



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:11 PM UTC

PDB ID : 3AEP / pdb_00003aep
Title : Reaction intermediate structure of Entamoeba histolytica methionine gamma-lyase 1 containing alpha-amino-alpha, beta-butenic acid-pyridoxal-5'-phosphate
Authors : Karaki, T.; Sato, D.; Shimizu, A.; Nozaki, T.; Harada, S.
Deposited on : 2010-02-10
Resolution : 2.28 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

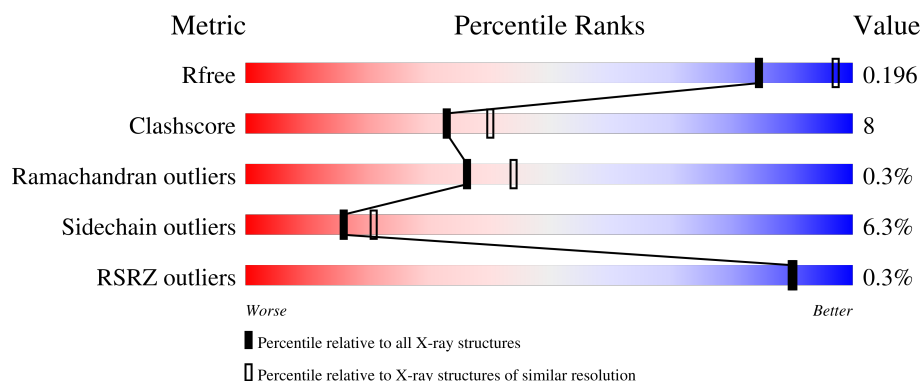
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	389	82% 14% ..
1	B	389	80% 17% ...
1	C	389	85% 13% ..
1	D	389	% 80% 16% ..

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
2	4LM	A	2001[B]	-	-	X	-
2	4LM	C	2004[B]	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12620 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.

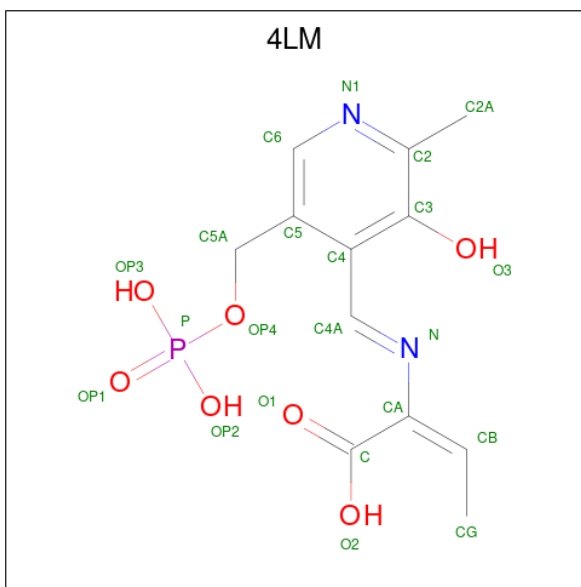
- Molecule 1 is a protein called Methionine gamma-lyase.

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	C	387	Total	C	N	O	S	0	1	0
			2952	1878	497	553	24			
1	D	384	Total	C	N	O	S	0	1	0
			2923	1859	492	548	24			

There are 4 discrepancies between the modelled and reference sequences:

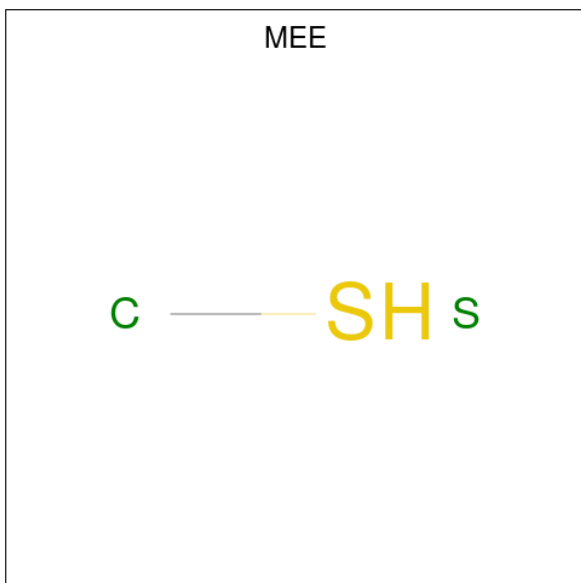
Chain	Residue	Modelled	Actual	Comment	Reference
A	308	LEU	SER	SEE REMARK 999	UNP Q86D28
B	808	LEU	SER	SEE REMARK 999	UNP Q86D28
C	1308	LEU	SER	SEE REMARK 999	UNP Q86D28
D	1808	LEU	SER	SEE REMARK 999	UNP Q86D28

- Molecule 2 is (2E)-2-{[(1E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}but-2-enoic acid (CCD ID: 4LM) (formula: C₁₂H₁₅N₂O₇P).



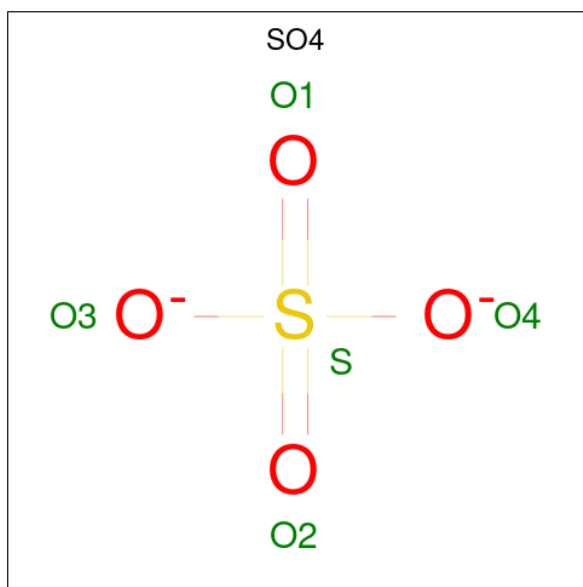
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			41	23	3	13	2		
2	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	C	1	Total	C	N	O	P	0	1
			41	23	3	13	2		
2	D	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

- Molecule 3 is METHANETHIOL (CCD ID: MEE) (formula: CH₄S).



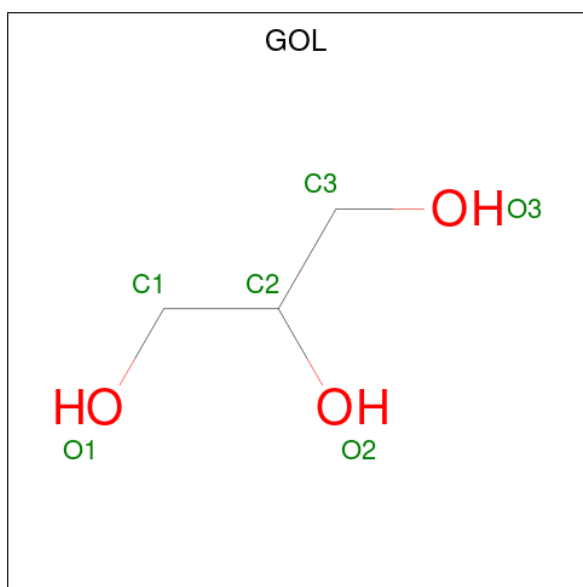
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	S	0	0
			2	1	1		
3	C	1	Total	C	S	0	0
			2	1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

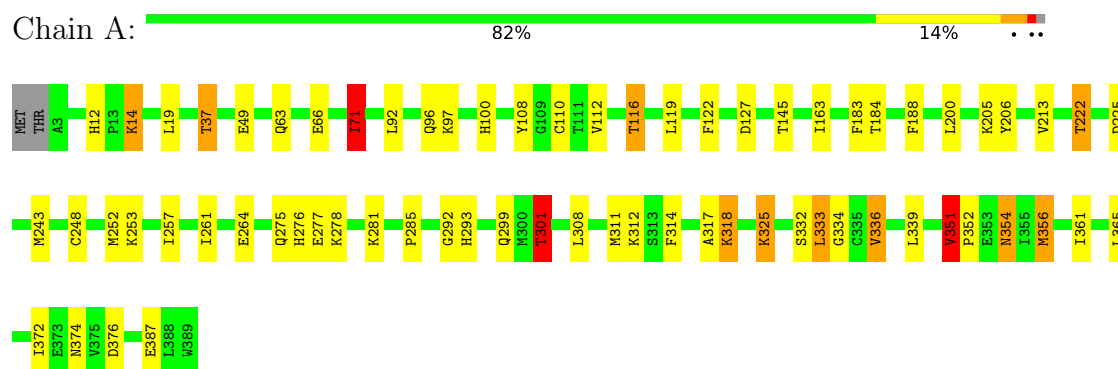
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	219	Total	O	0	0
			219	219		
6	B	132	Total	O	0	0
			132	132		
6	C	232	Total	O	0	0
			232	232		
6	D	111	Total	O	0	0
			111	111		

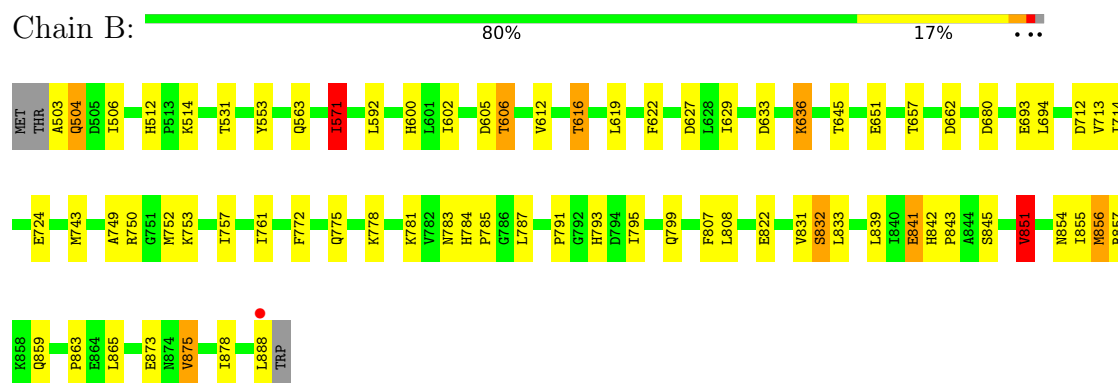
3 Residue-property plots

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.

