



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:37 am BST

PDB ID : 4L5Y
Title : Methylthioadenosine phosphorylase from *Schistosoma mansoni* in APO form
Authors : Torini, J.R.; DeMarco, R.; Brandao-Neto, J.; Pereira, H.M.
Deposited on : 2013-06-11
Resolution : 2.10 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
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

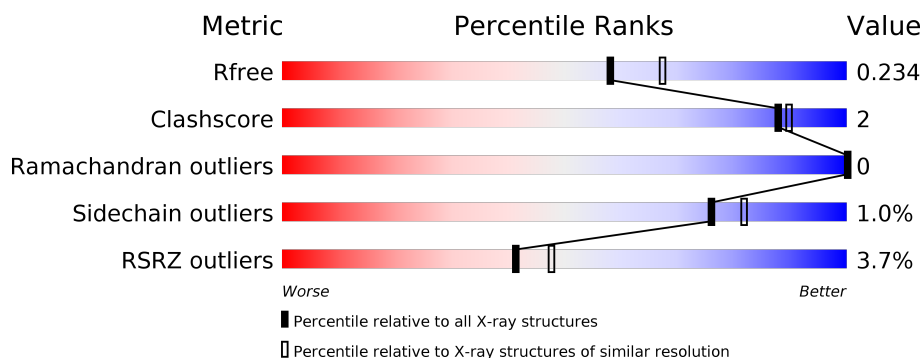
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	320	<div> <div>4%</div> <div>83%</div> <div>13%</div> </div>
1	B	320	<div> <div>4%</div> <div>83%</div> <div>12%</div> </div>
1	C	320	<div> <div>2%</div> <div>83%</div> <div>12%</div> </div>
1	D	320	<div> <div>5%</div> <div>83%</div> <div>12%</div> </div>
1	E	320	<div> <div>3%</div> <div>82%</div> <div>12%</div> </div>
1	F	320	<div> <div>%</div> <div>83%</div> <div>12%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13452 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 S-methyl-5'-thioadenosine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2075	1315	357	388	15			
1	B	282	Total	C	N	O	S	0	0	0
			2112	1342	364	391	15			
1	C	281	Total	C	N	O	S	0	0	0
			2121	1344	367	395	15			
1	D	281	Total	C	N	O	S	0	0	0
			2098	1336	359	388	15			
1	E	283	Total	C	N	O	S	0	0	0
			2127	1347	366	399	15			
1	F	281	Total	C	N	O	S	0	0	0
			2117	1343	363	395	16			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP I0B503
A	-19	GLY	-	EXPRESSION TAG	UNP I0B503
A	-18	SER	-	EXPRESSION TAG	UNP I0B503
A	-17	SER	-	EXPRESSION TAG	UNP I0B503
A	-16	HIS	-	EXPRESSION TAG	UNP I0B503
A	-15	HIS	-	EXPRESSION TAG	UNP I0B503
A	-14	HIS	-	EXPRESSION TAG	UNP I0B503
A	-13	HIS	-	EXPRESSION TAG	UNP I0B503
A	-12	HIS	-	EXPRESSION TAG	UNP I0B503
A	-11	HIS	-	EXPRESSION TAG	UNP I0B503
A	-10	SER	-	EXPRESSION TAG	UNP I0B503
A	-9	SER	-	EXPRESSION TAG	UNP I0B503
A	-8	GLY	-	EXPRESSION TAG	UNP I0B503
A	-7	LEU	-	EXPRESSION TAG	UNP I0B503
A	-6	VAL	-	EXPRESSION TAG	UNP I0B503
A	-5	PRO	-	EXPRESSION TAG	UNP I0B503
A	-4	ARG	-	EXPRESSION TAG	UNP I0B503

