



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:03 PM UTC

PDB ID : 7UCL / pdb_00007ucl
Title : SxtA Methyltransferase variant F458H in complex with Mn²⁺ and malonate
Authors : Lao, Y.; Smith, J.L.
Deposited on : 2022-03-16
Resolution : 2.09 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

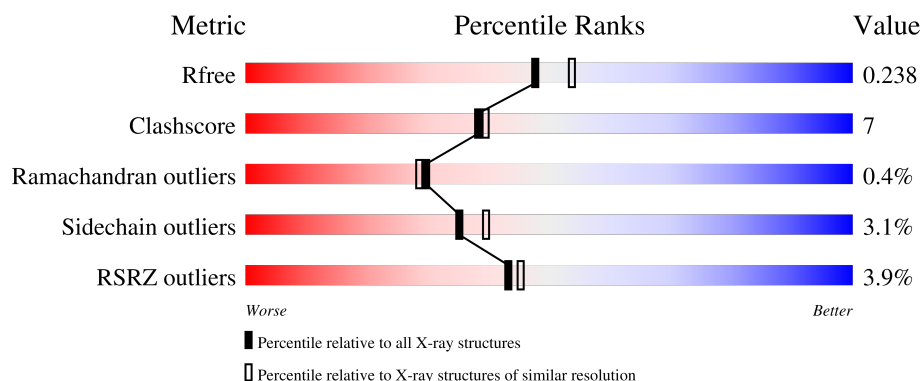
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	713	
1	B	713	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10088 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 Polyketide synthase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4923	3150	855	898	20			
1	B	616	Total	C	N	O	S	0	0	0
			4909	3145	852	892	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B3EYF9
A	-1	ASN	-	expression tag	UNP B3EYF9
A	0	ALA	-	expression tag	UNP B3EYF9
A	458	HIS	PHE	engineered mutation	UNP B3EYF9
B	-2	SER	-	expression tag	UNP B3EYF9
B	-1	ASN	-	expression tag	UNP B3EYF9
B	0	ALA	-	expression tag	UNP B3EYF9
B	458	HIS	PHE	engineered mutation	UNP B3EYF9

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		

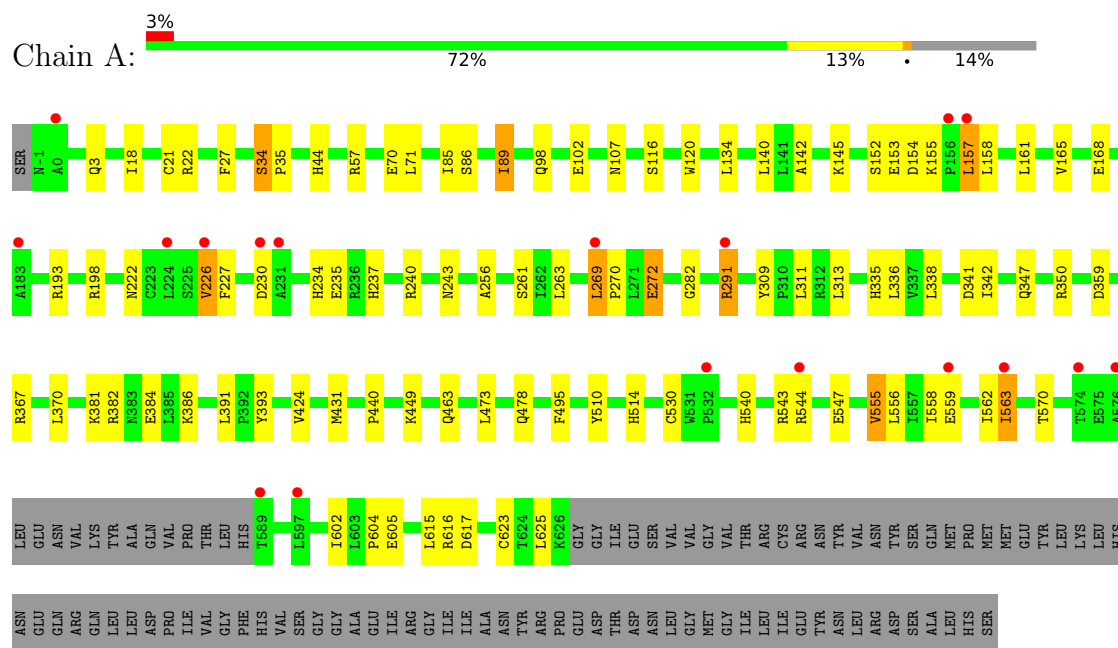
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		
4	B	109	Total	O	0	0
			109	109		