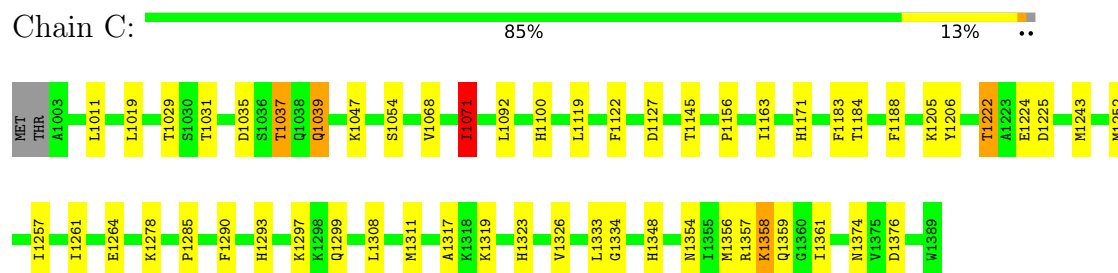
• Molecule 1: Methionine gamma-lyase



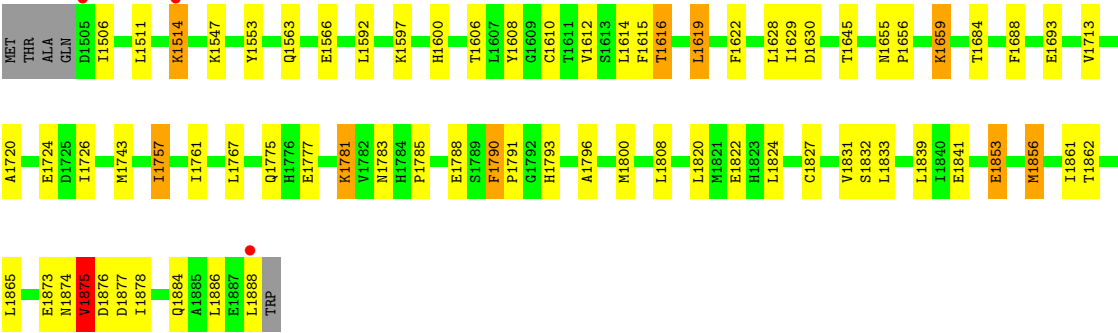
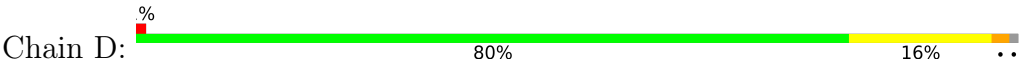
• Molecule 1: Methionine gamma-lyase



• 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	99.22Å 85.36Å 114.65Å 90.00° 101.99° 90.00°	Depositor
Resolution (Å)	39.89 – 2.28 39.89 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.89-2.28) 99.4 (39.89-2.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.198 0.155 , 0.196	Depositor DCC
R_{free} test set	4257 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12620	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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, MEE, 4LM, 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	0.93	0/3018	0.98	4/4080 (0.1%)
1	B	0.76	0/3001	0.94	3/4057 (0.1%)
1	C	0.93	0/3018	0.97	1/4080 (0.0%)
1	D	0.77	0/2987	0.93	3/4038 (0.1%)
All	All	0.85	0/12024	0.95	11/16255 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1071	ILE	CB-CA-C	-7.60	102.05	112.24
1	D	1875	VAL	CB-CA-C	-6.92	102.79	112.14
1	A	351	VAL	N-CA-CB	6.86	117.57	110.23
1	B	875	VAL	CB-CA-C	-6.76	103.18	112.04
1	A	71	ILE	CB-CA-C	-6.43	101.69	112.16
1	B	571	ILE	CB-CA-C	-6.14	103.75	112.22
1	A	301	THR	N-CA-C	-5.71	104.89	112.94
1	D	1790	PHE	CA-C-N	5.32	124.99	119.56
1	D	1790	PHE	C-N-CA	5.32	124.99	119.56
1	A	301	THR	N-CA-CB	-5.27	102.29	110.98
1	B	851	VAL	CB-CA-C	5.09	116.39	110.89

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	2952	0	2957	54	0
1	B	2937	0	2947	52	0
1	C	2952	0	2957	46	0
1	D	2923	0	2934	41	0
2	A	41	0	22	9	0
2	B	22	0	11	0	0
2	C	41	0	22	10	0
2	D	22	0	12	1	0
3	A	2	0	0	0	0
3	C	2	0	0	0	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	2	0
5	C	6	0	8	0	0
6	A	219	0	0	7	0
6	B	132	0	0	2	0
6	C	232	0	0	9	0
6	D	111	0	0	1	0
All	All	12620	0	11878	186	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 8.

