



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:12 PM UTC

PDB ID : 6AJG / pdb_00006ajg
Title : Crystal structure of mycolic acid transporter MmpL3 from Mycobacterium smegmatis complexed with SQ109
Authors : Zhang, B.; Li, J.; Yang, X.L.; Wu, L.J.; Yang, H.T.; Rao, Z.H.
Deposited on : 2018-08-27
Resolution : 2.60 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

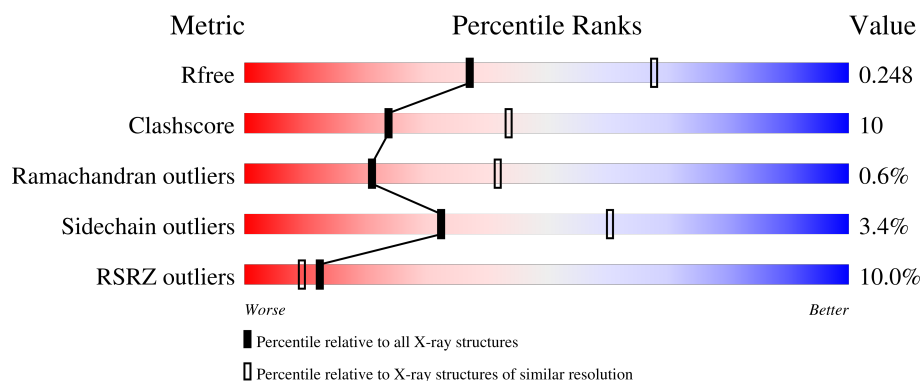
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	943	10% 78% 15% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7281 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 Drug exporters of the RND superfamily-like protein, Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	900	Total	C	N	O	S	0	0	0
			6952	4482	1182	1256	32			

There are 37 discrepancies between the modelled and reference sequences:

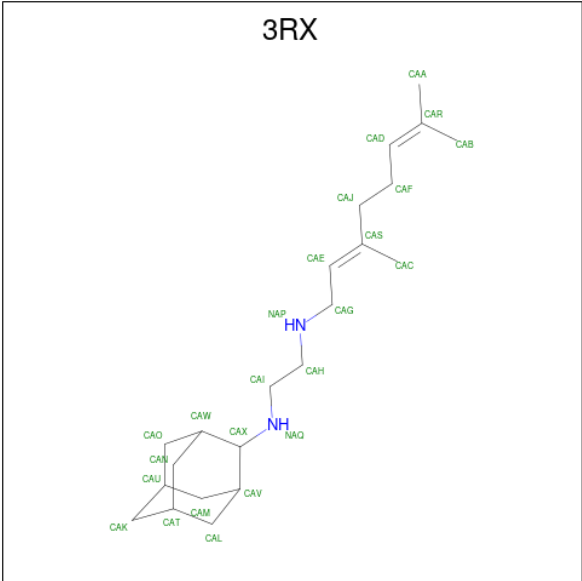
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	expression tag	UNP I7G2R2
A	-11	PRO	-	expression tag	UNP I7G2R2
A	-10	GLU	-	expression tag	UNP I7G2R2
A	-9	VAL	-	expression tag	UNP I7G2R2
A	-8	VAL	-	expression tag	UNP I7G2R2
A	-7	GLY	-	expression tag	UNP I7G2R2
A	-6	SER	-	expression tag	UNP I7G2R2
A	-5	TYR	-	expression tag	UNP I7G2R2
A	-4	PHE	-	expression tag	UNP I7G2R2
A	-3	GLN	-	expression tag	UNP I7G2R2
A	-2	SER	-	expression tag	UNP I7G2R2
A	-1	ASN	-	expression tag	UNP I7G2R2
A	0	ALA	-	expression tag	UNP I7G2R2
A	749	GLU	-	linker	UNP I7G2R2
A	750	PHE	-	linker	UNP I7G2R2
A	803	THR	CYS	engineered mutation	UNP D9IEF7
A	846	ALA	CYS	engineered mutation	UNP D9IEF7
A	911	GLU	-	expression tag	UNP D9IEF7
A	912	PHE	-	expression tag	UNP D9IEF7
A	913	HIS	-	expression tag	UNP D9IEF7
A	914	LEU	-	expression tag	UNP D9IEF7
A	915	GLY	-	expression tag	UNP D9IEF7
A	916	GLY	-	expression tag	UNP D9IEF7
A	917	ILE	-	expression tag	UNP D9IEF7
A	918	LYS	-	expression tag	UNP D9IEF7
A	919	ALA	-	expression tag	UNP D9IEF7
A	920	PHE	-	expression tag	UNP D9IEF7

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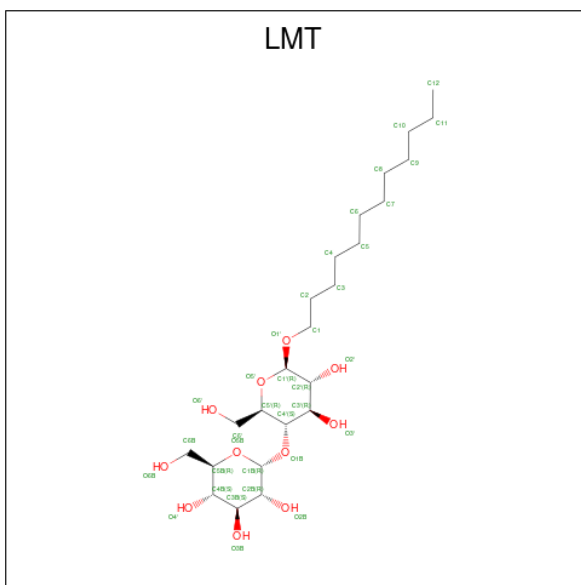
Chain	Residue	Modelled	Actual	Comment	Reference
A	921	HIS	-	expression tag	UNP D9IEF7
A	922	HIS	-	expression tag	UNP D9IEF7
A	923	HIS	-	expression tag	UNP D9IEF7
A	924	HIS	-	expression tag	UNP D9IEF7
A	925	HIS	-	expression tag	UNP D9IEF7
A	926	HIS	-	expression tag	UNP D9IEF7
A	927	HIS	-	expression tag	UNP D9IEF7
A	928	HIS	-	expression tag	UNP D9IEF7
A	929	HIS	-	expression tag	UNP D9IEF7
A	930	HIS	-	expression tag	UNP D9IEF7

- Molecule 2 is N-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-N'-[(1R,3S,5R,7R)-tricyclo[3.3.1.1 3,7]dec-2-yl]ethane-1,2-diamine (CCD ID: 3RX) (formula: C₂₂H₃₈N₂).



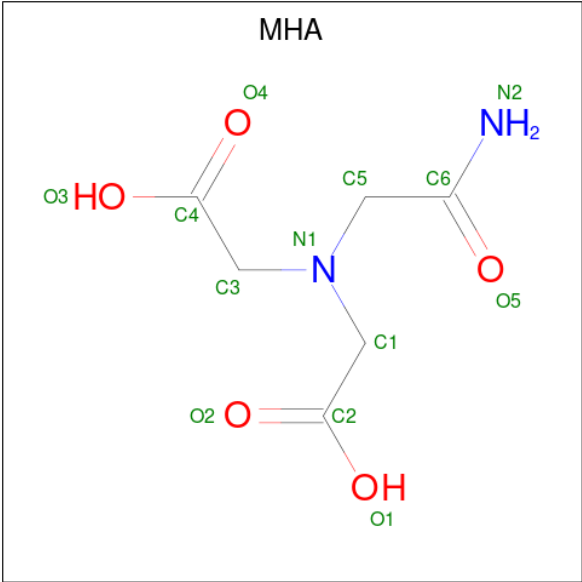
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			24	22	2		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 35	C 24	O 11	0	0
3	A	1	Total 35	C 24	O 11	0	0
3	A	1	Total 35	C 24	O 11	0	0
3	A	1	Total 35	C 24	O 11	0	0
3	A	1	Total 35	C 24	O 11	0	0
3	A	1	Total 28	C 17	O 11	0	0
3	A	1	Total 27	C 16	O 11	0	0
3	A	1	Total 35	C 24	O 11	0	0
3	A	1	Total 14	C 13	O 1	0	0

- Molecule 4 is (CARBAMOYLMETHYL-CARBOXYMETHYL-AMINO)-ACETIC ACID (CCD ID: MHA) (formula: $C_6H_{10}N_2O_5$).



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

3 Residue-property plots [i](#)

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

- Molecule 1: Drug exporters of the RND superfamily-like protein, Endolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.01Å 143.54Å 143.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.38 – 2.60 29.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.38-2.60) 98.2 (29.38-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.216 , 0.248 0.222 , 0.248	Depositor DCC
R_{free} test set	2645 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	71.9	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7281	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: 3RX, LMT, 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	0.37	0/7097	0.83	15/9642 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	GLN	N-CA-C	-13.38	96.69	111.14
1	A	352	THR	N-CA-C	12.42	124.36	111.07
1	A	818	GLN	N-CA-C	-7.72	102.50	112.23
1	A	392	ARG	N-CA-C	-7.70	104.38	114.31
1	A	654	MET	N-CA-C	-6.86	103.73	111.07
1	A	393	LEU	N-CA-C	-6.75	103.92	111.28
1	A	537	GLN	CA-C-N	6.20	124.13	119.66
1	A	537	GLN	C-N-CA	6.20	124.13	119.66
1	A	417	ILE	CA-C-N	-6.11	112.20	119.84
1	A	417	ILE	C-N-CA	-6.11	112.20	119.84
1	A	528	LYS	N-CA-C	5.97	117.59	111.14
1	A	422	LEU	N-CA-C	5.26	118.65	110.17
1	A	918	LYS	CA-C-N	-5.17	115.81	123.05
1	A	918	LYS	C-N-CA	-5.17	115.81	123.05
1	A	419	LEU	N-CA-C	-5.02	107.20	113.38

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	6952	0	7111	145	0
2	A	24	0	38	2	0
3	A	279	0	357	19	0
4	A	26	0	16	0	0
All	All	7281	0	7522	150	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 10.