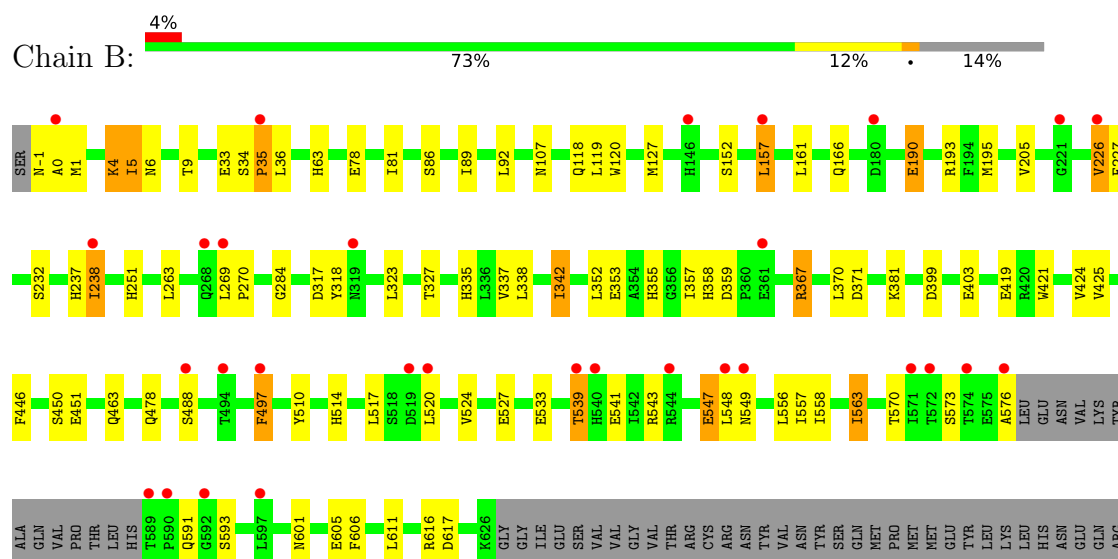
3 Residue-property plots

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: Polyketide synthase-related protein



• Molecule 1: Polyketide synthase-related protein



GLN
LEU
LEU
ASP
PRO
ILE
VAL
GLY
PHE
HIS
VAL
SER
GLY
GLY
ALA
GLU
ILE
ARG
GLY
ILE
ILE
ALA
ASN
TYR
ARG
PRO
GLU
ASP
THR
ASP
ASN
LEU
GLY
MET
GLY
ILE
ILE
LEU
ILE
GLU
TYR
ASN
LEU
ARG
ASP
SER
ALA
LEU
HIS
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.64Å 83.79Å 117.82Å 90.00° 103.09° 90.00°	Depositor
Resolution (Å)	47.34 – 2.09 47.34 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.34-2.09) 86.8 (47.34-2.09)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.02 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.239 0.206 , 0.238	Depositor DCC
R_{free} test set	1993 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10088	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: MN, MLI

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	0.39	0/5032	0.58	0/6825
1	B	0.39	0/5017	0.57	0/6804
All	All	0.39	0/10049	0.58	0/13629

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	SER	Peptide
1	A	367	ARG	Sidechain
1	B	367	ARG	Sidechain