All (186) 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:B:571:ILE:HD11	1:B:752:MET:HE1	1.43	1.00
2:C:2004[B]:4LM:CG	2:C:2004[B]:4LM:H4A	1.97	0.94
1:A:222:THR:HG21	6:A:3002:HOH:O	1.70	0.92
1:A:222:THR:HG22	1:A:225:ASP:H	1.32	0.92
2:A:2001[B]:4LM:CG	2:A:2001[B]:4LM:H4A	2.02	0.90
1:A:318:LYS:NZ	1:A:318:LYS:HB2	1.85	0.89
1:C:1092:LEU:HD21	1:C:1119:LEU:HD22	1.55	0.86
1:C:1222:THR:HG22	1:C:1225:ASP:H	1.43	0.83
1:D:1781:LYS:HE3	1:D:1783:ASN:HD21	1.45	0.81
2:C:2004[B]:4LM:H4A	2:C:2004[B]:4LM:HGB	1.62	0.79
1:A:188:PHE:HA	1:A:301:THR:HG22	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:ARG:HG3	6:B:3336:HOH:O	1.82	0.77
1:A:92:LEU:HD21	1:A:119:LEU:HD22	1.66	0.77
1:A:336:VAL:HG13	1:C:1011:LEU:HD22	1.66	0.77
1:A:71:ILE:HD11	1:A:252:MET:HE1	1.66	0.77
1:B:600:HIS:HD2	1:B:645:THR:OG1	1.70	0.75
2:A:2001[B]:4LM:H4A	2:A:2001[B]:4LM:HGB	1.68	0.75
1:C:1222:THR:HG21	6:C:3006:HOH:O	1.85	0.74
1:B:822:GLU:OE2	1:C:1037:THR:HG23	1.86	0.74
1:C:1278:LYS:HE2	6:C:3221:HOH:O	1.88	0.73
2:C:2004[B]:4LM:CG	2:C:2004[B]:4LM:C4A	2.66	0.73
1:D:1514:LYS:HD2	1:D:1514:LYS:H	1.53	0.72
1:B:781:LYS:HD3	1:B:783:ASN:HD21	1.53	0.72
1:C:1319:LYS:O	1:C:1323:HIS:HD2	1.73	0.70
1:A:112:VAL:O	1:A:116:THR:HB	1.89	0.70
1:A:318:LYS:NZ	1:A:318:LYS:CB	2.54	0.70
2:C:2004[B]:4LM:H4A	2:C:2004[B]:4LM:HGA	1.73	0.70
1:B:571:ILE:HD11	1:B:752:MET:CE	2.21	0.70
1:A:318:LYS:HB2	1:A:318:LYS:HZ3	1.55	0.69
1:B:605:ASP:OD1	1:B:606:THR:HG22	1.93	0.68
1:B:592:LEU:HD21	1:B:619:LEU:HD22	1.77	0.67
1:D:1592:LEU:HD21	1:D:1619:LEU:HD22	1.76	0.67
2:A:2001[B]:4LM:H4A	2:A:2001[B]:4LM:HGA	1.76	0.66
2:A:2001[B]:4LM:CG	2:A:2001[B]:4LM:C4A	2.70	0.66
1:A:37:THR:HG23	1:D:1822:GLU:OE1	1.96	0.65
1:A:205:LYS:HZ1	2:A:2001[B]:4LM:HGB	1.61	0.65
1:A:14:LYS:HE3	6:A:3506:HOH:O	1.96	0.65
1:C:1171:HIS:HD2	6:C:3061:HOH:O	1.80	0.65
1:D:1612:VAL:O	1:D:1616:THR:HB	1.98	0.64
1:A:100:HIS:HD2	1:A:145:THR:OG1	1.81	0.64
2:A:2001[B]:4LM:HG	1:D:1553:TYR:CE2	2.33	0.63
1:B:512:HIS:HE1	1:D:1873:GLU:OE1	1.81	0.63
1:B:612:VAL:O	1:B:616:THR:HB	1.98	0.63
1:C:1100:HIS:HE1	1:C:1127:ASP:OD2	1.81	0.62
1:A:318:LYS:HB2	1:A:318:LYS:HZ2	1.65	0.62
1:A:354:ASN:H	1:A:354:ASN:HD22	1.48	0.62
1:B:606:THR:HA	1:B:859:GLN:HE21	1.65	0.62
1:D:1684:THR:HG22	1:D:1688:PHE:HB2	1.82	0.61
1:C:1100:HIS:HD2	1:C:1145:THR:OG1	1.83	0.61
1:A:301:THR:HG23	6:A:3585:HOH:O	2.00	0.60
1:C:1358:LYS:HE2	6:C:3631:HOH:O	2.02	0.59
1:B:633:ASP:HB3	1:B:636:LYS:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:HIS:HE1	1:A:127:ASP:OD2	1.85	0.59
1:B:553:TYR:CE2	2:C:2004[B]:4LM:HG	2.38	0.59
1:B:842:HIS:HD2	1:B:845:SER:OG	1.86	0.57
1:A:301:THR:CG2	6:A:3585:HOH:O	2.52	0.57
1:B:743:MET:HE3	1:C:1243:MET:HE3	1.86	0.57
1:D:1514:LYS:HD2	1:D:1514:LYS:N	2.20	0.57
1:B:783:ASN:O	1:B:807:PHE:HB2	2.06	0.56
1:B:693:GLU:HG3	6:B:3417:HOH:O	2.04	0.56
1:B:842:HIS:HE1	1:B:863:PRO:O	1.88	0.56
2:A:2001[B]:4LM:HG	1:D:1553:TYR:CZ	2.40	0.56
1:A:336:VAL:HG13	1:C:1011:LEU:CD2	2.33	0.56
1:C:1035:ASP:H	1:C:1039:GLN:NE2	2.06	0.54
1:C:1068:VAL:HA	1:C:1071:ILE:HD11	1.87	0.54
1:C:1285:PRO:O	1:C:1293:HIS:HD2	1.89	0.54
1:D:1884:GLN:O	1:D:1888:LEU:HB2	2.08	0.54
1:A:308:LEU:HD21	1:A:365:LEU:HD13	1.88	0.54
1:B:785:PRO:O	1:B:793:HIS:HD2	1.91	0.54
1:C:1184:THR:HG22	1:C:1188:PHE:HB2	1.90	0.53
1:A:184:THR:HG22	1:A:188:PHE:HB2	1.91	0.53
1:A:285:PRO:O	1:A:293:HIS:HD2	1.92	0.53
1:A:318:LYS:CB	1:A:318:LYS:HZ3	2.19	0.52
1:B:600:HIS:HE1	1:B:627:ASP:OD2	1.92	0.52
1:D:1600:HIS:HD2	1:D:1645:THR:OG1	1.93	0.52
1:D:1630:ASP:OD2	1:D:1659:LYS:CE	2.57	0.52
1:C:1071:ILE:HD11	1:C:1252:MET:HE1	1.91	0.52
1:D:1781:LYS:HE3	1:D:1783:ASN:ND2	2.21	0.52
1:B:873:GLU:HG3	1:D:1511:LEU:HD12	1.92	0.52
1:D:1514:LYS:HD3	1:D:1566:GLU:HB3	1.92	0.52
1:B:808:LEU:HD21	1:B:865:LEU:HD13	1.91	0.51
1:A:97:LYS:HE3	1:D:1597:LYS:HE3	1.92	0.51
1:A:253:LYS:HE2	6:A:3597:HOH:O	2.10	0.51
1:B:714:ILE:CD1	1:C:1054:SER:HB2	2.41	0.51
1:D:1831:VAL:HG12	1:D:1841:GLU:HG3	1.94	0.50
1:B:714:ILE:HD12	1:C:1054:SER:HB2	1.93	0.50
1:A:336:VAL:HG22	1:A:372:ILE:CD1	2.43	0.49
1:C:1285:PRO:HA	1:C:1290:PHE:CD2	2.48	0.49
1:B:855:ILE:O	1:B:859:GLN:HG3	2.13	0.49
1:A:312:LYS:HB3	5:A:2011:GOL:H2	1.94	0.48
1:A:14:LYS:NZ	1:A:66:GLU:HB3	2.28	0.48
1:B:694:LEU:HD22	1:B:799:GLN:HG2	1.96	0.48
1:B:757:ILE:HG12	1:D:1761:ILE:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ILE:HD11	1:B:571:ILE:HG23	1.96	0.48
1:A:314:PHE:CZ	1:A:318:LYS:NZ	2.79	0.48
1:C:1311:MET:HG3	1:C:1317:ALA:HA	1.95	0.48
1:A:205:LYS:HD2	1:A:333:LEU:HG	1.96	0.48
1:B:781:LYS:HD3	1:B:783:ASN:ND2	2.26	0.48
1:B:851:VAL:HG22	1:B:856:MET:HG3	1.96	0.48
1:A:122:PHE:HB3	1:D:1622:PHE:HB3	1.96	0.47
1:B:602:ILE:HG23	1:B:629:ILE:HG12	1.96	0.47
1:C:1357:ARG:HA	6:C:3222:HOH:O	2.13	0.47
1:B:651:GLU:HG2	1:B:680:ASP:HB3	1.96	0.47
1:B:622:PHE:HB3	1:C:1122:PHE:HB3	1.95	0.47
1:A:71:ILE:HD11	1:A:252:MET:CE	2.40	0.47
1:B:657:THR:HA	1:B:808:LEU:HD22	1.95	0.47
1:C:1356:MET:HG2	1:C:1361:ILE:HB	1.95	0.47
1:B:784:HIS:HB3	1:B:787:LEU:HG	1.96	0.47
1:A:257:ILE:HG12	1:C:1261:ILE:HD11	1.96	0.47
1:C:1068:VAL:O	1:C:1071:ILE:HD12	2.14	0.47
1:C:1243:MET:CE	1:D:1743:MET:HE1	2.45	0.46
1:B:749:ALA:O	1:B:753:LYS:HD3	2.15	0.46
1:A:276:HIS:CE1	1:A:278:LYS:HG3	2.50	0.46
1:D:1874:ASN:HD21	1:D:1876:ASP:HB2	1.80	0.46
1:D:1796:ALA:HB1	1:D:1800:MET:HE2	1.98	0.46
1:C:1224:GLU:HB2	6:C:3094:HOH:O	2.16	0.46
1:C:1163:ILE:H	1:C:1299:GLN:HE22	1.64	0.46
1:D:1785:PRO:O	1:D:1793:HIS:HD2	1.99	0.46
1:D:1615:PHE:HA	1:D:1619:LEU:HG	1.98	0.46
1:A:292:GLY:HA2	6:A:3195:HOH:O	2.15	0.45
1:D:1790:PHE:HA	1:D:1791:PRO:HD3	1.84	0.45
1:A:261:ILE:HD11	1:C:1257:ILE:HG12	1.97	0.45
1:A:12:HIS:CE1	1:C:1326:VAL:O	2.70	0.45
1:D:1808:LEU:HD21	1:D:1865:LEU:HD13	1.97	0.45
1:B:750:ARG:O	1:B:753:LYS:HB2	2.17	0.45
1:B:553:TYR:CZ	2:C:2004[B]:4LM:HG	2.51	0.45
1:A:243:MET:HE2	1:A:243:MET:HB2	1.85	0.45
1:A:276:HIS:HE1	1:A:278:LYS:HG3	1.82	0.45
2:C:2004[B]:4LM:C4A	2:C:2004[B]:4LM:HGA	2.41	0.45
1:D:1862:THR:H	1:D:1865:LEU:HD12	1.82	0.45
1:B:531:THR:HG22	6:C:3076:HOH:O	2.16	0.45
1:C:1359:GLN:HE21	1:C:1361:ILE:HD12	1.80	0.45
1:D:1608:TYR:CE2	1:D:1610:CYS:HB2	2.51	0.45
1:C:1243:MET:HE1	1:D:1743:MET:CE	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2004[B]:4LM:HGB	2:C:2004[B]:4LM:C4A	2.39	0.45
1:D:1820:LEU:HD22	1:D:1886:LEU:HD21	1.98	0.44
1:A:243:MET:CE	1:B:743:MET:HE1	2.48	0.44
1:A:325:LYS:HD3	6:A:3527:HOH:O	2.16	0.44
5:A:2011:GOL:O3	5:A:2011:GOL:O1	2.34	0.44
1:D:1630:ASP:OD2	1:D:1659:LYS:HE2	2.18	0.44
1:D:1853:GLU:O	1:D:1856:MET:HB3	2.18	0.44
1:D:1875:VAL:HG22	6:D:3181:HOH:O	2.17	0.44
1:A:213:VAL:HG11	1:A:248:CYS:SG	2.58	0.43
1:A:96:GLN:O	1:A:97:LYS:C	2.60	0.43
1:D:1720:ALA:HB3	1:D:1726:ILE:HB	1.99	0.43
1:C:1319:LYS:O	1:C:1323:HIS:CD2	2.62	0.43
1:D:1874:ASN:HD22	1:D:1877:ASP:H	1.67	0.43
1:A:206:TYR:CE2	1:A:334:GLY:HA2	2.53	0.43
1:A:100:HIS:CE1	1:A:127:ASP:OD2	2.68	0.43
1:A:356:MET:HG2	1:A:361:ILE:HB	2.00	0.43
1:B:841:GLU:OE2	1:B:843:PRO:HA	2.19	0.43
1:B:662:ASP:HB2	1:B:795:ILE:HD13	2.02	0.42
1:C:1243:MET:CE	1:D:1743:MET:CE	2.96	0.42
1:A:354:ASN:HD22	1:A:354:ASN:N	2.14	0.42
1:A:108:TYR:CE2	1:A:110:CYS:HB2	2.54	0.42
1:D:1856:MET:HE2	1:D:1861:ILE:HB	2.02	0.42
1:B:761:ILE:HD11	1:D:1757:ILE:HG12	2.02	0.42
1:A:200:LEU:HD12	1:A:200:LEU:C	2.44	0.42
1:B:503:ALA:O	1:B:504:GLN:C	2.63	0.42
1:B:600:HIS:CD2	1:B:645:THR:OG1	2.61	0.42
1:C:1374:ASN:HD21	1:C:1376:ASP:HB2	1.85	0.42
1:A:374:ASN:HD21	1:A:376:ASP:HB2	1.85	0.41
2:D:2006:4LM:H4A	2:D:2006:4LM:HB	1.80	0.41
1:B:506:ILE:CD1	1:B:571:ILE:HG23	2.50	0.41
1:D:1655:ASN:HA	1:D:1656:PRO:HA	1.86	0.41
1:C:1206:TYR:CE1	1:C:1334:GLY:HA2	2.55	0.41
1:C:1299:GLN:NE2	6:C:3189:HOH:O	2.53	0.41
1:A:163:ILE:H	1:A:299:GLN:HE22	1.67	0.41
1:B:873:GLU:HB2	1:B:878:ILE:HD11	2.02	0.41
1:C:1243:MET:HE2	1:C:1243:MET:HB2	1.96	0.41
1:C:1205:LYS:HZ1	2:C:2004[A]:4LM:CB	2.33	0.41
1:C:1264:GLU:HG3	6:C:3663:HOH:O	2.21	0.41
1:D:1824:LEU:HD13	1:D:1827:CYS:HB2	2.01	0.41
1:B:606:THR:HB	1:B:859:GLN:HG2	2.03	0.41
1:B:772:PHE:HA	1:B:775:GLN:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2004[A]:4LM:H4A	2:C:2004[A]:4LM:HB	1.91	0.41
1:B:842:HIS:CD2	1:B:845:SER:OG	2.71	0.41
1:B:831:VAL:O	1:B:832:SER:CB	2.69	0.40
1:C:1100:HIS:CE1	1:C:1127:ASP:OD2	2.68	0.40
2:A:2001[B]:4LM:HGA	2:A:2001[B]:4LM:C4A	2.45	0.40
1:A:311:MET:HG3	1:A:317:ALA:HA	2.04	0.40
2:A:2001[B]:4LM:HGB	2:A:2001[B]:4LM:C4A	2.43	0.40
1:C:1092:LEU:HD21	1:C:1119:LEU:CD2	2.39	0.40
1:A:351:VAL:HA	1:A:352:PRO:HD3	1.94	0.40
1:B:712:ASP:HA	1:C:1029:THR:HA	2.03	0.40
1:C:1156:PRO:HD3	1:C:1348:HIS:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/389 (99%)	374 (97%)	11 (3%)	1 (0%)	36	44
1	B	385/389 (99%)	375 (97%)	8 (2%)	2 (0%)	24	29
1	C	386/389 (99%)	375 (97%)	11 (3%)	0	100	100
1	D	383/389 (98%)	374 (98%)	8 (2%)	1 (0%)	36	44
All	All	1540/1556 (99%)	1498 (97%)	38 (2%)	4 (0%)	36	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	854	ASN
1	B	832	SER
1	A	332	SER
1	D	1832	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	321/322 (100%)	298 (93%)	23 (7%)	13	16
1	B	320/322 (99%)	302 (94%)	18 (6%)	19	25
1	C	321/322 (100%)	308 (96%)	13 (4%)	28	40
1	D	319/322 (99%)	293 (92%)	26 (8%)	10	12
All	All	1281/1288 (100%)	1201 (94%)	80 (6%)	16	21

