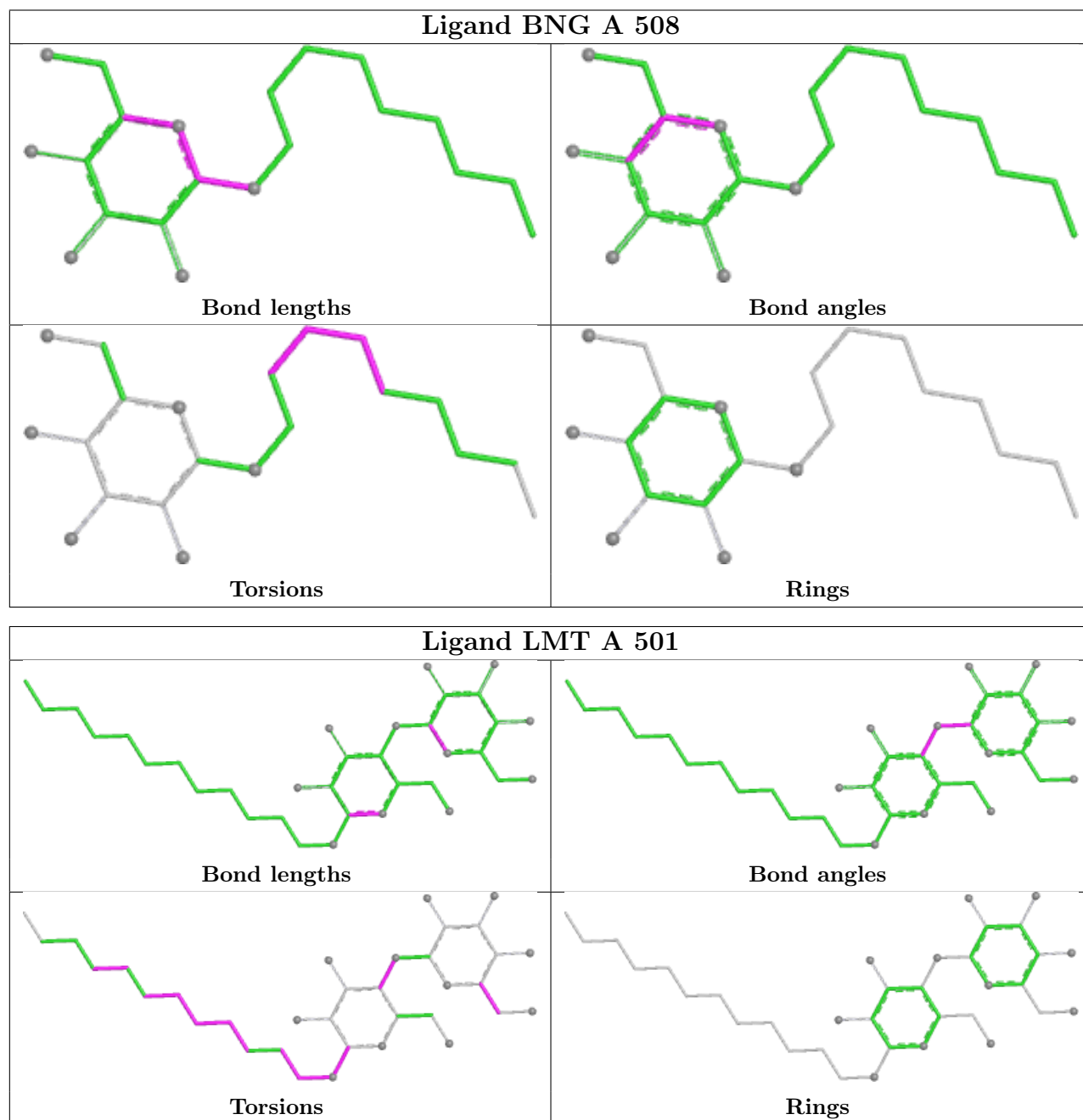
There are no ring outliers.

