Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2016 – 07:22 PM EST

PDB ID	:	4L5A
Title	:	Methylthioadenosine phosphorylase from Schistosoma mansoni in complex with tubercidin
Authors	:	Torini, J.R.; DeMarco, R.; Brandao-Neto, J.; Pereira, H.M.
Deposited on	:	2013-06-10
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

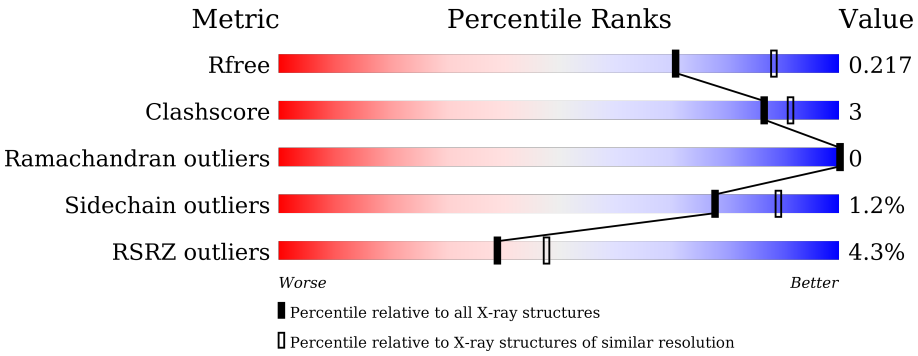
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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 <=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	5% 79% 9% 12%
1	B	320	5% 81% 6% 13%
1	C	320	2% 83% 6% 11%
1	D	320	2% 83% 5% 12%
1	E	320	4% 81% 6% 13%
1	F	320	5% 83% 5% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13566 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	282	Total	C	N	O	S	0	0	0
			2144	1361	370	396	17			
1	B	279	Total	C	N	O	S	0	0	0
			2129	1346	372	396	15			
1	C	284	Total	C	N	O	S	0	0	0
			2170	1378	375	401	16			
1	D	283	Total	C	N	O	S	0	0	0
			2155	1368	374	397	16			
1	E	279	Total	C	N	O	S	0	0	0
			2114	1342	369	388	15			
1	F	282	Total	C	N	O	S	0	0	0
			2149	1366	371	397	15			

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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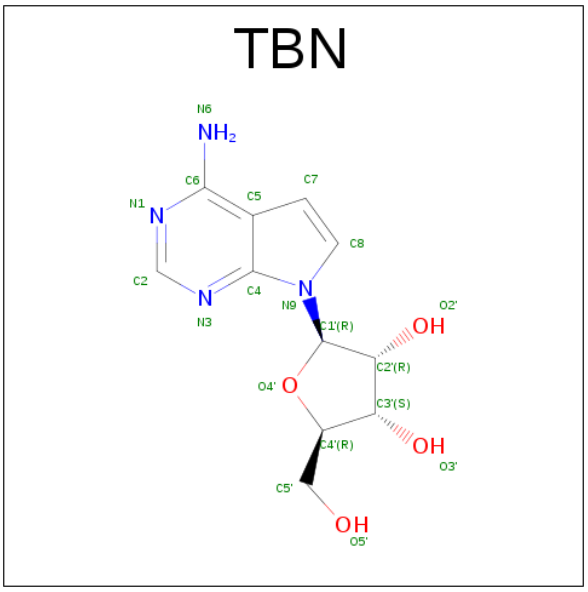
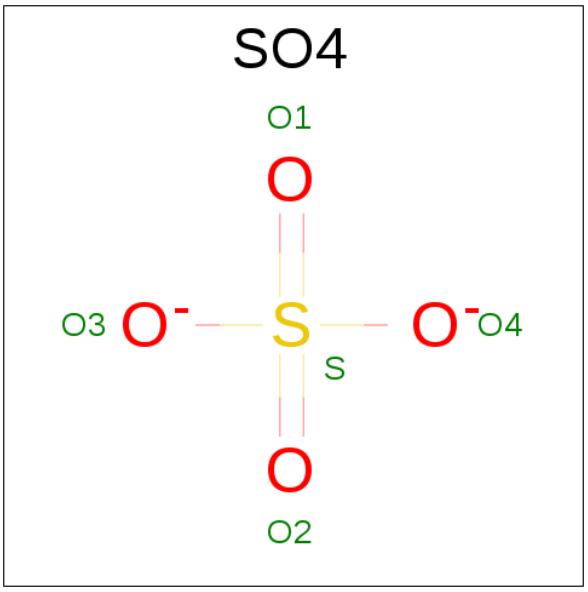
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP I0B503
E	-2	SER	-	EXPRESSION TAG	UNP I0B503
E	-1	HIS	-	EXPRESSION TAG	UNP I0B503
E	0	MET	-	EXPRESSION TAG	UNP I0B503
F	-20	MET	-	EXPRESSION TAG	UNP I0B503
F	-19	GLY	-	EXPRESSION TAG	UNP I0B503
F	-18	SER	-	EXPRESSION TAG	UNP 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 '2-(4-AMINO-PYRROLO[2,3-D]PYRIMIDIN-7-YL)-5-HYDROXYMETHYL-TETRAHYDRO-FURAN-3,4-DIOL (three-letter code: TBN) (formula: $C_{11}H_{14}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	11	4	4		
2	B	1	Total	C	N	O	0	0
			19	11	4	4		
2	C	1	Total	C	N	O	0	0
			19	11	4	4		
2	D	1	Total	C	N	O	0	0
			19	11	4	4		
2	E	1	Total	C	N	O	0	0
			19	11	4	4		
2	F	1	Total	C	N	O	0	0
			19	11	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