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	19	LEU
1	A	37	THR
1	A	49	GLU
1	A	63	GLN
1	A	71	ILE
1	A	116	THR
1	A	183	PHE
1	A	222	THR
1	A	264	GLU
1	A	275	GLN
1	A	277	GLU
1	A	281	LYS
1	A	301	THR
1	A	318	LYS
1	A	325	LYS
1	A	333	LEU
1	A	336	VAL
1	A	339	LEU
1	A	351	VAL
1	A	354	ASN
1	A	356	MET
1	A	387	GLU
1	B	504	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	514	LYS
1	B	563	GLN
1	B	571	ILE
1	B	606	THR
1	B	616	THR
1	B	636	LYS
1	B	713	VAL
1	B	724	GLU
1	B	778	LYS
1	B	791	PRO
1	B	833	LEU
1	B	839	LEU
1	B	841	GLU
1	B	851	VAL
1	B	856	MET
1	B	875	VAL
1	B	888	LEU
1	C	1019	LEU
1	C	1031	THR
1	C	1037	THR
1	C	1039	GLN
1	C	1047	LYS
1	C	1071	ILE
1	C	1183	PHE
1	C	1222	THR
1	C	1297	LYS
1	C	1308	LEU
1	C	1333	LEU
1	C	1354	ASN
1	C	1358	LYS
1	D	1506	ILE
1	D	1514	LYS
1	D	1547	LYS
1	D	1563	GLN
1	D	1606	THR
1	D	1614	LEU
1	D	1616	THR
1	D	1619	LEU
1	D	1628	LEU
1	D	1629	ILE
1	D	1659	LYS
1	D	1693	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1713	VAL
1	D	1724	GLU
1	D	1757	ILE
1	D	1767	LEU
1	D	1775	GLN
1	D	1777	GLU
1	D	1781	LYS
1	D	1788	GLU
1	D	1833	LEU
1	D	1839	LEU
1	D	1853	GLU
1	D	1856	MET
1	D	1875	VAL
1	D	1878	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	100	HIS
1	A	117	HIS
1	A	265	ASN
1	A	275	GLN
1	A	293	HIS
1	A	299	GLN
1	A	348	HIS
1	A	354	ASN
1	A	374	ASN
1	B	504	GLN
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	859	GLN
1	C	1028	GLN
1	C	1039	GLN
1	C	1063	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1100	HIS
1	C	1171	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	1359	GLN
1	C	1374	ASN
1	D	1528	GLN
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 [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](#)

14 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
2	4LM	A	2001[A]	-	21,22,22	1.55	3 (14%)	26,31,31	1.56	3 (11%)
2	4LM	C	2004[A]	-	21,22,22	1.50	2 (9%)	26,31,31	1.36	2 (7%)
4	SO4	D	2010	-	4,4,4	0.31	0	6,6,6	0.17	0
5	GOL	C	2012	-	5,5,5	0.44	0	5,5,5	0.20	0
4	SO4	A	2007	-	4,4,4	0.23	0	6,6,6	0.35	0
4	SO4	C	2009	-	4,4,4	0.18	0	6,6,6	0.18	0
3	MEE	A	2002	-	0,1,1	-	-	-	-	-
2	4LM	A	2001[B]	-	21,22,22	1.45	3 (14%)	26,31,31	1.66	4 (15%)
2	4LM	D	2006	-	21,22,22	1.42	2 (9%)	26,31,31	1.92	5 (19%)
2	4LM	B	2003	-	21,22,22	1.62	2 (9%)	26,31,31	1.87	4 (15%)
3	MEE	C	2005	-	0,1,1	-	-	-	-	-
5	GOL	A	2011	-	5,5,5	0.49	0	5,5,5	0.55	0
2	4LM	C	2004[B]	-	21,22,22	1.52	3 (14%)	26,31,31	1.53	3 (11%)
4	SO4	B	2008	-	4,4,4	0.27	0	6,6,6	0.14	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	4LM	A	2001[A]	-	-	2/15/17/17	0/1/1/1
2	4LM	C	2004[A]	-	-	0/15/17/17	0/1/1/1
5	GOL	C	2012	-	-	0/4/4/4	-
2	4LM	A	2001[B]	-	-	2/15/17/17	0/1/1/1
2	4LM	D	2006	-	-	2/15/17/17	0/1/1/1
2	4LM	B	2003	-	-	5/15/17/17	0/1/1/1
2	4LM	C	2004[B]	-	-	0/15/17/17	0/1/1/1
5	GOL	A	2011	-	-	4/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2003	4LM	CA-N	-5.62	1.35	1.41
2	C	2004[A]	4LM	CA-N	-4.95	1.35	1.41
2	D	2006	4LM	CA-N	-4.77	1.36	1.41
2	A	2001[A]	4LM	CA-N	-4.68	1.36	1.41
2	C	2004[B]	4LM	CA-N	-4.53	1.36	1.41
2	A	2001[B]	4LM	CA-N	-3.56	1.37	1.41
2	C	2004[A]	4LM	O2-C	-3.14	1.22	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2004[B]	4LM	O2-C	-3.14	1.22	1.30
2	A	2001[A]	4LM	O2-C	-2.82	1.22	1.30
2	A	2001[B]	4LM	O2-C	-2.82	1.22	1.30
2	A	2001[B]	4LM	C4-C5	-2.36	1.38	1.42
2	B	2003	4LM	O2-C	-2.36	1.24	1.30
2	C	2004[B]	4LM	CA-C	-2.31	1.45	1.48
2	A	2001[A]	4LM	C4-C5	-2.29	1.38	1.42
2	D	2006	4LM	O2-C	-2.05	1.25	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2006	4LM	O2-C-CA	6.85	124.39	113.40
2	B	2003	4LM	O2-C-CA	6.39	123.65	113.40
2	C	2004[B]	4LM	O2-C-CA	4.66	120.88	113.40
2	A	2001[B]	4LM	O2-C-CA	4.52	120.65	113.40
2	A	2001[A]	4LM	O2-C-CA	4.43	120.50	113.40
2	C	2004[A]	4LM	O2-C-CA	4.05	119.90	113.40
2	D	2006	4LM	O1-C-CA	-3.35	116.72	122.02
2	B	2003	4LM	O1-C-CA	-3.12	117.10	122.02
2	A	2001[B]	4LM	C4-C3-C2	2.93	121.79	120.14
2	C	2004[B]	4LM	C4A-N-CA	2.89	129.92	122.63
2	A	2001[A]	4LM	C4-C3-C2	2.82	121.73	120.14
2	A	2001[B]	4LM	C4A-N-CA	2.79	129.65	122.63
2	C	2004[A]	4LM	C4A-N-CA	2.69	129.40	122.63
2	A	2001[A]	4LM	C4A-N-CA	2.61	129.19	122.63
2	D	2006	4LM	OP4-C5A-C5	2.47	113.99	109.36
2	B	2003	4LM	OP4-C5A-C5	2.35	113.76	109.36
2	A	2001[B]	4LM	CG-CB-CA	-2.32	119.64	125.93
2	D	2006	4LM	OP2-P-OP4	-2.32	100.63	106.67
2	B	2003	4LM	C3-C2-N1	-2.22	118.16	120.96
2	D	2006	4LM	O2-C-O1	-2.14	118.80	123.90
2	C	2004[B]	4LM	CG-CB-CA	-2.13	120.17	125.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2011	GOL	O1-C1-C2-C3
5	A	2011	GOL	O1-C1-C2-O2
5	A	2011	GOL	C1-C2-C3-O3
2	A	2001[A]	4LM	C4-C5-C5A-OP4

Continued on next page...

Continued from previous page...