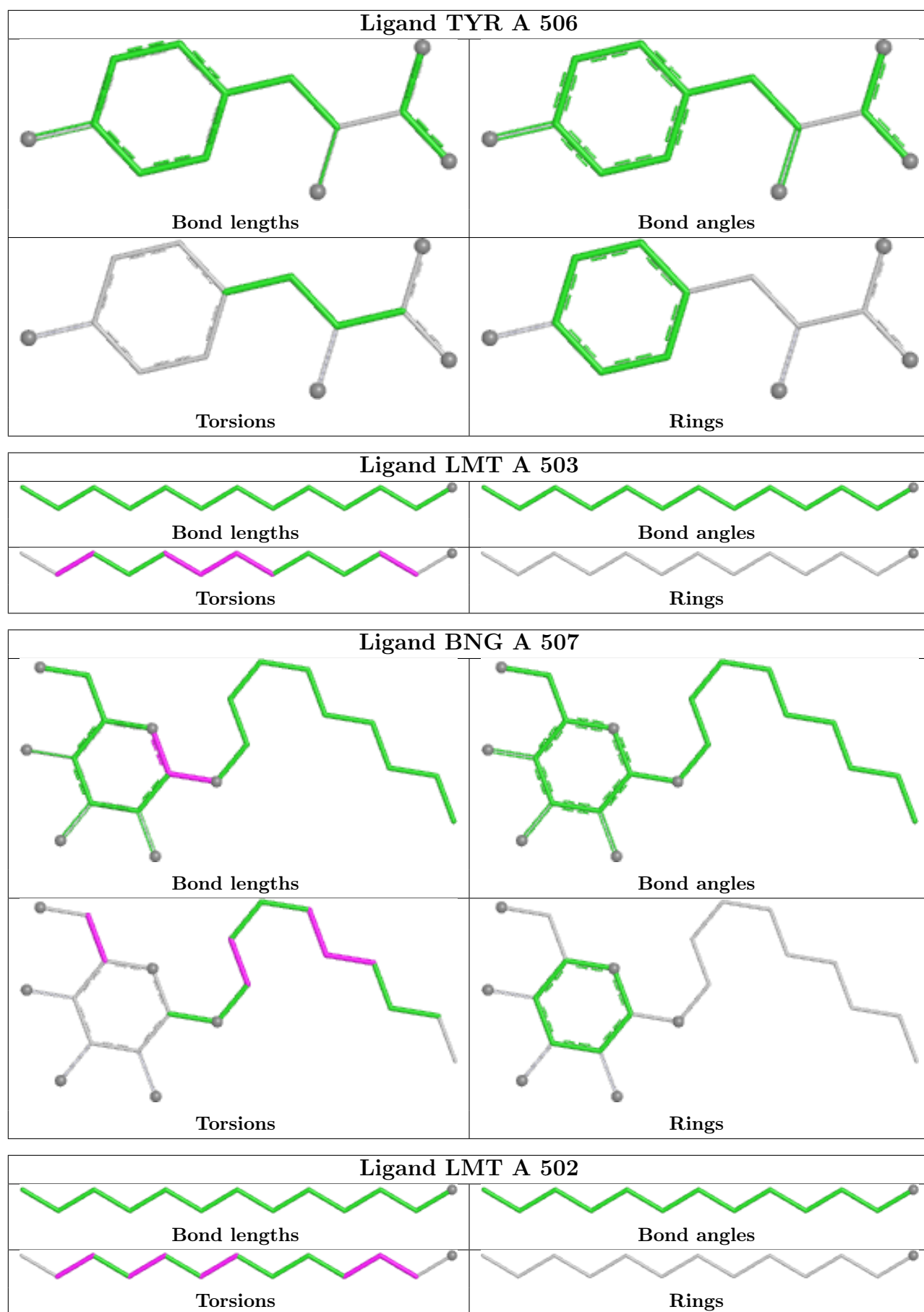
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	LMT	1	0
5	A	507	BNG	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 [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 [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	442/455 (97%)	-1.28	0 100 100	23, 35, 52, 69	0

There are no RSRZ outliers to report.

