



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:55 am BST

PDB ID : 3AEO
Title : Reaction intermediate structure of Entamoeba histolytica methionine gamma-lyase 1 containing methionine alpha, beta-enamine-pyridoxamine-5'-phosphate
Authors : Karaki, T.; Sato, D.; Shimizu, A.; Nozaki, T.; Harada, S.
Deposited on : 2010-02-10
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

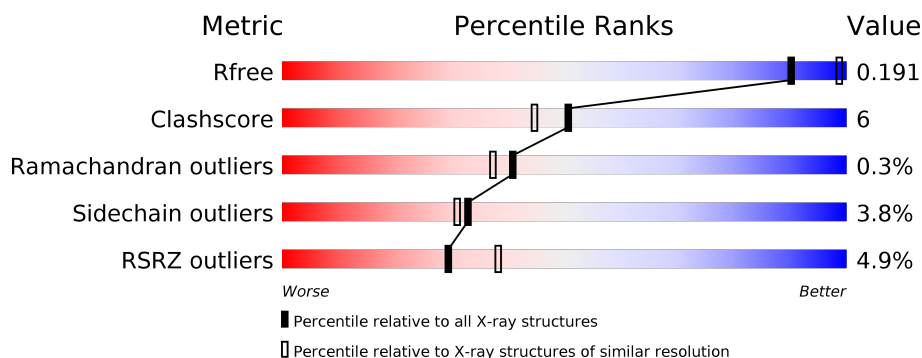
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	389	<div> <div>3%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	B	389	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	C	389	<div> <div>4%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	D	389	<div> <div>7%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12694 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.

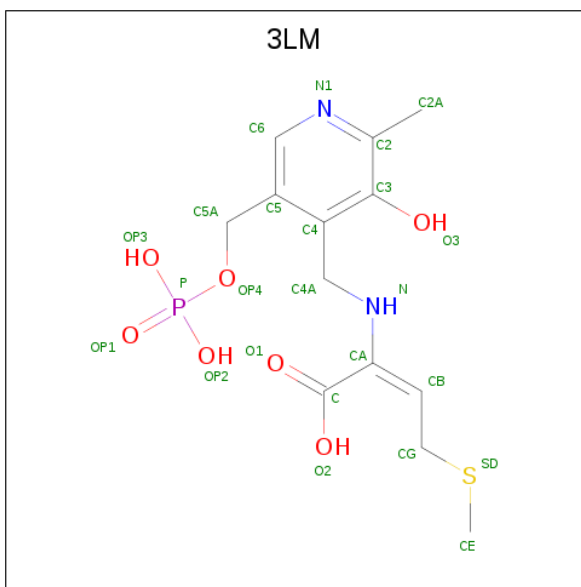
- Molecule 1 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	5	0
			2975	1894	499	556	26			
1	B	386	Total	C	N	O	S	0	4	0
			2951	1877	495	553	26			
1	C	387	Total	C	N	O	S	0	4	0
			2967	1889	498	555	25			
1	D	384	Total	C	N	O	S	0	4	0
			2937	1869	492	550	26			

There are 4 discrepancies between the modelled and reference sequences:

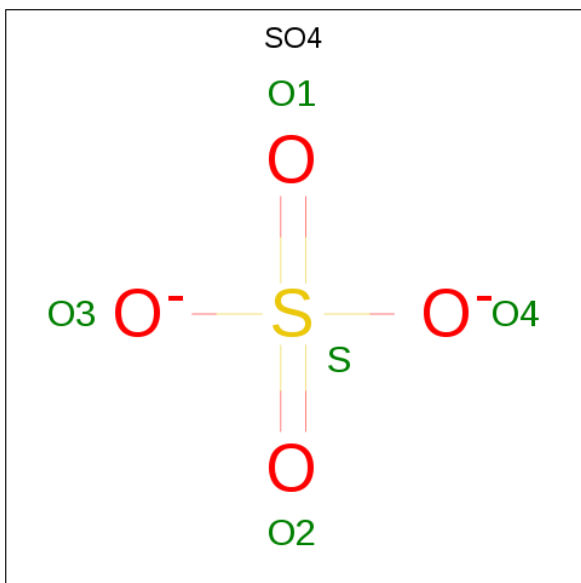
Chain	Residue	Modelled	Actual	Comment	Reference
A	308	LEU	SER	SEE REMARK 999	UNP Q86D28
B	808	LEU	SER	SEE REMARK 999	UNP Q86D28
C	1308	LEU	SER	SEE REMARK 999	UNP Q86D28
D	1808	LEU	SER	SEE REMARK 999	UNP Q86D28

- Molecule 2 is (2E)-2-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methylamino]-4-(methylsulfanyl)but-2-enoic acid (three-letter code: 3LM) (formula: C₁₃H₁₉N₂O₇PS).



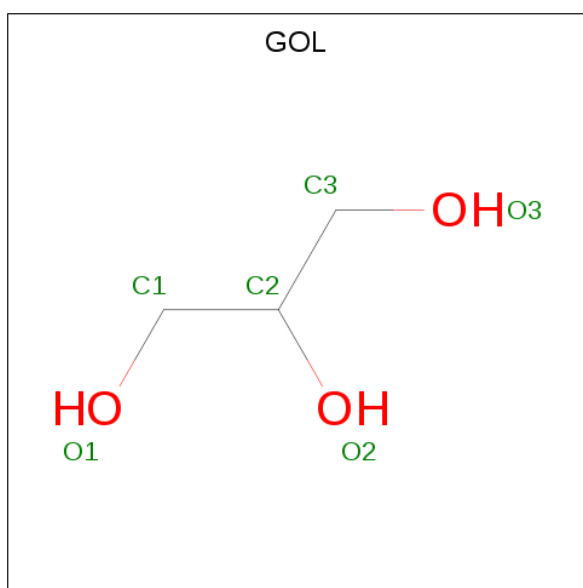
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			24	13	2	7	1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

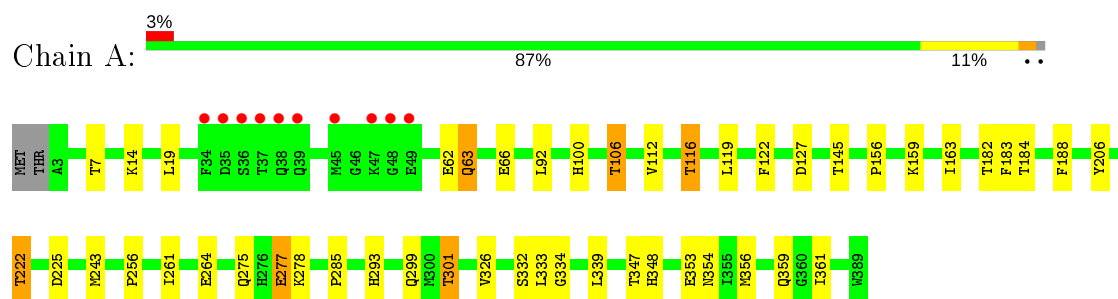
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	265	Total O 265 265	0	0
5	B	118	Total O 118 118	0	0
5	C	245	Total O 245 245	0	0
5	D	108	Total O 108 108	0	0