All (150) 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:398:MET:SD	1:A:729:LYS:HE2	1.63	1.38
1:A:731:LEU:CD2	1:A:734:ASP:HB3	1.62	1.28
1:A:731:LEU:HD22	1:A:734:ASP:CB	1.67	1.25
1:A:584:GLY:O	1:A:742:MET:HE3	1.38	1.20
1:A:398:MET:SD	1:A:729:LYS:CE	2.46	1.03
1:A:398:MET:HE1	1:A:665:ALA:O	1.65	0.95
1:A:628:MET:HG2	1:A:630:PRO:HD2	1.51	0.92
1:A:731:LEU:HD22	1:A:734:ASP:HB3	0.89	0.89
1:A:746:GLN:HG2	1:A:747:GLU:N	1.89	0.86
1:A:397:VAL:HB	1:A:404:PHE:CD2	2.12	0.84
1:A:747:GLU:O	1:A:748:LYS:C	2.20	0.84
1:A:914:LEU:HD12	1:A:914:LEU:O	1.81	0.80
1:A:653:ARG:HH22	3:A:1007:LMT:H6'2	1.43	0.79
1:A:207:THR:HG23	1:A:348:LEU:O	1.84	0.78
1:A:655:VAL:HG22	1:A:736:TRP:HZ3	1.49	0.78
1:A:348:LEU:N	1:A:348:LEU:HD23	1.99	0.77
1:A:397:VAL:HB	1:A:404:PHE:HD2	1.49	0.76
1:A:347:ALA:C	1:A:348:LEU:HD23	2.11	0.75
1:A:731:LEU:HD13	1:A:734:ASP:H	1.54	0.71
1:A:746:GLN:HG2	1:A:747:GLU:H	1.53	0.71
1:A:537:GLN:O	1:A:537:GLN:HG3	1.91	0.70
1:A:739:PRO:C	1:A:741:TRP:H	1.99	0.70
1:A:731:LEU:HD11	1:A:735:CYS:H	1.55	0.70
1:A:528:LYS:H	1:A:528:LYS:HD2	1.57	0.69
1:A:729:LYS:O	1:A:730:LEU:C	2.37	0.68
1:A:398:MET:CE	1:A:665:ALA:O	2.42	0.68
1:A:656:GLU:OE2	1:A:656:GLU:HA	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:HA	1:A:398:MET:HB2	1.77	0.67
1:A:731:LEU:O	1:A:731:LEU:HD12	1.94	0.66
1:A:746:GLN:O	1:A:747:GLU:CB	2.43	0.66
1:A:716:ALA:O	1:A:720:ARG:NH2	2.29	0.66
1:A:731:LEU:HD11	1:A:735:CYS:N	2.10	0.65
1:A:740:ARG:NH1	1:A:740:ARG:HA	2.11	0.65
1:A:399:LYS:O	1:A:401:PRO:HD3	1.97	0.65
1:A:399:LYS:C	1:A:401:PRO:HD3	2.24	0.63
1:A:664:THR:HG21	1:A:732:GLY:HA2	1.79	0.62
1:A:680:THR:HG21	3:A:1008:LMT:H5B	1.80	0.62
1:A:306:LEU:HD11	1:A:570:ILE:HD12	1.82	0.62
1:A:653:ARG:NH2	3:A:1007:LMT:H6'2	2.15	0.61
1:A:204:VAL:O	1:A:677:ARG:NH2	2.33	0.61
1:A:207:THR:HG21	1:A:346:ASP:HA	1.83	0.61
1:A:167:ARG:NH1	1:A:444:GLN:OE1	2.34	0.61
1:A:744:ARG:O	1:A:745:VAL:C	2.44	0.60
1:A:725:PRO:O	1:A:729:LYS:HG2	2.02	0.59
1:A:655:VAL:HA	1:A:736:TRP:CZ3	2.38	0.58
1:A:914:LEU:HD12	1:A:914:LEU:C	2.28	0.58
1:A:398:MET:HE1	1:A:665:ALA:C	2.28	0.58
1:A:664:THR:OG1	1:A:732:GLY:O	2.13	0.58
1:A:653:ARG:HH22	3:A:1007:LMT:C6B	2.14	0.58
1:A:288:ARG:HH11	3:A:1007:LMT:H1B	1.68	0.57
1:A:119:ASP:OD2	3:A:1002:LMT:O4'	2.22	0.57
1:A:731:LEU:CD1	1:A:735:CYS:H	2.18	0.57
1:A:721:MET:SD	3:A:1008:LMT:O4'	2.60	0.57
1:A:35:GLY:HA3	3:A:1006:LMT:H6E	1.86	0.57
1:A:580:PHE:CD1	1:A:589:PRO:HG2	2.39	0.57
3:A:1009:LMT:H6D	3:A:1010:LMT:H12	1.85	0.57
1:A:523:ARG:NH2	1:A:550:PRO:HG3	2.19	0.56
1:A:731:LEU:HD12	1:A:731:LEU:C	2.31	0.56
1:A:746:GLN:O	1:A:747:GLU:HB2	2.05	0.56
1:A:422:LEU:O	1:A:422:LEU:HD13	2.08	0.54
1:A:241:PHE:HD1	3:A:1003:LMT:H122	1.71	0.54
1:A:400:ARG:HB3	1:A:403:ALA:HB3	1.90	0.54
1:A:523:ARG:HH22	1:A:550:PRO:HG3	1.73	0.53
1:A:65:ARG:NH1	1:A:141:GLY:O	2.41	0.53
3:A:1006:LMT:H1B	3:A:1006:LMT:H6D	1.91	0.53
1:A:397:VAL:HG23	1:A:726:ALA:HB2	1.91	0.52
1:A:455:GLU:OE1	1:A:523:ARG:NH1	2.42	0.52
1:A:731:LEU:HD13	1:A:734:ASP:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PHE:O	1:A:313:LYS:NZ	2.43	0.51
1:A:398:MET:SD	1:A:729:LYS:CD	2.99	0.51
1:A:739:PRO:C	1:A:741:TRP:N	2.67	0.51
1:A:857:GLU:OE2	1:A:925:HIS:NE2	2.40	0.51
1:A:596:SER:HA	1:A:599:THR:HG22	1.92	0.51
1:A:604:MET:HE1	1:A:632:ILE:HG23	1.93	0.51
1:A:248:LEU:HD22	1:A:701:MET:HE1	1.94	0.50
1:A:680:THR:HG23	1:A:720:ARG:HH12	1.76	0.50
1:A:127:THR:OG1	1:A:129:ASP:OD1	2.25	0.50
1:A:745:VAL:HG12	1:A:745:VAL:O	2.12	0.50
1:A:584:GLY:C	1:A:742:MET:HE3	2.26	0.49
1:A:650:LEU:HD22	1:A:720:ARG:HG3	1.93	0.49
1:A:666:GLU:O	1:A:669:ARG:N	2.46	0.49
1:A:75:PRO:O	1:A:131:ARG:NH1	2.46	0.49
1:A:253:ILE:HD11	2:A:1001:3RX:HAJ	1.95	0.49
1:A:417:ILE:HG12	1:A:418:PRO:HD3	1.94	0.49
1:A:591:LYS:O	1:A:594:LEU:HB3	2.13	0.49
1:A:392:ARG:O	1:A:395:ASN:HB2	2.13	0.48
1:A:729:LYS:C	1:A:731:LEU:N	2.68	0.48
1:A:872:GLN:OE1	1:A:874:ARG:NH1	2.40	0.48
1:A:392:ARG:HA	1:A:395:ASN:OD1	2.13	0.48
1:A:398:MET:HE1	1:A:665:ALA:CA	2.43	0.48
1:A:731:LEU:HD22	1:A:734:ASP:HB2	1.82	0.48
1:A:349:GLY:O	1:A:352:THR:HG23	2.14	0.47
1:A:585:SER:OG	1:A:735:CYS:O	2.24	0.47
1:A:645:ASP:OD2	2:A:1001:3RX:NAP	2.47	0.47
1:A:747:GLU:O	1:A:749:GLU:N	2.48	0.47
1:A:453:ARG:HG3	3:A:1003:LMT:H6'1	1.97	0.47
1:A:731:LEU:HD21	1:A:734:ASP:HB3	1.77	0.47
1:A:63:ARG:HH22	1:A:143:ASP:HA	1.79	0.47
1:A:398:MET:SD	1:A:729:LYS:HD3	2.55	0.47
1:A:422:LEU:HD12	1:A:422:LEU:H	1.80	0.47
1:A:394:VAL:HG22	1:A:398:MET:HG3	1.95	0.46
3:A:1007:LMT:O3'	3:A:1007:LMT:O2B	2.27	0.46
1:A:740:ARG:HA	1:A:740:ARG:HH11	1.80	0.46
1:A:-2:SER:C	1:A:0:ALA:H	2.23	0.45
3:A:1002:LMT:H121	3:A:1003:LMT:H22	1.98	0.45
1:A:317:TYR:OH	3:A:1009:LMT:H6E	2.15	0.45
1:A:91:THR:HG23	1:A:108:TRP:HZ2	1.82	0.45
1:A:222:ILE:HD11	1:A:251:LEU:HB2	1.98	0.45
1:A:45:ASP:HB3	1:A:48:SER:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:HD12	1:A:330:SER:HB2	1.99	0.44
1:A:69:VAL:HB	1:A:137:ILE:HB	1.99	0.44
1:A:651:VAL:O	1:A:655:VAL:HG23	2.18	0.44
1:A:528:LYS:O	1:A:532:GLU:HG3	2.16	0.44
1:A:659:GLU:CD	1:A:659:GLU:C	2.85	0.44
1:A:207:THR:HG21	1:A:345:VAL:O	2.17	0.44
1:A:-4:PHE:O	1:A:-3:GLN:C	2.61	0.44
1:A:480:LYS:HB3	1:A:536:LEU:HD13	2.00	0.43
1:A:240:PHE:HB3	3:A:1003:LMT:H111	1.99	0.43
3:A:1005:LMT:H121	3:A:1005:LMT:H92	1.78	0.43
1:A:744:ARG:HD2	1:A:744:ARG:HA	1.60	0.43
1:A:662:MET:HE3	1:A:666:GLU:HG2	2.01	0.43
1:A:757:ARG:HG3	1:A:762:LEU:HB2	2.01	0.43
1:A:280:ARG:NH1	1:A:908:ASP:OD1	2.52	0.42
1:A:297:ILE:HG21	1:A:323:VAL:HG21	2.01	0.42
1:A:747:GLU:C	1:A:749:GLU:N	2.71	0.42
1:A:815:LEU:HD12	1:A:818:GLN:HE21	1.84	0.42
1:A:655:VAL:HG22	1:A:736:TRP:CZ3	2.39	0.42
1:A:119:ASP:HB3	1:A:122:VAL:HB	2.01	0.42
1:A:748:LYS:O	1:A:749:GLU:C	2.62	0.42
1:A:717:THR:OG1	1:A:718:ILE:N	2.53	0.42
1:A:247:THR:O	1:A:251:LEU:HB3	2.20	0.42
1:A:666:GLU:O	1:A:667:ALA:C	2.62	0.42
1:A:694:VAL:O	1:A:702:LYS:NZ	2.40	0.42
1:A:738:ALA:C	1:A:739:PRO:O	2.63	0.42
1:A:827:ILE:HD11	1:A:852:VAL:HG21	2.02	0.41
1:A:457:LEU:HD21	1:A:550:PRO:HB2	2.03	0.41
1:A:717:THR:HA	1:A:721:MET:HE2	2.01	0.41
1:A:392:ARG:HH22	1:A:669:ARG:HH11	1.69	0.41
1:A:628:MET:HE1	1:A:700:MET:SD	2.61	0.41
1:A:40:GLN:HB2	3:A:1003:LMT:H51	2.03	0.41
1:A:288:ARG:NH1	3:A:1007:LMT:H4'	2.36	0.41
1:A:631:MET:HE1	1:A:704:LEU:HB2	2.02	0.41
1:A:740:ARG:HH11	1:A:740:ARG:CA	2.34	0.41
1:A:422:LEU:HD13	1:A:422:LEU:C	2.46	0.40
1:A:691:GLY:O	1:A:694:VAL:HG22	2.21	0.40
1:A:729:LYS:O	1:A:731:LEU:N	2.54	0.40
1:A:461:MET:HE3	1:A:514:ARG:HB2	2.03	0.40
1:A:-4:PHE:O	1:A:-2:SER:OG	2.26	0.40
1:A:392:ARG:O	1:A:395:ASN:N	2.54	0.40
1:A:750:PHE:HB3	1:A:907:TRP:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	896/943 (95%)	862 (96%)	29 (3%)	5 (1%)	21	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	740	ARG
1	A	76	PRO
1	A	727	VAL
1	A	739	PRO
1	A	917	ILE

