wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 03:12 AM EDT

PDB ID	:	3AEM
Title	:	Reaction intermediate structure of Entamoeba histolytica methionine gamma-lyase 1 containing Michaelis complex and methionine imine-pyridoxamine-5'-phosphate
Authors	:	Karaki, T.; Sato, D.; Shimizu, A.; Nozaki, T.; Harada, S.
Deposited on	:	2010-02-10
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

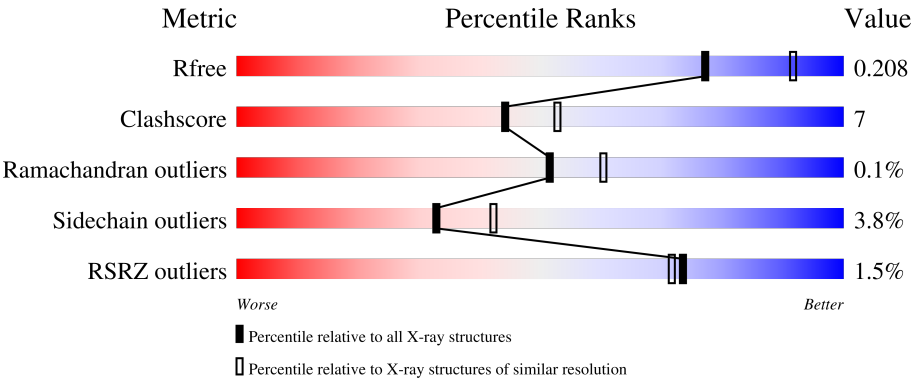
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	389	84% 13%
1	B	389	87% 11%
1	D	389	83% 14%
2	C	389	87% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MET	C	2003	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12782 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 Methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			2952	1878	497	553	24			
1	B	386	Total	C	N	O	S	0	1	0
			2937	1867	495	551	24			
1	D	384	Total	C	N	O	S	0	1	0
			2923	1859	492	548	24			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	LEU	SER	SEE REMARK 999	UNP Q86D28
B	808	LEU	SER	SEE REMARK 999	UNP Q86D28
D	1808	LEU	SER	SEE REMARK 999	UNP Q86D28

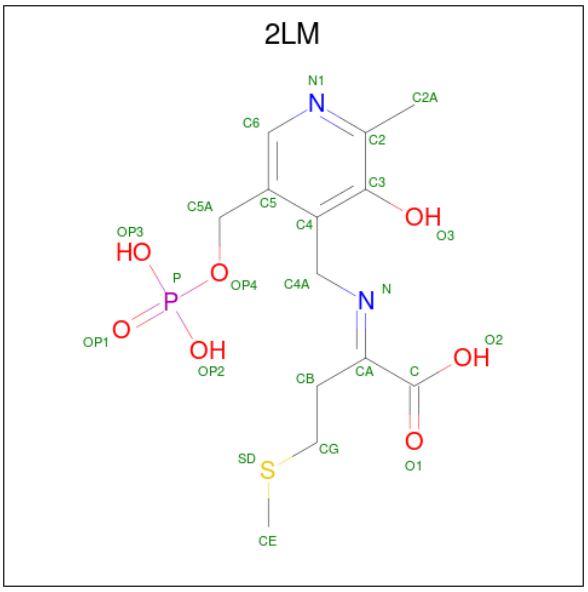
- Molecule 2 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	387	Total	C	N	O	P	S	0	1	0
			2967	1886	498	558	1	24			

There is a discrepancy between the modelled and reference sequences:

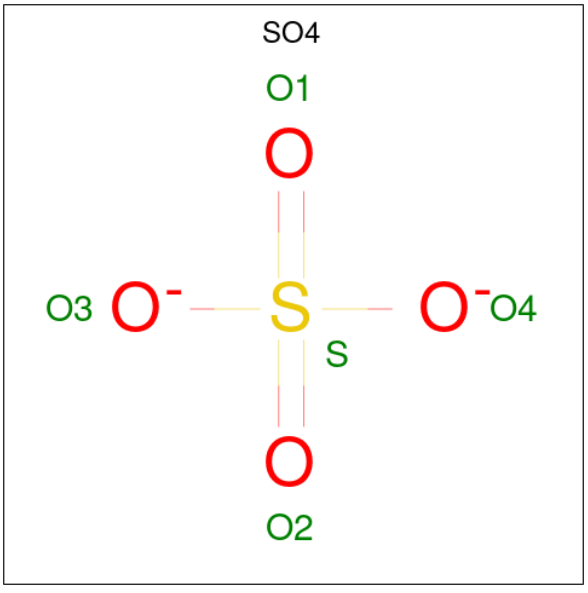
Chain	Residue	Modelled	Actual	Comment	Reference
C	1308	LEU	SER	SEE REMARK 999	UNP Q86D28