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	4923	0	4928	69	1
1	B	4909	0	4920	68	0
2	A	7	0	2	0	0
2	B	7	0	2	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	131	0	0	33	2
4	B	109	0	0	20	0
All	All	10088	0	9852	136	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (136) 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:18:ILE:O	4:A:901:HOH:O	1.69	1.09
1:A:235:GLU:OE2	4:A:902:HOH:O	1.94	0.86
1:B:157:LEU:O	4:B:901:HOH:O	1.96	0.83
1:A:256:ALA:HA	1:A:291:ARG:HH22	1.46	0.81
1:A:22:ARG:N	4:A:901:HOH:O	2.13	0.81
1:B:450:SER:OG	4:B:903:HOH:O	1.99	0.80
1:A:116:SER:O	4:A:903:HOH:O	1.99	0.79
1:A:240:ARG:NH2	4:A:902:HOH:O	2.14	0.79
1:B:119:LEU:N	4:B:905:HOH:O	2.16	0.78
1:A:602:ILE:O	4:A:905:HOH:O	2.04	0.75
1:B:563:ILE:HG21	4:B:1008:HOH:O	1.87	0.73
1:B:514:HIS:ND1	4:B:909:HOH:O	2.21	0.73
1:A:623:CYS:SG	4:A:1024:HOH:O	2.47	0.72
4:A:905:HOH:O	1:B:593:SER:OG	2.07	0.72
1:B:0:ALA:O	4:B:904:HOH:O	2.07	0.71
1:A:616:ARG:NH1	1:A:617:ASP:OD1	2.25	0.69
1:B:342:ILE:HD12	1:B:370:LEU:HG	1.75	0.69
1:B:478:GLN:NE2	4:B:911:HOH:O	2.23	0.68
1:B:269:LEU:HB2	1:B:270:PRO:HD3	1.76	0.67
1:A:27:PHE:HE2	4:A:901:HOH:O	1.77	0.67
1:A:44:HIS:ND1	4:A:907:HOH:O	2.28	0.67
1:A:198:ARG:NH1	4:A:909:HOH:O	2.29	0.66
1:A:543:ARG:NH1	4:A:906:HOH:O	2.17	0.66
1:A:543:ARG:NH1	4:A:908:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HB2	4:A:949:HOH:O	1.98	0.62
1:A:558:ILE:HG13	1:A:563:ILE:HG12	1.82	0.62
1:A:161:LEU:HB3	1:A:165:VAL:CG2	2.31	0.61
1:B:63:HIS:ND1	1:B:78:GLU:OE2	2.33	0.61
1:B:1:MET:HA	4:B:904:HOH:O	2.00	0.61
1:B:573:SER:HB3	1:B:593:SER:HB2	1.84	0.59
1:A:382:ARG:NH2	4:A:912:HOH:O	2.36	0.59
1:B:-1:ASN:C	1:B:1:MET:H	2.10	0.59
1:A:230:ASP:HB2	1:A:234:HIS:H	1.68	0.58
1:B:533:GLU:HG3	4:B:984:HOH:O	2.02	0.58
1:B:524:VAL:HG21	1:B:539:THR:HG22	1.87	0.57
1:B:34:SER:HB2	1:B:35:PRO:HD3	1.87	0.57
1:B:161:LEU:O	1:B:166:GLN:NE2	2.36	0.57
1:A:237:HIS:HD2	4:A:989:HOH:O	1.87	0.57
1:A:530:CYS:SG	4:A:905:HOH:O	2.31	0.56
1:B:338:LEU:HD21	1:B:355:HIS:CD2	2.39	0.56
1:B:421:TRP:O	1:B:425:VAL:HG23	2.05	0.56
1:B:353:GLU:OE2	1:B:358:HIS:ND1	2.39	0.56
1:B:107:ASN:HB3	4:B:1004:HOH:O	2.07	0.55
1:A:230:ASP:HB2	1:A:234:HIS:N	2.22	0.55
1:B:543:ARG:N	4:B:916:HOH:O	2.40	0.55
1:A:21:CYS:HB2	4:A:901:HOH:O	2.07	0.55
1:A:85:ILE:HG13	4:A:1028:HOH:O	2.06	0.54
1:A:227:PHE:N	4:A:904:HOH:O	2.01	0.54
1:B:488:SER:OG	4:B:906:HOH:O	2.18	0.54
1:A:256:ALA:HA	1:A:291:ARG:NH2	2.18	0.54
1:A:556:LEU:N	4:A:915:HOH:O	2.41	0.54
1:A:604:PRO:HB3	1:B:576:ALA:HA	1.89	0.54
1:B:237:HIS:HD2	4:B:951:HOH:O	1.90	0.53
1:A:558:ILE:HG22	1:A:559:GLU:HG2	1.90	0.53
1:A:193:ARG:NH1	4:A:913:HOH:O	2.38	0.53
1:B:323:LEU:HD22	1:B:337:VAL:HG13	1.91	0.52
1:B:367:ARG:HD2	1:B:371:ASP:OD2	2.09	0.52
1:B:317:ASP:OD1	1:B:318:TYR:N	2.42	0.52
1:A:89:ILE:HG12	1:A:134:LEU:HD22	1.90	0.52
1:A:540:HIS:O	1:A:544:ARG:HG2	2.10	0.51
1:A:85:ILE:HG13	4:A:1029:HOH:O	2.10	0.51
1:A:543:ARG:HD2	4:A:906:HOH:O	2.10	0.50
1:B:352:LEU:HD22	1:B:357:ILE:HD12	1.94	0.50
1:A:282:GLY:HA3	1:A:370:LEU:HD22	1.93	0.49
