



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:07 pm BST

PDB ID : 3AEN
Title : Reaction intermediate structure of Entamoeba histolytica methionine gamma-lyase 1 containing Michaelis complex and 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 : 2.00 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

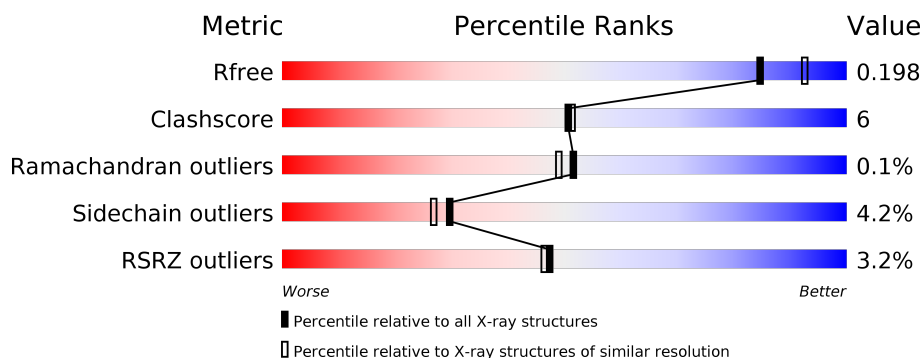
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 86% 12% .. </div> </div>
1	C	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 87% 10% .. </div> </div>
2	B	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 5% 85% 13% .. </div> </div>
2	D	389	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 5% 85% 13% .. </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MET	A	2001	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12758 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	P	S	0	1	0
			2967	1886	498	558	1	24			
1	C	387	Total	C	N	O	P	S	0	1	0
			2967	1886	498	558	1	24			

There are 2 discrepancies between the modelled and reference sequences:

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

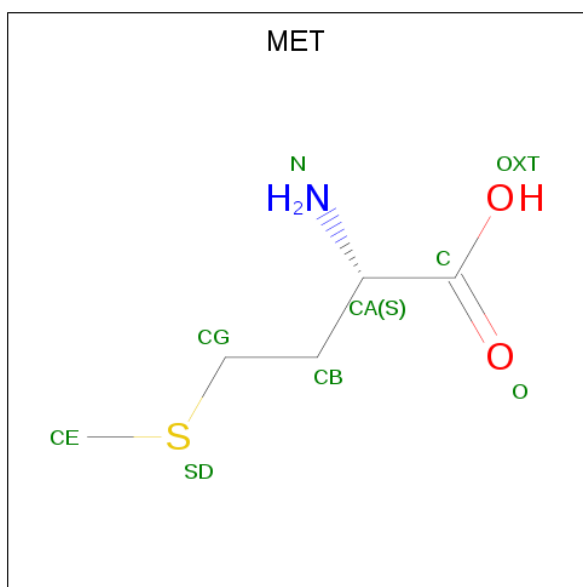
- Molecule 2 is a protein called Methionine gamma-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	386	Total	C	N	O	S	0	1	0
			2937	1867	495	551	24			
2	D	384	Total	C	N	O	S	0	1	0
			2923	1859	492	548	24			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



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

- Molecule 4 is SULFATE ION (three-letter code: 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		

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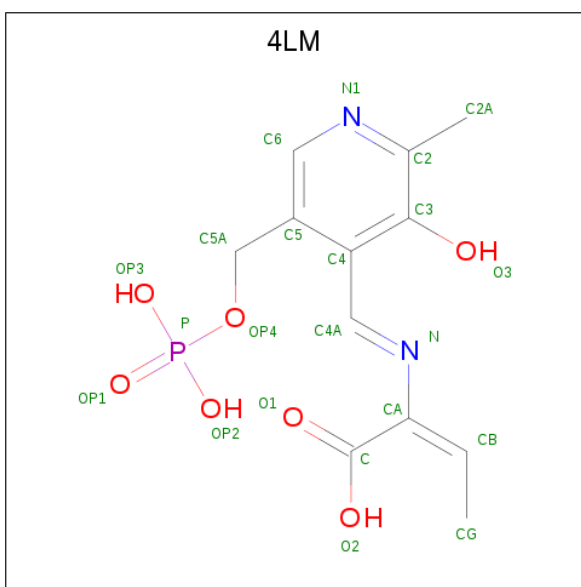
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
6	D	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

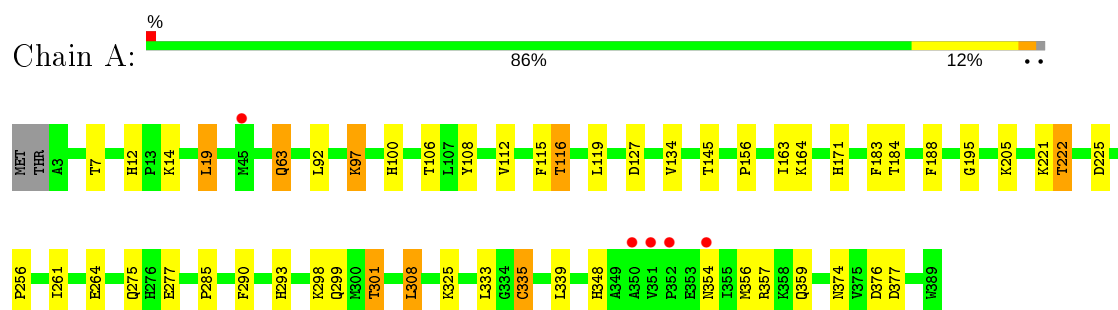
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	286	Total	O	0	0
			286	286		
7	B	158	Total	O	0	0
			158	158		
7	C	285	Total	O	0	0
			285	285		
7	D	145	Total	O	0	0
			145	145		