- Molecule 3 is (2E)-2-[({3-hydroxy-2-methyl-5-[(phosphonooxy)methyl]pyridin-4-yl}methyl)imino]-4-(methylsulfanyl)butanoic acid (three-letter code: 2LM) (formula: $C_{13}H_{19}N_2O_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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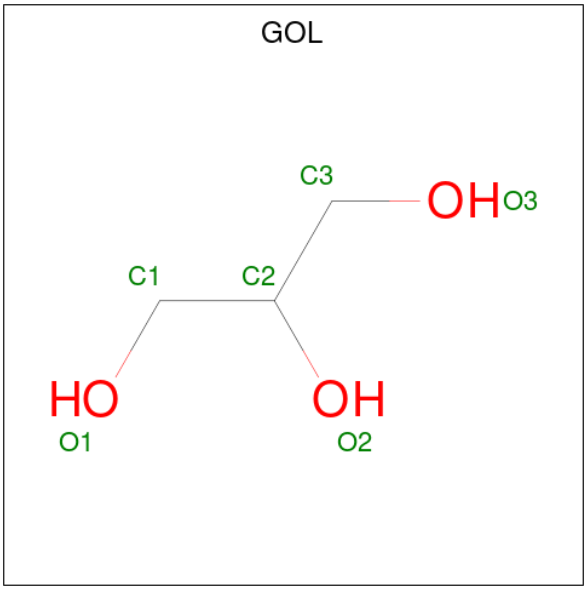
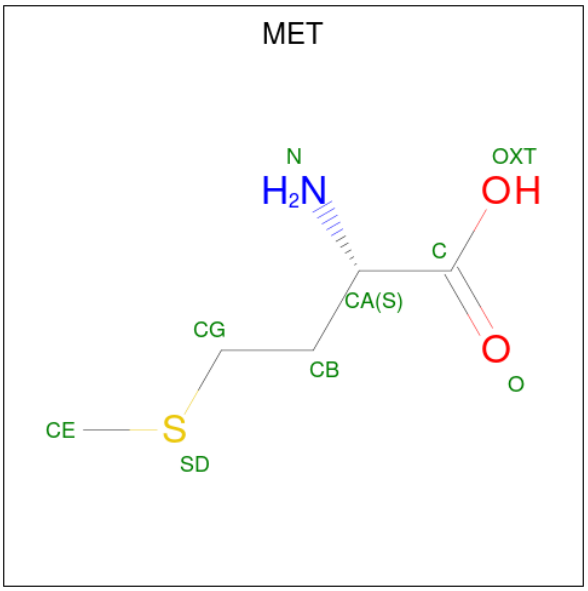
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O S 9 5 1 2 1	0	0

- Molecule 7 is water.

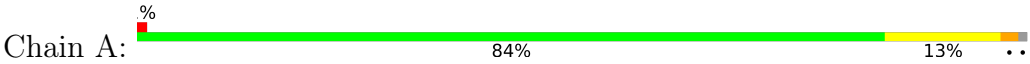
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	289	Total O 289 289	0	0
7	B	172	Total O 172 172	0	0
7	C	270	Total O 270 270	0	0
7	D	159	Total O 159 159	0	0

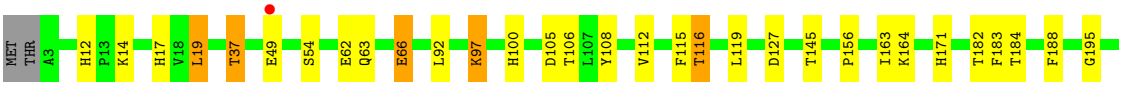
3 Residue-property plots (i)

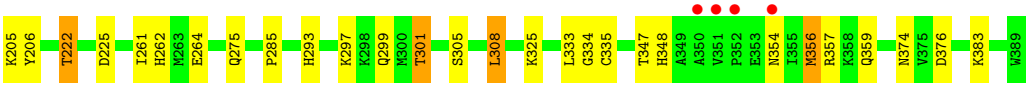
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Methionine gamma-lyase

Chain A:

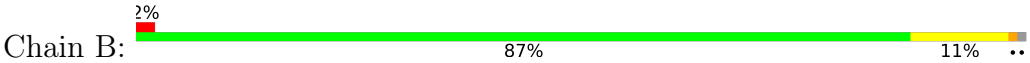


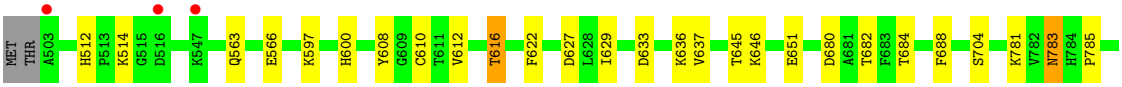


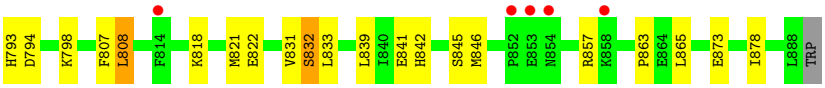


• Molecule 1: Methionine gamma-lyase

Chain B:

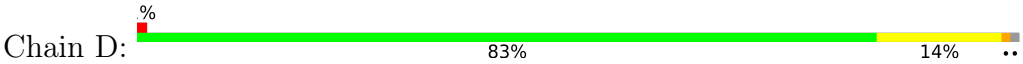


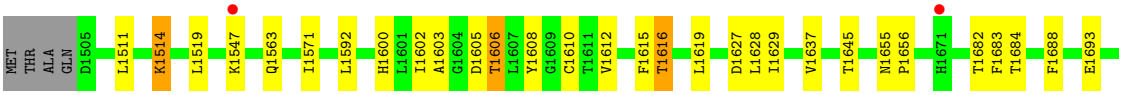


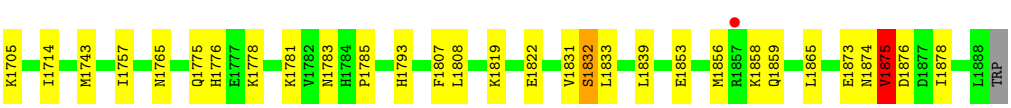


• Molecule 1: Methionine gamma-lyase

Chain D:

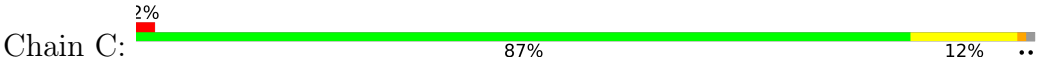


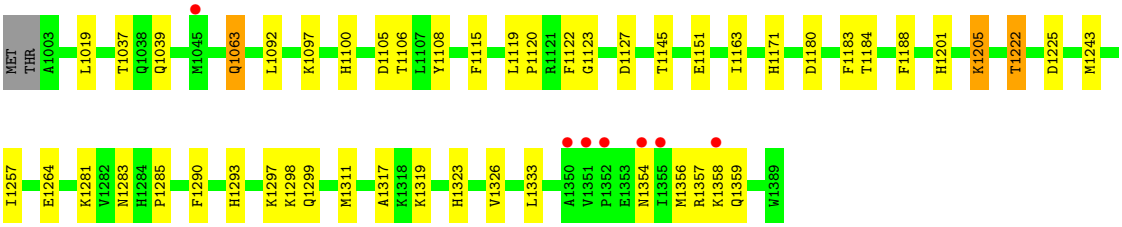




• Molecule 2: Methionine gamma-lyase

Chain C:




MET
THR
A1003
L1019
T1037
Q1038
Q1039
M1045
Q1063
L1092
K1097
H1100
D1105
T1106
L1107
Y1108
F1115
L1119
P1120
R1121
F1122
G1123
D1127
T1145
E1151
I1163
H1171
D1180
F1183
T1184
F1188
H1201
K1206
T1222
D1225
M1243
I1257
E1264
K1281
V1282
N1283
H1284
P1285
F1290
H1293
K1297
K1298
Q1299
M1311
A1317
K1318
K1319
H1323
V1326
L1333
A1350
V1351
P1352
E1353
N1354
I1355
M1356
R1357
K1358
Q1359
W1389

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.09Å 85.33Å 114.33Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	48.48 – 2.20 48.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.48-2.20) 99.7 (48.48-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.151 , 0.196 0.172 , 0.208	Depositor DCC
R_{free} test set	4752 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12782	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2LM, LLP, GOL, SO4

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	0.80	2/3018 (0.1%)	0.75	3/4080 (0.1%)
1	B	0.65	0/3001	0.67	1/4057 (0.0%)
1	D	0.63	0/2987	0.68	2/4038 (0.0%)
2	C	0.81	0/3008	0.74	0/4066
All	All	0.73	2/12014 (0.0%)	0.71	6/16241 (0.0%)

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
2	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	GLU	CG-CD	5.31	1.59	1.51
1	A	66	GLU	CG-CD	5.21	1.59	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1519	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	308	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	D	1875	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	19	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	808	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1201	HIS	Peptide

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	2952	0	2957	50	0
1	B	2937	0	2947	33	0
1	D	2923	0	2934	44	0
2	C	2967	0	2960	45	0
3	A	24	0	15	4	0
3	B	24	0	15	1	0
3	D	24	0	15	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
6	C	9	0	8	6	0
7	A	289	0	0	17	0
7	B	172	0	0	3	0
7	C	270	0	0	8	0
7	D	159	0	0	5	0
All	All	12782	0	11867	157	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 7.

The worst 5 of 157 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)
2:C:1205:LLP:H4'1	6:C:2003:MET:N	1.66	1.11
1:B:822:GLU:OE2	2:C:1037:THR:HG22	1.52	1.07
2:C:1205:LLP:C4'	6:C:2003:MET:N	2.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HG22	1:A:225:ASP:H	1.31	0.94
1:A:63:GLN:HG2	7:A:3525:HOH:O	1.67	0.93

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	386/389 (99%)	375 (97%)	11 (3%)	0	100	100
1	B	385/389 (99%)	374 (97%)	10 (3%)	1 (0%)	41	46
1	D	383/389 (98%)	375 (98%)	7 (2%)	1 (0%)	41	46
2	C	385/389 (99%)	375 (97%)	10 (3%)	0	100	100
All	All	1539/1556 (99%)	1499 (97%)	38 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1832	SER
1	B	832	SER

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	321/322 (100%)	307 (96%)	14 (4%)	28	35
1	B	320/322 (99%)	311 (97%)	9 (3%)	43	56
1	D	319/322 (99%)	305 (96%)	14 (4%)	28	35
2	C	320/321 (100%)	309 (97%)	11 (3%)	37	47
All	All	1280/1287 (100%)	1232 (96%)	48 (4%)	33	42

