



Full wwPDB X-ray Structure Validation Report

Jun 5, 2014 – 11:08 PM EDT

PDB ID : 4L5C
Title : Methylthioadenosine phosphorylase from *Schistosoma mansoni* in complex with adenine in space group P212121
Authors : Torini, J.R.; DeMarco, R.; Brandao-Neto, J.; Pereira, H.M.
Deposited on : 2013-06-10
Resolution : 2.08 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

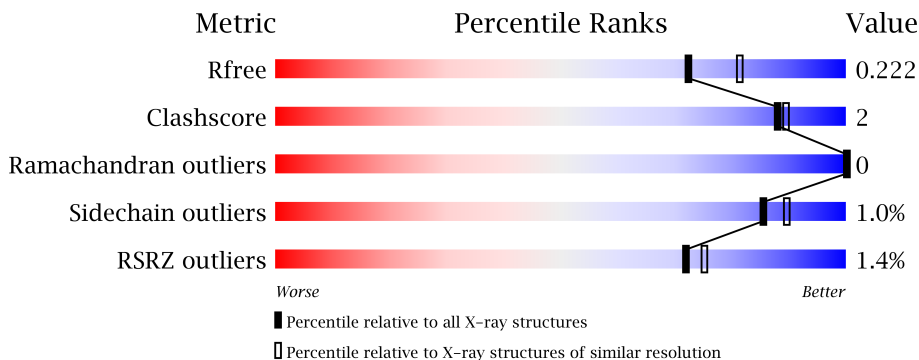
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.08 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}	66092	3396 (2.10-2.06)
Clashscore	79885	4085 (2.10-2.06)
Ramachandran outliers	78287	4045 (2.10-2.06)
Sidechain outliers	78261	4046 (2.10-2.06)
RSRZ outliers	66119	3397 (2.10-2.06)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	320	
1	B	320	
1	C	320	
1	D	320	
1	E	320	
1	F	320	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	E	302	-	X

2 Entry composition i

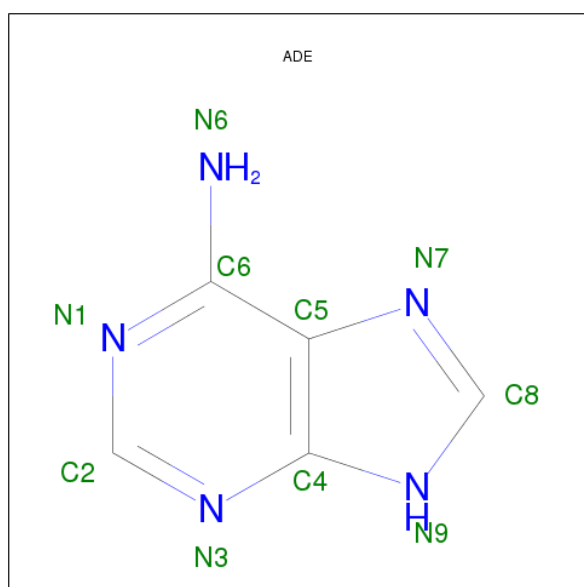
There are 4 unique types of molecules in this entry. The entry contains 14646 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-methyl-5'-thioadenosinephosphorylase.

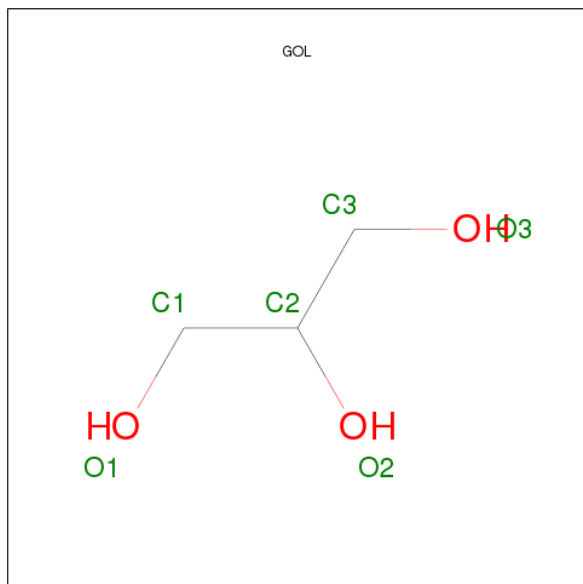
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2209	1399	385	408	17			
1	B	289	Total	C	N	O	S	0	0	0
			2214	1404	387	406	17			
1	C	290	Total	C	N	O	S	0	0	0
			2215	1406	386	406	17			
1	D	289	Total	C	N	O	S	21	0	0
			2209	1399	385	408	17			
1	E	289	Total	C	N	O	S	0	0	0
			2207	1402	384	404	17			
1	F	289	Total	C	N	O	S	0	0	0
			2206	1398	384	407	17			