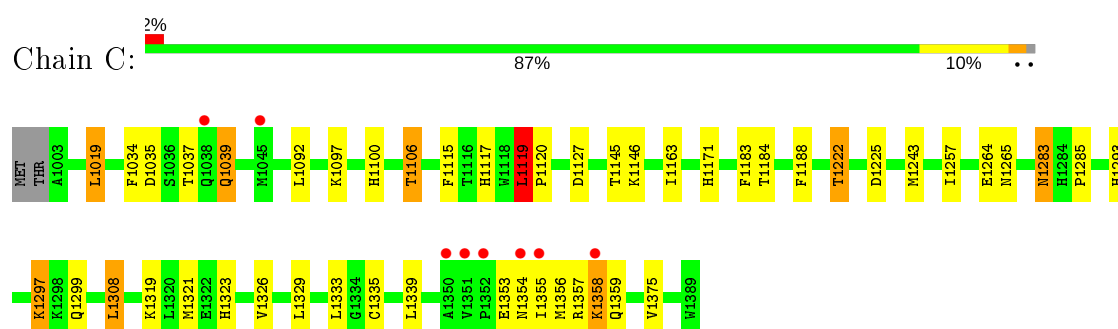
3 Residue-property plots [i](#)

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.

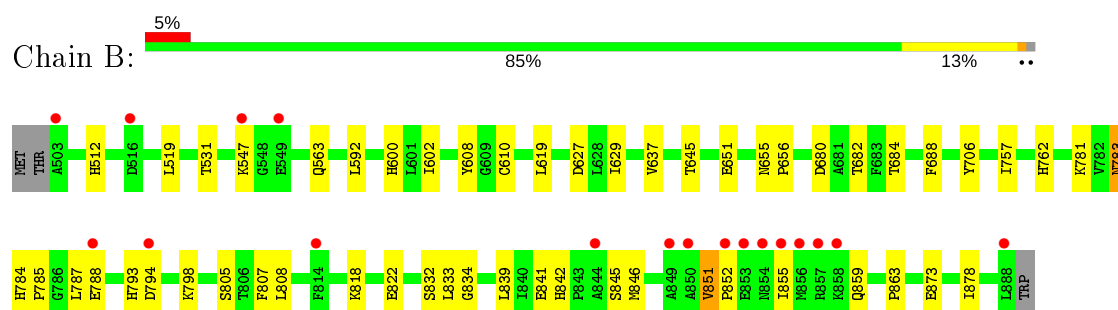
- Molecule 1: Methionine gamma-lyase



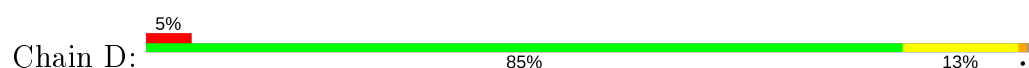
- Molecule 1: Methionine gamma-lyase

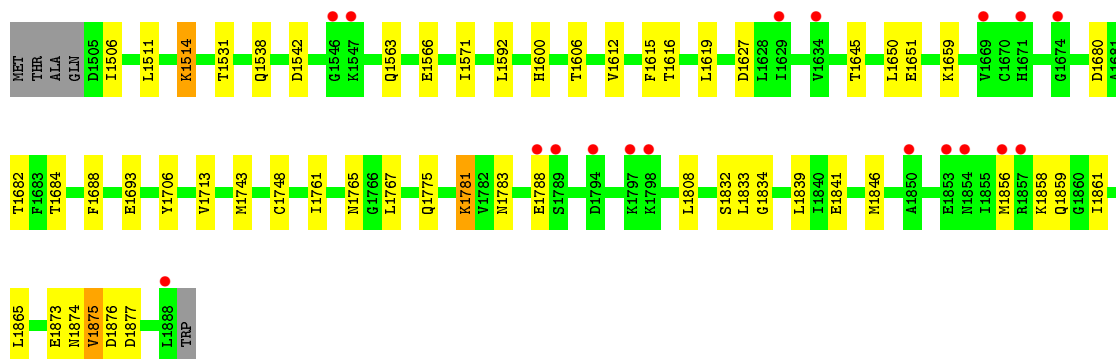


- Molecule 2: Methionine gamma-lyase



- Molecule 2: 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	99.16 Å 85.43 Å 114.75 Å 90.00° 101.90° 90.00°	Depositor
Resolution (Å)	46.92 – 2.00 46.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.92-2.00) 97.7 (46.92-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.00 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.166 , 0.198 0.166 , 0.198	Depositor DCC
R_{free} test set	6219 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.6	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	12758	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 5.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LLP, SO4, 4LM