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	738/777 (95%)	713 (97%)	25 (3%)	32	60

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	70	VAL
1	A	196	LEU

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Mol	Chain	Res	Type
1	A	348	LEU
1	A	350	VAL
1	A	352	THR
1	A	354	LEU
1	A	394	VAL
1	A	397	VAL
1	A	398	MET
1	A	399	LYS
1	A	421	GLN
1	A	422	LEU
1	A	537	GLN
1	A	647	GLU
1	A	653	ARG
1	A	656	GLU
1	A	659	GLU
1	A	663	SER
1	A	729	LYS
1	A	740	ARG
1	A	743	LYS
1	A	747	GLU
1	A	748	LYS
1	A	917	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	492	ASN
1	A	537	GLN
1	A	625	GLN
1	A	818	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	LMT	A	1008	-	28,28,36	1.26	2 (7%)	39,39,47	0.94	2 (5%)
3	LMT	A	1010	-	13,13,36	0.81	0	12,12,47	0.83	0
3	LMT	A	1002	-	36,36,36	1.15	2 (5%)	47,47,47	1.05	2 (4%)
2	3RX	A	1001	-	25,26,26	0.30	0	31,35,35	1.11	4 (12%)
3	LMT	A	1003	-	36,36,36	1.12	2 (5%)	47,47,47	1.04	3 (6%)
3	LMT	A	1005	-	36,36,36	1.18	3 (8%)	47,47,47	0.94	2 (4%)
3	LMT	A	1007	-	29,29,36	1.23	2 (6%)	40,40,47	1.05	4 (10%)
3	LMT	A	1009	-	36,36,36	1.14	3 (8%)	47,47,47	1.39	7 (14%)
3	LMT	A	1004	-	36,36,36	1.15	2 (5%)	47,47,47	0.89	1 (2%)
4	MHA	A	1011	-	12,12,12	1.29	1 (8%)	15,15,15	1.36	2 (13%)
3	LMT	A	1006	-	36,36,36	1.13	3 (8%)	47,47,47	1.09	3 (6%)
4	MHA	A	1012	-	12,12,12	1.31	1 (8%)	15,15,15	1.34	2 (13%)

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	LMT	A	1008	-	-	5/13/53/61	0/2/2/2
3	LMT	A	1010	-	-	4/11/11/61	-
3	LMT	A	1002	-	-	5/21/61/61	0/2/2/2
2	3RX	A	1001	-	-	3/15/43/43	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1003	-	-	10/21/61/61	0/2/2/2
3	LMT	A	1005	-	-	9/21/61/61	0/2/2/2
3	LMT	A	1007	-	-	3/14/54/61	0/2/2/2
3	LMT	A	1009	-	-	15/21/61/61	0/2/2/2
3	LMT	A	1004	-	-	7/21/61/61	0/2/2/2
4	MHA	A	1011	-	-	1/12/12/12	-
3	LMT	A	1006	-	-	15/21/61/61	0/2/2/2
4	MHA	A	1012	-	-	2/12/12/12	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1008	LMT	O5B-C1B	3.85	1.51	1.41
3	A	1005	LMT	O5B-C1B	3.78	1.51	1.41
3	A	1004	LMT	O5B-C1B	3.68	1.51	1.41
3	A	1002	LMT	O5B-C1B	3.63	1.51	1.41
3	A	1003	LMT	O5B-C1B	3.52	1.50	1.41
3	A	1007	LMT	O5B-C1B	3.52	1.50	1.41
3	A	1009	LMT	O5B-C1B	3.43	1.50	1.41
3	A	1009	LMT	O5'-C1'	3.31	1.50	1.41
3	A	1002	LMT	O5'-C1'	3.26	1.50	1.41
3	A	1006	LMT	O5B-C1B	3.23	1.50	1.41
3	A	1007	LMT	O5'-C1'	3.18	1.50	1.41
3	A	1006	LMT	O5'-C1'	3.15	1.49	1.41
3	A	1005	LMT	O5'-C1'	3.12	1.49	1.41
3	A	1004	LMT	O5'-C1'	3.11	1.49	1.41
4	A	1011	MHA	C6-N2	3.09	1.42	1.32
3	A	1008	LMT	O5'-C1'	3.09	1.49	1.41
4	A	1012	MHA	C6-N2	3.07	1.42	1.32
3	A	1003	LMT	O5'-C1'	2.97	1.49	1.41
3	A	1006	LMT	O5'-C5'	2.09	1.49	1.44
3	A	1009	LMT	O5'-C5'	2.07	1.49	1.44
3	A	1005	LMT	O5'-C5'	2.02	1.49	1.44