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP I0B503
A	-2	SER	-	EXPRESSION TAG	UNP I0B503
A	-1	HIS	-	EXPRESSION TAG	UNP I0B503
A	0	MET	-	EXPRESSION TAG	UNP I0B503
B	-20	MET	-	EXPRESSION TAG	UNP I0B503
B	-19	GLY	-	EXPRESSION TAG	UNP I0B503
B	-18	SER	-	EXPRESSION TAG	UNP I0B503
B	-17	SER	-	EXPRESSION TAG	UNP I0B503
B	-16	HIS	-	EXPRESSION TAG	UNP I0B503
B	-15	HIS	-	EXPRESSION TAG	UNP I0B503
B	-14	HIS	-	EXPRESSION TAG	UNP I0B503
B	-13	HIS	-	EXPRESSION TAG	UNP I0B503
B	-12	HIS	-	EXPRESSION TAG	UNP I0B503
B	-11	HIS	-	EXPRESSION TAG	UNP I0B503
B	-10	SER	-	EXPRESSION TAG	UNP I0B503
B	-9	SER	-	EXPRESSION TAG	UNP I0B503
B	-8	GLY	-	EXPRESSION TAG	UNP I0B503
B	-7	LEU	-	EXPRESSION TAG	UNP I0B503
B	-6	VAL	-	EXPRESSION TAG	UNP I0B503
B	-5	PRO	-	EXPRESSION TAG	UNP I0B503
B	-4	ARG	-	EXPRESSION TAG	UNP I0B503
B	-3	GLY	-	EXPRESSION TAG	UNP I0B503
B	-2	SER	-	EXPRESSION TAG	UNP I0B503
B	-1	HIS	-	EXPRESSION TAG	UNP I0B503
B	0	MET	-	EXPRESSION TAG	UNP I0B503
C	-20	MET	-	EXPRESSION TAG	UNP I0B503
C	-19	GLY	-	EXPRESSION TAG	UNP I0B503
C	-18	SER	-	EXPRESSION TAG	UNP I0B503
C	-17	SER	-	EXPRESSION TAG	UNP I0B503
C	-16	HIS	-	EXPRESSION TAG	UNP I0B503
C	-15	HIS	-	EXPRESSION TAG	UNP I0B503
C	-14	HIS	-	EXPRESSION TAG	UNP I0B503
C	-13	HIS	-	EXPRESSION TAG	UNP I0B503
C	-12	HIS	-	EXPRESSION TAG	UNP I0B503
C	-11	HIS	-	EXPRESSION TAG	UNP I0B503
C	-10	SER	-	EXPRESSION TAG	UNP I0B503
C	-9	SER	-	EXPRESSION TAG	UNP I0B503
C	-8	GLY	-	EXPRESSION TAG	UNP I0B503
C	-7	LEU	-	EXPRESSION TAG	UNP I0B503
C	-6	VAL	-	EXPRESSION TAG	UNP I0B503
C	-5	PRO	-	EXPRESSION TAG	UNP I0B503
C	-4	ARG	-	EXPRESSION TAG	UNP I0B503