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	0.82	2/3008 (0.1%)	0.75	3/4066 (0.1%)
1	C	0.80	0/3008	0.73	4/4066 (0.1%)
2	B	0.60	0/3001	0.62	0/4057
2	D	0.59	0/2987	0.64	0/4038
All	All	0.71	2/12004 (0.0%)	0.69	7/16227 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335[A]	CYS	CB-SG	-6.36	1.71	1.82
1	A	335[B]	CYS	CB-SG	-6.36	1.71	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1308	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	308	LEU	CA-CB-CG	5.57	128.11	115.30
1	C	1019	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	1308	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	A	19	LEU	CA-CB-CG	5.27	127.41	115.30
1	C	1119	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	19	LEU	CB-CG-CD2	5.15	119.76	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2967	0	2960	45	0
1	C	2967	0	2960	41	0
2	B	2937	0	2947	30	0
2	D	2923	0	2934	28	0
3	A	9	0	8	7	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	10	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	B	22	0	11	1	0
6	D	22	0	12	1	0
7	A	286	0	0	13	0
7	B	158	0	0	1	0
7	C	285	0	0	11	0
7	D	145	0	0	1	0
All	All	12758	0	11848	135	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 (135) 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:205:LLP:H4'1	3:A:2001:MET:N	1.51	1.21
1:A:205:LLP:C4'	3:A:2001:MET:N	2.21	1.03
2:B:822:GLU:OE2	1:C:1037:THR:HG22	1.61	0.99
1:C:1222:THR:HG22	1:C:1225:ASP:H	1.37	0.89
1:A:222:THR:HG22	1:A:225:ASP:H	1.37	0.88
2:D:1808:LEU:HD21	2:D:1865:LEU:HD13	1.59	0.83
1:C:1222:THR:HG21	7:C:3097:HOH:O	1.77	0.83
1:A:108:TYR:CE1	3:A:2001:MET:N	2.46	0.82
1:A:335[A]:CYS:SG	7:A:3590:HOH:O	2.37	0.82
1:A:108:TYR:OH	3:A:2001:MET:HG3	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HG2	7:A:3466:HOH:O	1.83	0.78
1:A:222:THR:HG21	7:A:3031:HOH:O	1.81	0.78
1:A:301:THR:HG23	7:A:3356:HOH:O	1.83	0.77
1:C:1321:MET:HE3	1:C:1329:LEU:CD1	2.15	0.76
1:A:188:PHE:HA	1:A:301:THR:HG22	1.67	0.75
1:A:112:VAL:O	1:A:116:THR:HB	1.86	0.74
2:D:1514:LYS:HE3	2:D:1566:GLU:HB3	1.70	0.74
1:C:1264:GLU:HG3	7:C:3423:HOH:O	1.88	0.73
1:A:261:ILE:HD11	1:C:1257:ILE:HG12	1.72	0.71
2:B:600:HIS:HE1	2:B:627:ASP:OD2	1.73	0.70
1:C:1335[A]:CYS:SG	7:C:3825:HOH:O	2.38	0.70
1:A:134:VAL:HG23	7:A:3564:HOH:O	1.92	0.69
2:B:512:HIS:HE1	2:D:1873:GLU:OE1	1.75	0.69
1:A:222:THR:CG2	1:A:225:ASP:H	2.08	0.67
1:C:1100:HIS:HD2	1:C:1145:THR:OG1	1.77	0.67
1:C:1171:HIS:HD2	7:C:3042:HOH:O	1.78	0.67
2:B:592:LEU:HD21	2:B:619:LEU:HD22	1.77	0.67
2:D:1592:LEU:HD21	2:D:1619:LEU:HD22	1.76	0.66
1:C:1285:PRO:O	1:C:1293:HIS:HD2	1.79	0.65
1:C:1319:LYS:O	1:C:1323:HIS:HD2	1.80	0.64
1:A:264:GLU:HG3	7:A:3278:HOH:O	1.97	0.64
2:D:1682:THR:HB	6:D:2003:4LM:H2A1	1.80	0.63
1:A:100:HIS:HD2	1:A:145:THR:OG1	1.82	0.62
2:D:1506:ILE:CG2	2:D:1571:ILE:HD13	2.31	0.61
2:B:757:ILE:HG12	2:D:1761:ILE:HD11	1.83	0.61
2:B:682:THR:HB	6:B:2002:4LM:H2A1	1.81	0.61
2:D:1600:HIS:HD2	2:D:1645:THR:OG1	1.84	0.61
2:B:600:HIS:HD2	2:B:645:THR:OG1	1.83	0.60
1:A:92:LEU:HD21	1:A:119:LEU:HD22	1.82	0.60
2:D:1765:ASN:ND2	2:D:1875:VAL:HG22	2.16	0.60
1:C:1100:HIS:HE1	1:C:1127:ASP:OD2	1.84	0.60
1:C:1321:MET:CE	1:C:1329:LEU:HD11	2.32	0.60
2:D:1684:THR:HG22	2:D:1688:PHE:HB2	1.84	0.59
1:C:1222:THR:CG2	1:C:1225:ASP:H	2.12	0.59
1:A:205:LLP:HE3	3:A:2001:MET:HA	1.85	0.59
1:A:301:THR:CG2	7:A:3356:HOH:O	2.45	0.58
1:C:1092:LEU:HD21	1:C:1119:LEU:HD22	1.84	0.58
1:A:100:HIS:HE1	1:A:127:ASP:OD2	1.87	0.58
1:A:374:ASN:HD21	1:A:376:ASP:HB2	1.69	0.58
1:C:1321:MET:HE3	1:C:1329:LEU:HD13	1.83	0.58
1:A:14:LYS:HE3	7:A:3367:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1874:ASN:HD21	2:D:1876:ASP:HB2	1.72	0.55
2:B:531:THR:HG22	7:C:3129:HOH:O	2.07	0.55
2:D:1506:ILE:HG21	2:D:1571:ILE:HD13	1.89	0.55
1:C:1321:MET:HE3	1:C:1329:LEU:HD11	1.86	0.54
2:B:794:ASP:O	2:B:798:LYS:HE2	2.08	0.54
2:B:783:ASN:O	2:B:807:PHE:HB2	2.08	0.54
2:B:600:HIS:CE1	2:B:627:ASP:OD2	2.59	0.53
1:A:357:ARG:HA	7:A:3241:HOH:O	2.08	0.53
1:A:163:ILE:H	1:A:299:GLN:HE22	1.56	0.53