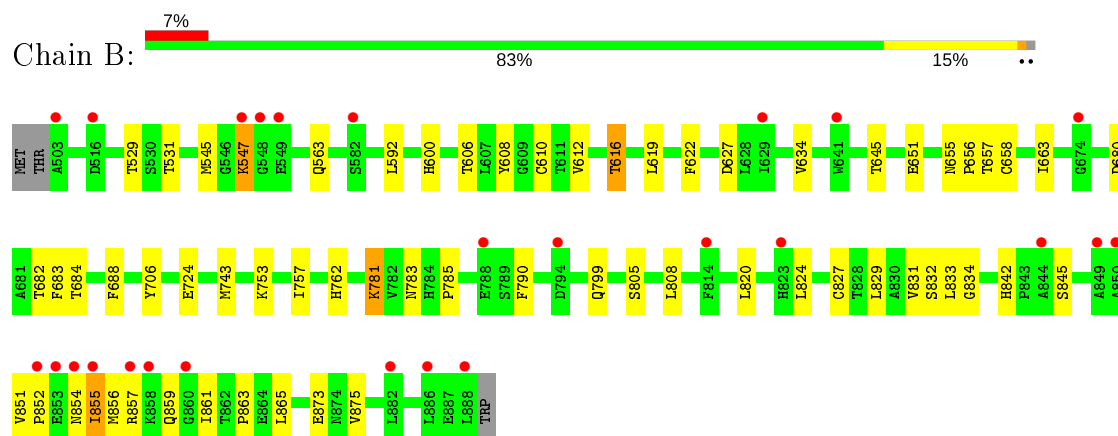
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

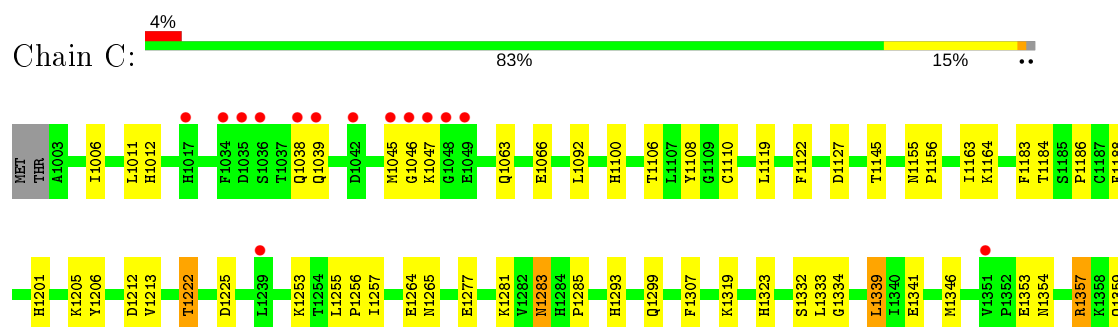
• Molecule 1: Methionine gamma-lyase

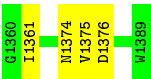


• Molecule 1: Methionine gamma-lyase

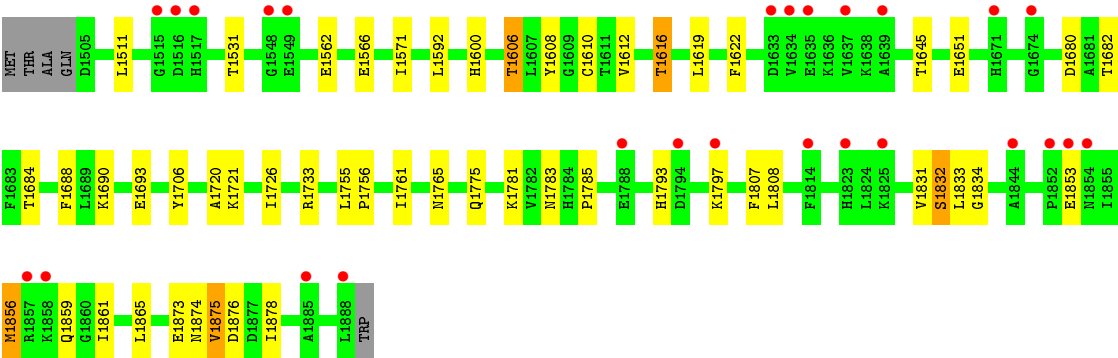
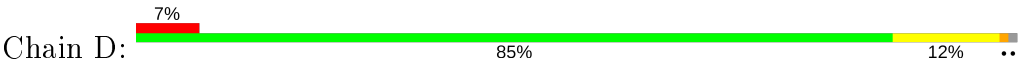


• Molecule 1: Methionine gamma-lyase





● Molecule 1: Methionine gamma-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.06 Å 85.70 Å 115.14 Å 90.00° 101.39° 90.00°	Depositor
Resolution (Å)	39.90 – 2.15 39.90 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.90-2.15) 98.5 (39.90-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.14 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.153 , 0.194 0.151 , 0.191	Depositor DCC
R_{free} test set	5110 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12694	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: GOL, SO4, 3LM

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	0.86	0/3050	0.75	0/4121
1	B	0.61	0/3024	0.63	0/4087
1	C	0.83	1/3042 (0.0%)	0.75	1/4111 (0.0%)
1	D	0.61	0/3010	0.64	1/4068 (0.0%)
All	All	0.74	1/12126 (0.0%)	0.70	2/16387 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1264	GLU	CG-CD	5.31	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1733	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	C	1339	LEU	CB-CG-CD1	5.00	119.50	111.00

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	2975	0	2989	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2951	0	2967	37	0
1	C	2967	0	2981	42	0
1	D	2937	0	2954	31	0
2	A	24	0	15	1	0
2	B	24	0	15	2	0
2	C	24	0	15	1	0
2	D	24	0	15	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
5	A	265	0	0	12	0
5	B	118	0	0	2	0
5	C	245	0	0	10	0
5	D	108	0	0	0	0
All	All	12694	0	11967	136	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 6.