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](#)

There are no oligosaccharides in this entry.

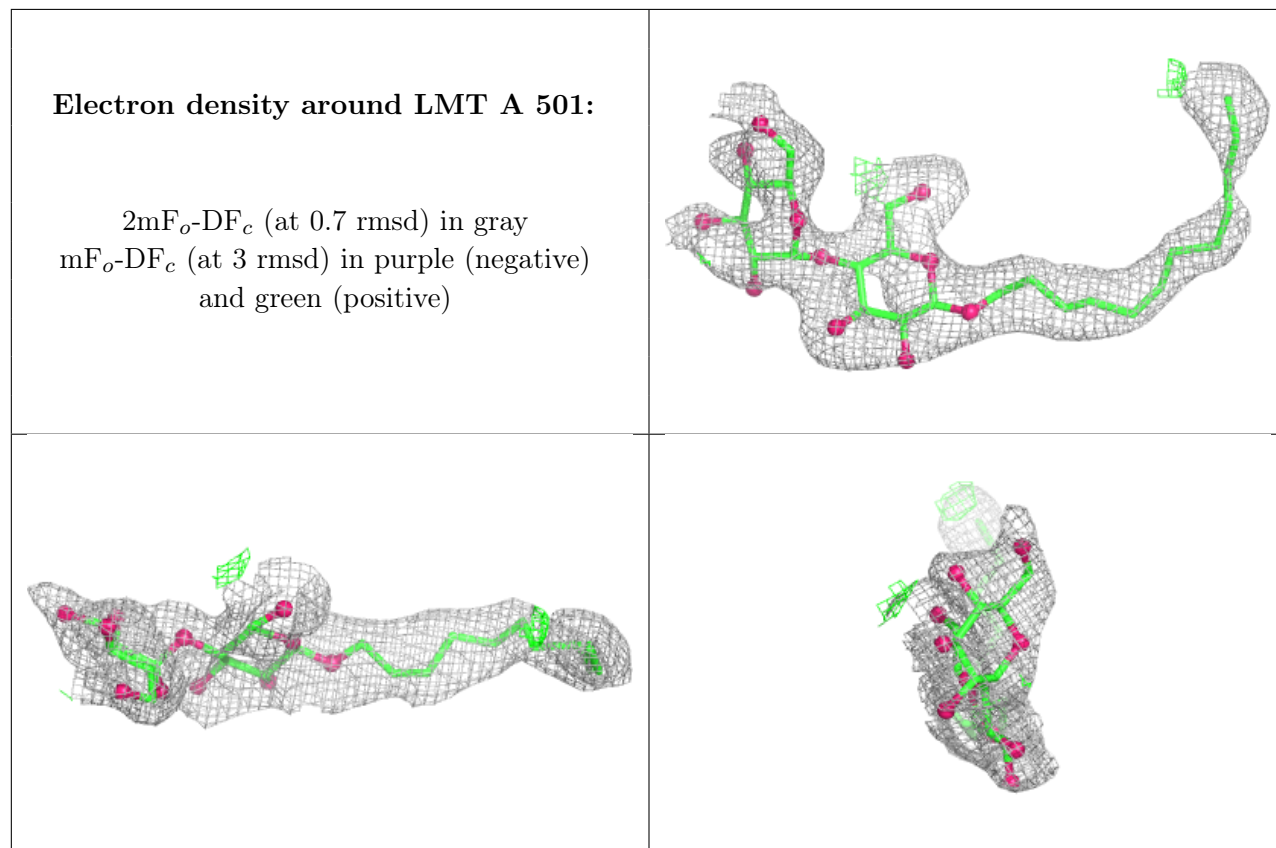
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	LMT	A	501	35/35	0.98	0.05	38,56,69,75	0
2	LMT	A	502	13/35	0.98	0.04	28,40,47,52	0
2	LMT	A	503	13/35	0.98	0.04	37,41,48,50	0
3	NA	A	504	1/1	0.98	0.07	28,28,28,28	0
5	BNG	A	507	21/21	0.98	0.05	28,44,58,59	0
5	BNG	A	508	21/21	0.98	0.05	36,46,60,63	0
3	NA	A	505	1/1	0.99	0.05	29,29,29,29	0
4	TYR	A	506	13/13	0.99	0.03	21,25,30,31	0