1:B:118:GLN:O	1:B:120:TRP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASN:OD1	4:B:907:HOH:O	2.20	0.48
1:A:269:LEU:HA	4:A:968:HOH:O	2.13	0.48
1:A:272:GLU:HG3	1:A:309:TYR:CE1	2.48	0.48
1:A:547:GLU:OE2	4:A:906:HOH:O	2.20	0.48
1:B:605:GLU:HB3	1:B:606:PHE:CD2	2.49	0.48
1:B:517:LEU:HD21	1:B:547:GLU:OE2	2.13	0.47
1:A:153:GLU:C	1:A:155:LYS:H	2.21	0.47
1:A:386:LYS:HE2	4:A:912:HOH:O	2.13	0.47
1:B:33:GLU:HB2	1:B:36:LEU:HD11	1.96	0.47
1:B:86:SER:O	1:B:89:ILE:HG12	2.14	0.47
1:A:269:LEU:HB2	1:A:270:PRO:HD3	1.97	0.47
1:B:616:ARG:NH1	1:B:617:ASP:OD1	2.47	0.47
1:B:327:THR:HG23	1:B:335:HIS:NE2	2.30	0.47
1:B:251:HIS:HE1	4:B:923:HOH:O	1.98	0.46
1:A:261:SER:HB3	1:A:431:MET:HE2	1.98	0.46
1:A:449:LYS:HD2	1:A:495:PHE:CZ	2.49	0.46
1:A:514:HIS:HD2	4:A:928:HOH:O	1.98	0.45
1:B:558:ILE:HG13	1:B:563:ILE:HG12	1.99	0.45
1:B:381:LYS:NZ	1:B:419:GLU:OE1	2.42	0.45
1:A:107:ASN:HB2	1:A:168:GLU:OE2	2.17	0.45
1:A:313:LEU:O	1:A:335:HIS:HA	2.17	0.45
1:B:510:TYR:HB2	1:B:556:LEU:HD21	1.99	0.45
1:B:78:GLU:OE1	1:B:78:GLU:N	2.48	0.45
1:B:611:LEU:HD13	4:B:1008:HOH:O	2.17	0.45
1:A:510:TYR:HB3	1:A:558:ILE:HD13	1.99	0.45
1:B:-1:ASN:C	1:B:1:MET:N	2.73	0.45
1:B:4:LYS:HD2	1:B:4:LYS:HA	1.61	0.45
1:B:81:ILE:HD13	1:B:127:MET:HG3	2.00	0.44
1:B:497:PHE:C	1:B:497:PHE:CD2	2.96	0.44
1:A:391:LEU:HD12	1:A:393:TYR:OH	2.18	0.44
1:B:556:LEU:HD23	1:B:557:ILE:N	2.31	0.44
1:B:359:ASP:N	1:B:359:ASP:OD1	2.50	0.44
1:B:226:VAL:HA	4:B:902:HOH:O	2.17	0.44
1:A:89:ILE:HD12	1:A:120:TRP:CZ3	2.52	0.43
1:A:57:ARG:HG3	1:A:440:PRO:HG3	2.00	0.43
1:A:347:GLN:OE1	1:A:350:ARG:NH2	2.50	0.43
1:A:359:ASP:OD1	1:A:359:ASP:N	2.44	0.43
1:B:399:ASP:OD2	1:B:403:GLU:HB2	2.19	0.43
1:A:240:ARG:NH1	1:A:243:ASN:OD1	2.51	0.43
1:B:446:PHE:HB2	1:B:497:PHE:HE1	1.84	0.43
1:A:152:SER:O	1:A:154:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLU:OE2	1:B:601:ASN:ND2	2.49	0.43
1:B:5:ILE:HG13	1:B:195:MET:HE1	2.01	0.42
1:A:341:ASP:OD1	1:A:342:ILE:N	2.52	0.42
1:A:142:ALA:O	1:A:145:LYS:HB2	2.20	0.42
1:B:446:PHE:CB	1:B:497:PHE:HE1	2.33	0.42
1:B:9:THR:HG23	1:B:205:VAL:HG11	2.02	0.42
1:A:615:LEU:HD22	4:A:915:HOH:O	2.19	0.42
1:B:548:LEU:HA	1:B:548:LEU:HD12	1.82	0.42
1:A:336:LEU:HG	1:A:338:LEU:HD13	2.01	0.41
1:A:381:LYS:HD3	1:A:384:GLU:OE2	2.19	0.41
1:A:473:LEU:HD22	1:A:625:LEU:HD12	2.02	0.41
1:A:70:GLU:O	1:A:71:LEU:HB2	2.20	0.41
1:A:263:LEU:HA	1:A:263:LEU:HD23	1.87	0.41
1:A:313:LEU:HD23	4:A:924:HOH:O	2.20	0.41
1:A:478:GLN:NE2	4:A:928:HOH:O	2.52	0.41
1:A:157:LEU:HG	1:A:158:LEU:HG	2.02	0.41
1:B:497:PHE:C	1:B:497:PHE:HD2	2.28	0.41
1:A:555:VAL:HG13	1:A:562:ILE:HG23	2.01	0.41
1:B:226:VAL:O	1:B:227:PHE:HB2	2.21	0.41
1:A:226:VAL:HA	4:A:904:HOH:O	2.21	0.41
1:B:190:GLU:HG3	1:B:193:ARG:NH2	2.36	0.41
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.89	0.41
1:B:227:PHE:N	4:B:902:HOH:O	1.98	0.41
1:B:237:HIS:ND1	1:B:238:ILE:HG23	2.36	0.41
1:B:284:GLY:HA3	4:B:983:HOH:O	2.20	0.41
1:B:611:LEU:HD23	1:B:611:LEU:HA	1.84	0.41
1:A:98:GLN:O	1:A:102:GLU:HG2	2.21	0.40
1:B:451:GLU:OE2	4:B:910:HOH:O	2.21	0.40
1:A:605:GLU:HB2	4:A:1027:HOH:O	2.21	0.40
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.93	0.40