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1283	ASN
1	D	1547	LYS
2	C	1297	LYS
2	C	1354	ASN
1	D	1571	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1348	HIS
1	D	1775	GLN
2	C	1354	ASN
1	D	1600	HIS
1	D	1793	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	LLP	C	1205	2	23,24,25	2.24	7 (30%)	25,32,34	1.56	2 (8%)

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	LLP	C	1205	2	-	5/16/17/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1205	LLP	O3-C3	-5.75	1.23	1.37
2	C	1205	LLP	CE-NZ	4.83	1.57	1.46
2	C	1205	LLP	C4'-NZ	3.72	1.39	1.27
2	C	1205	LLP	C4-C4'	3.12	1.52	1.46
2	C	1205	LLP	C2-N1	2.53	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1205	LLP	OP4-C5'-C5	5.09	119.05	109.35
2	C	1205	LLP	C4-C4'-NZ	-3.34	108.96	124.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1205	LLP	O-C-CA-CB
2	C	1205	LLP	CG-CD-CE-NZ
2	C	1205	LLP	C4-C4'-NZ-CE
2	C	1205	LLP	CD-CE-NZ-C4'
2	C	1205	LLP	C3-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1205	LLP	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	2005	-	4,4,4	0.11	0	6,6,6	0.36	0
6	MET	C	2003	-	7,8,8	1.80	1 (14%)	7,9,9	1.90	1 (14%)
4	SO4	C	2007	-	4,4,4	0.09	0	6,6,6	0.18	0
3	2LM	A	2001	-	22,24,24	2.21	2 (9%)	24,33,33	2.45	9 (37%)
3	2LM	B	2002	-	22,24,24	2.65	1 (4%)	24,33,33	1.72	3 (12%)
3	2LM	D	2004	-	22,24,24	2.71	2 (9%)	24,33,33	1.54	6 (25%)
5	GOL	C	2010	-	5,5,5	0.33	0	5,5,5	0.33	0
5	GOL	A	2009	-	5,5,5	0.39	0	5,5,5	0.40	0
4	SO4	B	2006	-	4,4,4	0.18	0	6,6,6	0.18	0
4	SO4	D	2008	-	4,4,4	0.14	0	6,6,6	0.09	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
6	MET	C	2003	-	-	3/8/8/8	-
5	GOL	C	2010	-	-	0/4/4/4	-
3	2LM	B	2002	-	-	12/18/19/19	0/1/1/1
3	2LM	D	2004	-	-	7/18/19/19	0/1/1/1
3	2LM	A	2001	-	-	10/18/19/19	0/1/1/1
5	GOL	A	2009	-	-	4/4/4/4	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2004	2LM	C4A-N	-11.81	1.29	1.46
3	B	2002	2LM	C4A-N	-11.72	1.29	1.46
3	A	2001	2LM	C4A-N	-9.34	1.32	1.46
6	C	2003	MET	OXT-C	-4.14	1.17	1.30
3	A	2001	2LM	O2-C	-2.21	1.24	1.30

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2001	2LM	C4A-N-CA	5.84	135.75	121.40
3	A	2001	2LM	CG-CB-CA	-4.79	104.41	112.52
3	A	2001	2LM	CE-SD-CG	4.67	116.45	100.40
3	B	2002	2LM	CE-SD-CG	4.46	115.72	100.40
3	A	2001	2LM	C3-C4-C5	-4.13	114.76	118.72

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	2LM	O2-C-CA-N
3	A	2001	2LM	O2-C-CA-CB
3	A	2001	2LM	C3-C4-C4A-N
3	A	2001	2LM	C5-C4-C4A-N
3	A	2001	2LM	C-CA-CB-CG

There are no ring outliers.