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:222:THR:HG22	1:A:225:ASP:H	1.39	0.86
1:D:1612:VAL:O	1:D:1616:THR:HB	1.76	0.84
1:C:1066[B]:GLU:HG2	5:C:3576:HOH:O	1.78	0.82
1:D:1781:LYS:HE3	1:D:1783:ASN:HD21	1.46	0.81
1:A:222:THR:HG21	5:A:3006:HOH:O	1.83	0.77
1:B:757:ILE:HG12	1:D:1761:ILE:HD11	1.65	0.77
1:C:1222:THR:HG21	5:C:3008:HOH:O	1.84	0.76
1:D:1600:HIS:HD2	1:D:1645:THR:OG1	1.68	0.75
1:B:612:VAL:O	1:B:616:THR:HB	1.87	0.74
1:B:592:LEU:HD21	1:B:619:LEU:HD22	1.70	0.73
1:A:92:LEU:HD21	1:A:119:LEU:HD22	1.69	0.73
1:B:600:HIS:HD2	1:B:645:THR:OG1	1.72	0.73
1:A:188:PHE:HA	1:A:301:THR:HG22	1.69	0.73
1:C:1222:THR:HG22	1:C:1225:ASP:H	1.53	0.72
1:A:301:THR:HG23	5:A:3184:HOH:O	1.91	0.71
1:A:100:HIS:HD2	1:A:145:THR:OG1	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1319:LYS:O	1:C:1323:HIS:HD2	1.75	0.70
1:C:1100:HIS:HD2	1:C:1145:THR:OG1	1.75	0.69
1:A:293:HIS:HE1	5:A:3416:HOH:O	1.74	0.69
1:B:873:GLU:HG3	1:D:1511:LEU:HD12	1.73	0.69
1:D:1765:ASN:ND2	1:D:1875:VAL:HG13	2.08	0.68
1:D:1808:LEU:HD21	1:D:1865:LEU:HD13	1.75	0.67
1:C:1092:LEU:HD21	1:C:1119:LEU:HD22	1.74	0.67
1:C:1100:HIS:HE1	1:C:1127:ASP:OD2	1.80	0.65
1:D:1592:LEU:HD21	1:D:1619:LEU:HD22	1.78	0.65
1:A:106:THR:HG21	5:A:3197:HOH:O	1.97	0.64
5:A:3396:HOH:O	1:D:1531:THR:HG22	1.99	0.62
1:B:600:HIS:HE1	1:B:627:ASP:OD2	1.82	0.61
1:A:112:VAL:O	1:A:116:THR:HB	2.01	0.60
1:A:277:GLU:OE1	1:A:278:LYS:HG2	2.01	0.60
1:C:1106:THR:HG22	1:C:1359:GLN:HG2	1.84	0.60
1:A:100:HIS:HE1	1:A:127:ASP:OD2	1.84	0.60
1:B:608:TYR:CE2	1:B:610:CYS:HB2	2.36	0.59
1:D:1684:THR:HG22	1:D:1688:PHE:HB2	1.84	0.59
5:B:3643:HOH:O	1:C:1110:CYS:SG	2.56	0.58
1:A:261:ILE:HD11	1:C:1257:ILE:HG12	1.84	0.58
1:C:1063:GLN:HG2	5:C:3165:HOH:O	2.05	0.57
1:C:1222:THR:CG2	1:C:1225:ASP:H	2.17	0.57
1:A:264:GLU:HG3	5:A:3573:HOH:O	2.06	0.55
1:A:264:GLU:HG3	5:A:3153:HOH:O	2.06	0.55
1:C:1011:LEU:HD23	1:C:1253[A]:LYS:HD2	1.88	0.54
1:A:353:GLU:HB3	5:A:3245:HOH:O	2.06	0.54
1:B:684:THR:HG22	1:B:688:PHE:HB2	1.90	0.54
1:A:301:THR:CG2	5:A:3184:HOH:O	2.51	0.53
1:C:1341:GLU:OE2	1:C:1346:MET:HB2	2.09	0.53
1:A:63:GLN:NE2	5:A:3641:HOH:O	2.40	0.53
1:D:1606:THR:HB	1:D:1859:GLN:HG2	1.89	0.53
1:C:1184:THR:HG22	1:C:1188:PHE:HB2	1.90	0.53
1:B:682:THR:HB	2:B:2002:3LM:H2A1	1.91	0.52
1:B:831:VAL:HG22	5:C:3059:HOH:O	2.10	0.52
1:C:1285:PRO:O	1:C:1293:HIS:HD2	1.93	0.51
1:C:1106:THR:HG21	5:C:3275:HOH:O	2.09	0.51
1:C:1281:LYS:HE3	5:C:3517:HOH:O	2.11	0.51
1:C:1108:TYR:CE2	1:C:1110:CYS:HB2	2.46	0.50
1:B:842:HIS:HE1	1:B:863:PRO:O	1.95	0.50
1:A:106:THR:HB	1:A:359:GLN:HG2	1.94	0.50
1:B:781:LYS:NZ	1:B:783:ASN:HD21	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1319:LYS:O	1:C:1323:HIS:CD2	2.61	0.49
1:C:1283:ASN:ND2	5:C:3676:HOH:O	2.46	0.49
1:B:808:LEU:HD21	1:B:865:LEU:HD22	1.94	0.49
1:D:1853:GLU:O	1:D:1856:MET:HB3	2.13	0.49
1:D:1682:THR:HB	2:D:2004:3LM:H2A1	1.94	0.48
1:D:1608:TYR:CE2	1:D:1610:CYS:HB2	2.48	0.48
1:C:1353:GLU:O	1:C:1357:ARG:HG2	2.12	0.48
1:C:1374:ASN:HD21	1:C:1376:ASP:HB2	1.79	0.48
1:D:1831:VAL:O	1:D:1832:SER:CB	2.62	0.47
1:A:163:ILE:H	1:A:299:GLN:HE22	1.61	0.47
1:B:855:ILE:O	1:B:859:GLN:HG2	2.14	0.47
1:D:1859:GLN:HB3	1:D:1861:ILE:CD1	2.45	0.47
1:A:264:GLU:CG	5:A:3153:HOH:O	2.63	0.47
1:A:206:TYR:CE2	1:A:334:GLY:HA2	2.50	0.47
1:C:1206:TYR:CE1	1:C:1334:GLY:HA2	2.50	0.47
1:D:1706:TYR:CE2	1:D:1834:GLY:HA2	2.49	0.47
1:A:184:THR:HG22	1:A:188:PHE:HB2	1.97	0.47
1:A:326:VAL:O	1:C:1012:HIS:CE1	2.68	0.47
1:B:600:HIS:CE1	1:B:627:ASP:OD2	2.66	0.47
1:D:1781:LYS:CE	1:D:1783:ASN:HD21	2.21	0.47
5:A:3117:HOH:O	1:D:1831:VAL:HG22	2.14	0.46
1:B:531:THR:HG22	5:C:3242:HOH:O	2.14	0.46
1:C:1281:LYS:HE2	5:C:3394:HOH:O	2.14	0.46
1:D:1651:GLU:HG3	1:D:1680:ASP:HB3	1.97	0.46
1:B:622:PHE:HB3	1:C:1122:PHE:HB3	1.97	0.46
1:C:1106:THR:HG22	1:C:1359:GLN:HA	1.96	0.46
1:D:1781:LYS:HE3	1:D:1783:ASN:ND2	2.24	0.46
1:A:156:PRO:HD3	1:A:348:HIS:CE1	2.51	0.45
1:A:285:PRO:O	1:A:293:HIS:HD2	1.99	0.45
1:B:842:HIS:HD2	1:B:845:SER:OG	1.99	0.45
1:A:243:MET:HE1	1:B:743:MET:CE	2.47	0.45
1:B:824:LEU:HD13	1:B:827:CYS:HB2	1.99	0.45
1:D:1873:GLU:HB2	1:D:1878:ILE:HD11	1.99	0.45
1:D:1562:GLU:O	1:D:1566[A]:GLU:HG3	2.17	0.45
1:B:655:ASN:HA	1:B:656:PRO:HA	1.85	0.45
1:C:1359:GLN:HE21	1:C:1361:ILE:HD12	1.81	0.45
1:C:1155:ASN:HA	1:C:1156:PRO:HA	1.79	0.44
1:D:1874:ASN:HD21	1:D:1876:ASP:HB2	1.82	0.44
1:A:243:MET:CE	1:B:743:MET:CE	2.96	0.44
1:A:62:GLU:O	1:A:66[A]:GLU:HG3	2.18	0.44
1:D:1785:PRO:O	1:D:1793:HIS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:THR:HB	2:A:2001:3LM:H2A1	2.00	0.44
1:C:1100:HIS:CE1	1:C:1127:ASP:OD2	2.66	0.44
1:C:1205:LYS:CE	2:C:2003:3LM:H4A	2.48	0.44
1:B:529:THR:HA	1:C:1212:ASP:HA	2.00	0.44
1:A:7:THR:HG22	1:A:256:PRO:HB2	1.99	0.43
1:D:1765:ASN:CG	1:D:1875:VAL:HG13	2.39	0.43
1:A:106:THR:HG23	1:A:159:LYS:HE2	2.00	0.43
1:C:1186:PRO:HD3	1:C:1201:HIS:CE1	2.54	0.43
1:C:1357:ARG:HA	5:C:3405:HOH:O	2.18	0.43
1:A:243:MET:CE	1:B:743:MET:HE1	2.48	0.43
1:B:651:GLU:HG2	1:B:680:ASP:HB3	2.00	0.43
1:B:753:LYS:HE2	5:B:3094:HOH:O	2.19	0.42
1:B:785:PRO:HA	1:B:790:PHE:CD2	2.54	0.42
1:C:1045:MET:N	1:C:1046:GLY:HA2	2.34	0.42
1:B:762:HIS:HB3	1:B:805:SER:HB3	2.00	0.42
1:A:261:ILE:CD1	1:C:1257:ILE:HG12	2.48	0.42
1:A:14:LYS:HA	1:A:14:LYS:HD3	1.88	0.42
1:A:356:MET:HG2	1:A:361:ILE:HB	2.02	0.42
1:B:545[A]:MET:HE3	1:B:547:LYS:HD3	2.01	0.42
1:C:1255:LEU:HB3	1:C:1256:PRO:HD3	2.02	0.41
1:B:657:THR:O	1:B:658:CYS:HB2	2.20	0.41
1:B:851:VAL:HA	1:B:852:PRO:HD2	1.92	0.41
1:D:1571:ILE:O	1:D:1690:LYS:HE3	2.20	0.41
1:B:854:ASN:ND2	1:B:854:ASN:H	2.19	0.41
1:C:1283:ASN:O	1:C:1307:PHE:HB2	2.21	0.41
1:C:1006:ILE:HA	1:C:1006:ILE:HD12	1.91	0.41
1:A:347:THR:OG1	1:A:348:HIS:HD2	2.03	0.41
1:B:608:TYR:CZ	2:B:2002:3LM:H4A1	2.56	0.41
1:D:1783:ASN:O	1:D:1807:PHE:HB2	2.21	0.41
1:B:861:ILE:HA	1:B:865:LEU:HD12	2.03	0.40
1:C:1265:ASN:ND2	1:C:1375:VAL:HB	2.36	0.40
1:A:122:PHE:HB3	1:D:1622:PHE:HB3	2.02	0.40
1:D:1720:ALA:HB3	1:D:1726:ILE:HB	2.03	0.40
1:B:663:ILE:H	1:B:799:GLN:HE22	1.68	0.40
1:B:606:THR:HG23	1:B:859:GLN:HB2	2.02	0.40
1:B:706:TYR:CE1	1:B:834:GLY:HA2	2.56	0.40
1:D:1755:LEU:HB3	1:D:1756:PRO:HD3	2.04	0.40
1:C:1163:ILE:H	1:C:1299:GLN:HE22	1.69	0.40