1:A:156:PRO:HD3	1:A:348:HIS:NE2	2.24	0.52
2:B:781:LYS:HD3	2:B:783:ASN:HD21	1.75	0.52
2:B:873:GLU:HB2	2:B:878:ILE:HD11	1.91	0.52
7:A:3112:HOH:O	2:D:1531:THR:HG22	2.09	0.52
1:C:1308:LEU:HB3	7:C:3318:HOH:O	2.10	0.51
1:A:261:ILE:CD1	1:C:1257:ILE:HG12	2.39	0.51
7:B:3571:HOH:O	1:C:1335[A]:CYS:SG	2.60	0.51
2:D:1841:GLU:OE2	2:D:1846:MET:HB2	2.10	0.51
1:C:1184:THR:HG22	1:C:1188:PHE:HB2	1.92	0.50
1:C:1163:ILE:H	1:C:1299:GLN:HE22	1.59	0.50
1:A:7:THR:HG22	1:A:256:PRO:HB2	1.95	0.49
1:A:171:HIS:HE1	1:A:195:GLY:O	1.96	0.49
2:B:818:LYS:HG3	1:C:1037:THR:HG21	1.94	0.48
2:D:1506:ILE:HG23	2:D:1571:ILE:HD13	1.95	0.48
2:B:651:GLU:HG2	2:B:680:ASP:HB3	1.95	0.48
2:D:1781:LYS:HE3	2:D:1783:ASN:HD21	1.78	0.48
1:A:156:PRO:HD3	1:A:348:HIS:CE1	2.48	0.48
1:C:1283:ASN:ND2	7:C:3756:HOH:O	2.47	0.48
1:C:1034:PHE:HA	1:C:1039:GLN:HE22	1.78	0.47
2:D:1650:LEU:HA	7:D:3291:HOH:O	2.14	0.47
2:D:1713:VAL:HG11	2:D:1748:CYS:SG	2.55	0.47
1:C:1035:ASP:H	1:C:1039:GLN:NE2	2.12	0.47
1:A:12:HIS:CE1	1:C:1326:VAL:O	2.67	0.47
2:D:1615:PHE:HA	2:D:1619:LEU:HG	1.96	0.47
2:D:1612:VAL:O	2:D:1616:THR:HB	2.13	0.47
2:B:608:TYR:CE2	2:B:610:CYS:HB2	2.49	0.47
1:A:184:THR:HG22	1:A:188:PHE:HB2	1.96	0.47
2:D:1600:HIS:HE1	2:D:1627:ASP:OD2	1.97	0.47
2:D:1651:GLU:HG2	2:D:1680:ASP:HB3	1.96	0.46
1:C:1297:LYS:HE2	7:C:3177:HOH:O	2.15	0.46
1:A:115:PHE:HA	1:A:119:LEU:HG	1.98	0.46
1:A:285:PRO:O	1:A:293:HIS:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:HG3	7:A:3113:HOH:O	2.16	0.45
1:A:374:ASN:ND2	1:A:376:ASP:HB2	2.30	0.45
2:D:1859:GLN:HB3	2:D:1861:ILE:CD1	2.46	0.45
1:A:97:LYS:HB3	1:A:97:LYS:HE3	1.76	0.45
2:B:855:ILE:O	2:B:859:GLN:HG3	2.17	0.45
1:C:1039:GLN:HE21	1:C:1039:GLN:HB3	1.59	0.45
1:C:1355:ILE:HG12	1:C:1358:LYS:HZ2	1.81	0.45
2:D:1874:ASN:HD22	2:D:1877:ASP:H	1.64	0.45
1:A:171:HIS:CE1	1:A:195:GLY:O	2.70	0.44
1:A:221:LYS:HD2	7:A:3724:HOH:O	2.18	0.44
1:C:1146:LYS:HE3	7:C:3191:HOH:O	2.18	0.44
1:C:1265:ASN:ND2	1:C:1375:VAL:HB	2.32	0.44
1:C:1319:LYS:O	1:C:1323:HIS:CD2	2.67	0.44
1:A:308:LEU:HB3	7:A:3307:HOH:O	2.16	0.44
1:A:108:TYR:CZ	3:A:2001:MET:N	2.84	0.44
1:A:108:TYR:HE1	3:A:2001:MET:N	2.06	0.43
1:C:1355:ILE:O	1:C:1359:GLN:HG3	2.18	0.43
2:D:1706:TYR:CE2	2:D:1834:GLY:HA2	2.53	0.43
1:C:1115:PHE:HA	1:C:1119:LEU:HG	2.01	0.43
1:C:1106:THR:HG21	7:C:3372:HOH:O	2.19	0.43
2:B:602:ILE:HG23	2:B:629:ILE:HG12	2.01	0.43
2:B:842:HIS:HD2	2:B:845:SER:OG	2.02	0.43
1:C:1117:HIS:HE1	7:C:3528:HOH:O	2.01	0.43
1:A:285:PRO:HA	1:A:290:PHE:CD2	2.53	0.42
1:C:1119:LEU:HB2	1:C:1120:PRO:HD3	2.01	0.42
1:C:1222:THR:HG22	1:C:1225:ASP:N	2.18	0.42
1:C:1353:GLU:O	1:C:1357:ARG:HG3	2.19	0.42
2:B:629:ILE:HD11	2:B:637:VAL:HA	2.02	0.42
1:A:100:HIS:CE1	1:A:127:ASP:OD2	2.70	0.42
1:A:106:THR:HA	1:A:359:GLN:HG2	2.02	0.42
2:B:784:HIS:HB3	2:B:787:LEU:HG	2.01	0.42
2:B:842:HIS:HE1	2:B:863:PRO:O	2.03	0.42
2:B:762:HIS:O	2:B:805:SER:HB3	2.20	0.41
2:B:785:PRO:O	2:B:793:HIS:HD2	2.03	0.41
1:C:1243:MET:CE	2:D:1743:MET:HE1	2.50	0.41
1:A:374:ASN:HD22	1:A:377:ASP:H	1.68	0.41
2:B:684:THR:HG22	2:B:688:PHE:HB2	2.02	0.41
2:B:655:ASN:HA	2:B:656:PRO:HA	1.88	0.41
2:B:706:TYR:CE1	2:B:834:GLY:HA2	2.56	0.41
2:D:1538:GLN:NE2	2:D:1542:ASP:OD1	2.52	0.41
2:B:851:VAL:HA	2:B:852:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:873:GLU:HG3	2:D:1511:LEU:HD12	2.03	0.40
2:B:841:GLU:OE2	2:B:846:MET:HB2	2.21	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	385/389 (99%)	374 (97%)	11 (3%)	0	100	100
1	C	385/389 (99%)	375 (97%)	10 (3%)	0	100	100
2	B	385/389 (99%)	375 (97%)	9 (2%)	1 (0%)	41	37
2	D	383/389 (98%)	374 (98%)	8 (2%)	1 (0%)	41	37
All	All	1538/1556 (99%)	1498 (97%)	38 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	832	SER
2	D	1832	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	320/321 (100%)	305 (95%)	15 (5%)	26	22
1	C	320/321 (100%)	306 (96%)	14 (4%)	28	25
2	B	320/322 (99%)	311 (97%)	9 (3%)	43	44
2	D	319/322 (99%)	305 (96%)	14 (4%)	28	25
All	All	1279/1286 (100%)	1227 (96%)	52 (4%)	30	28