All (3) 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)
4:A:1007:HOH:O	4:A:1012:HOH:O[2_555]	1.90	0.30
4:A:1007:HOH:O	4:A:1015:HOH:O[2_555]	1.98	0.22
1:A:222:ASN:O	1:A:544:ARG:NH2[2_555]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	612/713 (86%)	591 (97%)	18 (3%)	3 (0%)	24	22
1	B	612/713 (86%)	589 (96%)	21 (3%)	2 (0%)	36	36
All	All	1224/1426 (86%)	1180 (96%)	39 (3%)	5 (0%)	30	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	PRO
1	B	157	LEU
1	A	157	LEU
1	B	35	PRO
1	A	269	LEU

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	539/629 (86%)	526 (98%)	13 (2%)	43	49
1	B	535/629 (85%)	515 (96%)	20 (4%)	30	33
All	All	1074/1258 (85%)	1041 (97%)	33 (3%)	35	39

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

Mol	Chain	Res	Type
1	A	3	GLN

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Mol	Chain	Res	Type
1	A	34	SER
1	A	86	SER
1	A	89	ILE
1	A	140	LEU
1	A	226	VAL
1	A	272	GLU
1	A	291	ARG
1	A	424	VAL
1	A	463	GLN
1	A	555	VAL
1	A	563	ILE
1	A	570	THR
1	B	4	LYS
1	B	5	ILE
1	B	152	SER
1	B	190	GLU
1	B	226	VAL
1	B	232	SER
1	B	238	ILE
1	B	263	LEU
1	B	342	ILE
1	B	424	VAL
1	B	463	GLN
1	B	497	PHE
1	B	520	LEU
1	B	539	THR
1	B	541	GLU
1	B	547	GLU
1	B	549	ASN
1	B	563	ILE
1	B	570	THR
1	B	591	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	358	HIS
1	A	408	HIS
1	B	91	GLN
1	B	201	ASN
1	B	355	HIS

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Mol	Chain	Res	Type
1	B	362	ASN
1	B	549	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	MLI	A	801	3	6,6,6	1.92	1 (16%)	7,7,7	1.13	1 (14%)
2	MLI	B	801	3	6,6,6	1.60	1 (16%)	7,7,7	1.14	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	MLI	A	801	3	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	B	801	3	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	MLI	C1-C3	3.22	1.56	1.51
2	B	801	MLI	C1-C3	2.06	1.54	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	MLI	O6-C2-C1	-2.25	115.71	122.11

There are no chirality outliers.

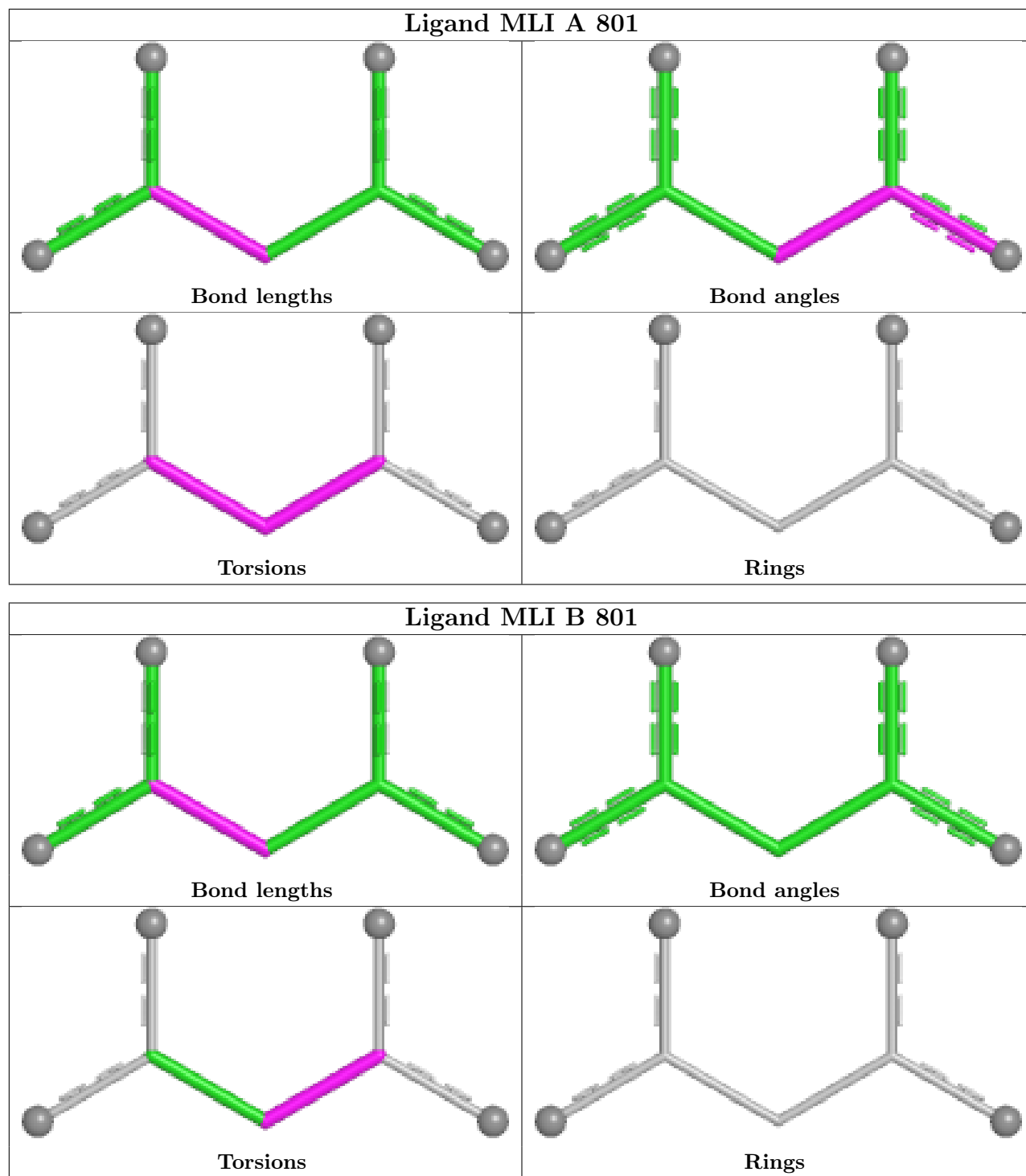
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	MLI	C3-C1-C2-O7
2	B	801	MLI	C3-C1-C2-O7
2	A	801	MLI	C3-C1-C2-O6
2	B	801	MLI	C3-C1-C2-O6
2	A	801	MLI	C2-C1-C3-O9
2	A	801	MLI	C2-C1-C3-O8