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1009	LMT	O1B-C4'-C3'	3.62	116.44	107.23
3	A	1002	LMT	C1B-O1B-C4'	-3.24	110.30	117.98
3	A	1007	LMT	O5B-C5B-C4B	3.13	115.33	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	LMT	C1B-O1B-C4'	-3.10	110.62	117.98
2	A	1001	3RX	CAC-CAS-CAJ	2.95	120.35	115.23
2	A	1001	3RX	CAI-NAQ-CAX	-2.93	109.98	114.03
3	A	1006	LMT	C1B-O5B-C5B	-2.90	108.06	113.72
3	A	1004	LMT	C1B-O1B-C4'	-2.85	111.21	117.98
3	A	1009	LMT	C1B-O5B-C5B	-2.81	108.24	113.72
3	A	1009	LMT	O5'-C5'-C4'	2.77	115.45	109.72
3	A	1005	LMT	O5'-C5'-C4'	2.74	115.38	109.72
3	A	1009	LMT	O1B-C1B-O5B	-2.59	103.87	110.69
3	A	1005	LMT	C1B-O1B-C4'	-2.51	112.02	117.98
3	A	1006	LMT	O5'-C5'-C4'	2.51	114.91	109.72
4	A	1012	MHA	C6-C5-N1	-2.48	109.87	114.42
4	A	1011	MHA	C5-C6-N2	2.41	120.47	115.61
3	A	1007	LMT	C1B-O1B-C4'	-2.38	112.33	117.98
3	A	1009	LMT	O1B-C4'-C5'	-2.33	103.37	109.48
3	A	1002	LMT	C1B-C2B-C3B	2.33	114.91	110.01
3	A	1009	LMT	O5'-C1'-C2'	2.30	115.09	110.37
3	A	1007	LMT	C3B-C4B-C5B	2.29	114.39	110.23
3	A	1003	LMT	O5'-C5'-C4'	2.26	114.39	109.72
3	A	1003	LMT	C2'-C3'-C4'	2.21	114.70	109.68
3	A	1007	LMT	C6B-C5B-C4B	-2.18	107.67	113.02
3	A	1006	LMT	O1B-C1B-O5B	-2.15	105.02	110.69
3	A	1008	LMT	C1B-O5B-C5B	2.14	117.89	113.72
3	A	1009	LMT	O5'-C5'-C6'	2.13	111.71	106.44
4	A	1011	MHA	C6-C5-N1	-2.13	110.53	114.42
2	A	1001	3RX	CAB-CAR-CAA	2.12	119.47	114.59
4	A	1012	MHA	C5-C6-N2	2.10	119.85	115.61
2	A	1001	3RX	CAH-CAI-NAQ	-2.10	107.63	111.06
3	A	1008	LMT	O5B-C5B-C4B	2.08	113.45	109.70

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	LMT	C2-C1-O1'-C1'
3	A	1009	LMT	O5'-C1'-O1'-C1
3	A	1009	LMT	C3'-C4'-O1B-C1B
3	A	1003	LMT	O5'-C5'-C6'-O6'
3	A	1009	LMT	O5B-C5B-C6B-O6B
3	A	1006	LMT	O5B-C5B-C6B-O6B
3	A	1008	LMT	O5B-C5B-C6B-O6B
3	A	1003	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	A	1002	LMT	O5B-C5B-C6B-O6B
2	A	1001	3RX	CAD-CAF-CAJ-CAS
3	A	1005	LMT	O5'-C5'-C6'-O6'
3	A	1009	LMT	O5B-C1B-O1B-C4'
3	A	1008	LMT	O5'-C5'-C6'-O6'
3	A	1009	LMT	C4B-C5B-C6B-O6B
3	A	1005	LMT	C4'-C5'-C6'-O6'
3	A	1006	LMT	C4B-C5B-C6B-O6B
3	A	1008	LMT	C4'-C5'-C6'-O6'
3	A	1007	LMT	C4'-C5'-C6'-O6'
3	A	1007	LMT	O5'-C5'-C6'-O6'
3	A	1002	LMT	C4B-C5B-C6B-O6B
3	A	1005	LMT	O5B-C5B-C6B-O6B
3	A	1003	LMT	O1'-C1-C2-C3
3	A	1006	LMT	C4'-C5'-C6'-O6'
3	A	1006	LMT	O5'-C5'-C6'-O6'
3	A	1009	LMT	C2B-C1B-O1B-C4'
2	A	1001	3RX	NAP-CAH-CAI-NAQ
3	A	1009	LMT	C2'-C1'-O1'-C1
3	A	1010	LMT	C4-C5-C6-C7
3	A	1008	LMT	C4B-C5B-C6B-O6B
3	A	1006	LMT	C6-C7-C8-C9
3	A	1006	LMT	C1-C2-C3-C4
3	A	1010	LMT	C1-C2-C3-C4
3	A	1004	LMT	C11-C10-C9-C8
3	A	1004	LMT	C7-C8-C9-C10
3	A	1009	LMT	C5-C6-C7-C8
3	A	1005	LMT	C4-C5-C6-C7
3	A	1003	LMT	C11-C10-C9-C8
3	A	1005	LMT	C2-C3-C4-C5
3	A	1009	LMT	C4-C5-C6-C7
3	A	1007	LMT	C2-C3-C4-C5
3	A	1006	LMT	C3'-C4'-O1B-C1B
3	A	1009	LMT	C3-C4-C5-C6
3	A	1010	LMT	O1'-C1-C2-C3
2	A	1001	3RX	CAI-CAH-NAP-CAG
3	A	1003	LMT	C6-C7-C8-C9
3	A	1006	LMT	C5'-C4'-O1B-C1B
3	A	1009	LMT	O5'-C5'-C6'-O6'
3	A	1003	LMT	C1-C2-C3-C4
3	A	1006	LMT	C3-C4-C5-C6
3	A	1004	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	1004	LMT	C4-C5-C6-C7
3	A	1008	LMT	C2-C1-O1'-C1'
3	A	1010	LMT	C9-C10-C11-C12
3	A	1003	LMT	C9-C10-C11-C12
3	A	1009	LMT	C1-C2-C3-C4
3	A	1004	LMT	C1-C2-C3-C4
3	A	1004	LMT	C4B-C5B-C6B-O6B
3	A	1006	LMT	C2-C1-O1'-C1'
3	A	1003	LMT	C2-C3-C4-C5
3	A	1002	LMT	C1-C2-C3-C4
3	A	1002	LMT	C5-C6-C7-C8
3	A	1006	LMT	C11-C10-C9-C8
3	A	1005	LMT	C4B-C5B-C6B-O6B
3	A	1003	LMT	C7-C8-C9-C10
3	A	1009	LMT	C2-C1-O1'-C1'
3	A	1006	LMT	C2'-C1'-O1'-C1
3	A	1006	LMT	C7-C8-C9-C10
4	A	1012	MHA	C2-C1-N1-C5
3	A	1005	LMT	C5-C6-C7-C8
4	A	1012	MHA	C2-C1-N1-C3
3	A	1005	LMT	C2-C1-O1'-C1'
3	A	1009	LMT	C11-C10-C9-C8
3	A	1009	LMT	C6-C7-C8-C9
3	A	1002	LMT	C2'-C1'-O1'-C1
3	A	1004	LMT	O5B-C5B-C6B-O6B
3	A	1006	LMT	O5'-C1'-O1'-C1
3	A	1006	LMT	C2-C3-C4-C5
4	A	1011	MHA	C2-C1-N1-C3
3	A	1005	LMT	C1-C2-C3-C4

There are no ring outliers.

9 monomers are involved in 21 short contacts:

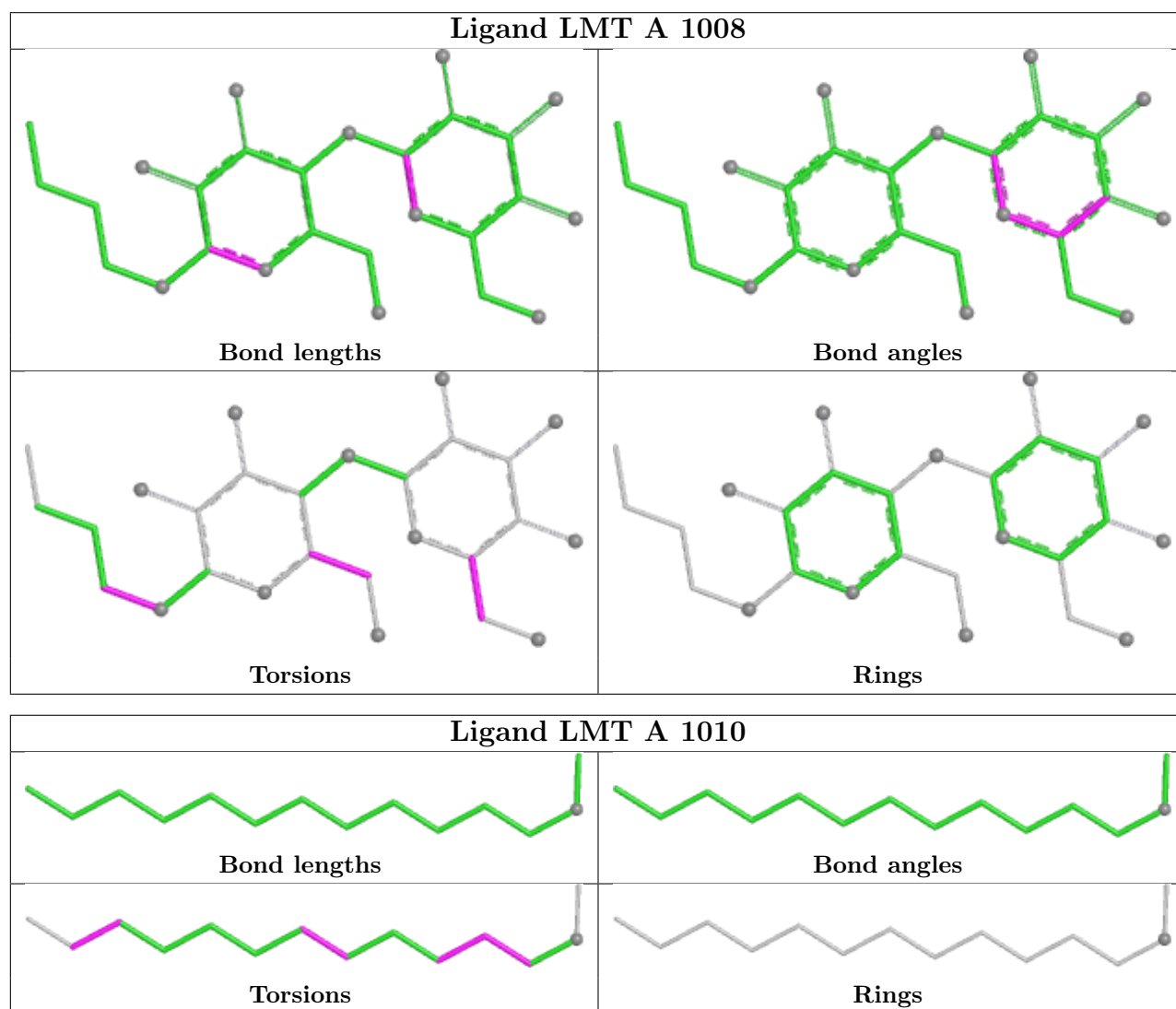
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1008	LMT	2	0
3	A	1010	LMT	1	0
3	A	1002	LMT	2	0
2	A	1001	3RX	2	0
3	A	1003	LMT	5	0
3	A	1005	LMT	1	0
3	A	1007	LMT	6	0
3	A	1009	LMT	2	0