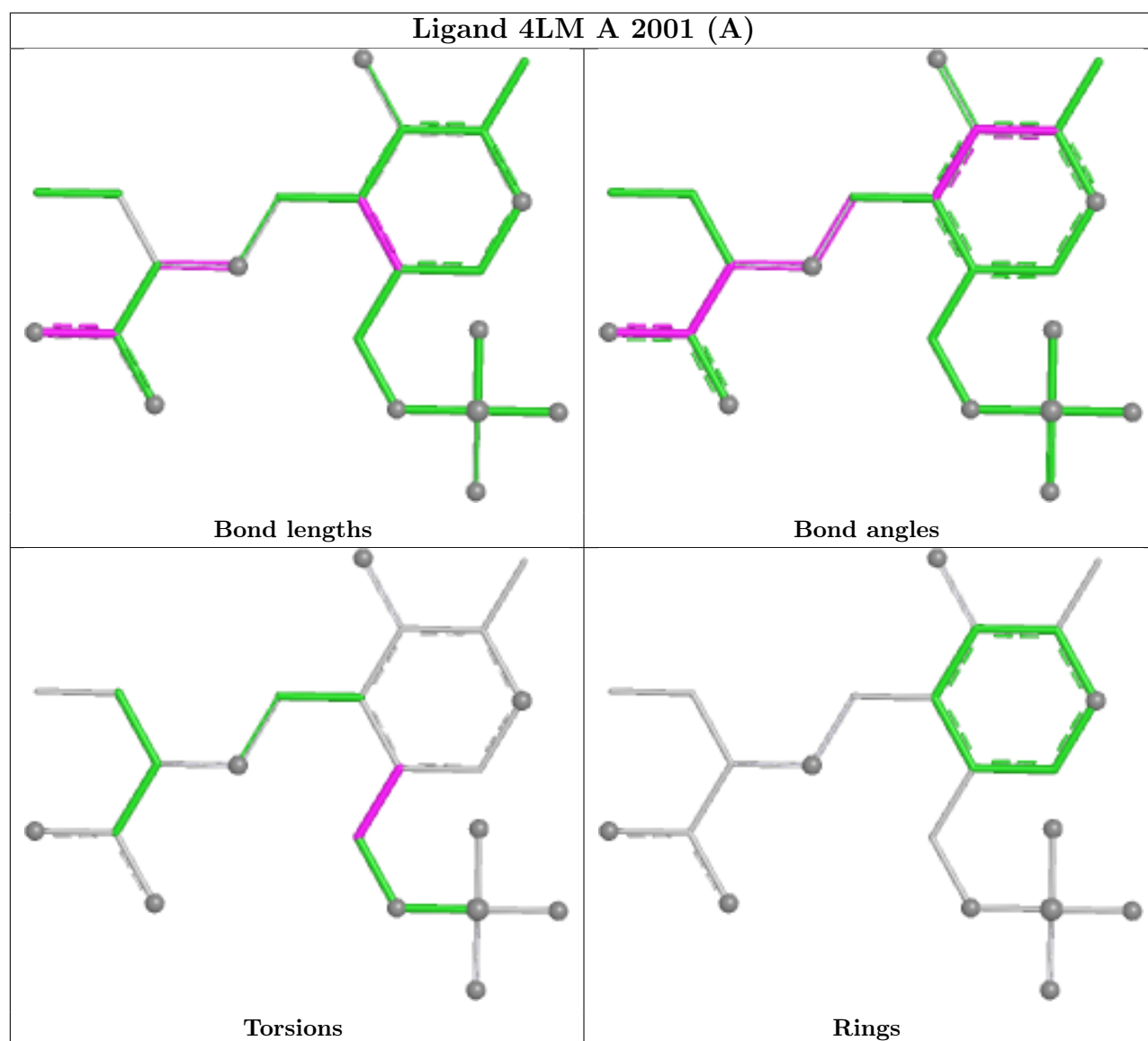
Mol	Chain	Res	Type	Atoms
2	A	2001[B]	4LM	C4-C5-C5A-OP4
2	D	2006	4LM	C4-C5-C5A-OP4
5	A	2011	GOL	O2-C2-C3-O3
2	A	2001[A]	4LM	C6-C5-C5A-OP4
2	A	2001[B]	4LM	C6-C5-C5A-OP4
2	B	2003	4LM	C6-C5-C5A-OP4
2	D	2006	4LM	C6-C5-C5A-OP4
2	B	2003	4LM	O2-C-CA-CB
2	B	2003	4LM	C4-C5-C5A-OP4
2	B	2003	4LM	N-CA-CB-CG
2	B	2003	4LM	O2-C-CA-N

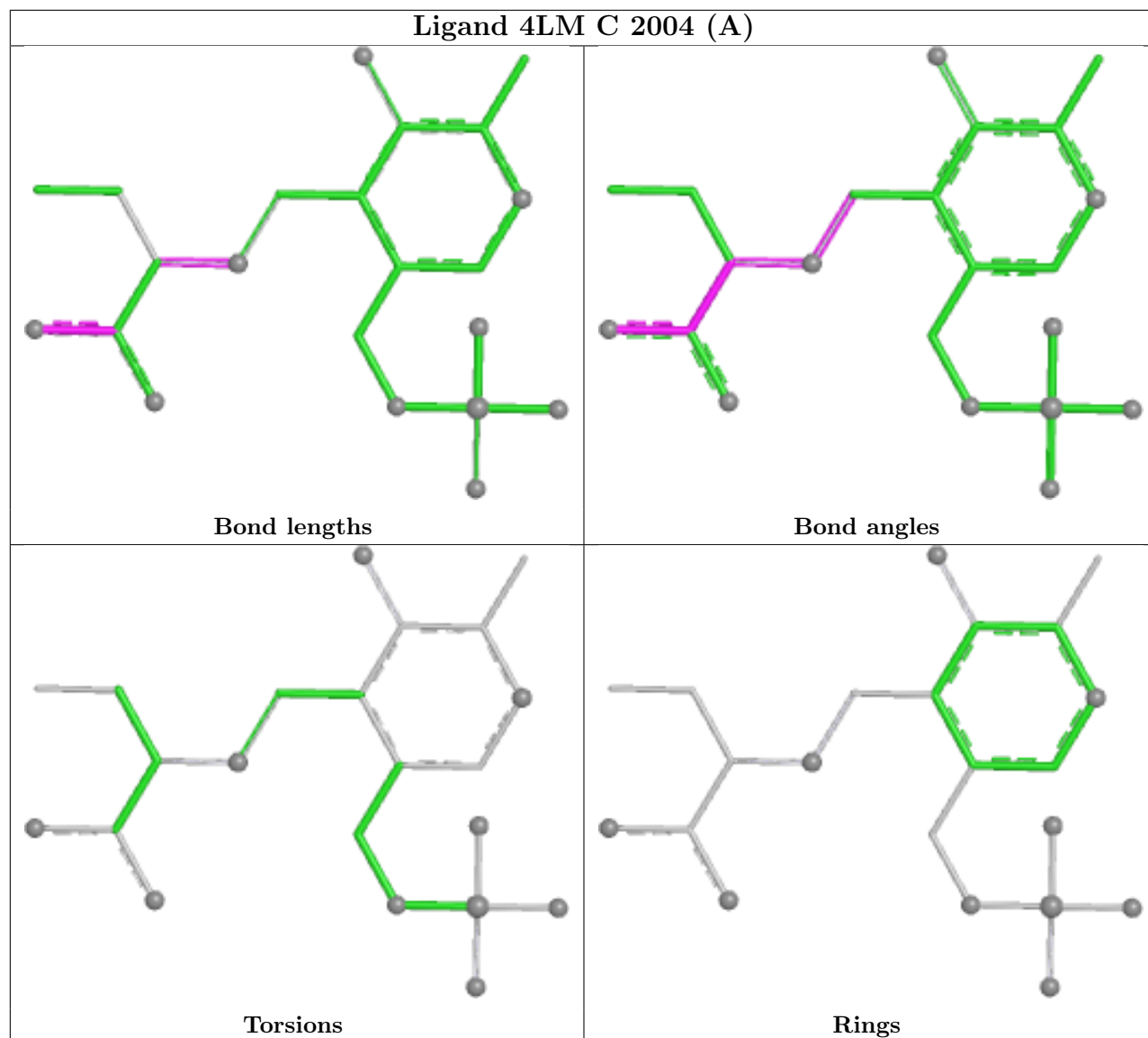
There are no ring outliers.

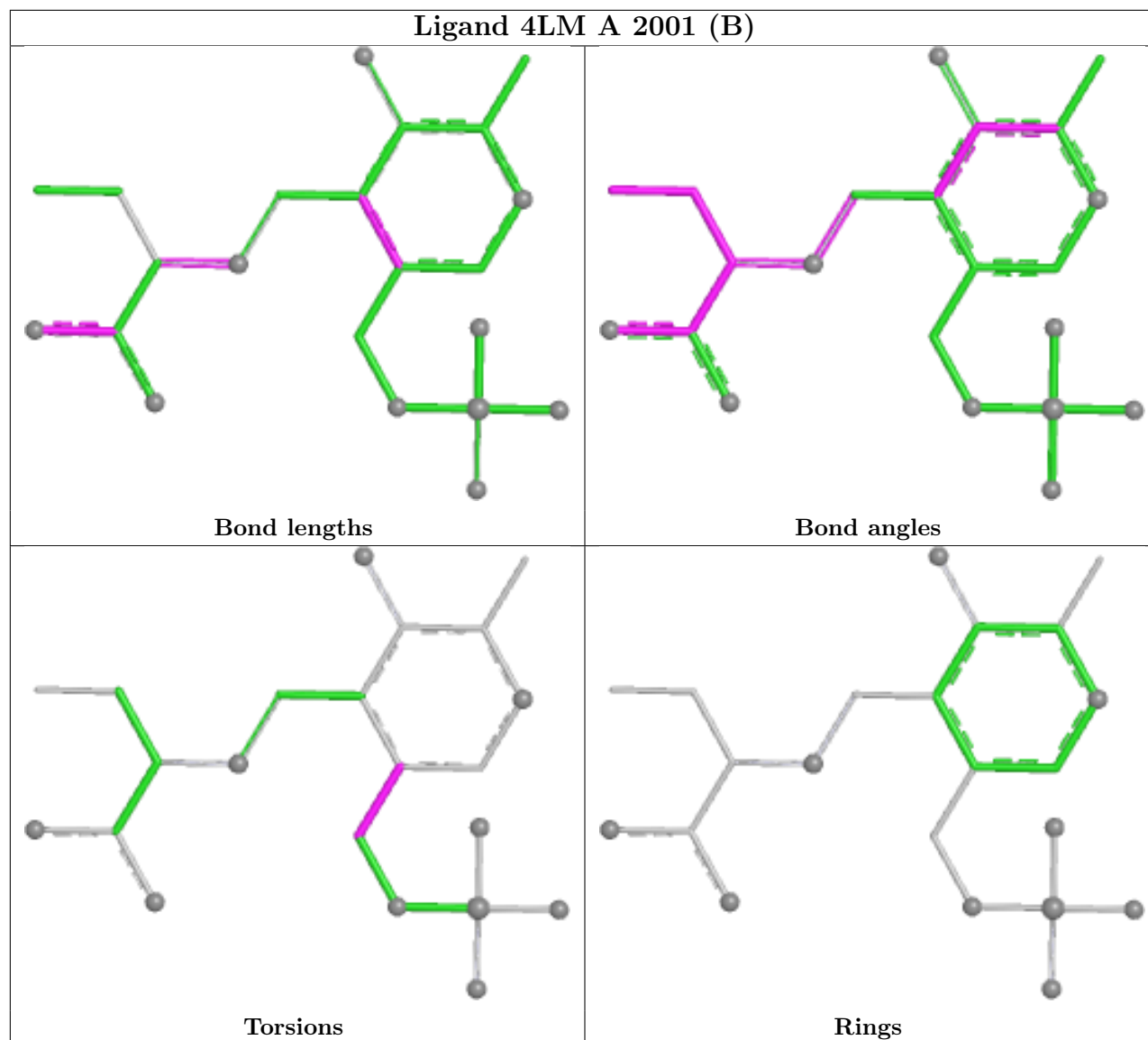
5 monomers are involved in 22 short contacts:

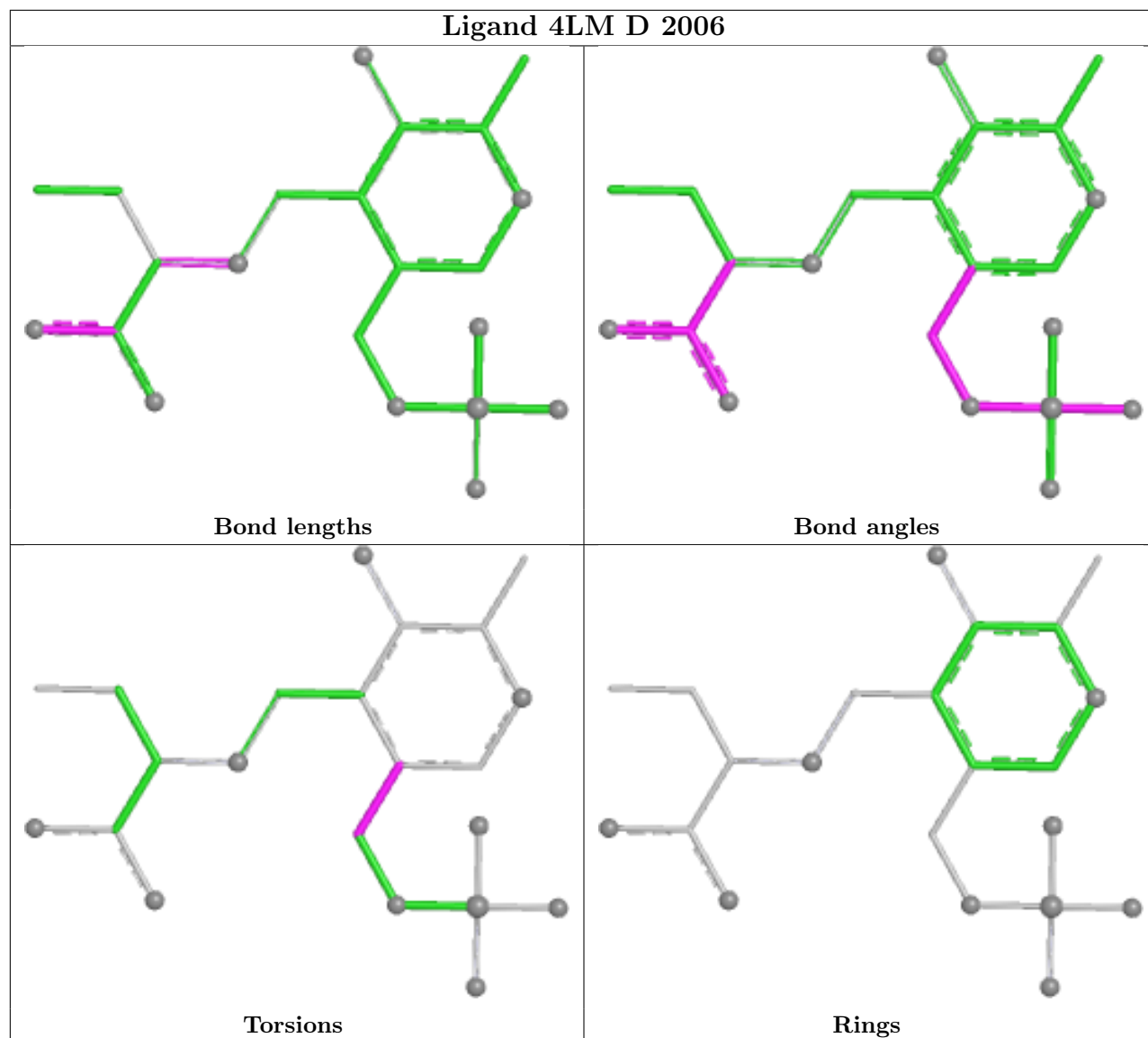
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2004[A]	4LM	2	0
2	A	2001[B]	4LM	9	0
2	D	2006	4LM	1	0
5	A	2011	GOL	2	0
2	C	2004[B]	4LM	8	0

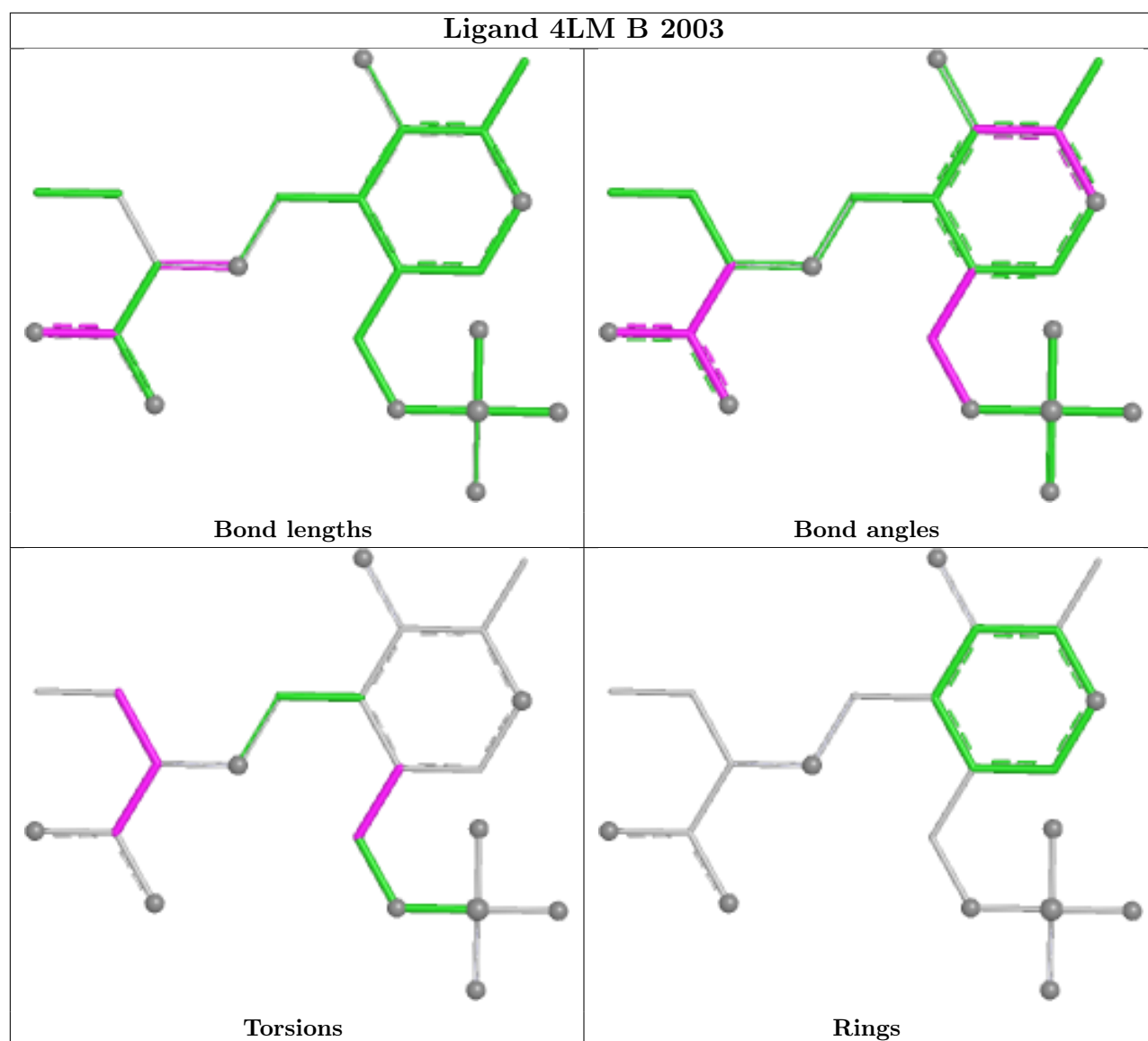
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