There are no ring outliers.

No monomer is involved in short contacts.

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

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	616/713 (86%)	0.40	18 (2%) 53 56	29, 49, 69, 114	0
1	B	616/713 (86%)	0.55	30 (4%) 35 37	35, 53, 73, 90	0
All	All	1232/1426 (86%)	0.47	48 (3%) 43 45	29, 51, 71, 114	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	576	ALA	6.3
1	B	590	PRO	4.1
1	B	548	LEU	3.8
1	B	574	THR	3.8
1	B	269	LEU	3.5
1	B	597	LEU	3.5
1	A	589	THR	3.4
1	B	589	THR	3.2
1	A	574	THR	3.0
1	A	231	ALA	3.0
1	B	497	PHE	2.8
1	A	224	LEU	2.8
1	A	563	ILE	2.7
1	A	269	LEU	2.6
1	A	597	LEU	2.6
1	A	156	PRO	2.6
1	B	221	GLY	2.5
1	A	576	ALA	2.5
1	A	559	GLU	2.4
1	B	35	PRO	2.4
1	A	183	ALA	2.4
1	A	230	ASP	2.4
1	A	157	LEU	2.4
1	B	549	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	226	VAL	2.3
1	B	0	ALA	2.3
1	B	488	SER	2.3
1	A	291	ARG	2.3
1	B	226	VAL	2.3
1	A	0	ALA	2.3
1	B	238	ILE	2.2
1	A	544	ARG	2.2
1	B	268	GLN	2.2
1	B	319	ASN	2.2
1	B	539	THR	2.2
1	B	540	HIS	2.2
1	B	361	GLU	2.1
1	B	572	THR	2.1
1	B	146	HIS	2.1
1	B	544	ARG	2.1
1	A	532	PRO	2.1
1	B	592	GLY	2.1
1	B	519	ASP	2.1
1	B	494	THR	2.1
1	B	571	ILE	2.1
1	B	157	LEU	2.0
1	B	520	LEU	2.0
1	B	180	ASP	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](#)

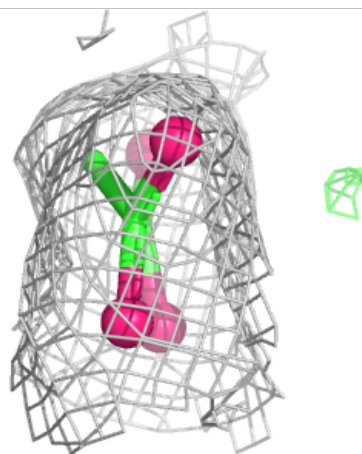
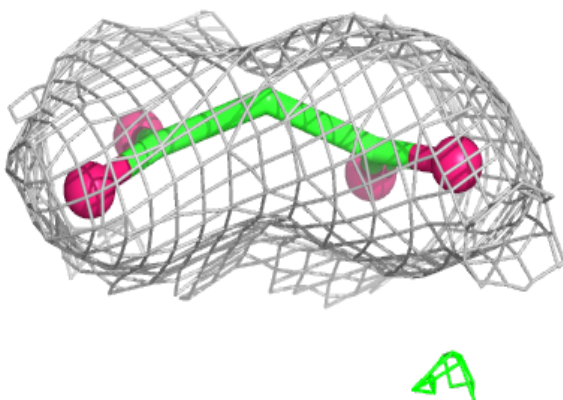
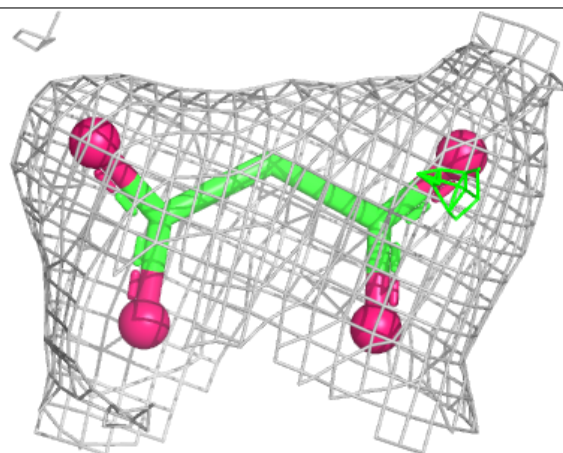
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MLI	B	801	7/7	0.95	0.08	38,44,47,52	0
2	MLI	A	801	7/7	0.96	0.07	37,38,43,50	0
3	MN	A	802	1/1	1.00	0.02	35,35,35,35	0
3	MN	B	802	1/1	1.00	0.01	36,36,36,36	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.