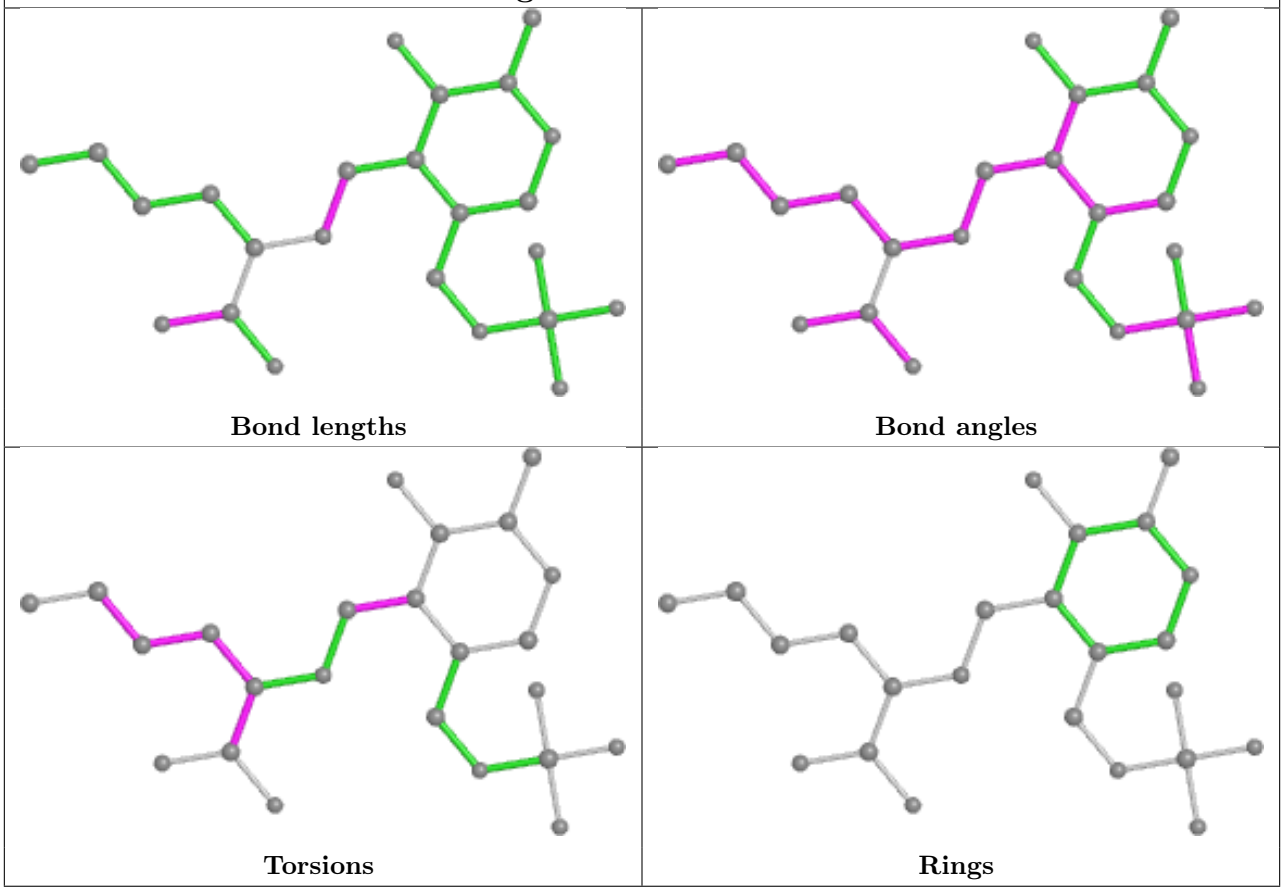
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2003	MET	6	0
3	A	2001	2LM	4	0
3	B	2002	2LM	1	0
3	D	2004	2LM	3	0

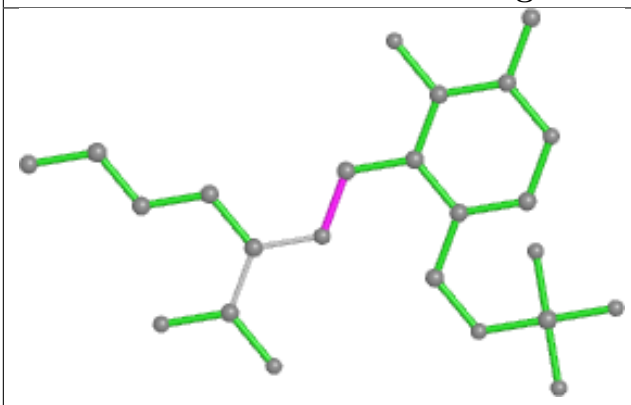
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