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: C₅H₅N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	C	1	Total	C	N	0	0
			10	5	5		
2	D	1	Total	C	N	0	0
			10	5	5		
2	E	1	Total	C	N	0	0
			10	5	5		
2	F	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

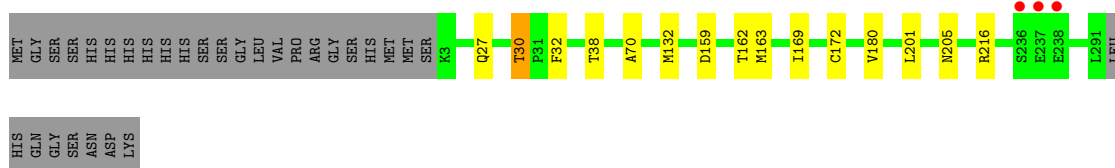
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	236	Total 236	O 236	0	0
4	B	216	Total 216	O 216	0	0
4	C	242	Total 242	O 242	0	0
4	D	220	Total 220	O 220	0	0
4	E	192	Total 192	O 192	0	0
4	F	184	Total 184	O 184	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

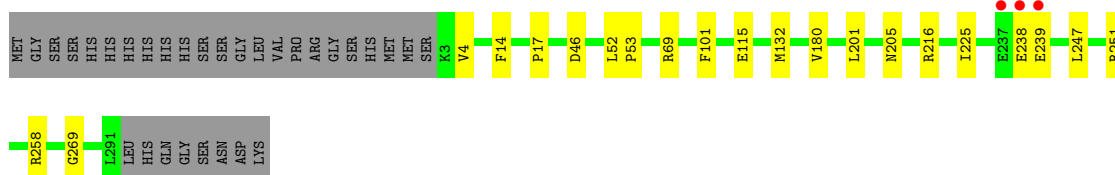
- Molecule 1: S-methyl-5'-thioadenosinephosphorylase

Chain A: 



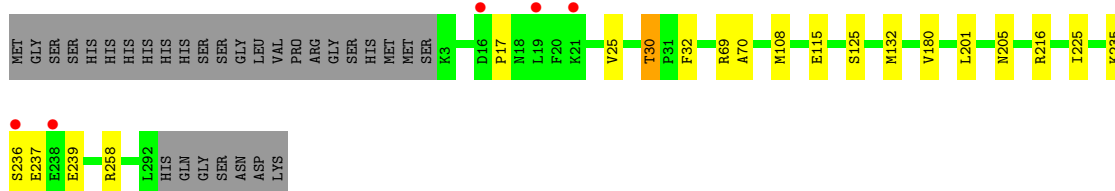
- Molecule 1: S-methyl-5'-thioadenosinephosphorylase

Chain B: 



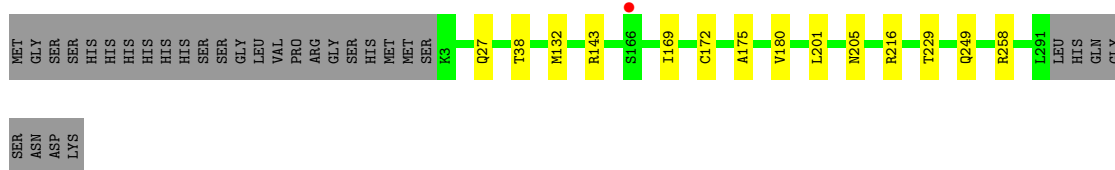
- Molecule 1: S-methyl-5'-thioadenosinephosphorylase

Chain C: 