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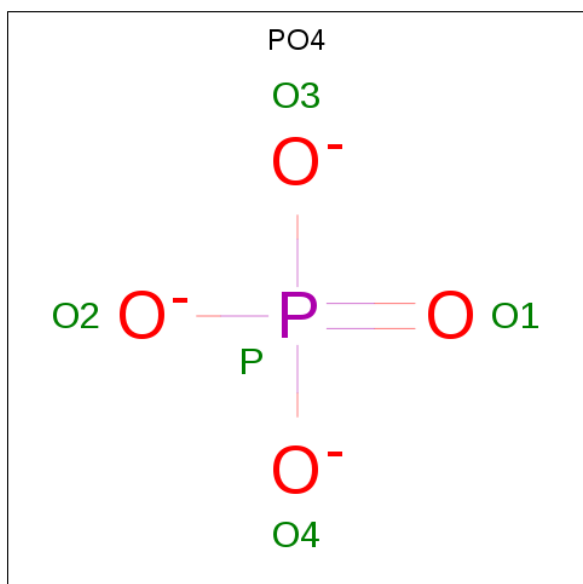
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	EXPRESSION TAG	UNP I0B503
C	-2	SER	-	EXPRESSION TAG	UNP I0B503
C	-1	HIS	-	EXPRESSION TAG	UNP I0B503
C	0	MET	-	EXPRESSION TAG	UNP I0B503
D	-20	MET	-	EXPRESSION TAG	UNP I0B503
D	-19	GLY	-	EXPRESSION TAG	UNP I0B503
D	-18	SER	-	EXPRESSION TAG	UNP I0B503
D	-17	SER	-	EXPRESSION TAG	UNP I0B503
D	-16	HIS	-	EXPRESSION TAG	UNP I0B503
D	-15	HIS	-	EXPRESSION TAG	UNP I0B503
D	-14	HIS	-	EXPRESSION TAG	UNP I0B503
D	-13	HIS	-	EXPRESSION TAG	UNP I0B503
D	-12	HIS	-	EXPRESSION TAG	UNP I0B503
D	-11	HIS	-	EXPRESSION TAG	UNP I0B503
D	-10	SER	-	EXPRESSION TAG	UNP I0B503
D	-9	SER	-	EXPRESSION TAG	UNP I0B503
D	-8	GLY	-	EXPRESSION TAG	UNP I0B503
D	-7	LEU	-	EXPRESSION TAG	UNP I0B503
D	-6	VAL	-	EXPRESSION TAG	UNP I0B503
D	-5	PRO	-	EXPRESSION TAG	UNP I0B503
D	-4	ARG	-	EXPRESSION TAG	UNP I0B503
D	-3	GLY	-	EXPRESSION TAG	UNP I0B503
D	-2	SER	-	EXPRESSION TAG	UNP I0B503
D	-1	HIS	-	EXPRESSION TAG	UNP I0B503
D	0	MET	-	EXPRESSION TAG	UNP I0B503
E	-20	MET	-	EXPRESSION TAG	UNP I0B503
E	-19	GLY	-	EXPRESSION TAG	UNP I0B503
E	-18	SER	-	EXPRESSION TAG	UNP I0B503
E	-17	SER	-	EXPRESSION TAG	UNP I0B503
E	-16	HIS	-	EXPRESSION TAG	UNP I0B503
E	-15	HIS	-	EXPRESSION TAG	UNP I0B503
E	-14	HIS	-	EXPRESSION TAG	UNP I0B503
E	-13	HIS	-	EXPRESSION TAG	UNP I0B503
E	-12	HIS	-	EXPRESSION TAG	UNP I0B503
E	-11	HIS	-	EXPRESSION TAG	UNP I0B503
E	-10	SER	-	EXPRESSION TAG	UNP I0B503
E	-9	SER	-	EXPRESSION TAG	UNP I0B503
E	-8	GLY	-	EXPRESSION TAG	UNP I0B503
E	-7	LEU	-	EXPRESSION TAG	UNP I0B503
E	-6	VAL	-	EXPRESSION TAG	UNP I0B503
E	-5	PRO	-	EXPRESSION TAG	UNP I0B503
E	-4	ARG	-	EXPRESSION TAG	UNP I0B503