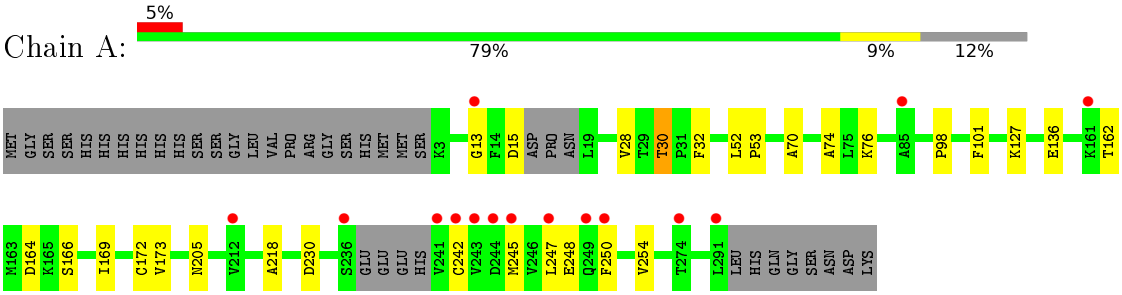
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	82	Total O 82 82	0	0
4	C	114	Total O 114 114	0	0
4	D	80	Total O 80 80	0	0
4	E	114	Total O 114 114	0	0
4	F	87	Total O 87 87	0	0

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 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.

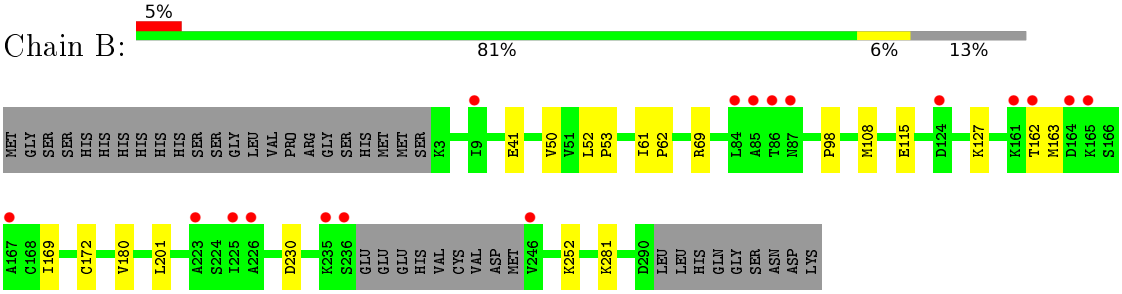
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain A:



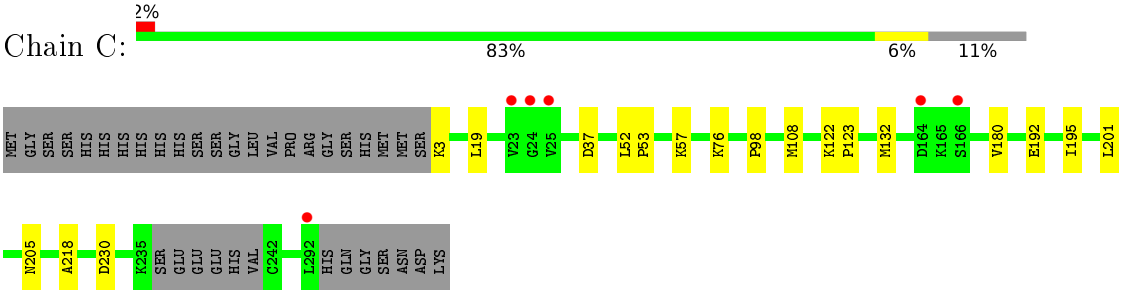
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain B:



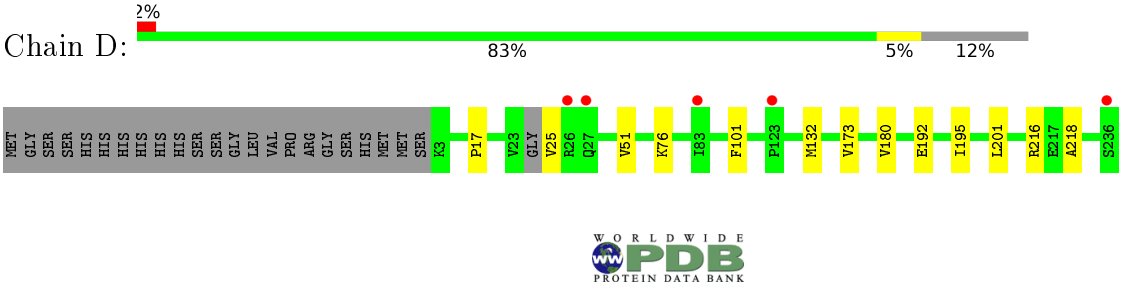
- Molecule 1: S-methyl-5'-thioadenosine phosphorylase

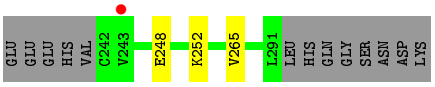
Chain C:



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

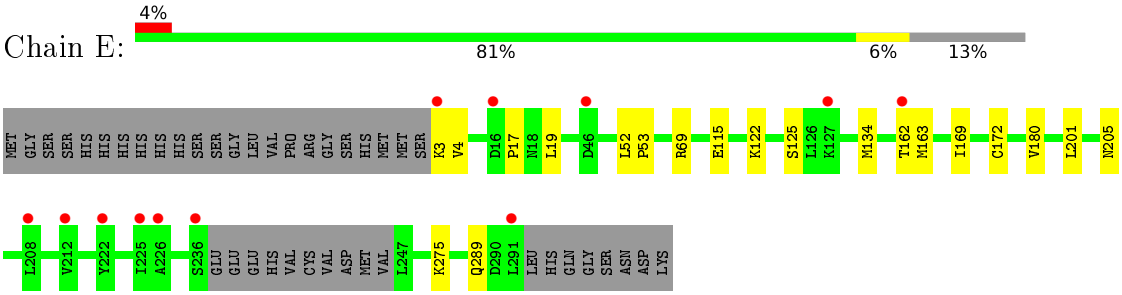
Chain D:





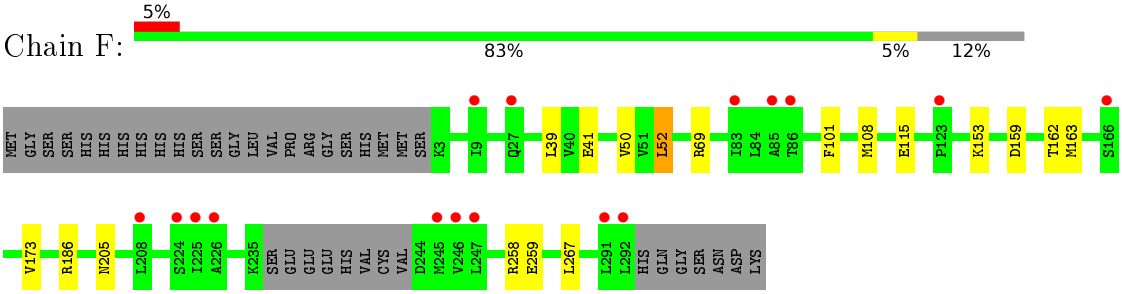
• Molecule 1: S-methyl-5'-thioadenosine phosphorylase

