



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:51 am GMT

PDB ID : 3T94
Title : Crystal structure of 5'-deoxy-5'-methylthioadenosine phosphorylase (MTAP)
II complexed with 5'-deoxy-5'-methylthioadenosine and sulfate
Authors : Zhang, Y.; Ealick, S.E.
Deposited on : 2011-08-02
Resolution : 1.45 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

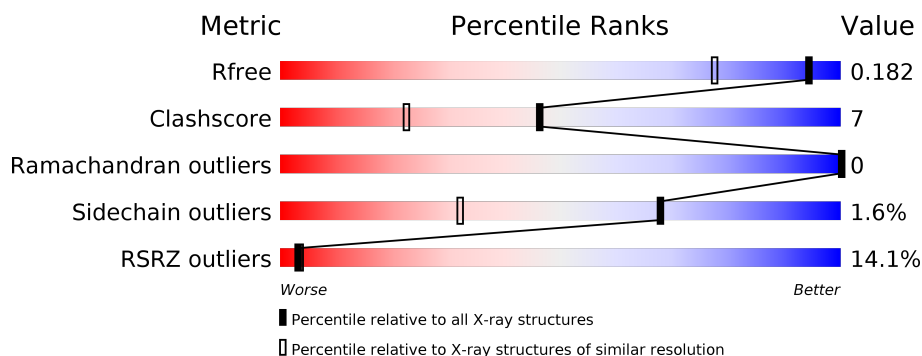
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	100719	1510 (1.48-1.44)
Clashscore	112137	1573 (1.48-1.44)
Ramachandran outliers	110173	1555 (1.48-1.44)
Sidechain outliers	110143	1555 (1.48-1.44)
RSRZ outliers	101464	1516 (1.48-1.44)

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 $\leq 5\%$. 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	270	<div> <div>14%</div> <div>89%</div> <div>11%</div> </div>
1	B	270	<div> <div>14%</div> <div>85%</div> <div>15%</div> </div>
1	C	270	<div> <div>13%</div> <div>86%</div> <div>14%</div> </div>
1	D	270	<div> <div>16%</div> <div>84%</div> <div>16%</div> </div>
1	E	270	<div> <div>13%</div> <div>85%</div> <div>15%</div> </div>
1	F	270	<div> <div>15%</div> <div>89%</div> <div>11%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	271[A]	-	-	-	X
3	SO4	A	271[B]	-	-	-	X
3	SO4	B	272	-	-	-	X
3	SO4	D	271[A]	-	-	-	X
3	SO4	D	271[B]	-	-	-	X

2 Entry composition [i](#)

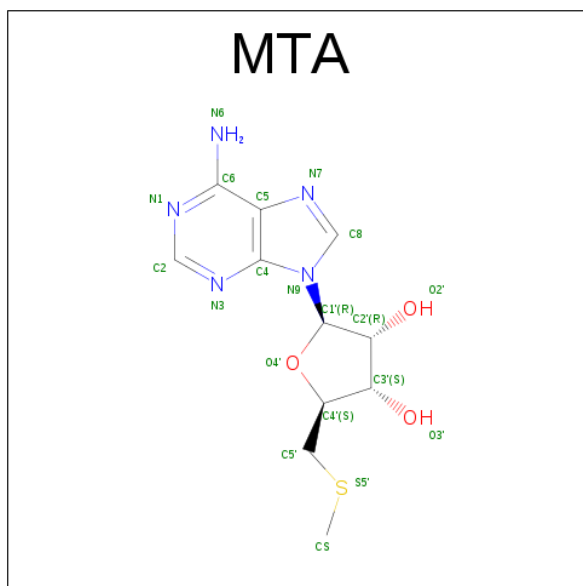
There are 4 unique types of molecules in this entry. The entry contains 14787 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 5'-methylthioadenosine phosphorylase (MtaP).

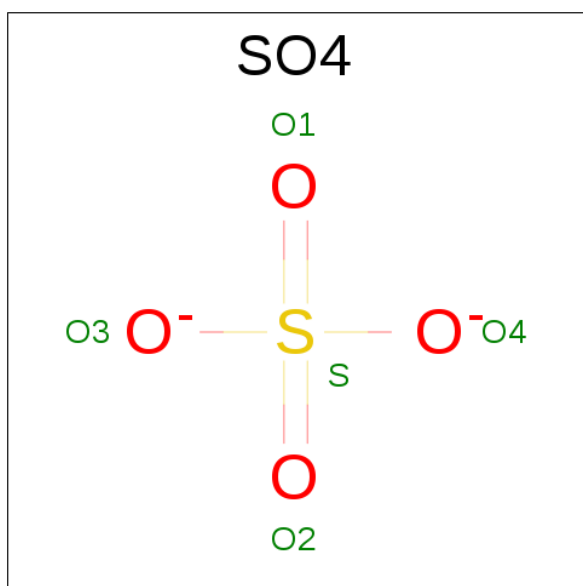
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	13	0
			2145	1375	361	390	19			
1	B	270	Total	C	N	O	S	0	23	0
			2237	1433	374	410	20			
1	C	270	Total	C	N	O	S	0	23	0
			2246	1445	371	410	20			
1	D	270	Total	C	N	O	S	0	22	0
			2226	1427	376	404	19			
1	E	270	Total	C	N	O	S	0	31	0
			2286	1465	385	417	19			
1	F	270	Total	C	N	O	S	0	17	0
			2185	1403	364	399	19			