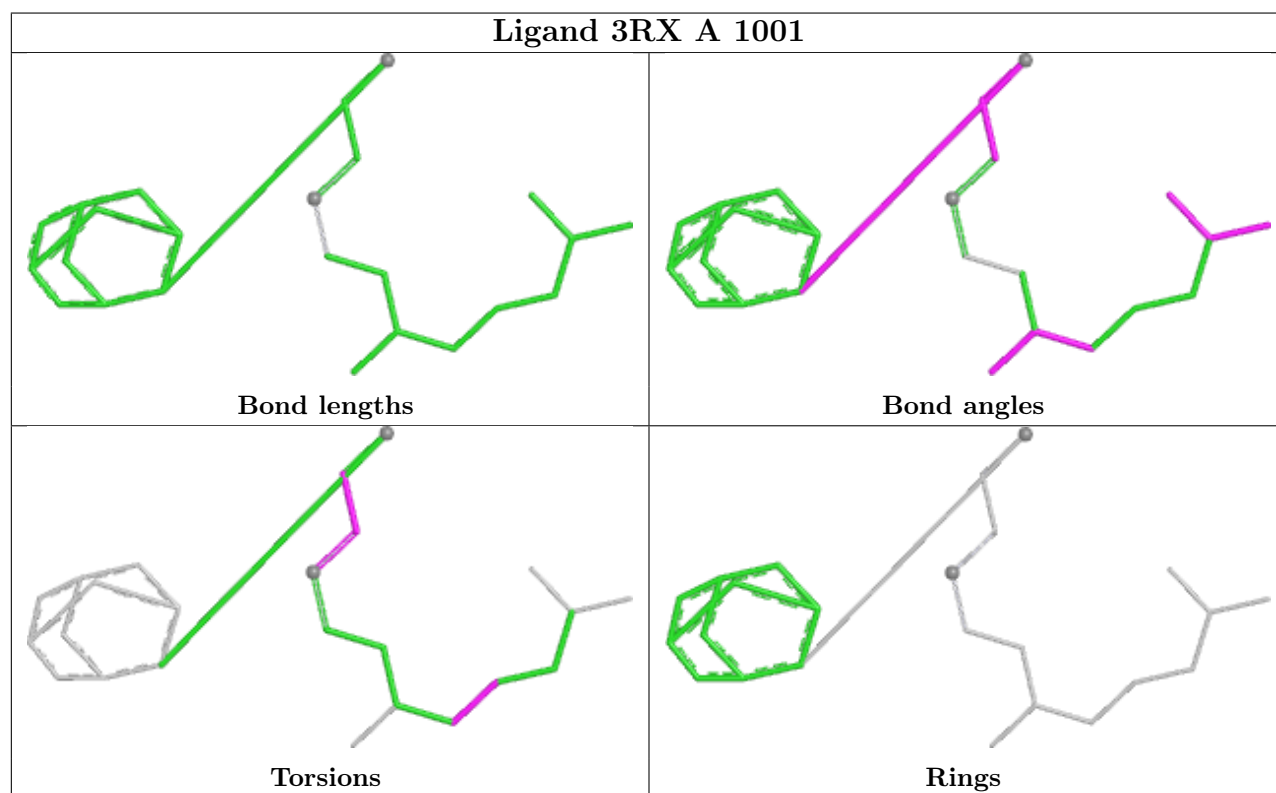
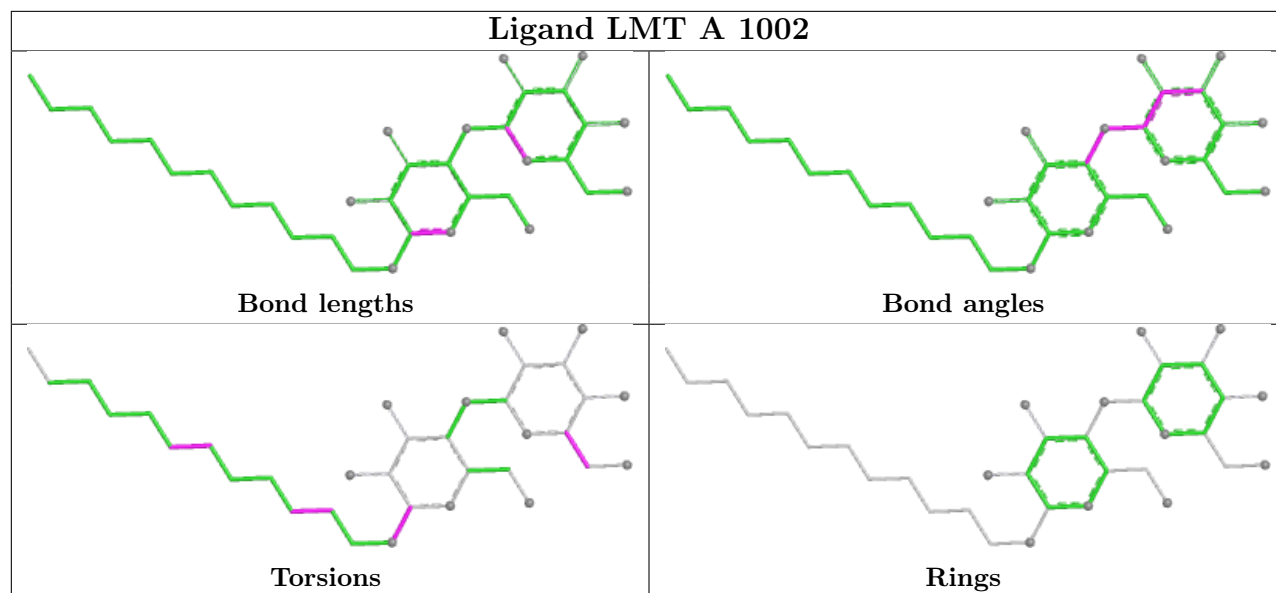
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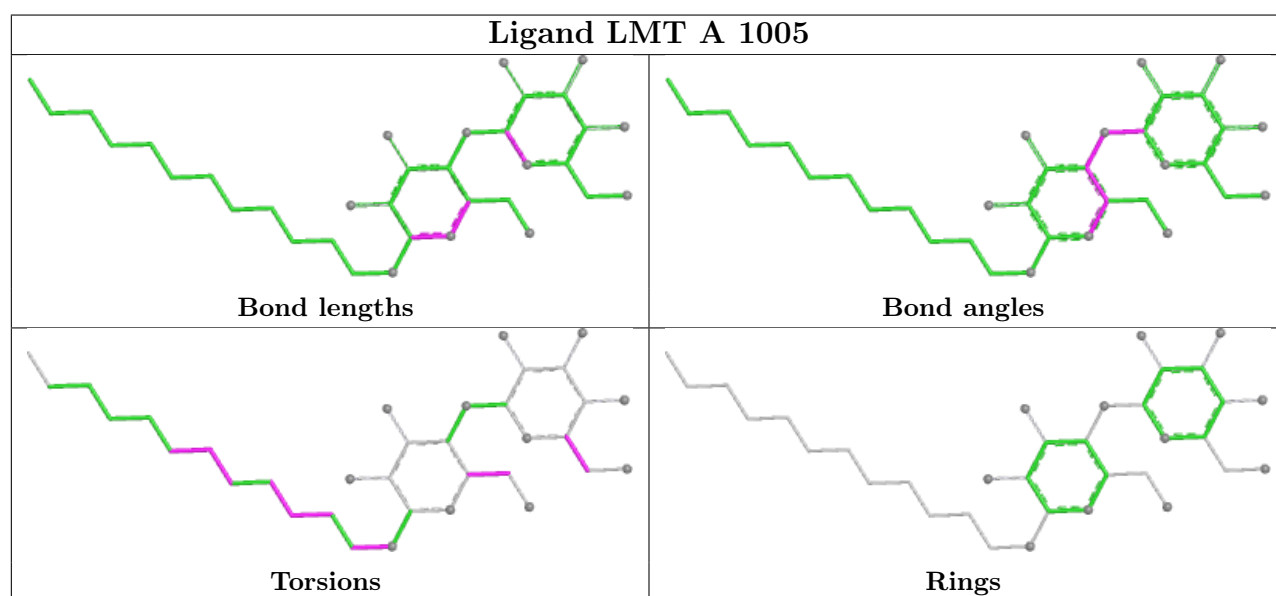
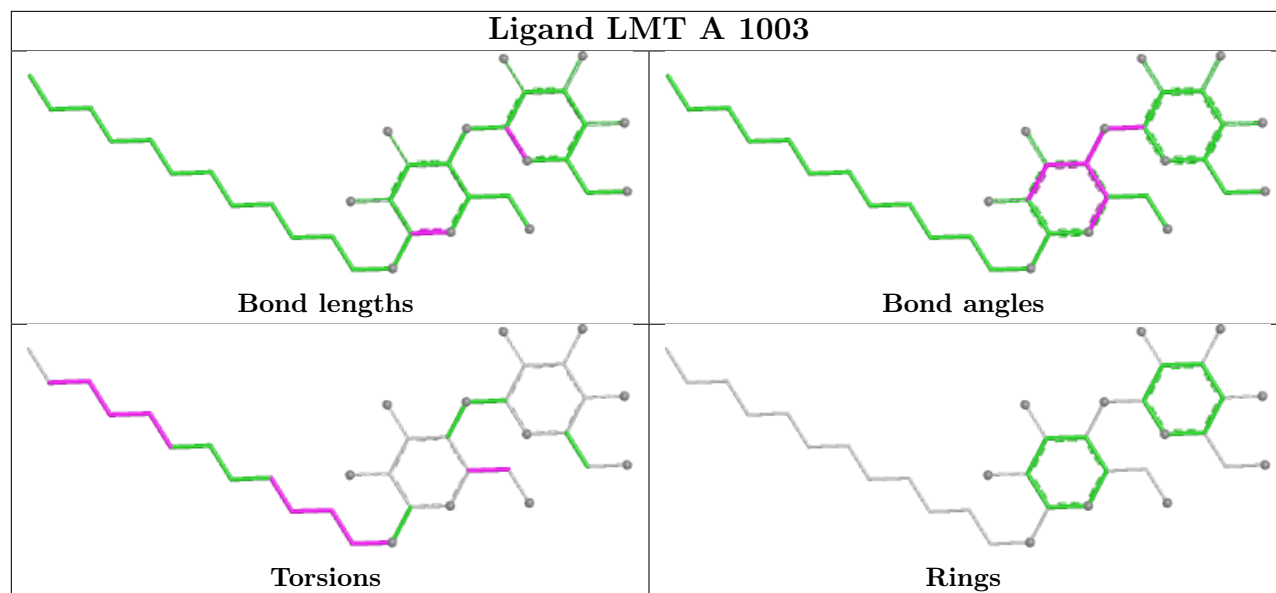
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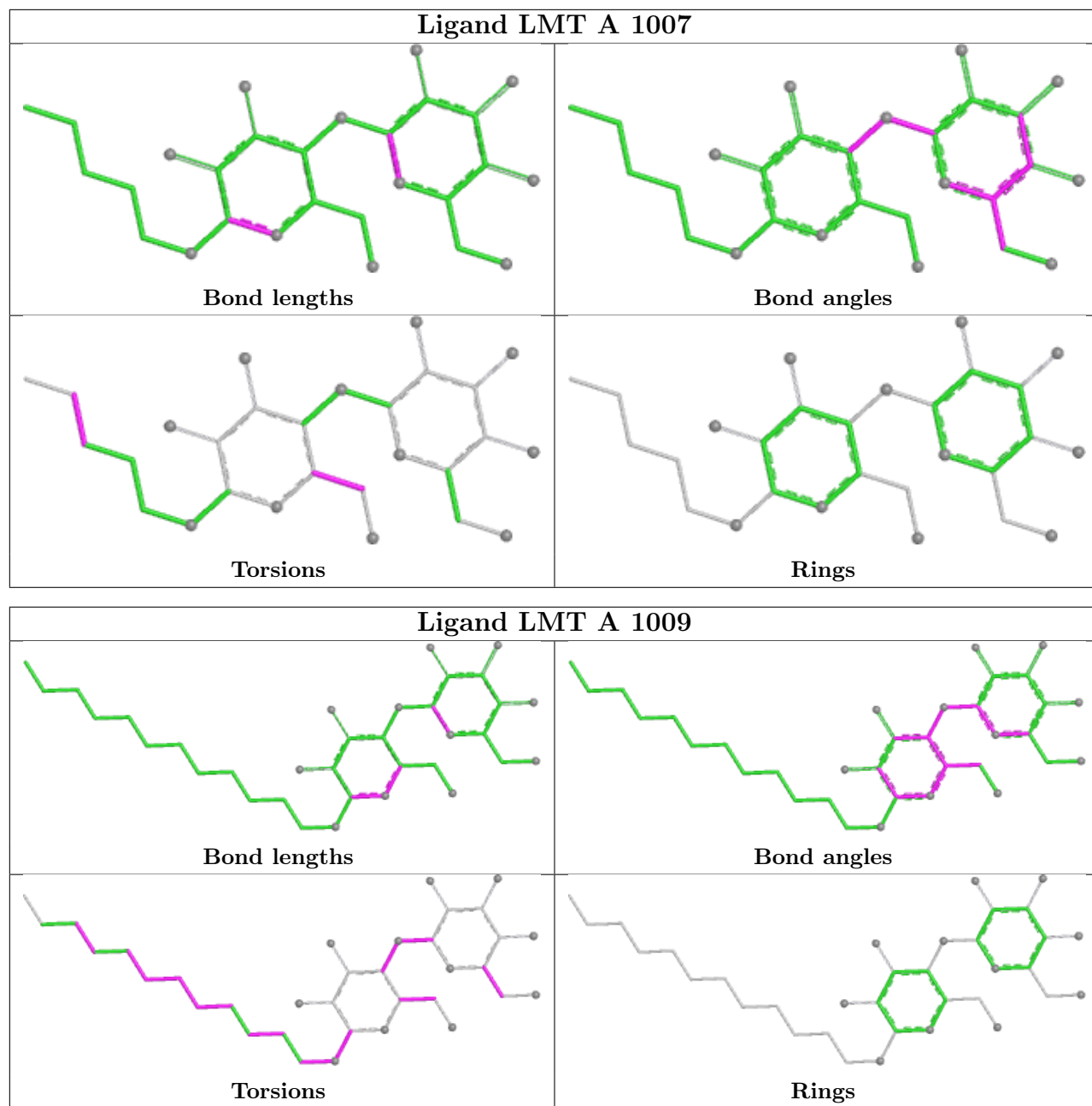
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1006	LMT	2	0