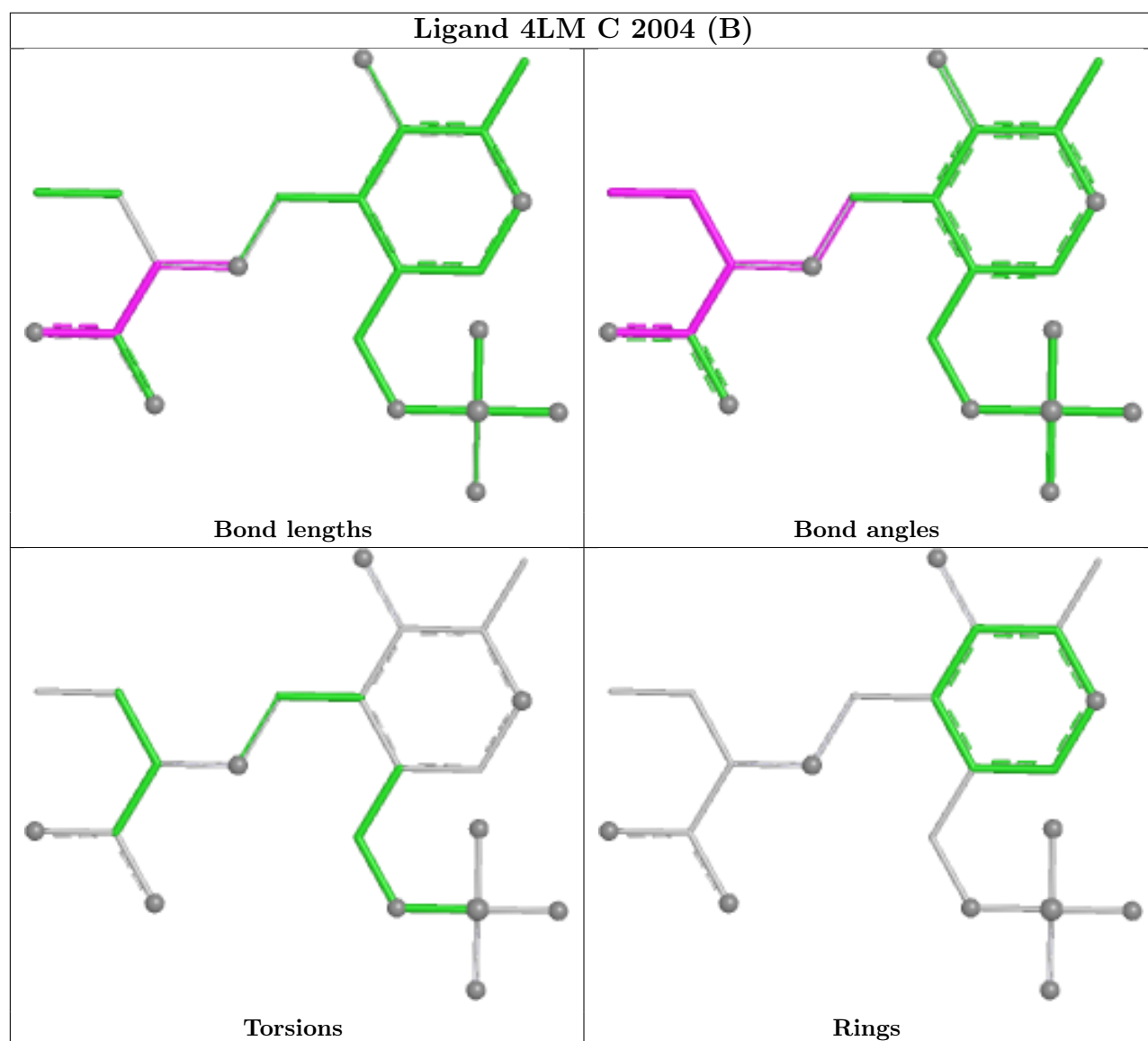












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/389 (99%)	-0.80	0 100 100	12, 21, 42, 61	2 (0%)
1	B	386/389 (99%)	-0.46	1 (0%) 90 90	18, 36, 63, 79	2 (0%)
1	C	387/389 (99%)	-0.77	0 100 100	12, 22, 44, 61	2 (0%)
1	D	384/389 (98%)	-0.45	3 (0%) 82 84	17, 38, 65, 79	1 (0%)
All	All	1544/1556 (99%)	-0.62	4 (0%) 90 90	12, 27, 60, 79	7 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	888	LEU	3.2
1	D	1888	LEU	2.9
1	D	1514	LYS	2.3
1	D	1505	ASP	2.1

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](#)

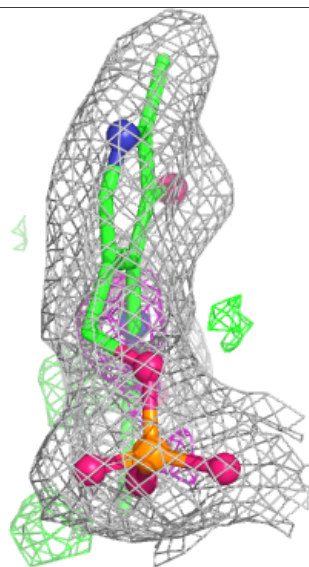
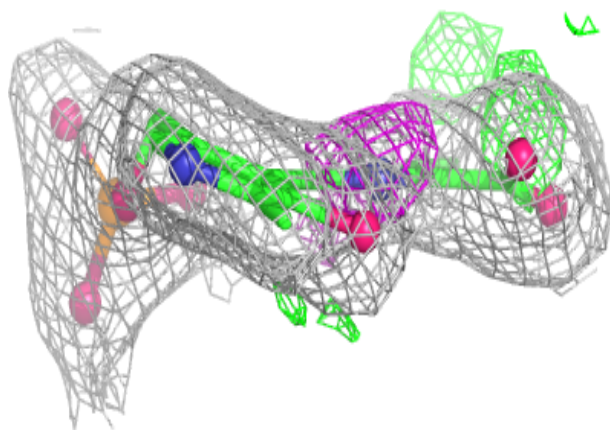
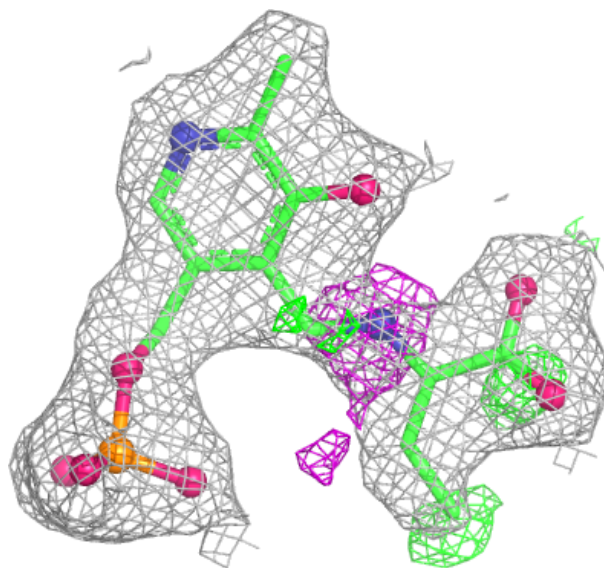
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	SO4	D	2010	5/5	0.85	0.08	83,83,84,84	0
3	MEE	A	2002	2/2	0.87	0.20	57,57,57,57	0
3	MEE	C	2005	2/2	0.88	0.20	63,63,63,63	0
4	SO4	B	2008	5/5	0.89	0.07	79,79,80,80	0
5	GOL	A	2011	6/6	0.90	0.12	57,59,59,61	0
4	SO4	C	2009	5/5	0.91	0.13	71,72,73,73	0
5	GOL	C	2012	6/6	0.91	0.11	58,58,60,61	0
4	SO4	A	2007	5/5	0.93	0.09	67,67,68,68	0
2	4LM	C	2004[A]	22/22	0.94	0.08	18,22,27,28	19
2	4LM	C	2004[B]	22/22	0.94	0.08	18,23,27,28	19
2	4LM	A	2001[A]	22/22	0.95	0.07	17,21,25,26	19
2	4LM	A	2001[B]	22/22	0.95	0.07	17,21,26,27	19
2	4LM	B	2003	22/22	0.97	0.07	25,37,38,39	0
2	4LM	D	2006	22/22	0.97	0.07	23,37,38,38	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.

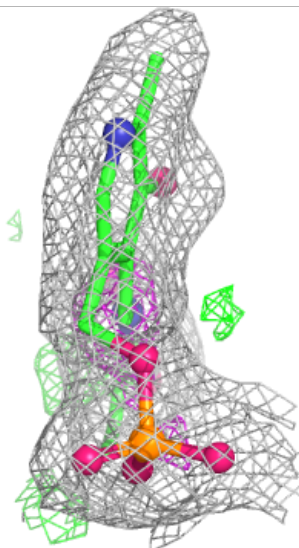
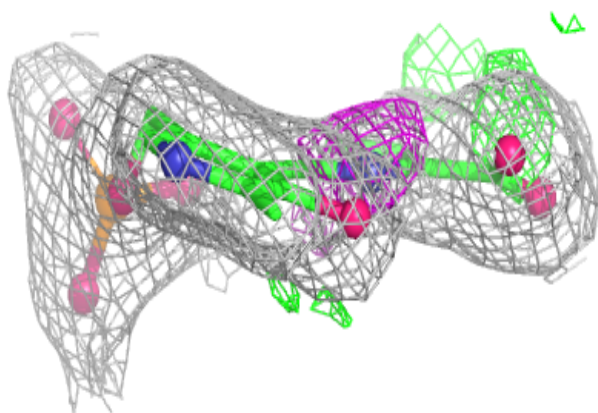
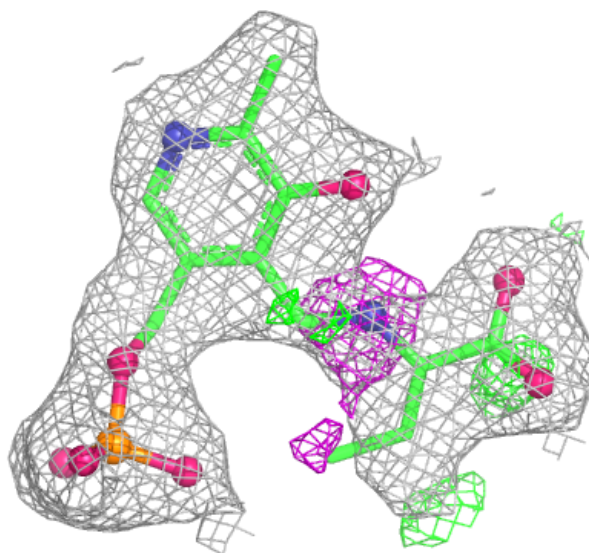
Electron density around 4LM C 2004 (A):