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	63	GLN
1	A	97	LYS
1	A	116	THR
1	A	164	LYS
1	A	183	PHE
1	A	222	THR
1	A	275	GLN
1	A	277	GLU
1	A	301	THR
1	A	325	LYS
1	A	333	LEU
1	A	339	LEU
1	A	354	ASN
1	A	356	MET
2	B	519	LEU
2	B	547	LYS
2	B	563	GLN
2	B	783	ASN
2	B	788	GLU
2	B	808	LEU
2	B	833	LEU
2	B	839	LEU
2	B	851	VAL
1	C	1019	LEU
1	C	1039	GLN
1	C	1097	LYS
1	C	1106	THR
1	C	1119	LEU
1	C	1183	PHE
1	C	1222	THR
1	C	1283	ASN
1	C	1297	LYS

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Mol	Chain	Res	Type
1	C	1333	LEU
1	C	1339	LEU
1	C	1354	ASN
1	C	1356	MET
1	C	1358	LYS
2	D	1514	LYS
2	D	1563	GLN
2	D	1606	THR
2	D	1659	LYS
2	D	1693	GLU
2	D	1767	LEU
2	D	1775	GLN
2	D	1781	LYS
2	D	1788	GLU
2	D	1833	LEU
2	D	1839	LEU
2	D	1856	MET
2	D	1858	LYS
2	D	1875	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) 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	374	ASN
2	B	512	HIS
2	B	517	HIS
2	B	528	GLN
2	B	563	GLN
2	B	600	HIS
2	B	760	GLN
2	B	765	ASN
2	B	783	ASN
2	B	793	HIS
2	B	799	GLN
2	B	842	HIS

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Mol	Chain	Res	Type
1	C	1028	GLN
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	1354	ASN
1	C	1359	GLN
1	C	1374	ASN
2	D	1528	GLN
2	D	1600	HIS
2	D	1617	HIS
2	D	1765	ASN
2	D	1775	GLN
2	D	1783	ASN
2	D	1793	HIS
2	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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	205	1	23,24,25	2.12	7 (30%)	25,32,34	1.59	4 (16%)
1	LLP	C	1205	1	23,24,25	2.07	6 (26%)	25,32,34	1.69	5 (20%)

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
1	LLP	A	205	1	-	6/16/17/19	0/1/1/1
1	LLP	C	1205	1	-	5/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1205	LLP	O3-C3	-6.21	1.22	1.37
1	A	205	LLP	O3-C3	-5.65	1.23	1.37
1	A	205	LLP	CE-NZ	4.80	1.57	1.46
1	C	1205	LLP	CE-NZ	3.33	1.54	1.46
1	C	1205	LLP	C4'-NZ	3.29	1.38	1.27
1	C	1205	LLP	C4-C4'	3.01	1.52	1.46
1	A	205	LLP	C4'-NZ	2.63	1.36	1.27
1	A	205	LLP	C2-N1	2.60	1.38	1.33
1	A	205	LLP	CD-CE	2.48	1.60	1.51
1	A	205	LLP	C4-C4'	2.31	1.51	1.46
1	A	205	LLP	CG-CB	2.23	1.61	1.52
1	C	1205	LLP	C6-N1	2.21	1.39	1.34
1	C	1205	LLP	C2-N1	2.01	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	LLP	C4-C4'-NZ	-4.11	105.43	124.31
1	C	1205	LLP	OP4-C5'-C5	4.00	116.98	109.35
1	A	205	LLP	OP4-C5'-C5	3.84	116.67	109.35
1	C	1205	LLP	C4-C3-C2	3.76	122.52	120.19
1	C	1205	LLP	C4-C4'-NZ	-3.02	110.45	124.31
1	C	1205	LLP	OP4-P-OP1	-2.82	98.57	106.47
1	A	205	LLP	OP4-P-OP1	-2.65	99.05	106.47
1	C	1205	LLP	CD-CE-NZ	2.46	116.95	110.93
1	A	205	LLP	OP3-P-OP2	2.13	115.77	107.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	205	LLP	O-C-CA-CB
1	C	1205	LLP	O-C-CA-CB
1	C	1205	LLP	C4-C4'-NZ-CE
1	A	205	LLP	CG-CD-CE-NZ
1	C	1205	LLP	CG-CD-CE-NZ
1	A	205	LLP	C3-C4-C4'-NZ
1	C	1205	LLP	C3-C4-C4'-NZ
1	A	205	LLP	C5-C4-C4'-NZ
1	A	205	LLP	CA-CB-CG-CD
1	A	205	LLP	CD-CE-NZ-C4'
1	C	1205	LLP	CD-CE-NZ-C4'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	205	LLP	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	C	2006	-	4,4,4	0.18	0	6,6,6	0.68	0
6	4LM	B	2002	-	19,22,22	0.95	0	21,31,31	1.08	0
5	GOL	A	2010	-	5,5,5	0.36	0	5,5,5	0.28	0
4	SO4	B	2005	-	4,4,4	0.15	0	6,6,6	0.14	0
6	4LM	D	2003	-	19,22,22	1.11	0	21,31,31	1.18	1 (4%)
4	SO4	A	2004	-	4,4,4	0.12	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	2008	-	4,4,4	0.15	0	6,6,6	0.14	0
4	SO4	C	2007	-	4,4,4	0.15	0	6,6,6	0.25	0
5	GOL	C	2011	-	5,5,5	0.35	0	5,5,5	0.41	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	4LM	B	2002	-	-	2/11/17/17	0/1/1/1
6	4LM	D	2003	-	-	0/11/17/17	0/1/1/1
5	GOL	C	2011	-	-	0/4/4/4	-
5	GOL	A	2010	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2003	4LM	OP2-P-OP4	-2.03	101.33	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2010	GOL	C1-C2-C3-O3
5	A	2010	GOL	O2-C2-C3-O3
6	B	2002	4LM	C4-C5-C5A-OP4
6	B	2002	4LM	C6-C5-C5A-OP4