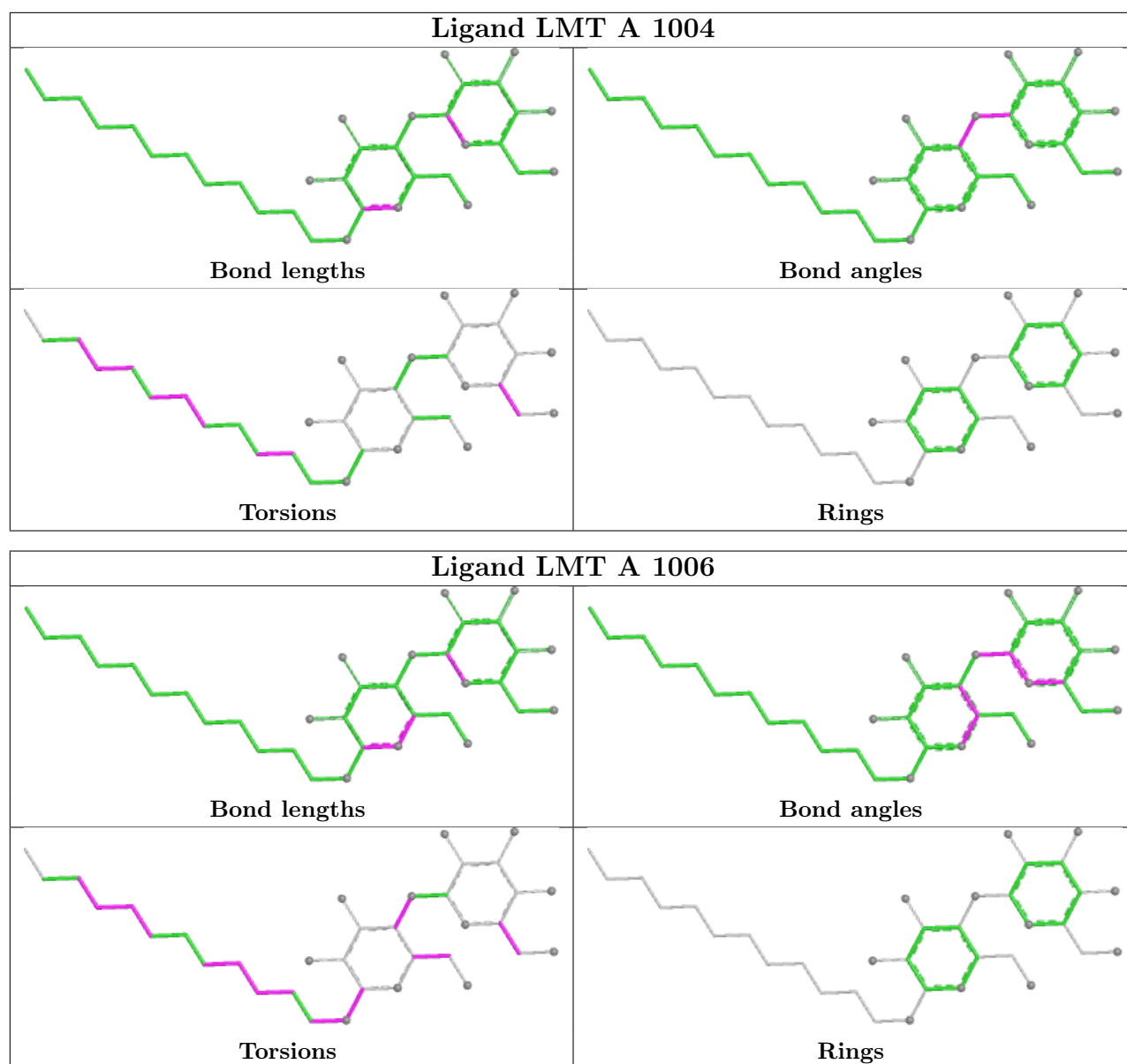
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	900/943 (95%)	0.60	90 (10%) 12 9	53, 79, 149, 205	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TRP	8.4
1	A	652	SER	6.1
1	A	741	TRP	5.8
1	A	739	PRO	5.7
1	A	736	TRP	5.6
1	A	743	LYS	5.6
1	A	738	ALA	5.5
1	A	745	VAL	4.9
1	A	583	PHE	4.9
1	A	655	VAL	4.8
1	A	653	ARG	4.5
1	A	171	LEU	4.3
1	A	399	LYS	4.2
1	A	391	GLY	4.1
1	A	674	THR	4.0
1	A	730	LEU	4.0
1	A	732	GLY	3.9
1	A	353	LEU	3.8
1	A	81	VAL	3.8
1	A	647	GLU	3.8
1	A	727	VAL	3.8
1	A	786	PRO	3.8
1	A	354	LEU	3.7
1	A	64	ASP	3.7
1	A	785	SER	3.5
1	A	392	ARG	3.5
1	A	729	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	580	PHE	3.5
1	A	914	LEU	3.5
1	A	249	ILE	3.4
1	A	656	GLU	3.4
1	A	733	ASP	3.3
1	A	4	TRP	3.3
1	A	665	ALA	3.3
1	A	700	MET	3.2
1	A	128	GLN	3.1
1	A	14	TYR	3.1
1	A	735	CYS	3.1
1	A	1	MET	3.0
1	A	915	GLY	3.0
1	A	748	LYS	2.9
1	A	917	ILE	2.9
1	A	584	GLY	2.9
1	A	483	THR	2.9
1	A	928	HIS	2.9
1	A	740	ARG	2.8
1	A	390	TRP	2.8
1	A	393	LEU	2.8
1	A	659	GLU	2.8
1	A	742	MET	2.8
1	A	734	ASP	2.8
1	A	857	GLU	2.8
1	A	421	GLN	2.7
1	A	219	GLY	2.7
1	A	7	ARG	2.7
1	A	644	THR	2.7
1	A	187	LYS	2.7
1	A	649	PHE	2.7
1	A	804	ASN	2.6
1	A	12	PHE	2.6
1	A	77	ASP	2.6
1	A	913	HIS	2.6
1	A	-4	PHE	2.6
1	A	11	GLN	2.5
1	A	523	ARG	2.5
1	A	837	TYR	2.5
1	A	599	THR	2.4
1	A	540	HIS	2.4
1	A	670	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	731	LEU	2.4
1	A	628	MET	2.4
1	A	537	GLN	2.4
1	A	63	ARG	2.4
1	A	389	PHE	2.3
1	A	528	LYS	2.3
1	A	747	GLU	2.3
1	A	163	GLY	2.3
1	A	579	MET	2.2
1	A	401	PRO	2.2
1	A	561	PHE	2.2
1	A	437	ALA	2.2
1	A	240	PHE	2.2
1	A	133	THR	2.1
1	A	406	ALA	2.1
1	A	209	ILE	2.1
1	A	926	HIS	2.0
1	A	918	LYS	2.0
1	A	67	SER	2.0
1	A	594	LEU	2.0
1	A	929	HIS	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](#)