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.07Å 82.68Å 150.56Å 90.00° 101.34° 90.00°	Depositor
Resolution (Å)	29.20 – 2.30 28.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.20-2.30) 92.8 (28.90-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.189 , 0.219 0.186 , 0.217	Depositor DCC
R_{free} test set	4042 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13566	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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 33.78 % 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 7.5741e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, TBN

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	0/2185	0.42	0/2962
1	B	0.23	0/2172	0.42	0/2944
1	C	0.23	0/2213	0.42	0/3001
1	D	0.23	0/2197	0.42	0/2979
1	E	0.24	0/2157	0.43	0/2926
1	F	0.24	0/2192	0.44	0/2973
All	All	0.24	0/13116	0.42	0/17785

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

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	2144	0	2138	16	0
1	B	2129	0	2110	12	0
1	C	2170	0	2165	11	0
1	D	2155	0	2145	9	0
1	E	2114	0	2103	10	0
1	F	2149	0	2143	12	0
2	A	19	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	19	0	14	1	0
2	C	19	0	14	1	0
2	D	19	0	14	1	0
2	E	19	0	14	1	0
2	F	19	0	14	1	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	84	0	0	0	0
4	B	82	0	0	0	0
4	C	114	0	0	1	0
4	D	80	0	0	1	0
4	E	114	0	0	0	0
4	F	87	0	0	0	0
All	All	13566	0	12888	71	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 3.