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP I0B503
E	-2	SER	-	EXPRESSION TAG	UNP I0B503
E	-1	HIS	-	EXPRESSION TAG	UNP I0B503
E	0	MET	-	EXPRESSION TAG	UNP I0B503
F	-20	MET	-	EXPRESSION TAG	UNP I0B503
F	-19	GLY	-	EXPRESSION TAG	UNP I0B503
F	-18	SER	-	EXPRESSION TAG	UNP I0B503
F	-17	SER	-	EXPRESSION TAG	UNP I0B503
F	-16	HIS	-	EXPRESSION TAG	UNP I0B503
F	-15	HIS	-	EXPRESSION TAG	UNP I0B503
F	-14	HIS	-	EXPRESSION TAG	UNP I0B503
F	-13	HIS	-	EXPRESSION TAG	UNP I0B503
F	-12	HIS	-	EXPRESSION TAG	UNP I0B503
F	-11	HIS	-	EXPRESSION TAG	UNP I0B503
F	-10	SER	-	EXPRESSION TAG	UNP I0B503
F	-9	SER	-	EXPRESSION TAG	UNP I0B503
F	-8	GLY	-	EXPRESSION TAG	UNP I0B503
F	-7	LEU	-	EXPRESSION TAG	UNP I0B503
F	-6	VAL	-	EXPRESSION TAG	UNP I0B503
F	-5	PRO	-	EXPRESSION TAG	UNP I0B503
F	-4	ARG	-	EXPRESSION TAG	UNP I0B503
F	-3	GLY	-	EXPRESSION TAG	UNP I0B503
F	-2	SER	-	EXPRESSION TAG	UNP I0B503
F	-1	HIS	-	EXPRESSION TAG	UNP I0B503
F	0	MET	-	EXPRESSION TAG	UNP I0B503

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

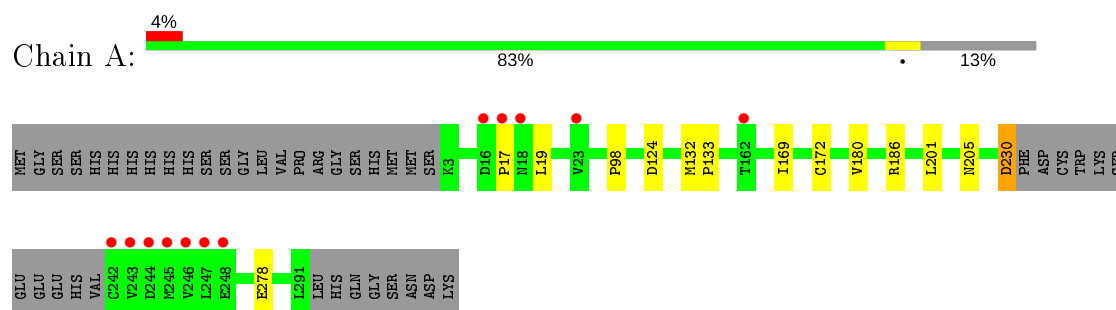
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	129	Total O 129 129	0	0
3	B	129	Total O 129 129	0	0
3	C	126	Total O 126 126	0	0
3	D	99	Total O 99 99	0	0
3	E	130	Total O 130 130	0	0
3	F	159	Total O 159 159	0	0

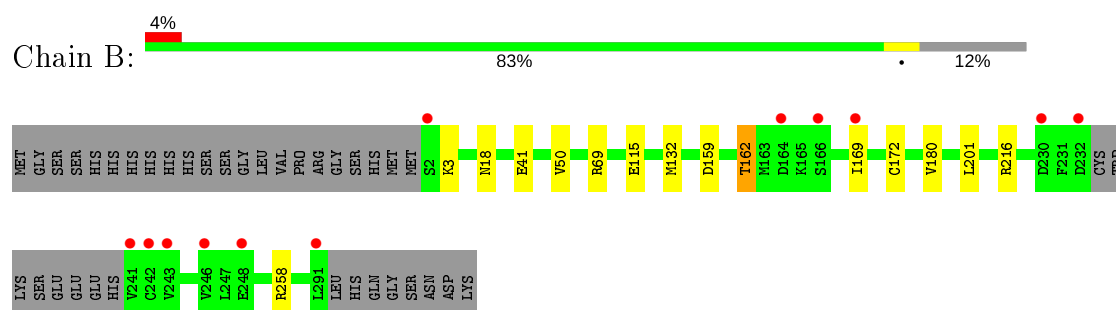
3 Residue-property plots [i](#)

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.