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($\text{\AA}^2$)	Q<0.9
3	LMT	A	1008	27/35	0.53	0.19	83,115,141,144	0
3	LMT	A	1006	35/35	0.70	0.25	99,140,151,152	0

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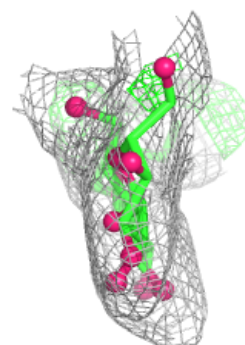
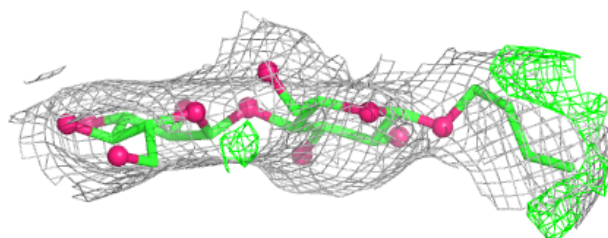
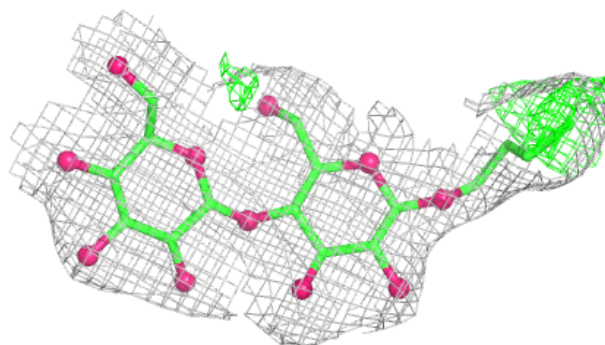
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	A	1009	35/35	0.76	0.16	82,136,151,153	0
3	LMT	A	1005	35/35	0.78	0.19	71,132,142,143	0
3	LMT	A	1003	35/35	0.86	0.21	77,130,138,144	0
3	LMT	A	1007	28/35	0.87	0.15	110,123,132,140	0
4	MHA	A	1011	13/13	0.88	0.12	75,82,92,93	0
3	LMT	A	1010	14/35	0.89	0.23	68,89,121,130	0
4	MHA	A	1012	13/13	0.90	0.10	67,75,89,91	0
3	LMT	A	1002	35/35	0.92	0.14	52,115,143,145	0
3	LMT	A	1004	35/35	0.93	0.11	71,86,108,113	0
2	3RX	A	1001	24/24	0.96	0.15	81,90,96,98	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.

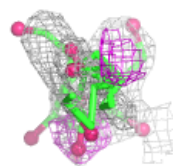
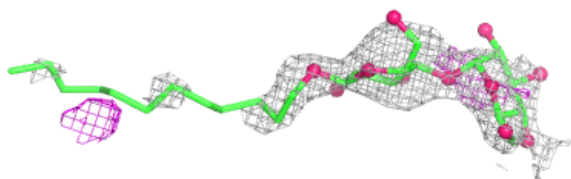
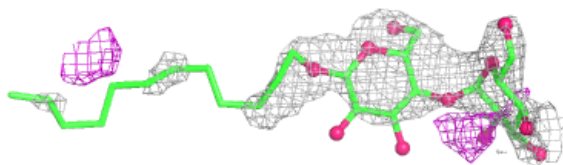
Electron density around LMT A 1008:

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

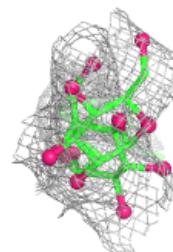
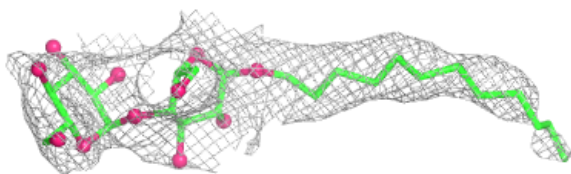
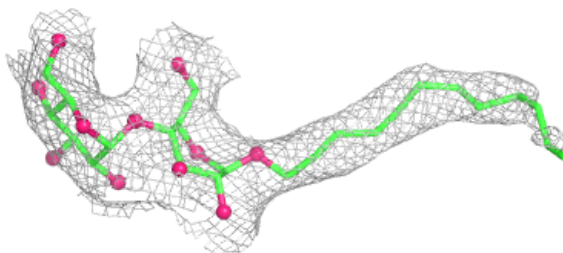


Electron density around LMT A 1006:

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

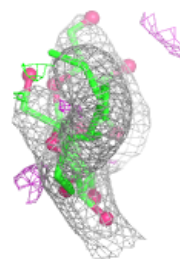
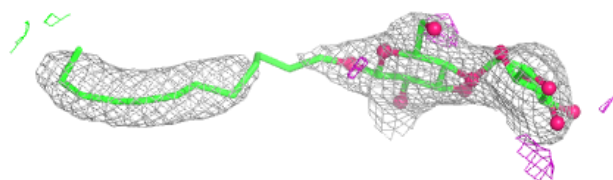
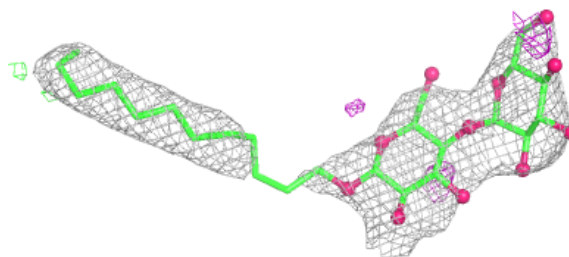
**Electron density around LMT A 1009:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