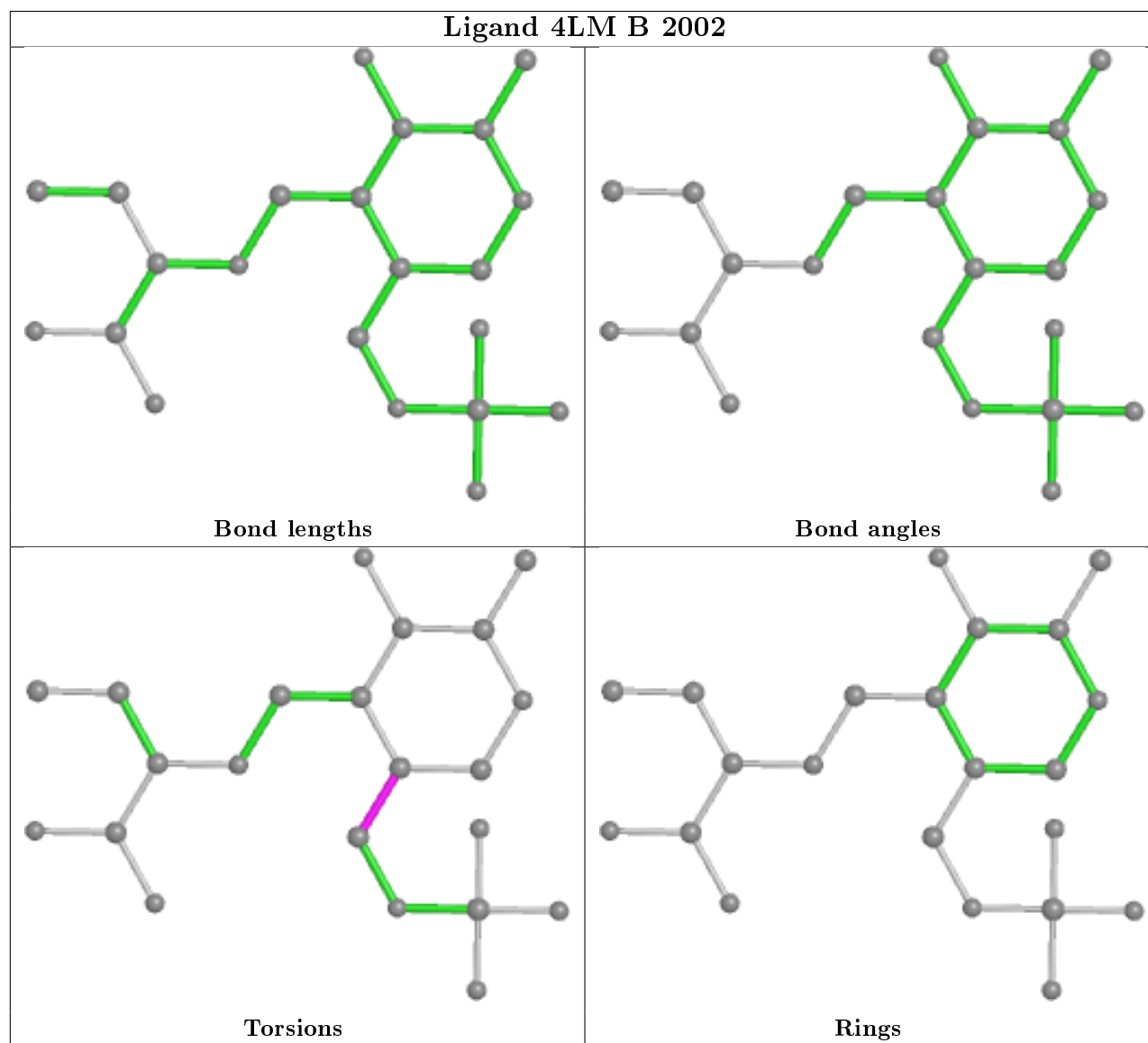
There are no ring outliers.