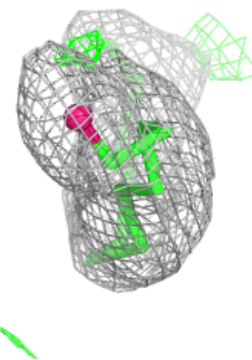
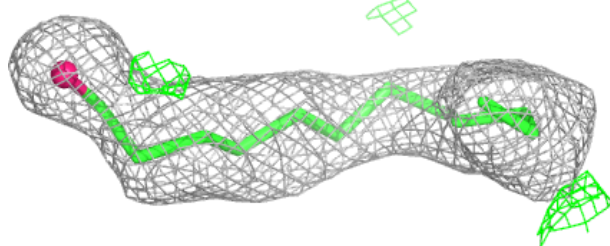
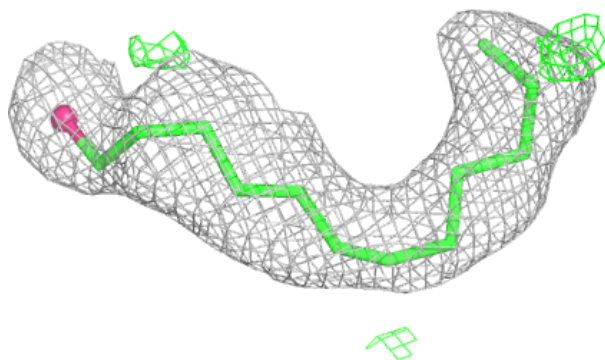
The following is a graphical depiction of the model fit to experimental electron density of all

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.

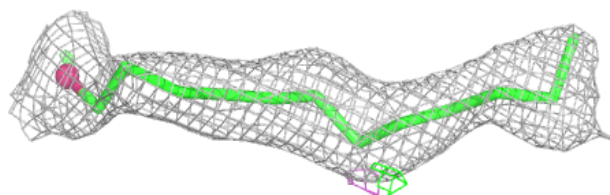
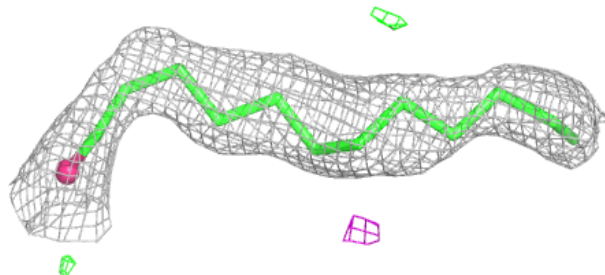


Electron density around LMT A 502:

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

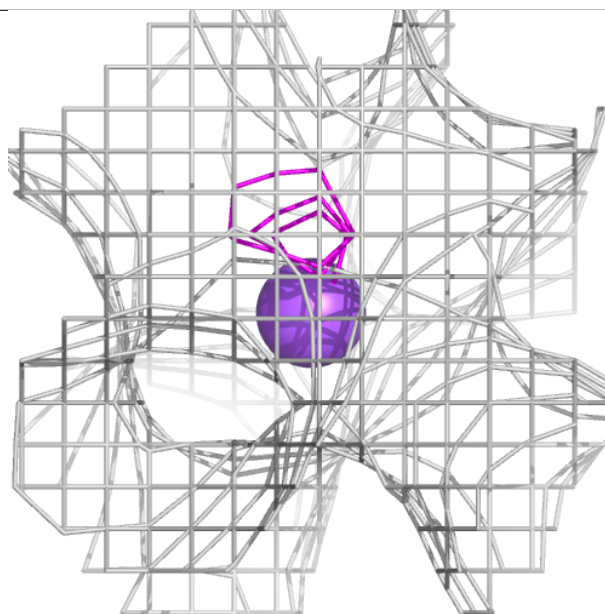
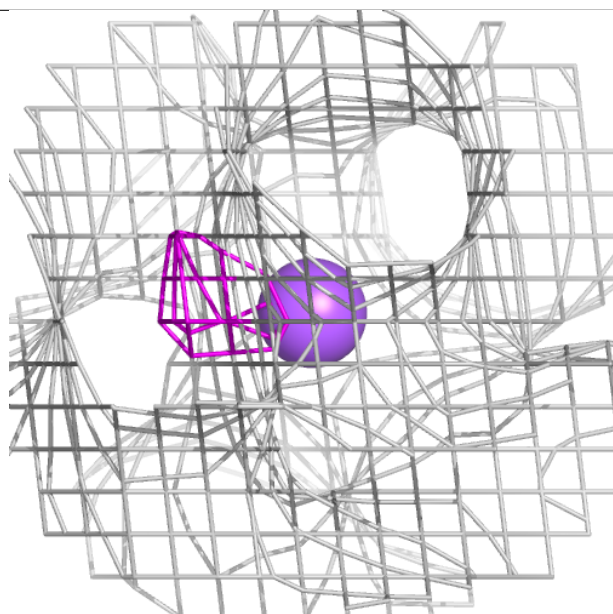
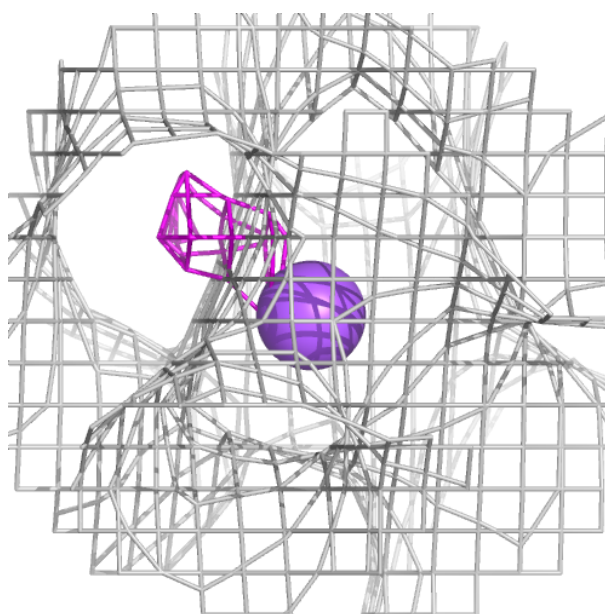
**Electron density around LMT A 503:**

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



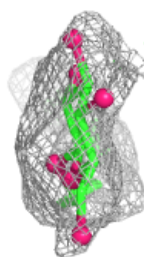
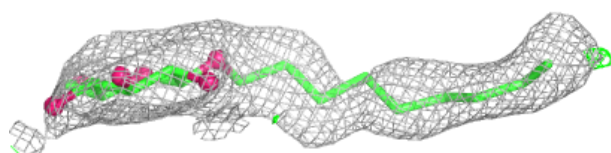
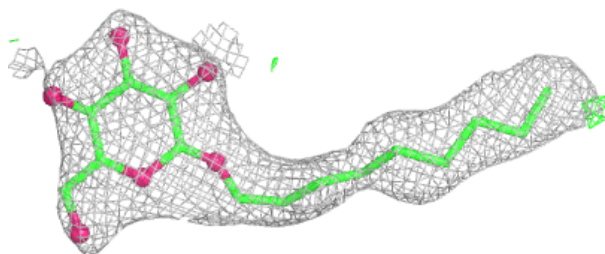
Electron density around NA A 504:

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

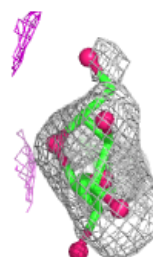
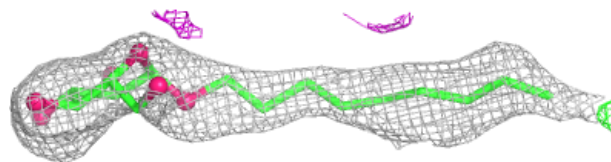
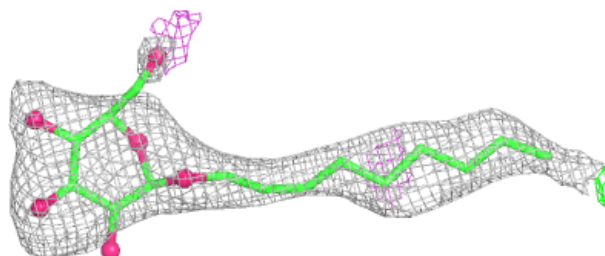


Electron density around BNG A 507:

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

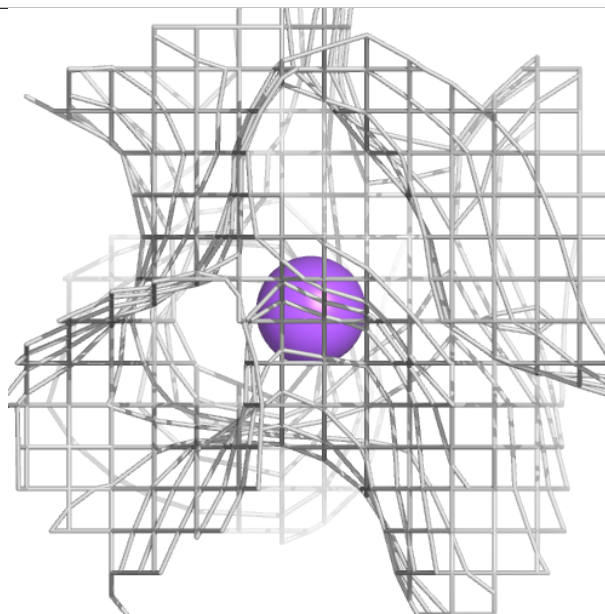
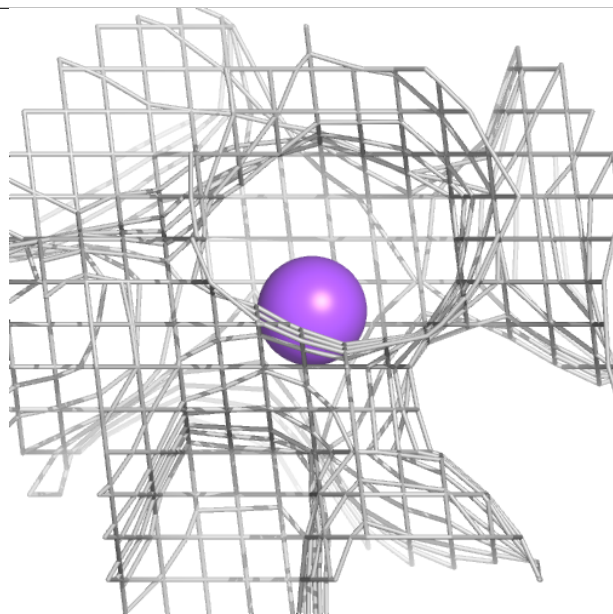
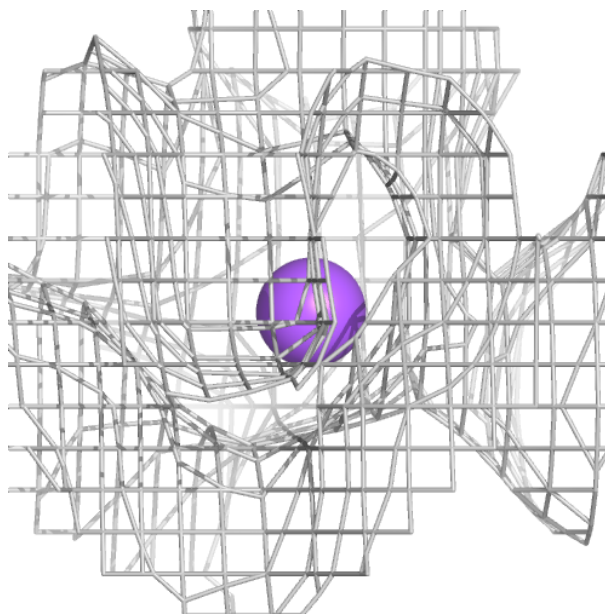
**Electron density around BNG A 508:**