There are no symmetry-related clashes.

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	390/389 (100%)	380 (97%)	9 (2%)	1 (0%)	41	37
1	B	388/389 (100%)	376 (97%)	11 (3%)	1 (0%)	41	37
1	C	389/389 (100%)	375 (96%)	13 (3%)	1 (0%)	41	37
1	D	386/389 (99%)	376 (97%)	9 (2%)	1 (0%)	41	37
All	All	1553/1556 (100%)	1507 (97%)	42 (3%)	4 (0%)	41	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1832	SER
1	C	1332	SER
1	B	832	SER
1	A	332	SER

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	325/322 (101%)	313 (96%)	12 (4%)	34	32
1	B	323/322 (100%)	309 (96%)	14 (4%)	29	27
1	C	324/322 (101%)	311 (96%)	13 (4%)	31	29
1	D	322/322 (100%)	313 (97%)	9 (3%)	43	44
All	All	1294/1288 (100%)	1246 (96%)	48 (4%)	33	32

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	63	GLN
1	A	106	THR
1	A	116	THR
1	A	183	PHE
1	A	222	THR
1	A	275	GLN
1	A	277	GLU
1	A	301	THR
1	A	333	LEU
1	A	339	LEU
1	A	354	ASN
1	B	547	LYS
1	B	563	GLN
1	B	616	THR
1	B	634	VAL
1	B	683	PHE
1	B	724	GLU
1	B	781	LYS
1	B	820	LEU
1	B	829	LEU
1	B	833	LEU
1	B	855	ILE
1	B	856	MET
1	B	857	ARG
1	B	875	VAL
1	C	1038	GLN
1	C	1039	GLN
1	C	1047	LYS
1	C	1164	LYS
1	C	1183	PHE
1	C	1213	VAL
1	C	1222	THR
1	C	1277	GLU
1	C	1283	ASN
1	C	1333	LEU
1	C	1339	LEU
1	C	1354	ASN
1	C	1357	ARG
1	D	1606	THR
1	D	1616	THR
1	D	1693	GLU

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Mol	Chain	Res	Type
1	D	1721	LYS
1	D	1775	GLN
1	D	1797	LYS
1	D	1833	LEU
1	D	1856	MET
1	D	1875	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	28	GLN
1	A	100	HIS
1	A	265	ASN
1	A	275	GLN
1	A	293	HIS
1	A	299	GLN
1	A	348	HIS
1	A	374	ASN
1	B	512	HIS
1	B	528	GLN
1	B	563	GLN
1	B	600	HIS
1	B	765	ASN
1	B	783	ASN
1	B	793	HIS
1	B	799	GLN
1	B	842	HIS
1	B	854	ASN
1	C	1038	GLN
1	C	1039	GLN
1	C	1100	HIS
1	C	1265	ASN
1	C	1283	ASN
1	C	1293	HIS
1	C	1299	GLN
1	C	1323	HIS
1	C	1348	HIS
1	C	1354	ASN
1	C	1359	GLN
1	C	1374	ASN
1	D	1528	GLN

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Mol	Chain	Res	Type
1	D	1600	HIS
1	D	1617	HIS
1	D	1765	ASN
1	D	1783	ASN
1	D	1793	HIS
1	D	1874	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	SO4	C	2007	-	4,4,4	0.12	0	6,6,6	0.25	0
2	3LM	B	2002	-	20,24,24	2.79	4 (20%)	23,33,33	1.70	3 (13%)
4	GOL	A	2009	-	5,5,5	0.38	0	5,5,5	0.64	0
2	3LM	C	2003	-	20,24,24	2.78	5 (25%)	23,33,33	2.13	7 (30%)
3	SO4	B	2006	-	4,4,4	0.18	0	6,6,6	0.19	0
3	SO4	A	2005	-	4,4,4	0.08	0	6,6,6	0.35	0
3	SO4	D	2008	-	4,4,4	0.16	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	2010	-	5,5,5	0.34	0	5,5,5	0.58	0
2	3LM	A	2001	-	20,24,24	2.77	5 (25%)	23,33,33	1.85	7 (30%)
2	3LM	D	2004	-	20,24,24	2.68	4 (20%)	23,33,33	1.59	4 (17%)