All (71) 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:30:THR:HG22	1:A:32:PHE:H	1.44	0.82
1:D:265:VAL:O	4:D:448:HOH:O	2.04	0.74
1:E:162:THR:HG23	1:E:163:MET:HG3	1.77	0.66
1:C:180:VAL:HB	1:C:201:LEU:HD13	1.76	0.65
1:B:180:VAL:HB	1:B:201:LEU:HD13	1.78	0.65
1:A:30:THR:HG21	1:A:70:ALA:HA	1.79	0.64
1:D:180:VAL:HB	1:D:201:LEU:HD13	1.82	0.62
2:A:301:TBN:O3'	3:A:302:SO4:O1	2.18	0.61
1:B:41:GLU:HG2	1:B:50:VAL:HG22	1.83	0.61
1:A:98:PRO:HG3	1:A:230:ASP:HA	1.87	0.57
1:E:180:VAL:HB	1:E:201:LEU:HD13	1.87	0.57
1:D:192:GLU:HG2	1:F:108:MET:HG2	1.88	0.56
1:D:132:MET:HE2	1:D:216:ARG:HG2	1.88	0.55
1:D:101:PHE:HB2	1:D:173:VAL:HG22	1.89	0.53
1:F:159:ASP:HB3	1:F:162:THR:HG22	1.91	0.52
1:B:98:PRO:HG3	1:B:230:ASP:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:ARG:HD2	1:F:115:GLU:CB	2.40	0.52
1:B:162:THR:HG23	1:B:163:MET:HG3	1.91	0.51
1:C:3:LYS:N	4:C:430:HOH:O	2.44	0.50
1:C:52:LEU:HD12	1:C:53:PRO:HD2	1.94	0.50
1:F:41:GLU:HG2	1:F:50:VAL:HG22	1.93	0.50
1:F:153:LYS:HD3	1:F:259:GLU:HB3	1.93	0.50
1:C:37:ASP:OD2	1:C:57:LYS:HG2	2.11	0.50
2:D:301:TBN:H2'	2:D:301:TBN:N3	2.27	0.49
1:C:98:PRO:HG3	1:C:230:ASP:HA	1.95	0.49
2:B:301:TBN:H2'	2:B:301:TBN:N3	2.27	0.48
1:F:39:LEU:HD13	1:F:52:LEU:HB3	1.96	0.48
2:C:301:TBN:N3	2:C:301:TBN:H2'	2.28	0.47
1:F:69:ARG:HD2	1:F:115:GLU:HB2	1.95	0.47
1:B:108:MET:HG2	1:C:192:GLU:HG2	1.97	0.47
1:A:15:ASP:HA	1:A:53:PRO:HB3	1.98	0.46
1:A:13:GLY:HA3	1:A:250:PHE:CE2	2.50	0.46
2:E:301:TBN:N3	2:E:301:TBN:H2'	2.30	0.46
1:F:159:ASP:O	1:F:163:MET:HG2	2.16	0.46
2:A:301:TBN:N3	2:A:301:TBN:H2'	2.31	0.45
1:B:69:ARG:HD2	1:B:115:GLU:CB	2.46	0.45
1:E:134:MET:HG3	1:F:186:ARG:HD2	1.97	0.45
1:A:169:ILE:O	1:A:172:CYS:HB3	2.16	0.45
1:A:76:LYS:HD2	1:A:218:ALA:HB1	1.98	0.45
1:E:17:PRO:HB2	1:E:19:LEU:HD13	1.98	0.45
1:A:28:VAL:HG21	1:A:74:ALA:HB1	1.98	0.45
1:A:242:CYS:SG	1:A:245:MET:HG2	2.57	0.44
1:F:101:PHE:HB2	1:F:173:VAL:HG22	1.98	0.44
1:E:69:ARG:NH2	1:E:125:SER:OG	2.46	0.44
1:E:69:ARG:HD2	1:E:115:GLU:CB	2.48	0.44
1:B:127:LYS:HD3	1:B:127:LYS:HA	1.81	0.44
1:D:17:PRO:HG2	1:D:51:VAL:HG11	2.00	0.44
2:F:301:TBN:N3	2:F:301:TBN:H2'	2.33	0.43
1:C:76:LYS:HD2	1:C:218:ALA:HB1	2.01	0.43
1:D:76:LYS:HD2	1:D:218:ALA:HB1	1.99	0.43
1:E:3:LYS:HA	1:E:4:VAL:HA	1.54	0.43
1:B:52:LEU:HA	1:B:53:PRO:HD3	1.89	0.42
1:A:164:ASP:OD2	1:A:166:SER:OG	2.28	0.42
1:A:162:THR:HB	1:F:258:ARG:NE	2.34	0.42
1:C:122:LYS:HA	1:C:123:PRO:HD3	1.92	0.42
1:A:250:PHE:O	1:A:254:VAL:HG23	2.19	0.42
1:D:248:GLU:O	1:D:252:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PHE:CD2	1:A:254:VAL:HG22	2.55	0.42
1:E:52:LEU:HD12	1:E:53:PRO:HD2	2.02	0.42
1:A:127:LYS:HA	1:A:127:LYS:HD3	1.88	0.42
1:B:169:ILE:O	1:B:172:CYS:HB3	2.20	0.41
1:C:52:LEU:HA	1:C:53:PRO:HD3	1.93	0.41
1:A:52:LEU:HD12	1:A:53:PRO:HD2	2.03	0.41
1:E:275:LYS:HB2	1:E:275:LYS:HE2	1.77	0.41
1:E:169:ILE:O	1:E:172:CYS:HB3	2.20	0.41
1:D:195:ILE:HD12	1:F:108:MET:HG3	2.03	0.41
1:A:101:PHE:HB2	1:A:173:VAL:HG22	2.01	0.41
1:B:61:ILE:HA	1:B:62:PRO:HD2	1.97	0.41
1:B:108:MET:HG3	1:C:195:ILE:HD12	2.03	0.40
1:B:69:ARG:HD2	1:B:115:GLU:HB3	2.02	0.40
1:C:132:MET:HE2	1:C:132:MET:HB3	1.80	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	276/320 (86%)	273 (99%)	3 (1%)	0	100	100
1	B	275/320 (86%)	271 (98%)	4 (2%)	0	100	100
1	C	280/320 (88%)	277 (99%)	3 (1%)	0	100	100
1	D	277/320 (87%)	275 (99%)	2 (1%)	0	100	100
1	E	275/320 (86%)	271 (98%)	4 (2%)	0	100	100
1	F	278/320 (87%)	275 (99%)	3 (1%)	0	100	100
All	All	1661/1920 (86%)	1642 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	234/274 (85%)	229 (98%)	5 (2%)	61 78
1	B	231/274 (84%)	229 (99%)	2 (1%)	84 93
1	C	236/274 (86%)	233 (99%)	3 (1%)	76 87
1	D	234/274 (85%)	233 (100%)	1 (0%)	93 97
1	E	228/274 (83%)	225 (99%)	3 (1%)	76 87
1	F	233/274 (85%)	230 (99%)	3 (1%)	76 87
All	All	1396/1644 (85%)	1379 (99%)	17 (1%)	78 89