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	E	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	F	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	1
			10	8	2		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	1
			10	8	2		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

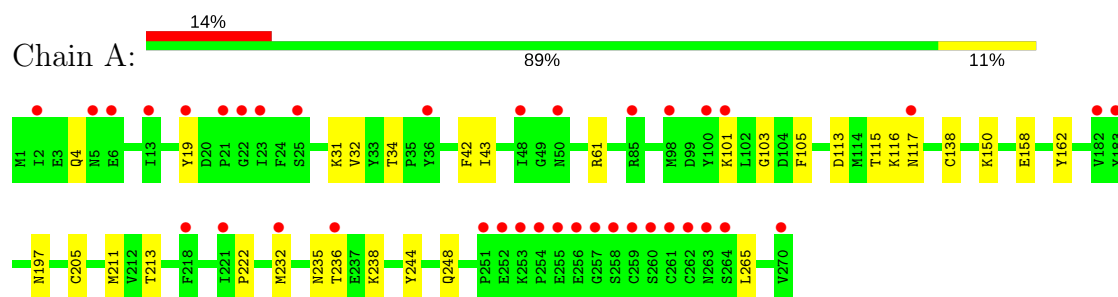
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	1
			196	196		
4	B	230	Total	O	0	0
			230	230		
4	C	208	Total	O	0	0
			208	208		
4	D	219	Total	O	0	0
			219	219		
4	E	221	Total	O	0	1
			222	222		
4	F	202	Total	O	0	0
			202	202		

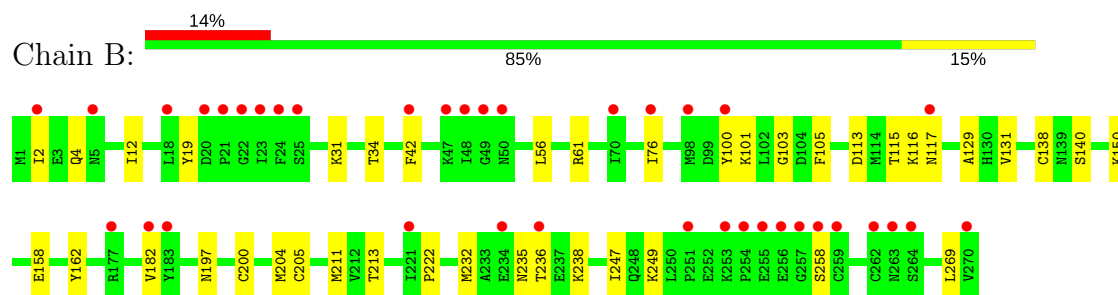
3 Residue-property plots

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

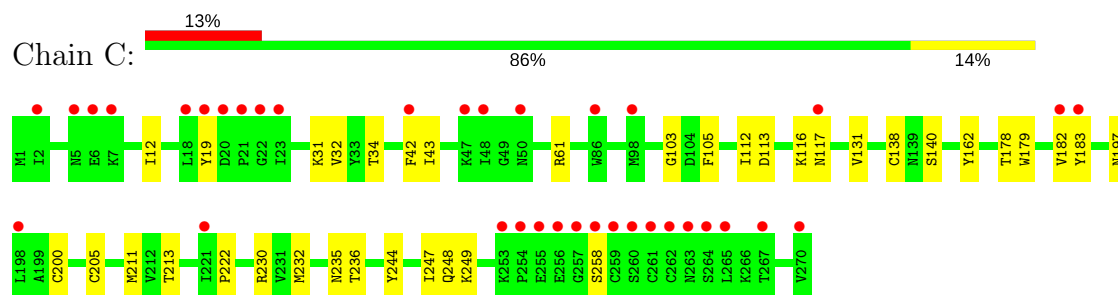
- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)