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	3LM	C	2003	-	-	6/13/19/19	0/1/1/1
2	3LM	B	2002	-	-	7/13/19/19	0/1/1/1
4	GOL	A	2009	-	-	0/4/4/4	-
2	3LM	A	2001	-	-	6/13/19/19	0/1/1/1
4	GOL	C	2010	-	-	2/4/4/4	-
2	3LM	D	2004	-	-	6/13/19/19	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	3LM	C3-C2	8.51	1.49	1.40
2	C	2003	3LM	C3-C2	7.88	1.48	1.40
2	D	2004	3LM	C3-C2	7.82	1.48	1.40
2	B	2002	3LM	C3-C2	7.78	1.48	1.40
2	D	2004	3LM	C3-C4	6.43	1.49	1.40
2	B	2002	3LM	C5-C4	6.30	1.49	1.40
2	B	2002	3LM	C3-C4	6.04	1.49	1.40
2	C	2003	3LM	C5-C4	5.88	1.48	1.40
2	A	2001	3LM	C5-C4	5.35	1.48	1.40
2	D	2004	3LM	C5-C4	4.98	1.47	1.40
2	C	2003	3LM	C3-C4	4.73	1.47	1.40
2	A	2001	3LM	C3-C4	4.61	1.47	1.40
2	C	2003	3LM	C-CA	-4.02	1.46	1.52
2	A	2001	3LM	C-CA	-3.65	1.46	1.52
2	A	2001	3LM	CA-N	3.08	1.37	1.34
2	C	2003	3LM	CA-N	2.74	1.37	1.34
2	B	2002	3LM	C-CA	-2.71	1.48	1.52
2	D	2004	3LM	C-CA	-2.44	1.48	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2003	3LM	C3-C4-C5	-4.19	114.70	118.72
2	C	2003	3LM	C4A-C4-C3	4.08	124.41	120.04
2	D	2004	3LM	CE-SD-CG	3.87	113.08	99.97
2	A	2001	3LM	CE-SD-CG	3.83	112.93	99.97
2	C	2003	3LM	C4-C4A-N	3.55	118.47	111.22
2	C	2003	3LM	CE-SD-CG	3.54	111.95	99.97
2	D	2004	3LM	C4A-C4-C3	3.49	123.78	120.04
2	B	2002	3LM	CE-SD-CG	3.42	111.53	99.97
2	B	2002	3LM	C4A-C4-C3	3.41	123.69	120.04
2	A	2001	3LM	C2A-C2-C3	-3.25	116.88	120.89
2	A	2001	3LM	C4A-C4-C3	3.15	123.41	120.04
2	C	2003	3LM	C2A-C2-N1	3.00	123.54	117.67
2	A	2001	3LM	C3-C4-C5	-2.99	115.85	118.72
2	B	2002	3LM	C6-N1-C2	2.92	124.58	119.17
2	D	2004	3LM	C3-C4-C5	-2.89	115.95	118.72
2	C	2003	3LM	OP2-P-OP4	-2.67	99.62	106.73
2	A	2001	3LM	C2A-C2-N1	2.64	122.82	117.67
2	C	2003	3LM	C2A-C2-C3	-2.53	117.76	120.89
2	A	2001	3LM	C4-C4A-N	2.15	115.62	111.22
2	A	2001	3LM	OP2-P-OP4	-2.08	101.20	106.73
2	D	2004	3LM	OP3-P-OP2	2.06	115.52	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2003	3LM	C5-C4-C4A-N
2	C	2003	3LM	N-CA-CB-CG
2	B	2002	3LM	C-CA-N-C4A
2	B	2002	3LM	CB-CA-N-C4A
2	B	2002	3LM	C5-C4-C4A-N
2	B	2002	3LM	N-CA-CB-CG
2	A	2001	3LM	C3-C4-C4A-N
2	A	2001	3LM	C5-C4-C4A-N
2	A	2001	3LM	N-CA-CB-CG
2	D	2004	3LM	C5-C4-C4A-N
2	D	2004	3LM	N-CA-CB-CG
2	B	2002	3LM	CB-CG-SD-CE
2	A	2001	3LM	CB-CG-SD-CE
2	C	2003	3LM	C-CA-N-C4A
2	A	2001	3LM	C-CA-N-C4A
2	D	2004	3LM	C-CA-N-C4A
2	C	2003	3LM	CB-CG-SD-CE

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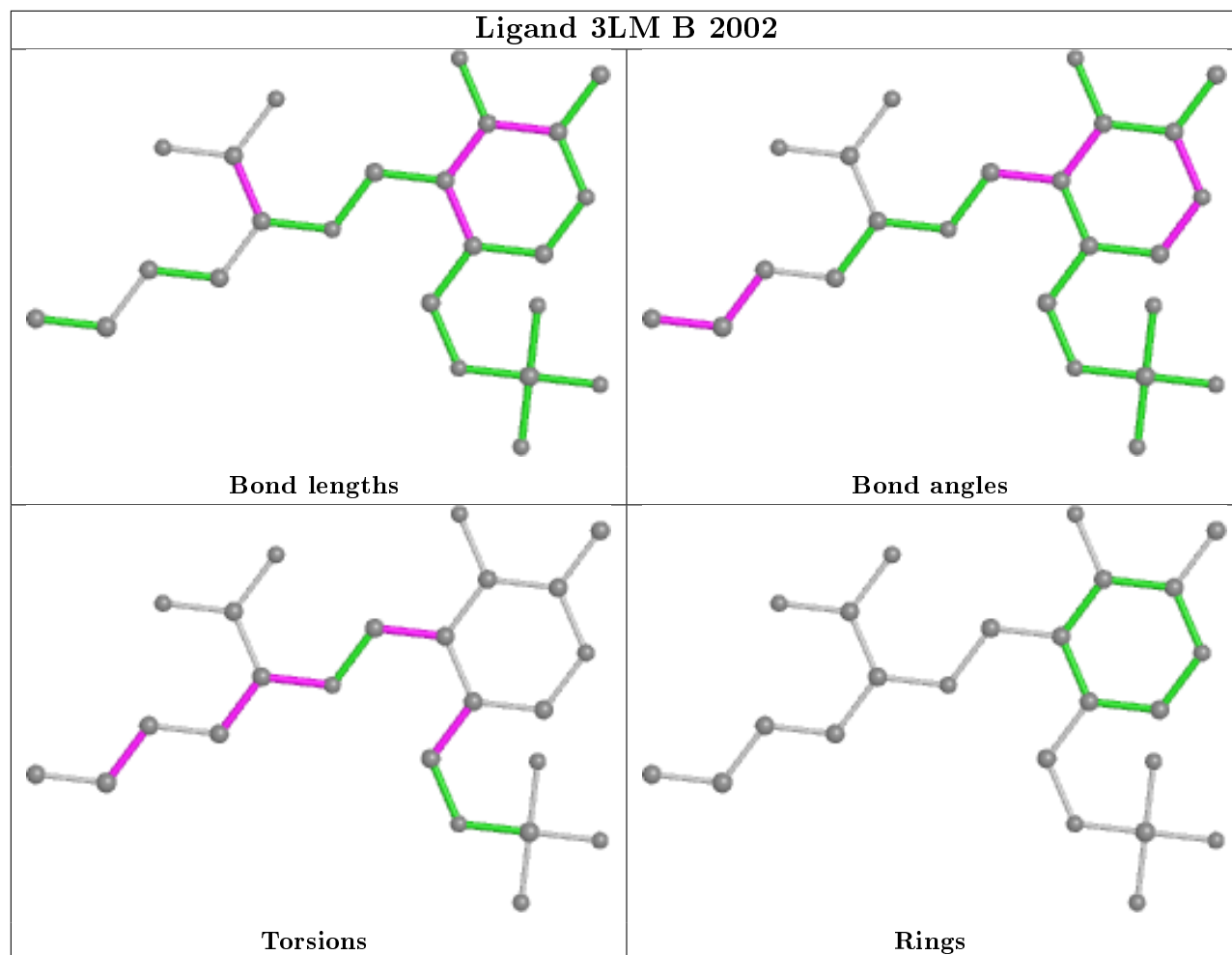
Mol	Chain	Res	Type	Atoms
2	C	2003	3LM	C3-C4-C4A-N
2	B	2002	3LM	C4-C5-C5A-OP4
2	C	2003	3LM	CB-CA-N-C4A
2	A	2001	3LM	CB-CA-N-C4A
2	D	2004	3LM	CB-CA-N-C4A
2	D	2004	3LM	CB-CG-SD-CE
2	B	2002	3LM	C3-C4-C4A-N
2	D	2004	3LM	C3-C4-C4A-N
4	C	2010	GOL	O1-C1-C2-C3
4	C	2010	GOL	O1-C1-C2-O2