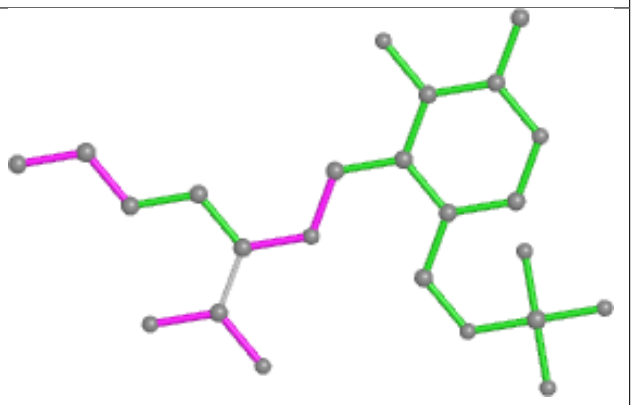
Ligand 2LM A 2001



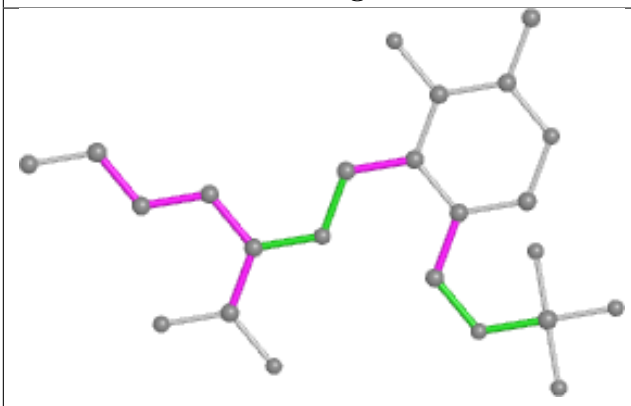
Ligand 2LM B 2002



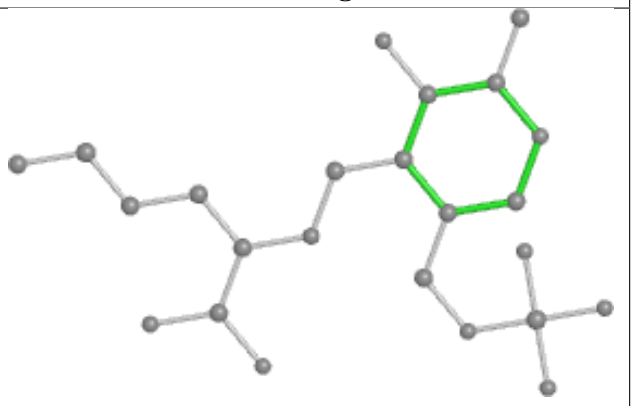
Bond lengths



Bond angles

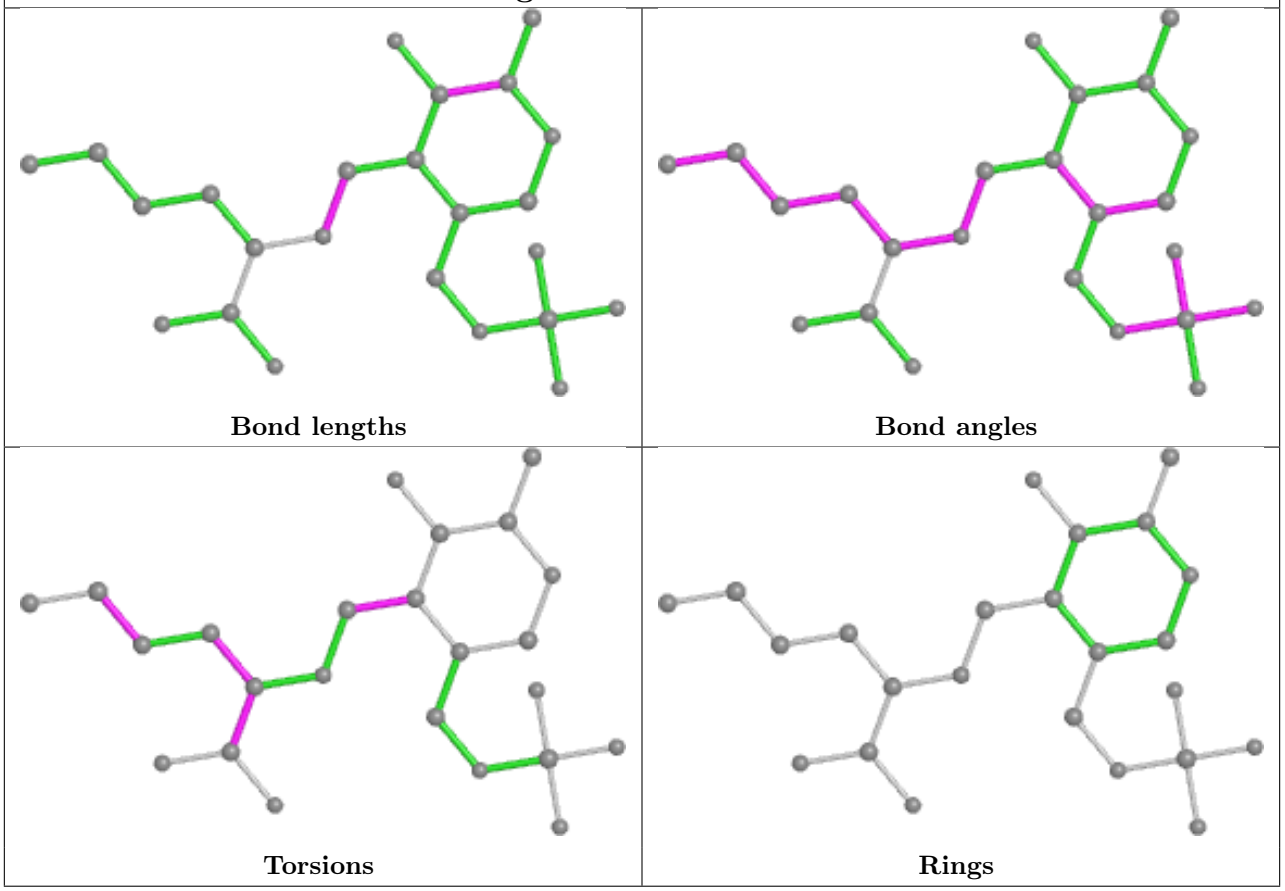


Torsions



Rings

Ligand 2LM D 2004



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, 95^{th} 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	387/389 (99%)	-0.40	5 (1%)	77	75	17, 28, 62, 88	1 (0%)
1	B	386/389 (99%)	-0.05	8 (2%)	63	61	20, 48, 92, 121	1 (0%)
1	D	384/389 (98%)	0.10	3 (0%)	86	85	21, 54, 97, 118	0
2	C	386/389 (99%)	-0.41	7 (1%)	68	66	18, 29, 63, 93	1 (0%)
All	All	1543/1556 (99%)	-0.19	23 (1%)	73	72	17, 36, 88, 121	3 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1351	VAL	4.2
2	C	1350	ALA	3.6
1	B	854	ASN	3.4
1	B	503	ALA	3.2
1	B	858	LYS	3.0