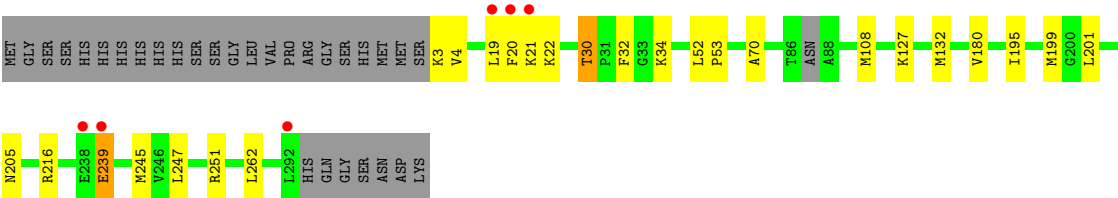
- Molecule 1: S-methyl-5'-thioadenosinephosphorylase

Chain D: 



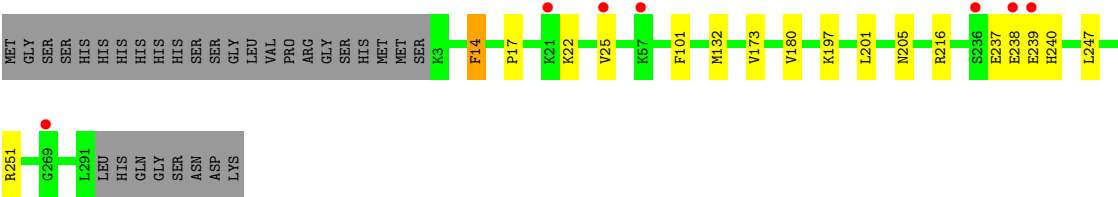
- Molecule 1: S-methyl-5'-thioadenosinephosphorylase

Chain E:



• Molecule 1: S-methyl-5'-thioadenosinephosphorylase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.58Å 135.71Å 145.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.22 – 2.08 59.22 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.22-2.08) 99.8 (59.22-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.08Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.191 , 0.222 0.191 , 0.222	Depositor DCC
R_{free} test set	6146 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 122450 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14646	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.82 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4443e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ADE

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	0.22	0/2254	0.39	0/3057
1	B	0.21	0/2259	0.39	0/3061
1	C	0.22	0/2260	0.39	0/3064
1	D	0.21	0/2254	0.39	0/3057
1	E	0.22	0/2251	0.40	0/3050
1	F	0.21	0/2251	0.39	0/3053
All	All	0.22	0/13529	0.39	0/18342