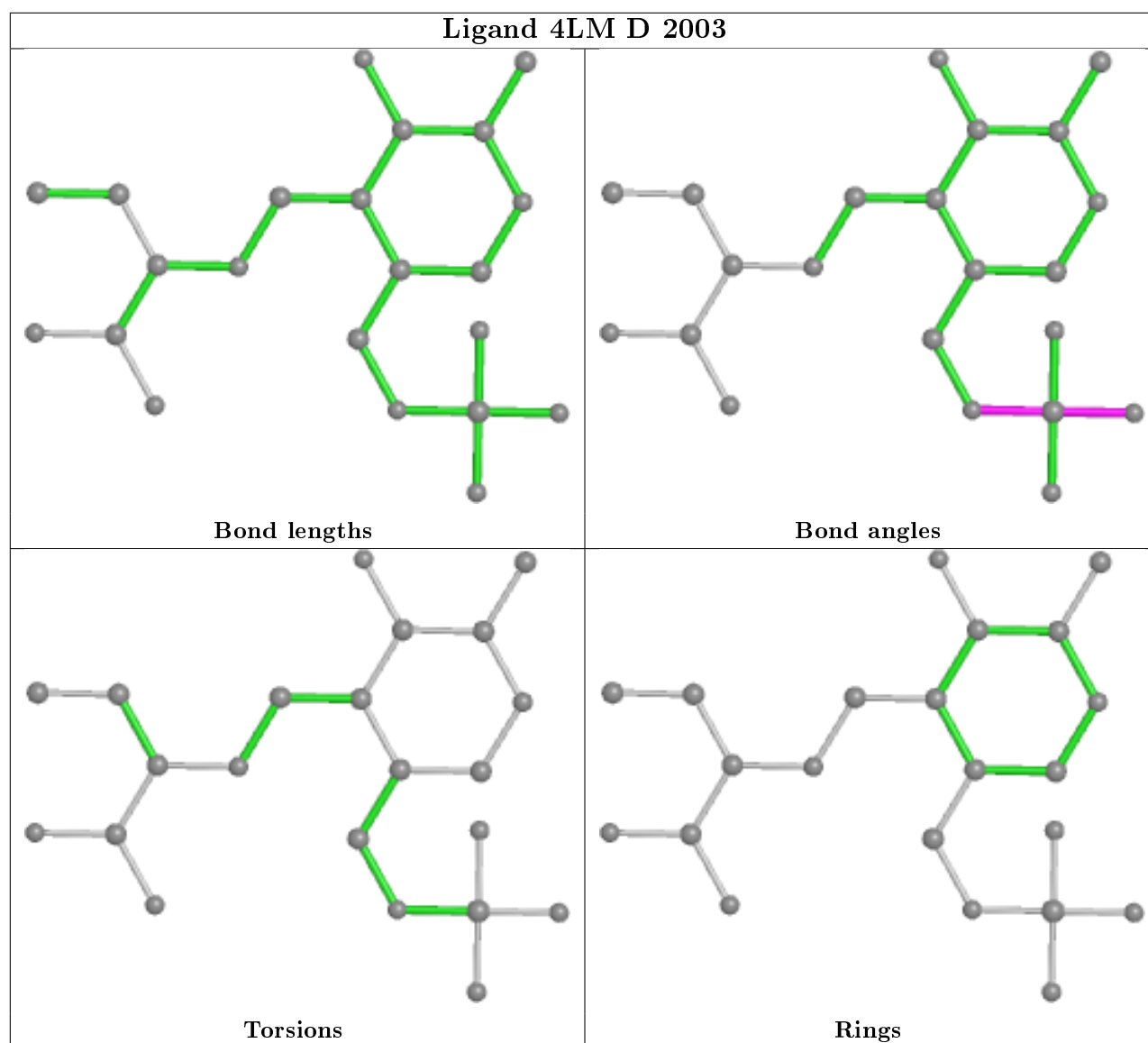
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2002	4LM	1	0
6	D	2003	4LM	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	386/389 (99%)	-0.31	5 (1%) 77 76	13, 21, 44, 66	1 (0%)
1	C	386/389 (99%)	-0.34	8 (2%) 63 62	14, 20, 43, 72	1 (0%)
2	B	386/389 (99%)	-0.06	18 (4%) 31 30	18, 36, 63, 80	1 (0%)
2	D	384/389 (98%)	0.01	18 (4%) 31 30	17, 39, 66, 80	0
All	All	1542/1556 (99%)	-0.17	49 (3%) 47 46	13, 27, 61, 80	3 (0%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1351	VAL	5.1
2	B	503	ALA	4.2
2	B	854	ASN	4.0
1	C	1354	ASN	3.9
2	B	788	GLU	3.9
1	A	351	VAL	3.6
2	B	814	PHE	3.5
2	B	850	ALA	3.4
2	D	1671	HIS	3.3
2	D	1854	ASN	3.2
2	D	1634	VAL	3.1
1	A	45	MET	3.1
2	D	1788	GLU	3.0
1	C	1352	PRO	3.0
2	B	857	ARG	2.9
2	D	1888	LEU	2.9
2	D	1853	GLU	2.9
2	D	1794	ASP	2.9
2	D	1857	ARG	2.9
1	A	352	PRO	2.8
1	C	1045	MET	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	855	ILE	2.8
2	B	853	GLU	2.7
2	D	1789	SER	2.7
1	C	1355	ILE	2.7
2	D	1798	LYS	2.7
2	B	516	ASP	2.6
1	A	354	ASN	2.6
1	C	1350	ALA	2.5
2	D	1797	LYS	2.5
2	B	547	LYS	2.5
2	B	888	LEU	2.5
1	C	1358	LYS	2.4
2	D	1547	LYS	2.4
2	B	856	MET	2.4
2	D	1674	GLY	2.4
1	A	350	ALA	2.3
2	B	794	ASP	2.3
2	D	1546	GLY	2.3
2	B	844	ALA	2.3
2	D	1850	ALA	2.3
2	D	1669	VAL	2.2
2	B	852	PRO	2.2
2	D	1856	MET	2.1
2	B	849	ALA	2.1
1	C	1038	GLN	2.1
2	B	858	LYS	2.1
2	D	1629	ILE	2.0
2	B	549	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	LLP	A	205	24/25	0.98	0.15	12,16,19,19	6
1	LLP	C	1205	24/25	0.98	0.12	15,17,19,23	6