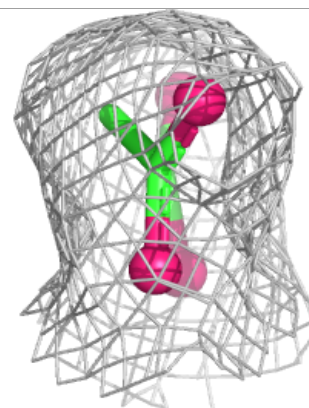
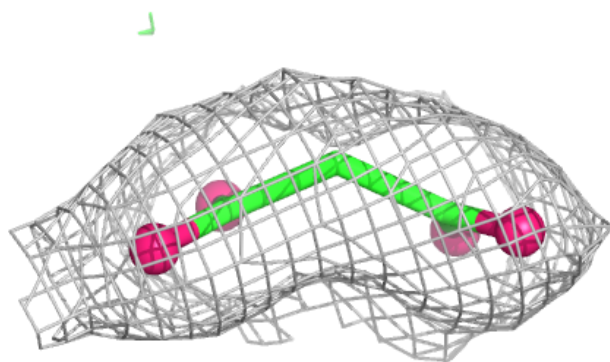
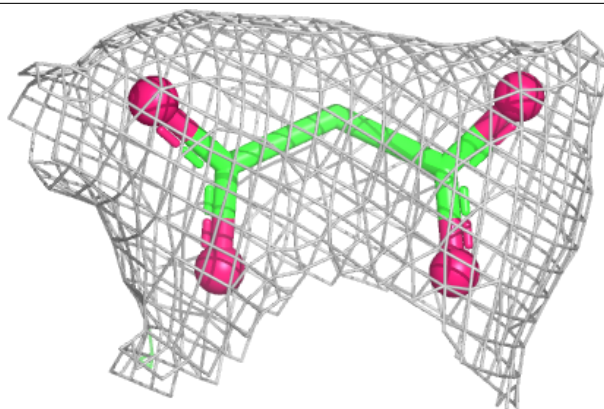
Electron density around MLI B 801:

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



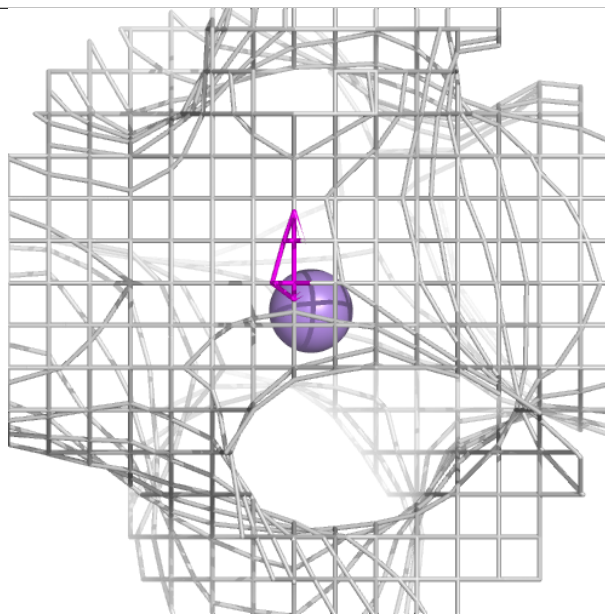
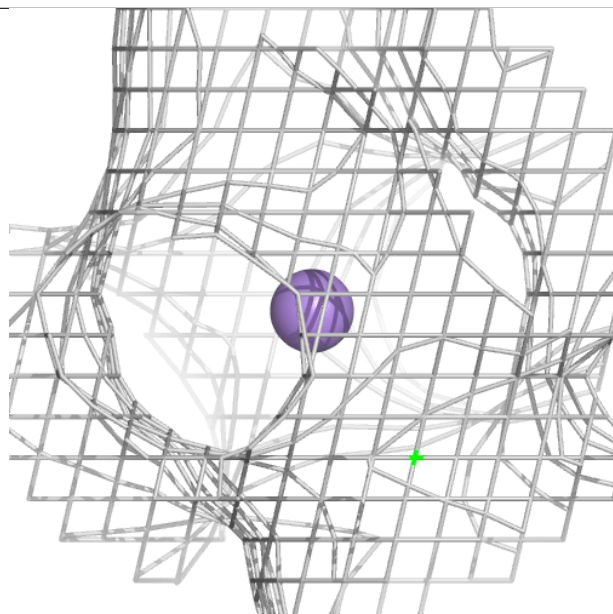
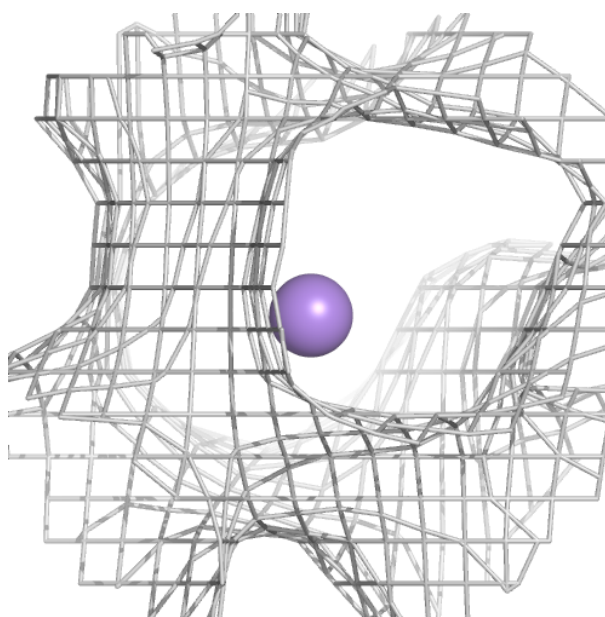
Electron density around MLI A 801:

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



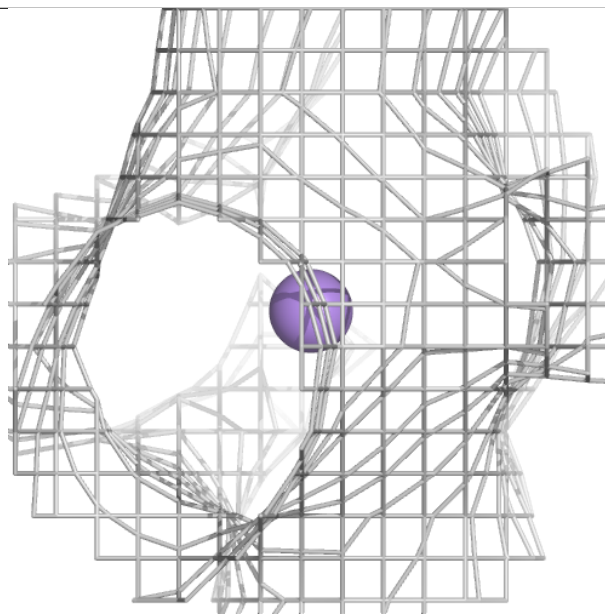
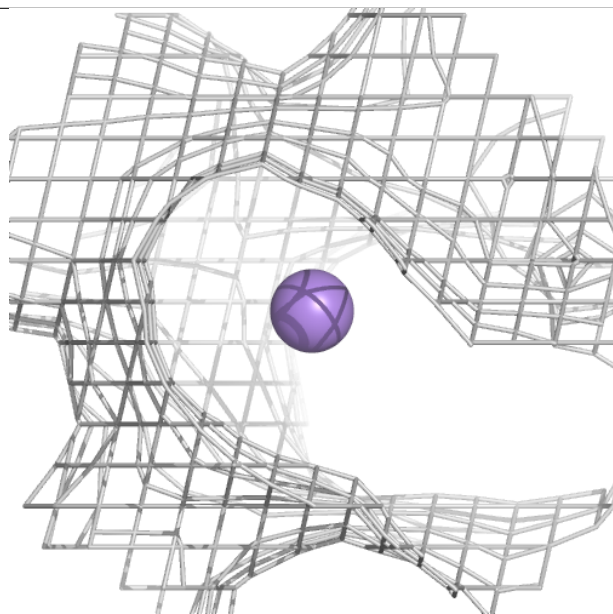
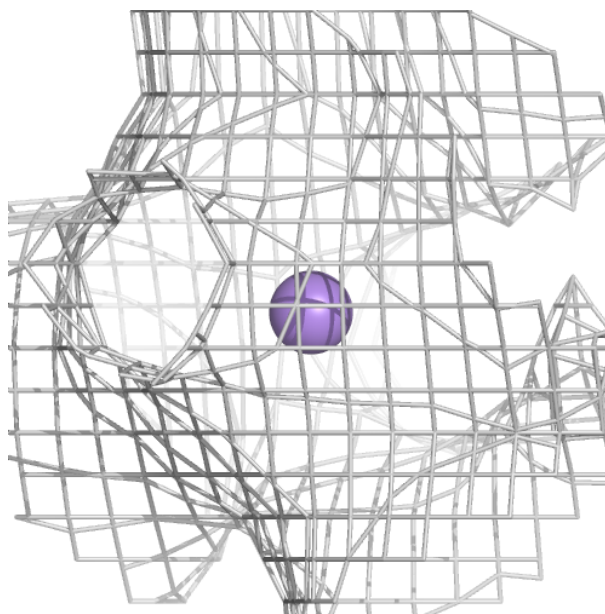
Electron density around MN A 802:

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



Electron density around MN B 802:

$2mF_o-DF_c$ (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.