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2209	0	2205	9	0
1	B	2214	0	2225	12	0
1	C	2215	0	2221	12	0
1	D	2209	0	2205	7	0
1	E	2207	0	2214	15	0
1	F	2206	0	2201	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
3	E	6	0	8	0	0
4	A	236	0	0	0	0
4	B	216	0	0	2	0
4	C	242	0	0	1	0
4	D	220	0	0	1	0
4	E	192	0	0	1	0
4	F	184	0	0	1	0
All	All	14646	0	13343	64	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (64) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:17:PRO:O	1:B:258:ARG:NH1	2.23	0.70
1:E:239:GLU:HB2	1:E:245:MET:HE1	1.76	0.66
1:E:30:THR:HG21	1:E:70:ALA:HA	1.77	0.66
1:D:180:VAL:HB	1:D:201:LEU:HD13	1.78	0.65
1:A:180:VAL:HB	1:A:201:LEU:HD13	1.80	0.63
1:F:180:VAL:HB	1:F:201:LEU:HD13	1.78	0.63
1:C:30:THR:HG21	1:C:70:ALA:HA	1.81	0.63
1:E:180:VAL:HB	1:E:201:LEU:HD13	1.82	0.61
1:D:132:MET:HE2	1:D:216:ARG:HG2	1.82	0.61
1:E:3:LYS:HD3	1:E:4:VAL:H	1.66	0.60
1:C:69:ARG:NH2	1:C:125:SER:OG	2.35	0.60
1:B:180:VAL:HB	1:B:201:LEU:HD13	1.85	0.59
1:A:30:THR:HG21	1:A:70:ALA:HA	1.84	0.59
1:E:132:MET:HE2	1:E:216:ARG:HG2	1.86	0.57
1:C:132:MET:HE2	1:C:216:ARG:HG2	1.86	0.57
1:D:27:GLN:HG2	1:D:38:THR:HG22	1.87	0.56
1:A:132:MET:HE2	1:A:216:ARG:HG2	1.86	0.56
1:F:132:MET:HE2	1:F:216:ARG:HG2	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:20:PHE:HB3	1:E:21:LYS:C	2.27	0.55
1:E:34:LYS:NZ	4:E:519:HOH:O	2.41	0.54
1:C:30:THR:HG23	1:C:32:PHE:H	1.72	0.54
1:A:162:THR:HG23	1:A:163:MET:HG3	1.90	0.53
1:E:247:LEU:O	1:E:251:ARG:HG2	2.09	0.52
1:A:27:GLN:HG2	1:A:38:THR:HG22	1.92	0.52
1:D:258:ARG:NH2	4:D:582:HOH:O	2.43	0.52
1:B:132:MET:HE2	1:B:216:ARG:HG2	1.92	0.51
1:A:30:THR:CG2	1:A:32:PHE:H	2.24	0.51
1:C:30:THR:CG2	1:C:32:PHE:H	2.24	0.51
1:E:20:PHE:HB3	1:E:22:LYS:N	2.28	0.48
1:A:159:ASP:HB3	1:A:162:THR:HG22	1.95	0.48
1:E:30:THR:HG23	1:E:32:PHE:H	1.79	0.48
1:C:235:LYS:NZ	4:C:557:HOH:O	2.46	0.48
1:E:30:THR:CG2	1:E:32:PHE:H	2.27	0.47
1:B:69:ARG:HD2	1:B:115:GLU:CB	2.44	0.47
1:F:22:LYS:HE2	1:F:25:VAL:HG23	1.96	0.47
1:E:19:LEU:HB3	1:E:262:LEU:HD21	1.98	0.46
1:A:30:THR:HG22	1:A:32:PHE:H	1.81	0.46
1:B:4:VAL:HG21	1:B:269:GLY:HA2	1.99	0.45
1:D:143:ARG:NH2	1:D:175:ALA:O	2.48	0.45
1:B:69:ARG:HD2	1:B:115:GLU:HB3	1.99	0.44
4:B:489:HOH:O	1:C:108:MET:SD	2.60	0.44
1:C:235:LYS:HB3	1:C:236:SER:H	1.60	0.43
1:C:17:PRO:O	1:C:258:ARG:NH1	2.50	0.43
1:B:258:ARG:NE	4:B:609:HOH:O	2.37	0.43
1:C:69:ARG:HD2	1:C:115:GLU:CB	2.49	0.42
1:C:180:VAL:HB	1:C:201:LEU:HD13	1.99	0.42
1:B:46:ASP:N	1:B:46:ASP:OD1	2.45	0.42
1:F:197:LYS:NZ	4:F:550:HOH:O	2.51	0.42
1:B:238:GLU:HA	1:B:239:GLU:HA	1.75	0.42
1:D:169:ILE:O	1:D:172:CYS:HB3	2.19	0.42
1:E:52:LEU:HD12	1:E:53:PRO:HD2	2.01	0.42
1:F:238:GLU:HA	1:F:239:GLU:HA	1.72	0.42
1:E:195:ILE:O	1:E:199:MET:HG3	2.20	0.42
1:A:169:ILE:O	1:A:172:CYS:HB3	2.20	0.42
1:F:101:PHE:HB2	1:F:173:VAL:HG22	2.02	0.42
1:F:247:LEU:O	1:F:251:ARG:HG3	2.19	0.42
1:B:247:LEU:O	1:B:251:ARG:HG3	2.21	0.41
1:E:127:LYS:HA	1:E:127:LYS:HD3	1.88	0.41
1:D:229:THR:HA	1:D:249:GLN:HG2	2.03	0.41
1:B:101:PHE:HB3	1:B:225:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:52:LEU:HD12	1:B:53:PRO:HD2	2.02	0.40
1:F:237:GLU:HA	1:F:240:HIS:CE1	2.56	0.40
1:C:237:GLU:O	1:C:239:GLU:HA	2.22	0.40
1:F:14:PHE:CE1	1:F:17:PRO:HA	2.56	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	287/320 (90%)	282 (98%)	5 (2%)	0	100	100
1	B	287/320 (90%)	283 (99%)	4 (1%)	0	100	100
1	C	288/320 (90%)	284 (99%)	4 (1%)	0	100	100
1	D	287/320 (90%)	283 (99%)	4 (1%)	0	100	100
1	E	285/320 (89%)	279 (98%)	6 (2%)	0	100	100
1	F	287/320 (90%)	283 (99%)	4 (1%)	0	100	100
All	All	1721/1920 (90%)	1694 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	242/274 (88%)	240 (99%)	2 (1%)	89	93
1	B	243/274 (89%)	241 (99%)	2 (1%)	89	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	242/274 (88%)	238 (98%)	4 (2%)	73	77
1	D	242/274 (88%)	241 (100%)	1 (0%)	95	97
1	E	241/274 (88%)	237 (98%)	4 (2%)	73	77
1	F	241/274 (88%)	239 (99%)	2 (1%)	89	93
All	All	1451/1644 (88%)	1436 (99%)	15 (1%)	85	89