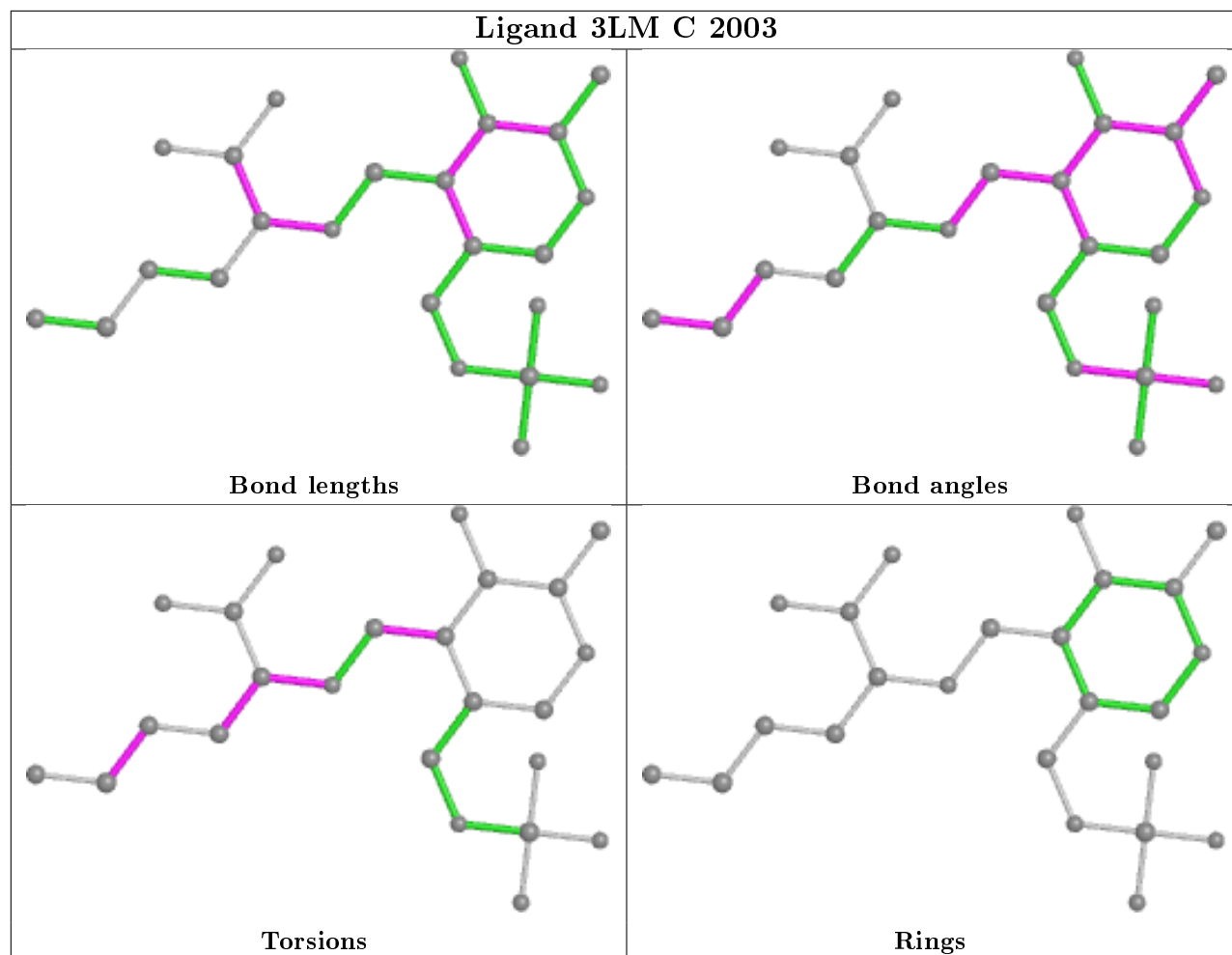
There are no ring outliers.

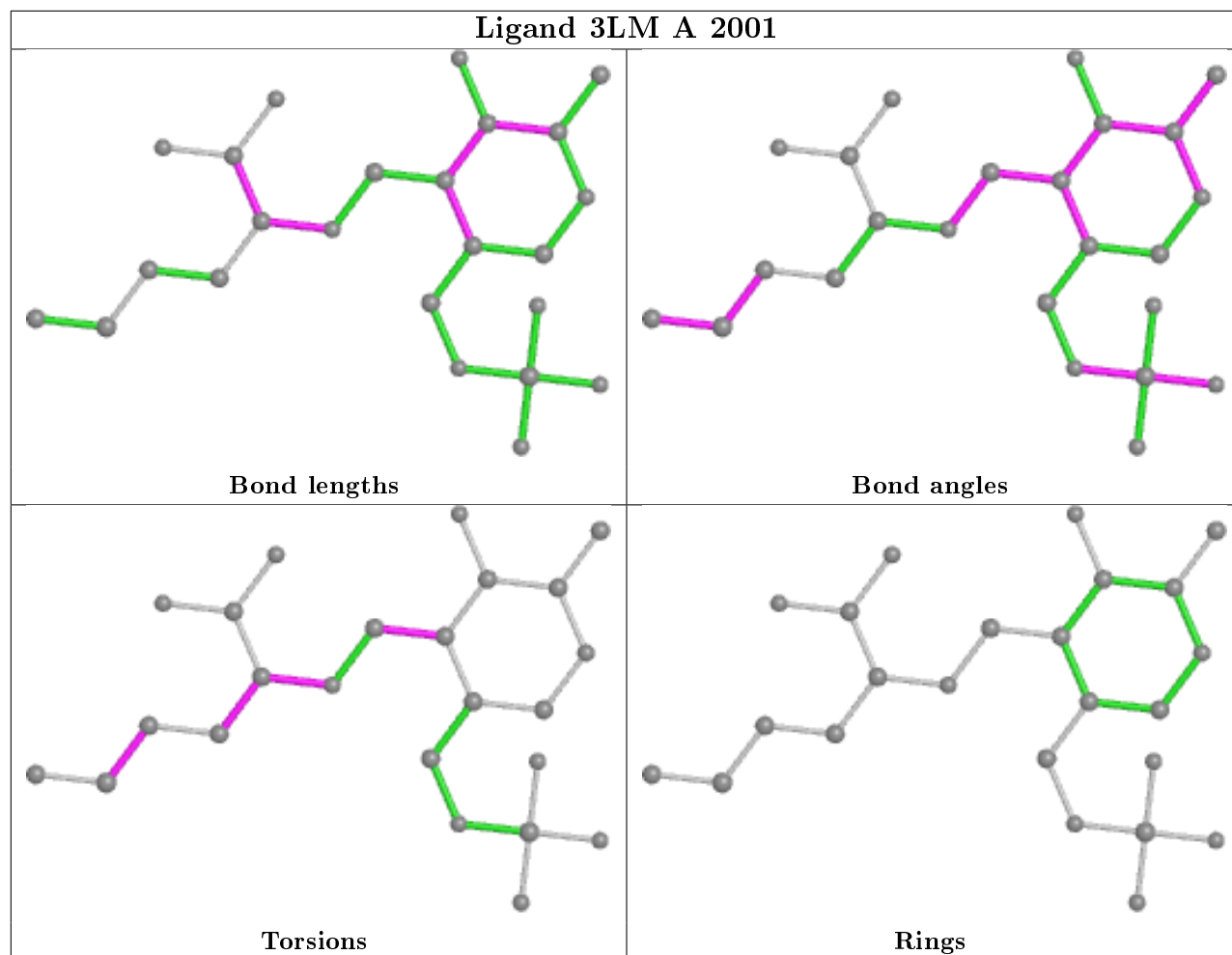
4 monomers are involved in 5 short contacts:

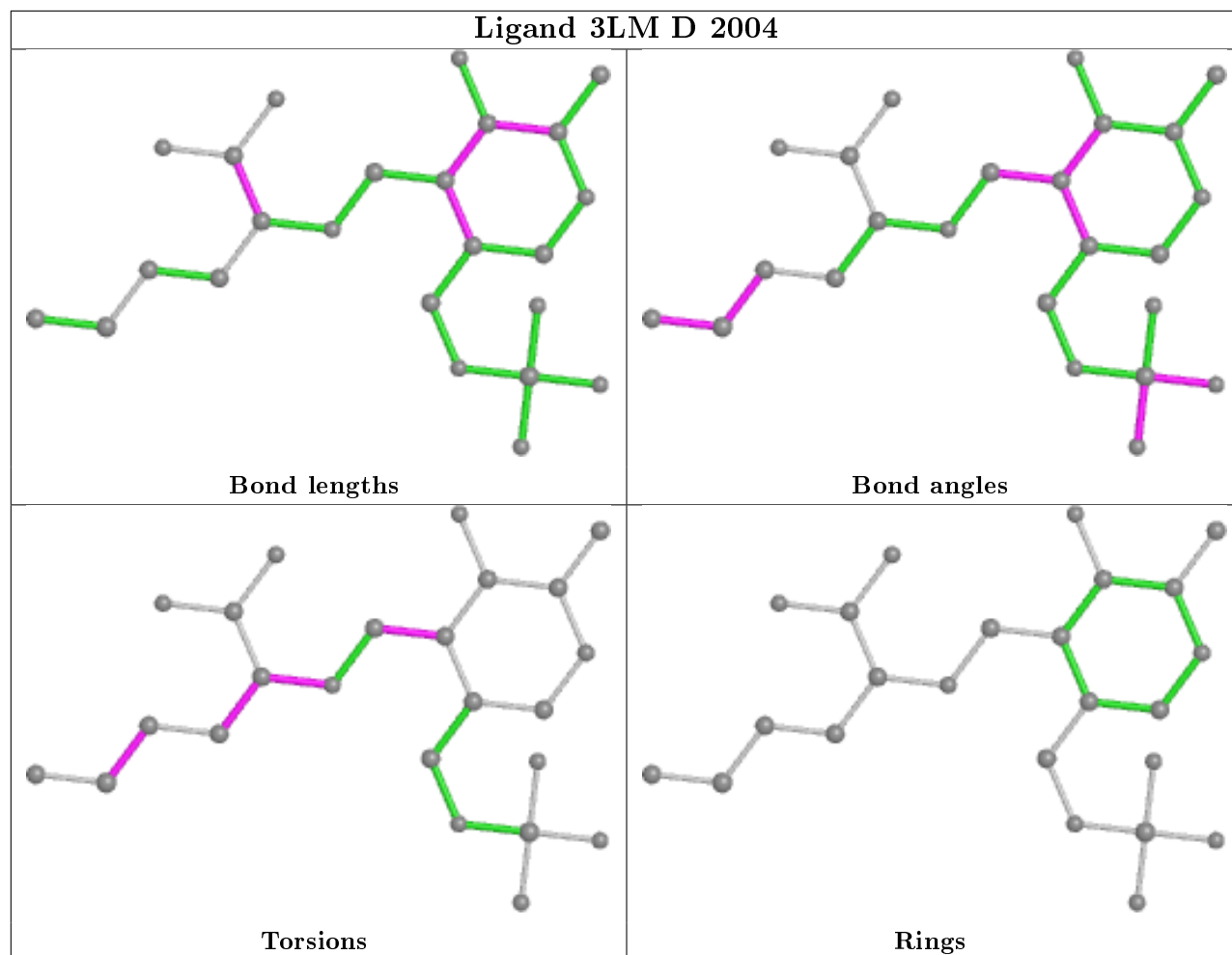
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	3LM	2	0
2	C	2003	3LM	1	0
2	A	2001	3LM	1	0
2	D	2004	3LM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	387/389 (99%)	-0.33	10 (2%) 56 64	12, 20, 46, 64	1 (0%)
1	B	386/389 (99%)	0.33	26 (6%) 17 24	18, 46, 87, 109	1 (0%)
1	C	387/389 (99%)	-0.31	14 (3%) 42 51	13, 22, 53, 74	0
1	D	384/389 (98%)	0.24	26 (6%) 17 24	18, 44, 79, 94	0
All	All	1544/1556 (99%)	-0.02	76 (4%) 29 38	12, 30, 76, 109	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	888	LEU	5.1
1	B	857	ARG	5.1
1	C	1045	MET	4.4
1	B	854	ASN	4.2
1	B	844	ALA	4.1
1	D	1516	ASP	4.1
1	A	45[A]	MET	4.0
1	B	674	GLY	4.0
1	D	1854	ASN	3.9
1	A	49	GLU	3.8
1	D	1515	GLY	3.8
1	B	853	GLU	3.8
1	B	855	ILE	3.7
1	D	1857	ARG	3.6
1	B	858	LYS	3.5
1	C	1047	LYS	3.5
1	D	1517	HIS	3.5
1	B	788	GLU	3.4
1	B	503	ALA	3.4
1	B	814	PHE	3.3
1	C	1048	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	547	LYS	3.2
1	D	1814	PHE	3.2
1	D	1634	VAL	3.2
1	A	35	ASP	3.2
1	D	1671	HIS	3.2
1	A	37	THR	3.2
1	B	516	ASP	3.1
1	D	1639	ALA	3.1
1	D	1858	LYS	3.0
1	D	1794	ASP	2.9
1	D	1853	GLU	2.9
1	B	852	PRO	2.9
1	C	1049	GLU	2.9
1	D	1788	GLU	2.8
1	C	1036	SER	2.8
1	A	38	GLN	2.8
1	B	549	GLU	2.8
1	D	1823	HIS	2.7
1	D	1852	PRO	2.7
1	C	1351	VAL	2.7
1	A	36	SER	2.7
1	C	1035	ASP	2.6
1	B	850	ALA	2.5
1	D	1635	GLU	2.5
1	C	1038	GLN	2.5
1	C	1034	PHE	2.5
1	D	1888	LEU	2.4
1	A	48	GLY	2.4
1	B	629	ILE	2.4
1	C	1017	HIS	2.4
1	D	1549	GLU	2.4
1	B	886	LEU	2.4
1	B	823	HIS	2.4
1	B	641	TRP	2.4
1	C	1039	GLN	2.3
1	D	1674	GLY	2.3
1	A	47	LYS	2.3
1	B	849	ALA	2.3
1	C	1239	LEU	2.3
1	B	882	LEU	2.2
1	B	860	GLY	2.2
1	D	1633	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	39	GLN	2.2
1	A	34	PHE	2.2
1	D	1637	VAL	2.2
1	B	548	GLY	2.2
1	D	1548	GLY	2.1
1	D	1844	ALA	2.1
1	D	1825	LYS	2.1
1	B	582	SER	2.1
1	C	1046	GLY	2.1
1	D	1885	ALA	2.0
1	D	1797	LYS	2.0
1	C	1042	ASP	2.0
1	B	794	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

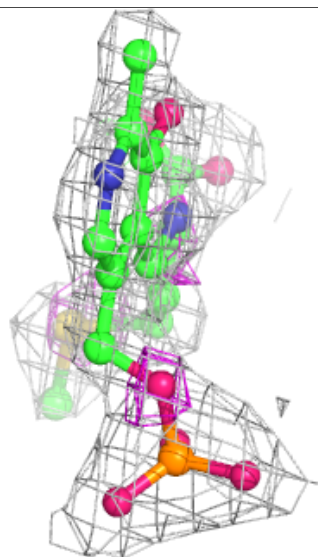
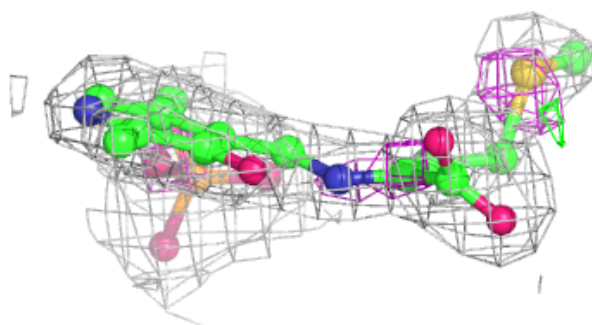
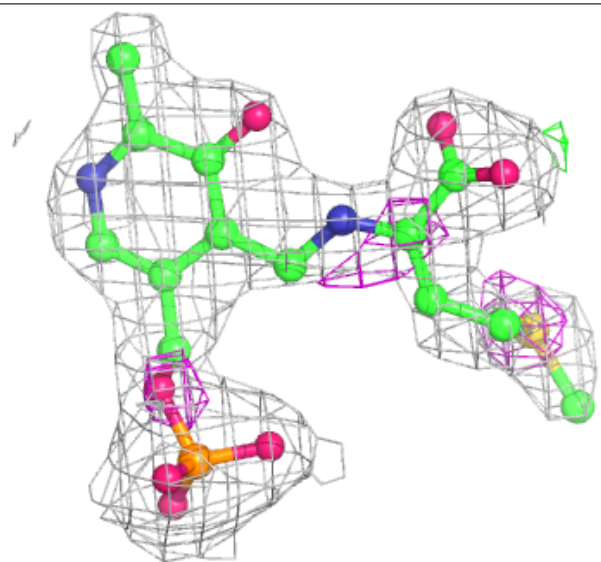
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	C	2010	6/6	0.90	0.12	47,50,52,54	0
4	GOL	A	2009	6/6	0.91	0.12	50,52,52,55	0
3	SO4	B	2006	5/5	0.93	0.24	87,87,88,88	0
3	SO4	A	2005	5/5	0.93	0.14	62,63,64,64	0
3	SO4	C	2007	5/5	0.93	0.16	63,64,64,64	0
3	SO4	D	2008	5/5	0.94	0.28	83,83,84,84	0
2	3LM	B	2002	24/24	0.95	0.17	29,45,58,63	0
2	3LM	D	2004	24/24	0.96	0.16	26,40,52,59	0
2	3LM	C	2003	24/24	0.97	0.14	15,22,38,45	0
2	3LM	A	2001	24/24	0.98	0.12	13,19,36,45	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.