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	136	GLU
1	A	205	ASN
1	A	247	LEU
1	A	248	GLU
1	B	252	LYS
1	B	281	LYS
1	C	19	LEU
1	C	108	MET
1	C	205	ASN
1	D	25	VAL
1	E	122	LYS
1	E	205	ASN
1	E	289	GLN
1	F	52	LEU
1	F	205	ASN
1	F	267	LEU

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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	TBN	A	301	-	19,21,21	1.22	2 (10%)	20,31,31	2.58	2 (10%)
3	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.13	0
2	TBN	B	301	-	19,21,21	1.24	2 (10%)	20,31,31	2.48	2 (10%)
3	SO4	B	302	-	4,4,4	0.21	0	6,6,6	0.07	0
2	TBN	C	301	-	19,21,21	1.21	2 (10%)	20,31,31	2.44	2 (10%)
3	SO4	C	302	-	4,4,4	0.18	0	6,6,6	0.07	0
2	TBN	D	301	-	19,21,21	1.20	2 (10%)	20,31,31	2.40	2 (10%)
3	SO4	D	302	-	4,4,4	0.19	0	6,6,6	0.11	0
2	TBN	E	301	-	19,21,21	1.21	2 (10%)	20,31,31	2.45	2 (10%)
3	SO4	E	302	-	4,4,4	0.22	0	6,6,6	0.13	0
2	TBN	F	301	-	19,21,21	1.23	2 (10%)	20,31,31	2.50	2 (10%)
3	SO4	F	302	-	4,4,4	0.18	0	6,6,6	0.10	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	TBN	A	301	-	-	0/2/22/22	0/3/3/3
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	TBN	B	301	-	-	0/2/22/22	0/3/3/3
3	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	TBN	C	301	-	-	0/2/22/22	0/3/3/3
3	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	TBN	D	301	-	-	0/2/22/22	0/3/3/3
3	SO4	D	302	-	-	0/0/0/0	0/0/0/0
2	TBN	E	301	-	-	0/2/22/22	0/3/3/3
3	SO4	E	302	-	-	0/0/0/0	0/0/0/0
2	TBN	F	301	-	-	0/2/22/22	0/3/3/3
3	SO4	F	302	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	TBN	C8-N9	-2.32	1.33	1.37
2	D	301	TBN	C8-N9	-2.29	1.33	1.37
2	B	301	TBN	C8-N9	-2.29	1.33	1.37
2	A	301	TBN	C8-N9	-2.24	1.33	1.37
2	C	301	TBN	C8-N9	-2.20	1.33	1.37
2	E	301	TBN	C8-N9	-2.09	1.33	1.37
2	B	301	TBN	C6-N6	3.46	1.48	1.34
2	F	301	TBN	C6-N6	3.46	1.48	1.34
2	D	301	TBN	C6-N6	3.46	1.48	1.34
2	E	301	TBN	C6-N6	3.48	1.48	1.34
2	A	301	TBN	C6-N6	3.49	1.48	1.34
2	C	301	TBN	C6-N6	3.54	1.48	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	TBN	N3-C2-N1	-10.20	120.86	128.87
2	B	301	TBN	N3-C2-N1	-10.04	120.99	128.87
2	E	301	TBN	N3-C2-N1	-10.02	121.00	128.87
2	F	301	TBN	N3-C2-N1	-9.96	121.05	128.87
2	C	301	TBN	N3-C2-N1	-9.82	121.16	128.87
2	D	301	TBN	N3-C2-N1	-9.80	121.18	128.87
2	A	301	TBN	C8-N9-C1'	-4.66	121.59	125.55
2	F	301	TBN	C8-N9-C1'	-4.44	121.78	125.55
2	B	301	TBN	C8-N9-C1'	-4.14	122.04	125.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	TBN	C8-N9-C1'	-4.12	122.05	125.55
2	E	301	TBN	C8-N9-C1'	-3.83	122.30	125.55
2	D	301	TBN	C8-N9-C1'	-3.76	122.36	125.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	TBN	2	0
3	A	302	SO4	1	0
2	B	301	TBN	1	0
2	C	301	TBN	1	0
2	D	301	TBN	1	0
2	E	301	TBN	1	0
2	F	301	TBN	1	0

5.7 Other polymers

There are no such residues in this entry.