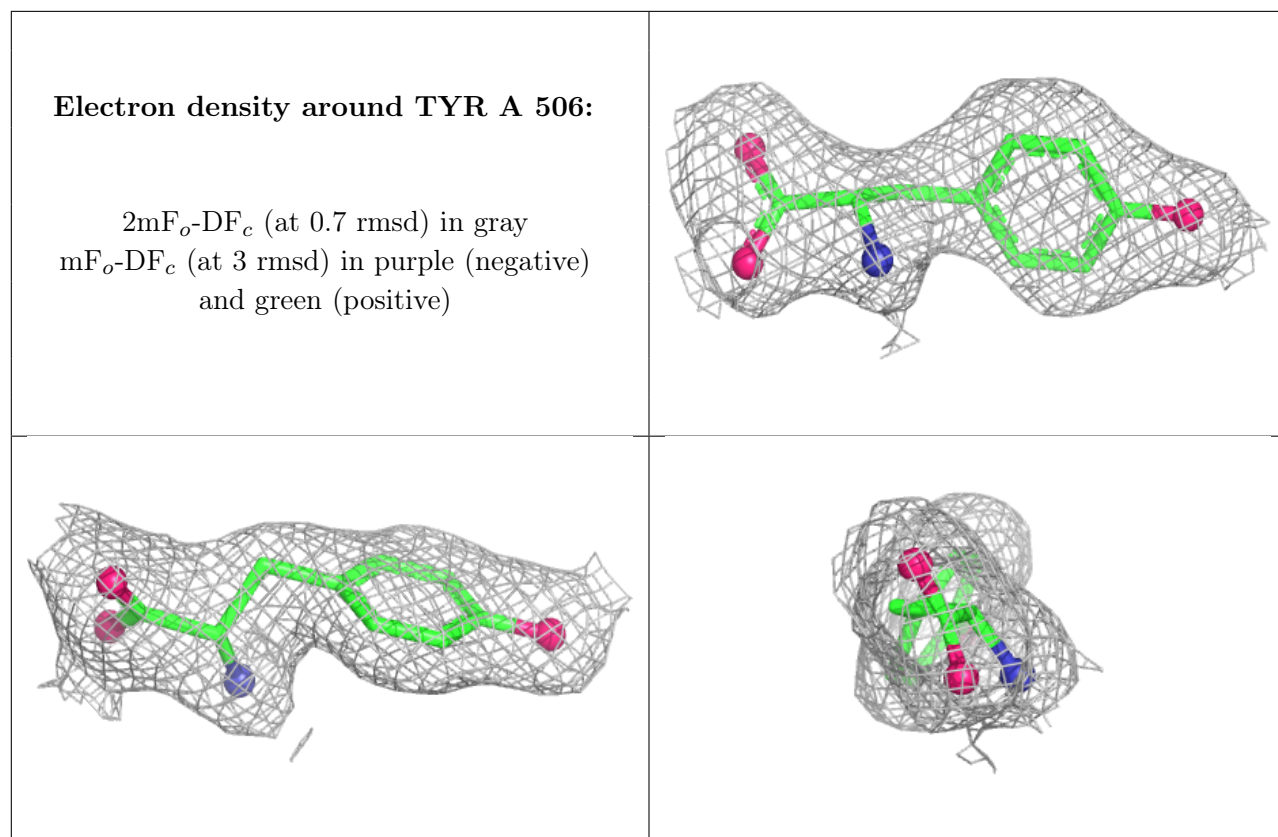
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NA A 505:

$2mF_o-DF_c$ (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.