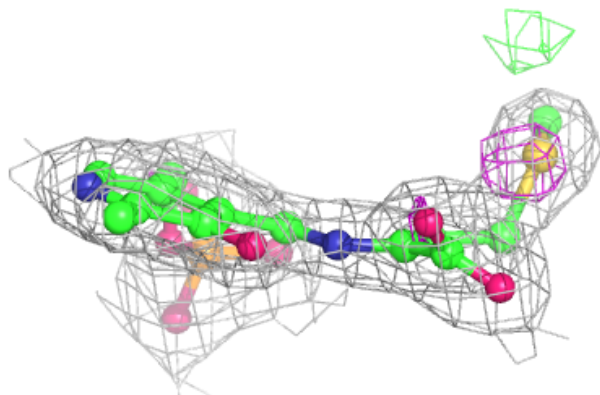
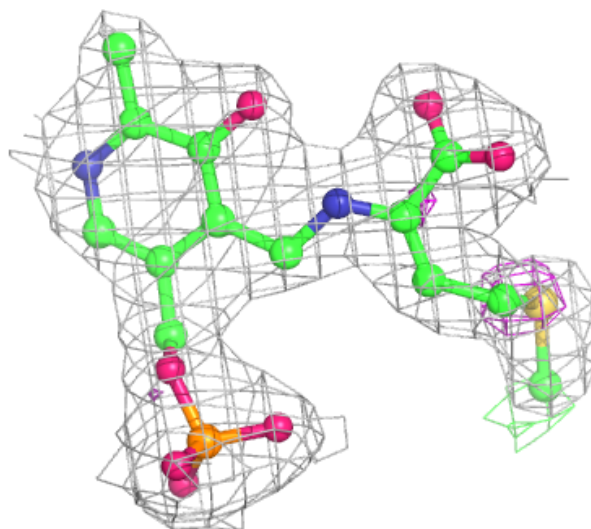
Electron density around 3LM B 2002:

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



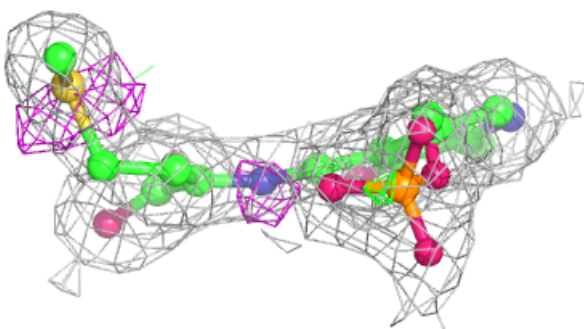
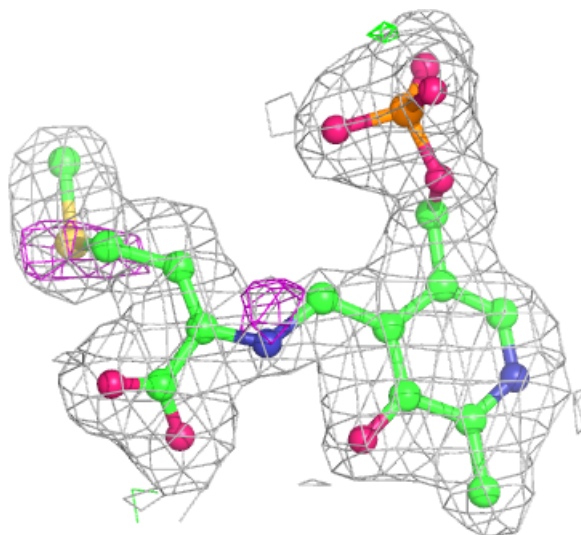
Electron density around 3LM D 2004:

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



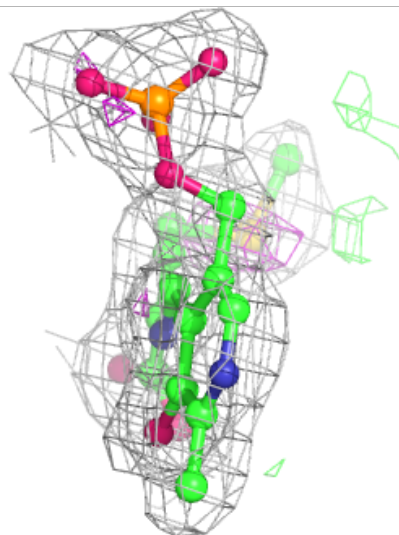
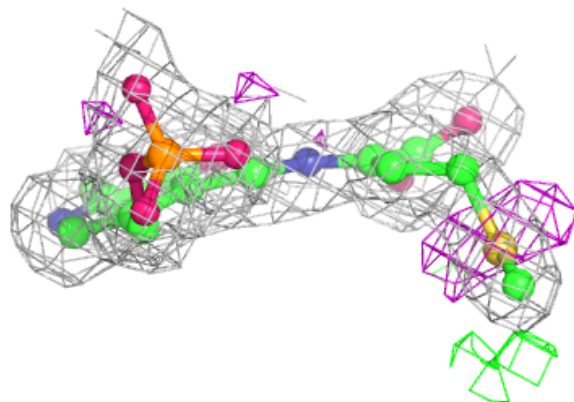
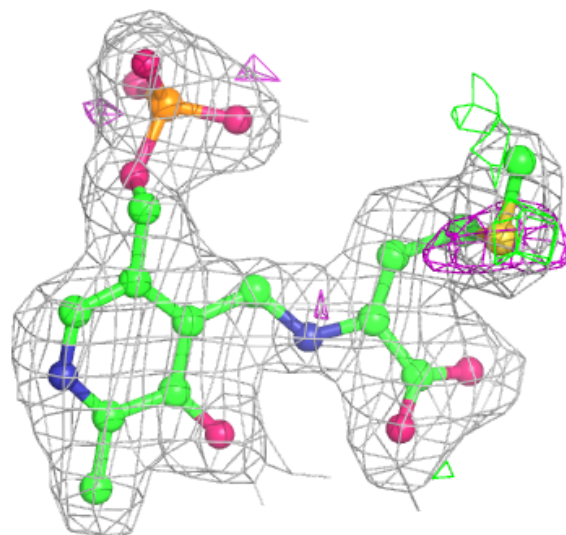
Electron density around 3LM C 2003:

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



Electron density around 3LM 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.