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, 95^{th} 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	282/320 (88%)	0.30	15 (5%)	30	39	22, 37, 67, 93	0
1	B	279/320 (87%)	0.19	17 (6%)	25	33	21, 34, 66, 87	0
1	C	284/320 (88%)	-0.04	6 (2%)	67	74	20, 33, 59, 97	0
1	D	283/320 (88%)	0.05	6 (2%)	67	74	21, 38, 59, 79	0
1	E	279/320 (87%)	0.05	12 (4%)	39	48	19, 31, 61, 80	0
1	F	282/320 (88%)	0.19	16 (5%)	27	36	22, 35, 64, 96	0
All	All	1689/1920 (87%)	0.12	72 (4%)	39	48	19, 34, 62, 97	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	MET	7.8
1	A	244	ASP	6.4
1	C	292	LEU	5.8
1	A	243	VAL	4.8
1	F	291	LEU	4.1
1	D	236	SER	4.1
1	A	247	LEU	3.9
1	F	245	MET	3.8
1	B	225	ILE	3.8
1	A	236	SER	3.6
1	F	292	LEU	3.5
1	F	246	VAL	3.4
1	B	165	LYS	3.4
1	A	13	GLY	3.2
1	B	167	ALA	3.2
1	A	291	LEU	3.2
1	B	162	THR	3.1
1	D	123	PRO	3.1
1	B	236	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	166	SER	3.1
1	A	242	CYS	3.0
1	C	23	VAL	3.0
1	F	85	ALA	2.9
1	B	9	ILE	2.9
1	A	85	ALA	2.9
1	B	223	ALA	2.9
1	F	9	ILE	2.8
1	F	166	SER	2.8
1	A	241	VAL	2.7
1	E	212	VAL	2.6
1	D	27	GLN	2.6
1	F	226	ALA	2.6
1	F	208	LEU	2.6
1	F	123	PRO	2.6
1	F	247	LEU	2.6
1	C	25	VAL	2.6
1	D	243	VAL	2.6
1	E	222	TYR	2.6
1	E	226	ALA	2.6
1	E	162	THR	2.5
1	C	24	GLY	2.5
1	E	236	SER	2.5
1	E	291	LEU	2.4
1	B	161	LYS	2.4
1	E	208	LEU	2.4
1	E	225	ILE	2.3
1	E	46	ASP	2.3
1	B	124	ASP	2.3
1	B	246	VAL	2.3
1	E	3	LYS	2.3
1	A	249	GLN	2.3
1	A	161	LYS	2.3
1	F	224	SER	2.2
1	B	85	ALA	2.2
1	B	226	ALA	2.2
1	B	87	ASN	2.2
1	A	250	PHE	2.2
1	B	164	ASP	2.2
1	E	16	ASP	2.2
1	F	225	ILE	2.2
1	B	235	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	83	ILE	2.1
1	C	164	ASP	2.1
1	F	83	ILE	2.1
1	D	26	ARG	2.0
1	A	274	THR	2.0
1	A	212	VAL	2.0
1	B	86	THR	2.0
1	F	27	GLN	2.0
1	F	86	THR	2.0
1	B	84	LEU	2.0
1	E	127	LYS	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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	TBN	C	301	19/19	0.96	0.12	-0.46	20,26,39,43	0
2	TBN	A	301	19/19	0.92	0.14	-0.51	24,35,47,48	0
2	TBN	F	301	19/19	0.96	0.11	-0.72	28,33,40,41	0
2	TBN	D	301	19/19	0.96	0.11	-0.81	32,33,40,42	0
3	SO4	D	302	5/5	0.98	0.12	-1.00	29,36,38,38	0
2	TBN	E	301	19/19	0.97	0.10	-1.19	27,29,38,39	0
2	TBN	B	301	19/19	0.96	0.10	-1.26	31,36,39,41	0
3	SO4	F	302	5/5	0.99	0.11	-1.33	31,31,34,35	0
3	SO4	B	302	5/5	0.99	0.10	-1.50	24,32,34,34	0
3	SO4	E	302	5/5	0.99	0.08	-1.77	29,30,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	C	302	5/5	1.00	0.09	-1.91	19,24,27,27	0
3	SO4	A	302	5/5	0.96	0.11	-2.09	42,44,49,50	0

6.5 Other polymers (i)

There are no such residues in this entry.