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



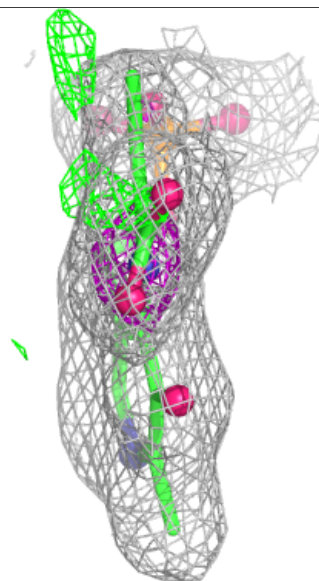
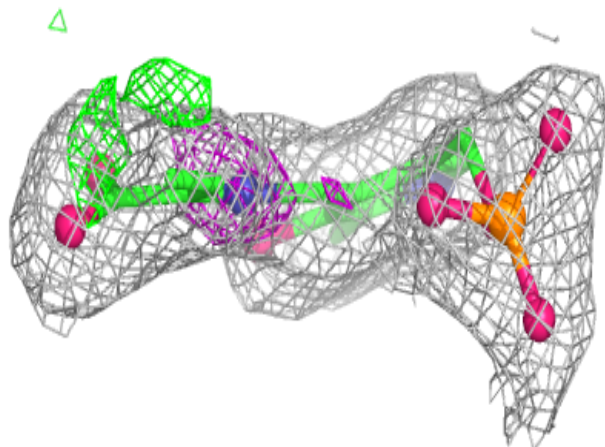
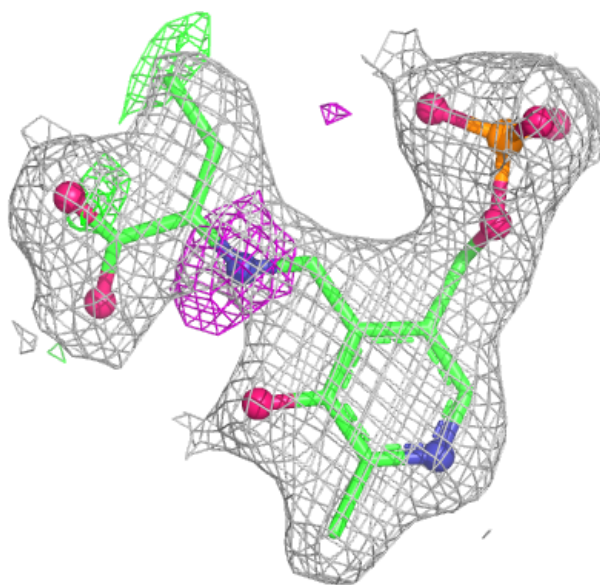
Electron density around 4LM C 2004 (B):

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



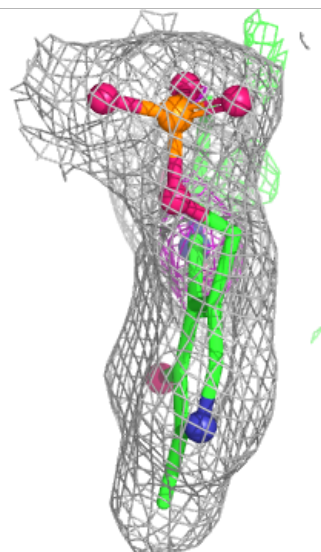
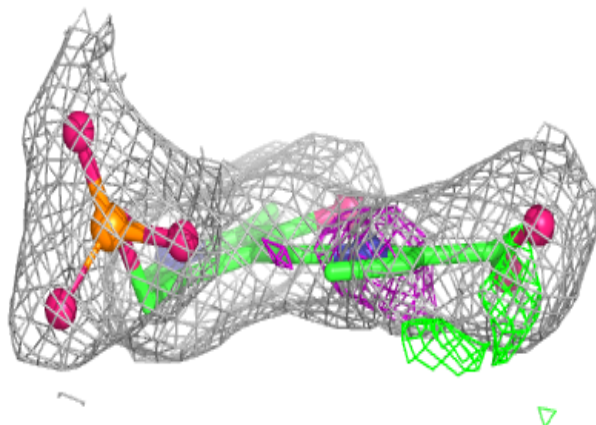
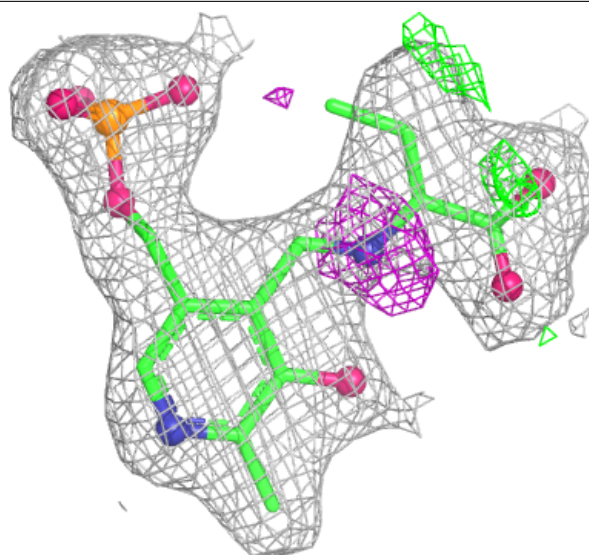
Electron density around 4LM A 2001 (A):

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



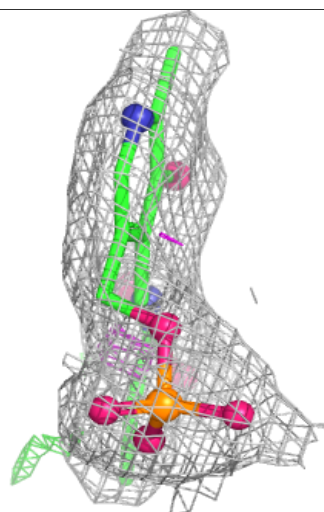
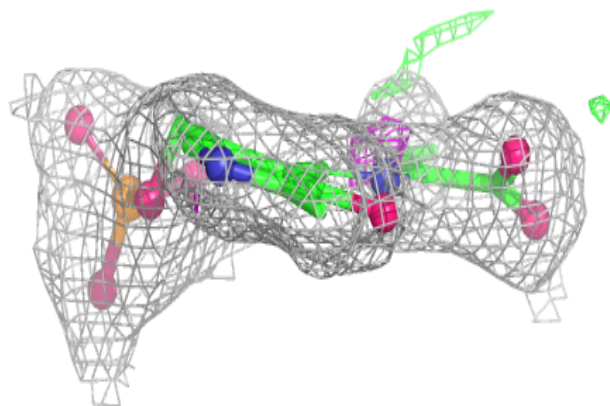
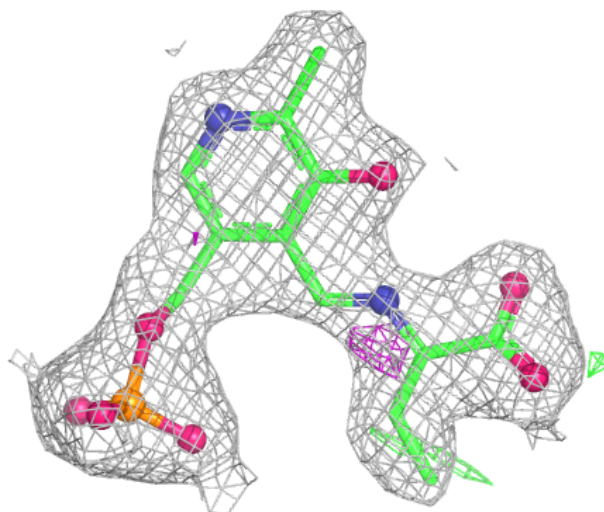
Electron density around 4LM A 2001 (B):

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



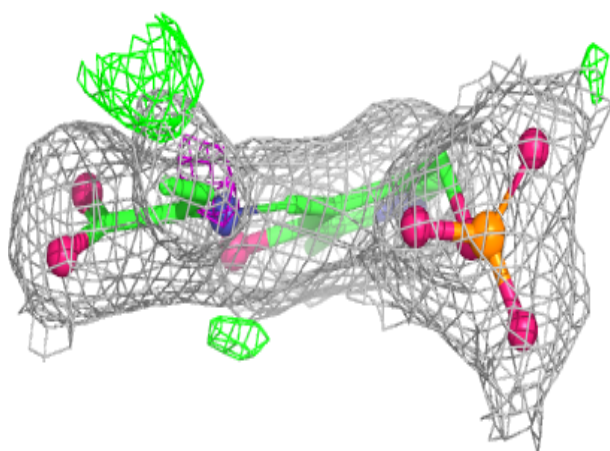
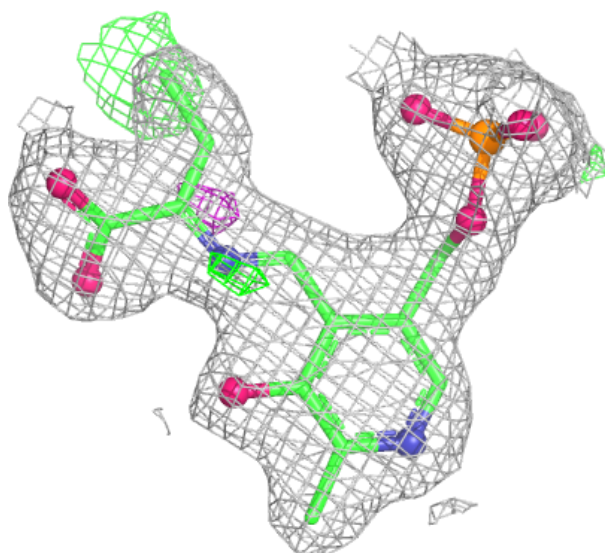
Electron density around 4LM B 2003:

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



Electron density around 4LM D 2006:

$2mF_o-DF_c$ (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.