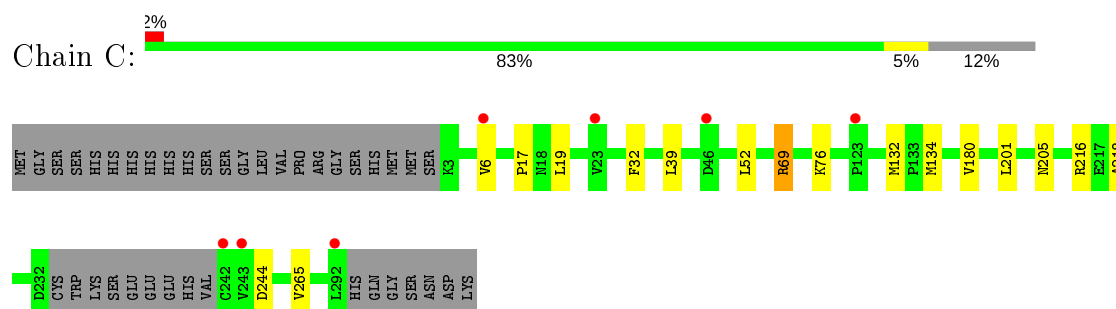
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase



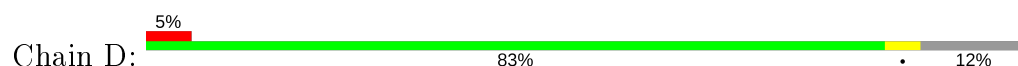
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

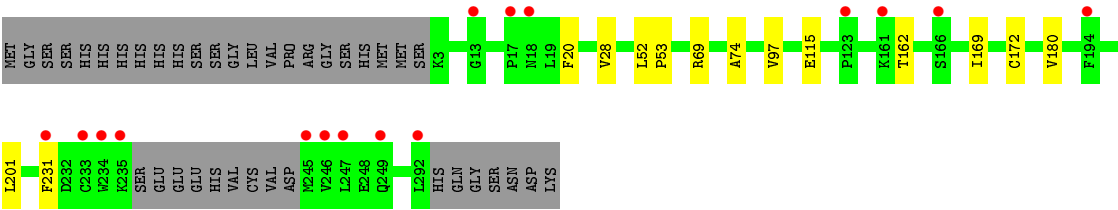


- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

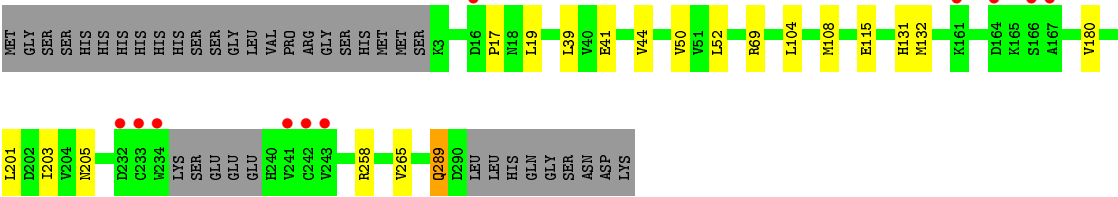
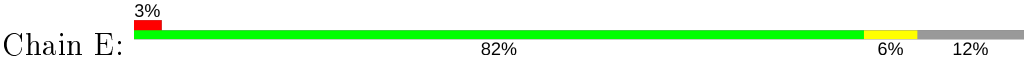


- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

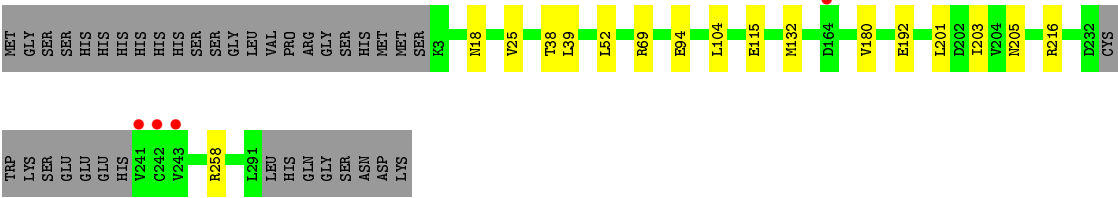
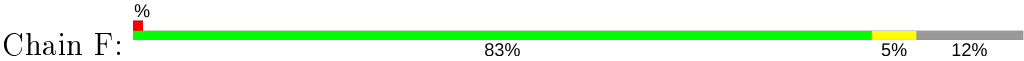




● Molecule 1: S-methyl-5'-thioadenosine phosphorylase



● Molecule 1: S-methyl-5'-thioadenosine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.63 Å 82.40 Å 150.29 Å 90.00° 101.60° 90.00°	Depositor
Resolution (Å)	19.93 – 2.10 19.93 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.93-2.10) 98.6 (19.93-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.09 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.184 , 0.227 0.190 , 0.234	Depositor DCC
R_{free} test set	5581 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13452	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 29.89 % 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 1.4357e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PO4

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	0.24	0/2115	0.43	0/2874
1	B	0.24	0/2153	0.44	0/2924
1	C	0.23	0/2162	0.43	0/2935
1	D	0.24	0/2141	0.42	0/2912
1	E	0.25	0/2168	0.42	0/2945
1	F	0.25	0/2158	0.44	0/2931
All	All	0.24	0/12897	0.43	0/17521

There are no bond length outliers.

There are no bond angle outliers.

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	2075	0	2021	6	0
1	B	2112	0	2067	11	0
1	C	2121	0	2091	9	0
1	D	2098	0	2034	7	0
1	E	2127	0	2085	10	0
1	F	2117	0	2074	9	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	129	0	0	0	0
3	B	129	0	0	0	0
3	C	126	0	0	0	0
3	D	99	0	0	0	0
3	E	130	0	0	0	0
3	F	159	0	0	1	0
All	All	13452	0	12372	49	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 2.