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

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, 95^{th} 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	LLP	C	1205	24/25	0.98	0.11	19,22,24,31	6

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

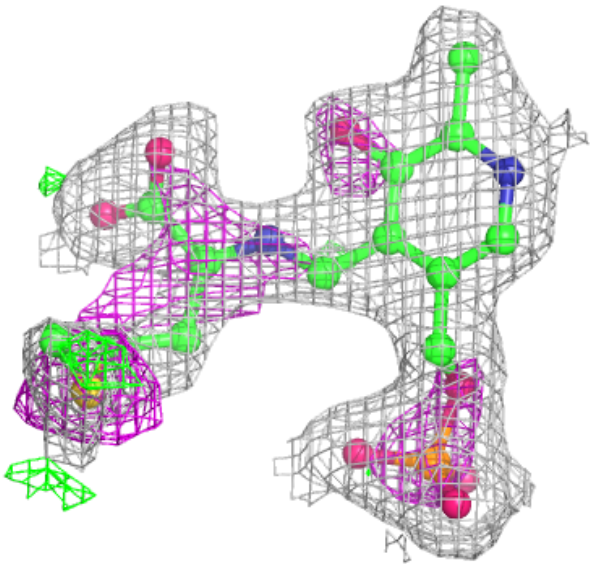
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

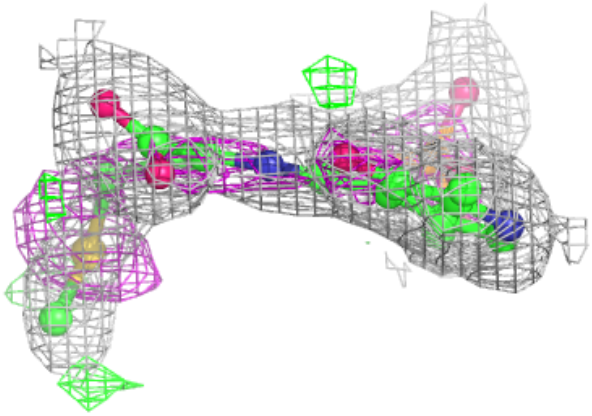
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	2009	6/6	0.84	0.17	42,45,46,47	0
6	MET	C	2003	9/9	0.87	0.21	25,30,42,45	0
5	GOL	C	2010	6/6	0.92	0.14	38,42,43,43	0
4	SO4	C	2007	5/5	0.94	0.25	58,59,60,60	0
4	SO4	B	2006	5/5	0.94	0.28	71,71,72,72	0
3	2LM	B	2002	24/24	0.95	0.13	17,30,40,52	0
4	SO4	D	2008	5/5	0.95	0.33	72,72,72,73	0
3	2LM	D	2004	24/24	0.95	0.14	19,31,40,52	0
4	SO4	A	2005	5/5	0.95	0.25	58,59,60,60	0
3	2LM	A	2001	24/24	0.95	0.12	7,17,33,43	0

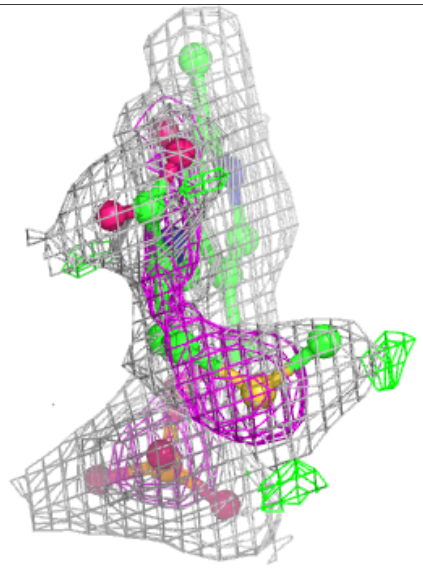
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2LM B 2002:

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

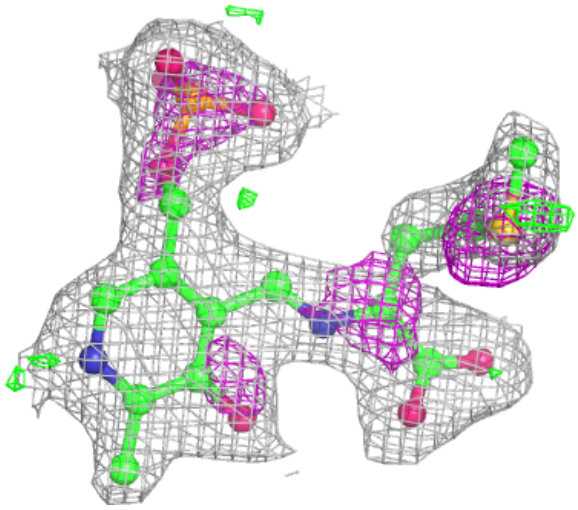


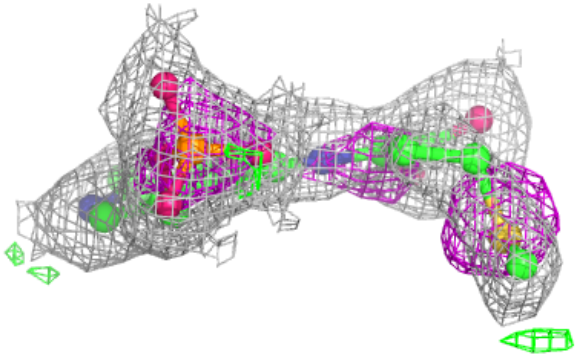


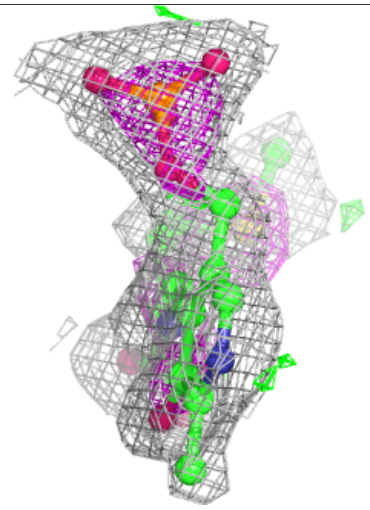


Electron density around 2LM D 2004:

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

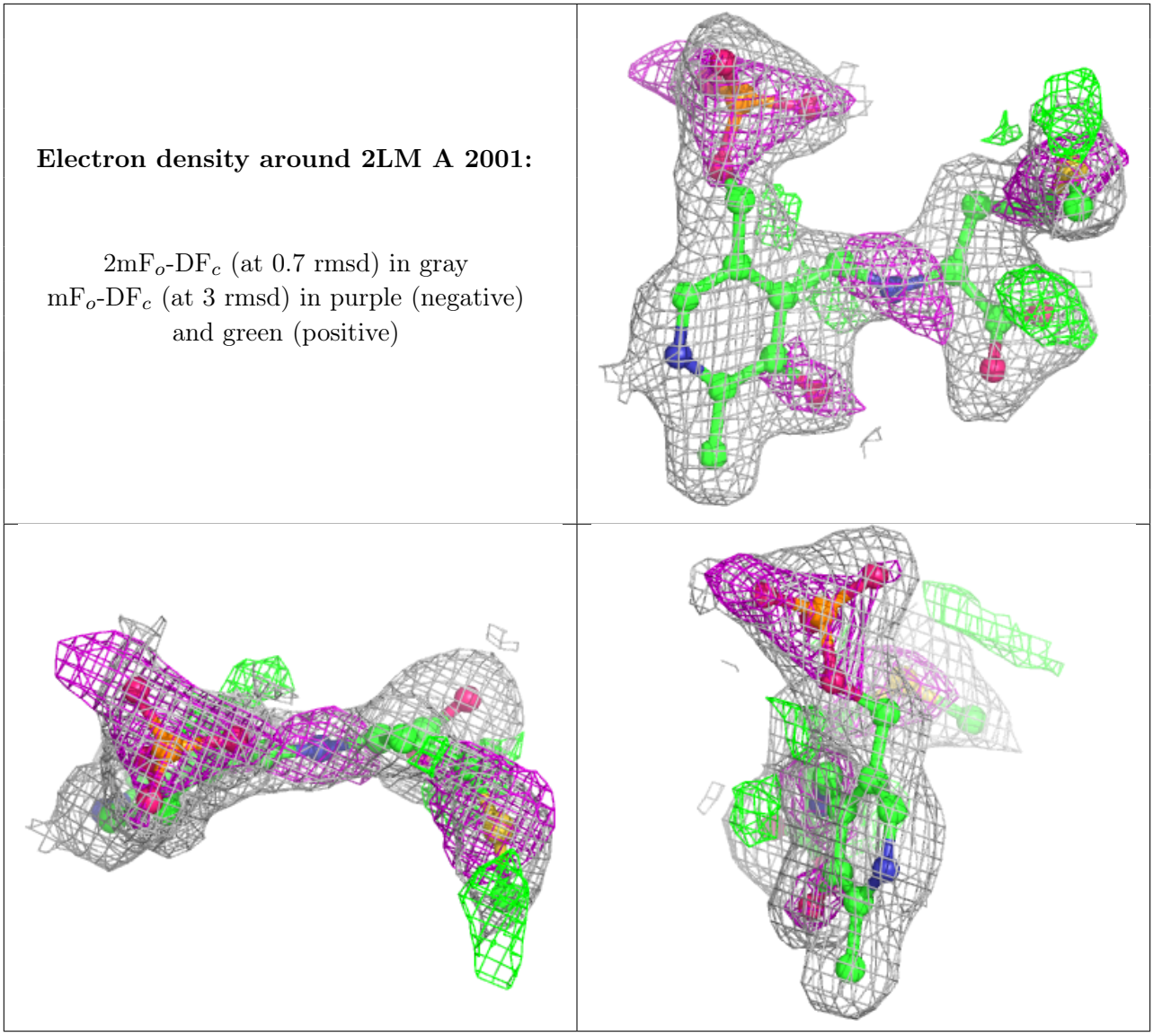






Electron density around 2LM A 2001:

$2mF_o$-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.