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

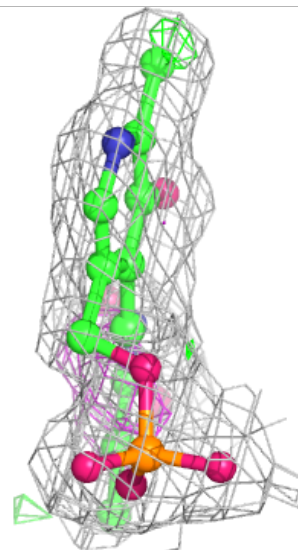
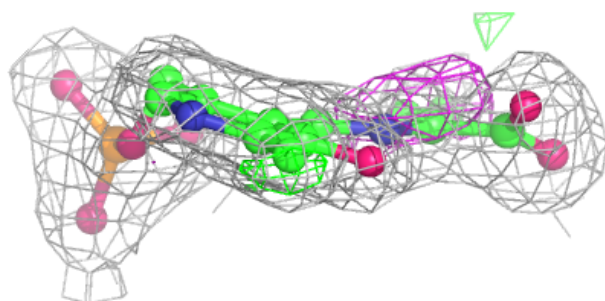
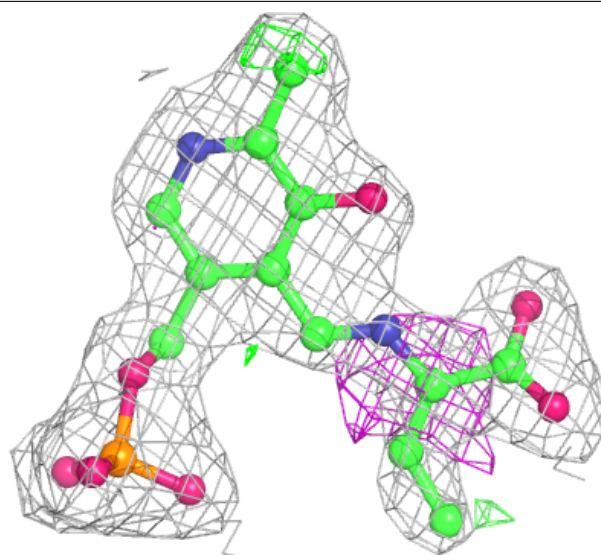
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MET	A	2001	9/9	0.84	0.34	19,22,35,39	9
5	GOL	A	2010	6/6	0.94	0.10	42,43,44,44	0
5	GOL	C	2011	6/6	0.94	0.10	42,43,43,45	0
6	4LM	B	2002	22/22	0.95	0.11	21,33,36,37	0
6	4LM	D	2003	22/22	0.95	0.11	25,33,37,37	0
4	SO4	A	2004	5/5	0.96	0.15	62,62,63,63	0
4	SO4	B	2005	5/5	0.96	0.21	82,82,82,83	0
4	SO4	D	2008	5/5	0.96	0.29	73,74,75,75	0
4	SO4	C	2007	5/5	0.97	0.17	65,65,66,66	0
4	SO4	C	2006	5/5	0.98	0.09	35,36,38,41	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.

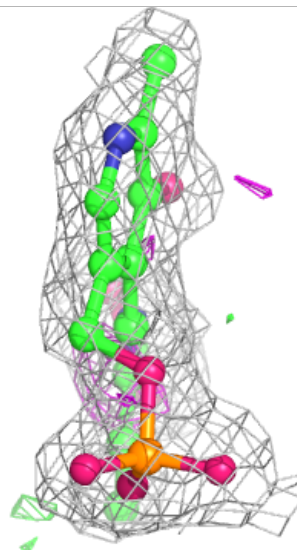
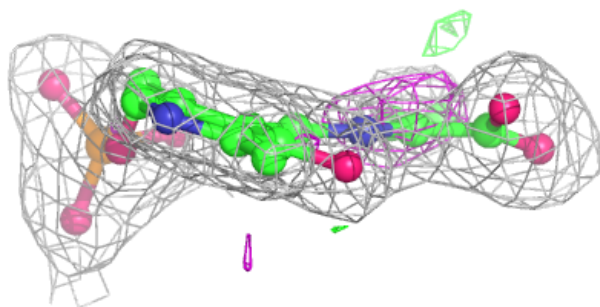
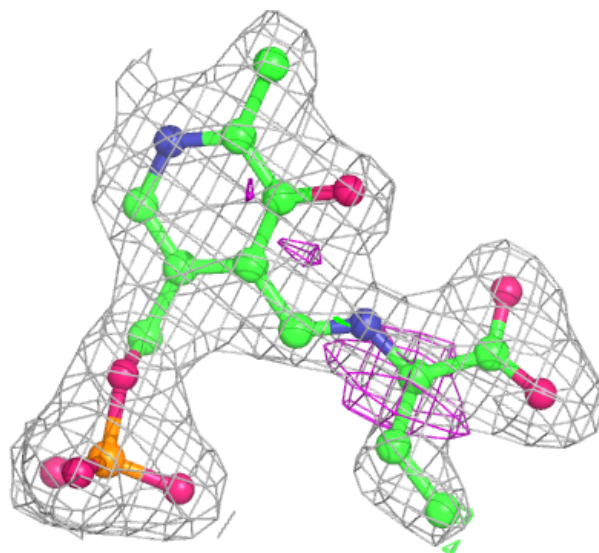
Electron density around 4LM B 2002:

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



Electron density around 4LM D 2003:

$2mF_o-DF_c$ (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.