All (49) 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:C:180:VAL:HB	1:C:201:LEU:HD13	1.73	0.71
1:C:32:PHE:HB3	1:C:69:ARG:HD3	1.75	0.68
1:F:180:VAL:HB	1:F:201:LEU:HD13	1.76	0.66
1:E:17:PRO:HB2	1:E:19:LEU:HD13	1.85	0.58
1:F:25:VAL:HG13	1:F:38:THR:HG21	1.85	0.58
1:A:17:PRO:HB2	1:A:19:LEU:HD13	1.86	0.58
1:F:104:LEU:HD21	1:F:203:ILE:HD11	1.85	0.56
1:B:41:GLU:HG2	1:B:50:VAL:HG22	1.87	0.56
1:E:69:ARG:HD2	1:E:115:GLU:CB	2.37	0.55
1:B:180:VAL:HB	1:B:201:LEU:HD13	1.89	0.55
1:D:180:VAL:HB	1:D:201:LEU:HD13	1.89	0.55
1:B:18:ASN:O	1:B:258:ARG:NH2	2.40	0.55
1:E:39:LEU:HD22	1:E:52:LEU:HB2	1.88	0.55
1:E:41:GLU:HG2	1:E:50:VAL:HG22	1.87	0.54
1:A:98:PRO:HG3	1:A:230:ASP:HB2	1.90	0.54
1:B:69:ARG:HD2	1:B:115:GLU:CB	2.38	0.54
1:B:132:MET:HE2	1:B:216:ARG:HG2	1.90	0.54
1:B:159:ASP:HB3	1:B:162:THR:HG22	1.89	0.53
1:B:258:ARG:NH1	1:D:162:THR:HG23	2.25	0.52
1:A:180:VAL:HB	1:A:201:LEU:HD13	1.91	0.51
1:E:69:ARG:HD2	1:E:115:GLU:HB2	1.91	0.51
1:D:52:LEU:HD12	1:D:53:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:MET:HE2	1:C:216:ARG:HG2	1.92	0.50
1:F:132:MET:HE2	1:F:216:ARG:HG2	1.94	0.49
1:E:44:VAL:HB	1:E:265:VAL:HG11	1.94	0.49
1:F:18:ASN:O	1:F:258:ARG:NH2	2.46	0.48
1:C:39:LEU:HD22	1:C:52:LEU:HB2	1.95	0.48
1:F:39:LEU:HD22	1:F:52:LEU:HB2	1.94	0.48
1:E:104:LEU:HD21	1:E:203:ILE:HD11	1.94	0.48
1:E:180:VAL:HB	1:E:201:LEU:HD13	1.96	0.48
1:A:186:ARG:HD2	1:C:134:MET:HG3	1.95	0.48
1:D:169:ILE:O	1:D:172:CYS:HB3	2.14	0.48
1:B:69:ARG:HD2	1:B:115:GLU:HB3	1.96	0.47
1:C:6:VAL:HG11	1:C:265:VAL:HG22	1.98	0.46
1:B:258:ARG:HH11	1:B:258:ARG:HB3	1.80	0.46
1:B:69:ARG:HD2	1:B:115:GLU:HB2	1.97	0.46
1:D:69:ARG:HD2	1:D:115:GLU:CB	2.46	0.45
1:F:94:GLU:HG2	3:F:506:HOH:O	2.15	0.45
1:D:97:VAL:HG12	1:D:231:PHE:HZ	1.82	0.44
1:E:131:HIS:HD2	1:E:289:GLN:HG3	1.84	0.43
1:E:108:MET:HG2	1:F:192:GLU:HG2	2.01	0.43
1:C:244:ASP:OD1	1:C:244:ASP:N	2.52	0.42
1:B:169:ILE:O	1:B:172:CYS:HB3	2.19	0.42
1:A:132:MET:HE3	1:A:133:PRO:HD2	2.02	0.42
1:C:76:LYS:HD2	1:C:218:ALA:HB1	2.02	0.42
1:A:169:ILE:O	1:A:172:CYS:HB3	2.20	0.42
1:F:69:ARG:HD2	1:F:115:GLU:CB	2.50	0.41
1:C:17:PRO:HB3	1:C:19:LEU:HD13	2.03	0.41
1:D:28:VAL:HG21	1:D:74:ALA:HB1	2.02	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	274/320 (86%)	273 (100%)	1 (0%)	0	100	100
1	B	278/320 (87%)	276 (99%)	2 (1%)	0	100	100
1	C	277/320 (87%)	276 (100%)	1 (0%)	0	100	100
1	D	277/320 (87%)	272 (98%)	5 (2%)	0	100	100
1	E	279/320 (87%)	274 (98%)	5 (2%)	0	100	100
1	F	277/320 (87%)	275 (99%)	2 (1%)	0	100	100
All	All	1662/1920 (87%)	1646 (99%)	16 (1%)	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	217/274 (79%)	213 (98%)	4 (2%)	59	65
1	B	221/274 (81%)	219 (99%)	2 (1%)	78	84
1	C	227/274 (83%)	225 (99%)	2 (1%)	78	84
1	D	218/274 (80%)	217 (100%)	1 (0%)	88	92
1	E	227/274 (83%)	223 (98%)	4 (2%)	59	65
1	F	225/274 (82%)	224 (100%)	1 (0%)	91	94
All	All	1335/1644 (81%)	1321 (99%)	14 (1%)	76	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASP
1	A	205	ASN
1	A	230	ASP
1	A	278	GLU
1	B	3	LYS
1	B	162	THR
1	C	69	ARG