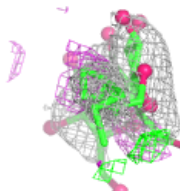
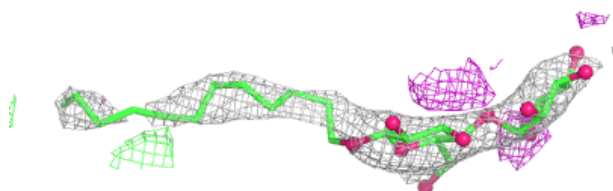
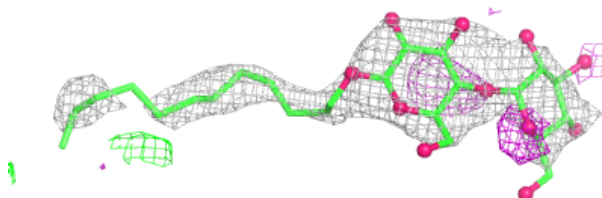


Electron density around LMT A 1005:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

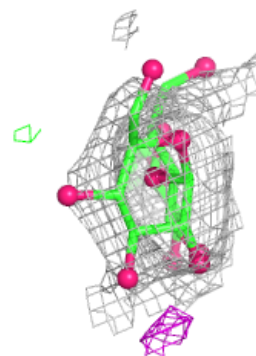
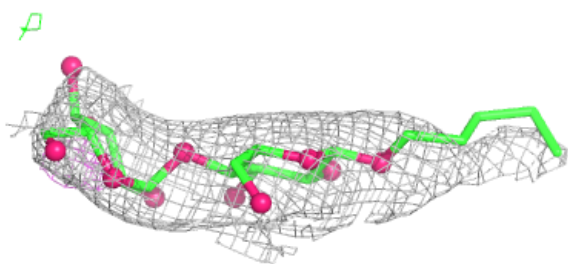
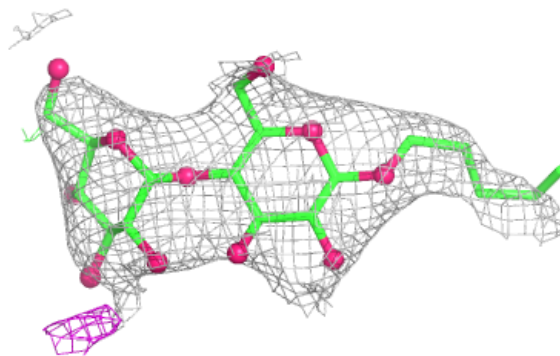
**Electron density around LMT A 1003:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

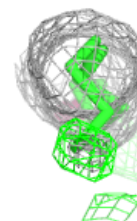
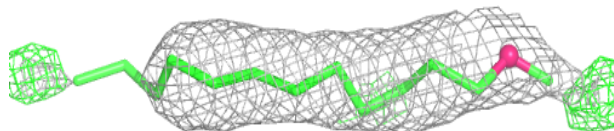
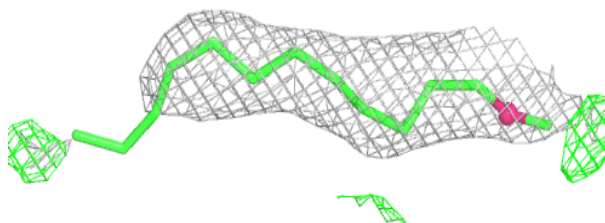


Electron density around LMT A 1007:

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

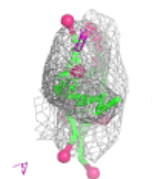
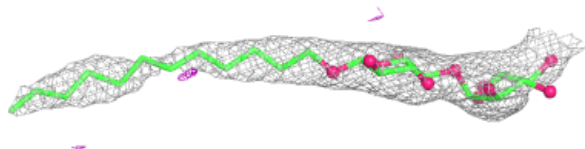
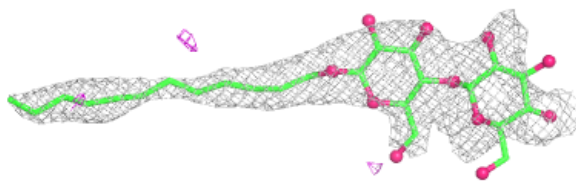
**Electron density around LMT A 1010:**

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

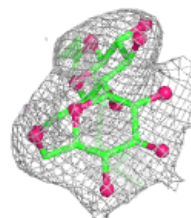
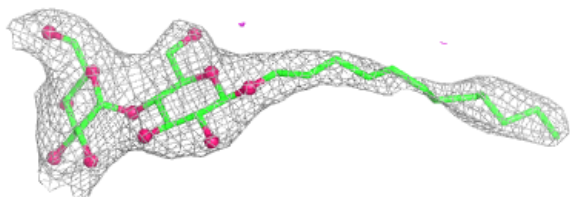
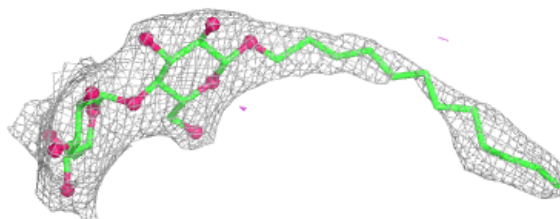


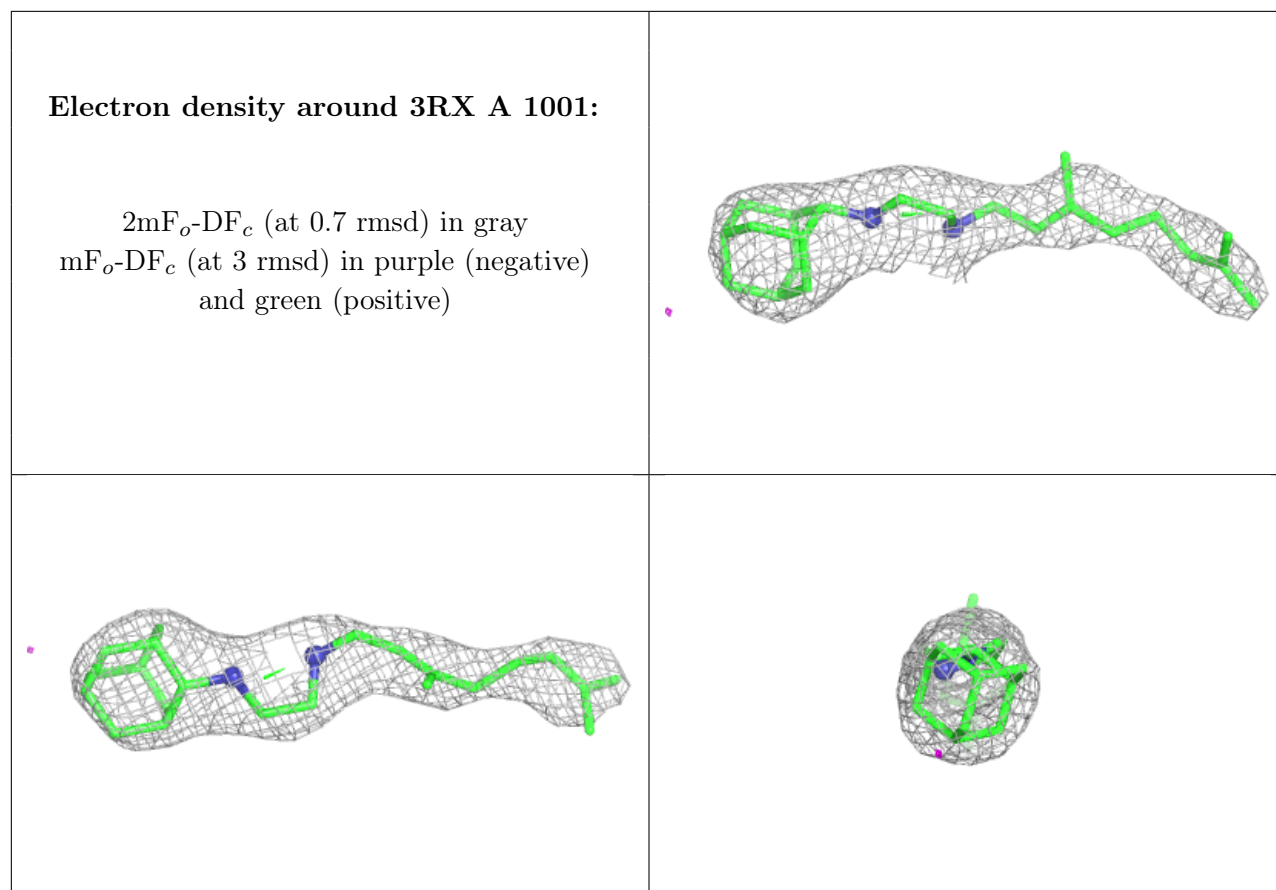
Electron density around LMT A 1002:

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

**Electron density around LMT A 1004:**

$2mF_o-DF_c$ (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.