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	205	ASN
1	B	14	PHE
1	B	205	ASN
1	C	25	VAL
1	C	30	THR
1	C	205	ASN
1	C	225	ILE
1	D	205	ASN
1	E	30	THR
1	E	108	MET
1	E	205	ASN
1	E	239	GLU
1	F	14	PHE
1	F	205	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/320 (90%)	-0.42	3 (1%) 79 82	10, 18, 42, 96	0
1	B	289/320 (90%)	-0.24	3 (1%) 79 82	11, 23, 45, 116	0
1	C	290/320 (90%)	-0.32	5 (1%) 67 70	11, 22, 50, 105	0
1	D	285/320 (89%)	-0.40	1 (0%) 90 92	13, 21, 42, 72	0
1	E	289/320 (90%)	-0.12	6 (2%) 60 65	14, 26, 59, 128	0
1	F	289/320 (90%)	-0.10	7 (2%) 56 60	14, 28, 62, 114	0
All	All	1731/1920 (90%)	-0.27	25 (1%) 72 75	10, 22, 52, 128	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	238	GLU	8.4
1	B	238	GLU	7.5
1	F	238	GLU	5.5
1	C	238	GLU	5.1
1	A	238	GLU	4.0
1	E	20	PHE	3.8
1	F	25	VAL	3.7
1	B	239	GLU	3.3
1	A	236	SER	2.8
1	D	166	SER	2.7
1	F	57	LYS	2.7
1	F	239	GLU	2.6
1	C	21	LYS	2.6
1	F	236	SER	2.5
1	C	236	SER	2.5
1	E	19	LEU	2.5
1	F	21	LYS	2.4
1	E	21	LYS	2.3
1	E	292	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	269	GLY	2.1
1	B	237	GLU	2.1
1	C	16	ASP	2.1
1	C	19	LEU	2.1
1	E	239	GLU	2.0
1	A	237	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	E	302	6/6	0.14	2.58	18,21,24,28	0
3	GOL	D	303	6/6	0.12	0.42	32,33,35,36	0
3	GOL	B	302	6/6	0.10	0.30	15,18,20,22	0
3	GOL	A	302	6/6	0.09	-0.07	14,14,18,20	0
2	ADE	D	301	10/10	0.08	-0.50	18,20,23,24	0
2	ADE	C	301	10/10	0.07	-0.56	11,14,17,18	0
2	ADE	E	301	10/10	0.08	-0.79	16,20,24,24	0
3	GOL	D	302	6/6	0.08	-0.82	16,18,19,20	0
3	GOL	C	302	6/6	0.07	-1.21	17,21,25,26	0
2	ADE	A	301	10/10	0.07	-1.62	10,16,18,18	0
2	ADE	B	301	10/10	0.07	-1.75	10,13,15,16	0
2	ADE	F	301	10/10	0.07	-2.24	12,15,19,19	0

6.5 Other polymers ⓘ

There are no such residues in this entry.