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Mol	Chain	Res	Type
1	C	205	ASN
1	D	20	PHE
1	E	132	MET
1	E	205	ASN
1	E	258	ARG
1	E	289	GLN
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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	PO4	D	301	-	4,4,4	0.83	0	6,6,6	0.42	0
2	PO4	B	301	-	4,4,4	0.86	0	6,6,6	0.49	0
2	PO4	A	301	-	4,4,4	0.94	0	6,6,6	0.51	0
2	PO4	C	301	-	4,4,4	0.86	0	6,6,6	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	F	301	-	4,4,4	0.90	0	6,6,6	0.52	0
2	PO4	E	301	-	4,4,4	0.94	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	278/320 (86%)	-0.14	12 (4%) 35 41	16, 29, 59, 85	0
1	B	282/320 (88%)	-0.11	12 (4%) 35 41	18, 32, 60, 88	0
1	C	281/320 (87%)	-0.16	7 (2%) 57 62	19, 33, 58, 85	0
1	D	281/320 (87%)	0.07	16 (5%) 23 29	19, 32, 63, 93	0
1	E	283/320 (88%)	-0.14	11 (3%) 39 45	19, 31, 67, 84	0
1	F	281/320 (87%)	-0.24	4 (1%) 75 78	18, 28, 53, 73	0
All	All	1686/1920 (87%)	-0.12	62 (3%) 41 48	16, 31, 60, 93	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	241	VAL	8.8
1	A	243	VAL	6.8
1	D	292	LEU	6.1
1	D	245	MET	5.3
1	A	18	ASN	4.9
1	B	291	LEU	4.8
1	E	233	CYS	4.7
1	C	242	CYS	4.6
1	D	234	TRP	4.6
1	A	242	CYS	4.5
1	E	241	VAL	4.2
1	D	246	VAL	4.1
1	B	242	CYS	4.1
1	B	246	VAL	3.7
1	B	241	VAL	3.6
1	B	169	ILE	3.6
1	D	231	PHE	3.6
1	A	246	VAL	3.6
1	B	166	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	242	CYS	3.5
1	A	244	ASP	3.4
1	B	243	VAL	3.4
1	E	166	SER	3.4
1	A	245	MET	3.3
1	D	249	GLN	3.2
1	E	243	VAL	3.1
1	D	166	SER	3.1
1	D	18	ASN	3.1
1	C	23	VAL	3.1
1	A	247	LEU	3.0
1	C	243	VAL	3.0
1	D	235	LYS	3.0
1	D	247	LEU	3.0
1	F	243	VAL	2.9
1	E	234	TRP	2.9
1	D	13	GLY	2.9
1	C	292	LEU	2.8
1	F	242	CYS	2.8
1	B	2	SER	2.8
1	D	233	CYS	2.8
1	C	123	PRO	2.8
1	D	17	PRO	2.8
1	E	164	ASP	2.8
1	A	248	GLU	2.7
1	B	230	ASP	2.6
1	A	23	VAL	2.6
1	C	46	ASP	2.6
1	B	164	ASP	2.5
1	D	194	PHE	2.5
1	F	164	ASP	2.5
1	A	16	ASP	2.4
1	D	123	PRO	2.4
1	D	161	LYS	2.4
1	E	161	LYS	2.3
1	E	167	ALA	2.3
1	E	16	ASP	2.3
1	A	162	THR	2.1
1	A	17	PRO	2.1
1	C	6	VAL	2.1
1	B	232	ASP	2.1
1	B	248	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	232	ASP	2.0

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 carbohydrates 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(Å ²)	Q<0.9
2	PO4	D	301	5/5	0.98	0.13	33,37,39,43	0
2	PO4	B	301	5/5	0.99	0.05	24,25,25,27	0
2	PO4	A	301	5/5	0.99	0.07	27,28,29,31	0
2	PO4	C	301	5/5	0.99	0.07	31,32,34,35	0
2	PO4	F	301	5/5	0.99	0.06	25,26,29,30	0
2	PO4	E	301	5/5	0.99	0.06	29,29,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.