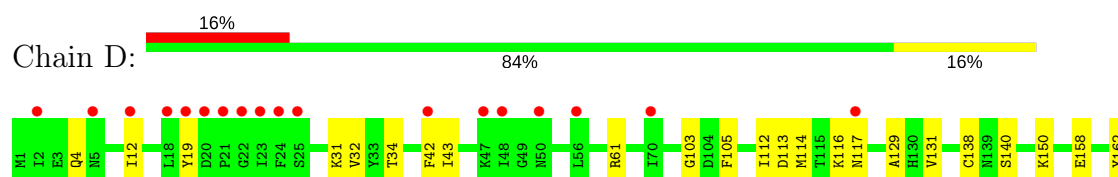
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- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)

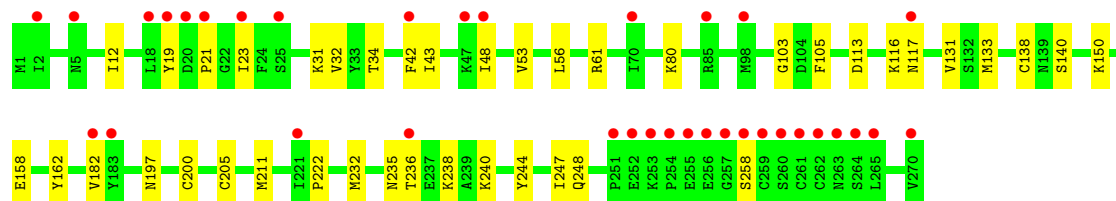
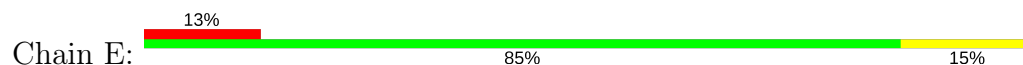


- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)

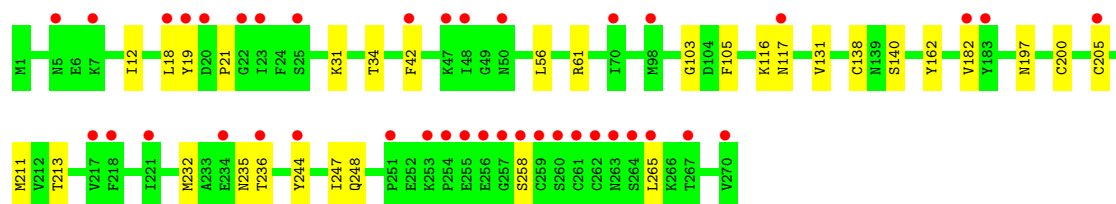




- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)



- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.16Å 138.09Å 96.56Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	39.67 – 1.45 39.67 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.67-1.45) 97.0 (39.67-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 1.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.169 , 0.185 0.165 , 0.182	Depositor DCC
R_{free} test set	20889 reflections (6.93%)	DCC
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.000 for -1/2*h-1/2*k-l,1/2*h+1/2*k-l,1/2 *h-1/2*k 0.000 for -1/2*h-1/2*k+l,1/2*h+1/2*k+l,-1 /2*h+1/2*k 0.000 for -1/2*h+1/2*k+l,-1/2*h+1/2*k-l,- 1/2*h-1/2*k 0.000 for -1/2*h+1/2*k-l,-1/2*h+1/2*k+l,1 /2*h+1/2*k 0.041 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.034 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/ 2*h+1/2*k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2 *h-1/2*k 0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1 /2*h+1/2*k 0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14787	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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.

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.06 % 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 9.0813e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MTA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2191	0.55	0/2969
1	B	0.33	0/2284	0.58	1/3095 (0.0%)
1	C	0.32	0/2294	0.56	0/3106
1	D	0.31	0/2273	0.54	0/3080
1	E	0.33	0/2332	0.56	1/3158 (0.0%)
1	F	0.31	0/2231	0.54	1/3023 (0.0%)
All	All	0.32	0/13605	0.55	3/18431 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	56	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	56	LEU	CA-CB-CG	5.11	127.05	115.30
1	E	56	LEU	CA-CB-CG	5.07	126.97	115.30

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	2145	0	2102	29	0
1	B	2237	0	2190	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2246	0	2208	37	0
1	D	2226	0	2188	46	0
1	E	2286	0	2262	37	0
1	F	2185	0	2154	28	0
2	A	20	0	15	1	0
2	B	20	0	15	0	0
2	C	20	0	15	1	0
2	D	20	0	15	1	0
2	E	20	0	15	1	0
2	F	20	0	15	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
4	A	196	0	0	2	0
4	B	230	0	0	3	0
4	C	208	0	0	2	0
4	D	219	0	0	1	0
4	E	222	0	0	2	0
4	F	202	0	0	1	0
All	All	14787	0	13194	192	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 7.

All (192) 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:F:12[B]:ILE:HD11	1:F:247:ILE:HD11	1.48	0.92
1:B:12[A]:ILE:HD11	1:B:247:ILE:HD11	1.52	0.90
1:E:131[B]:VAL:HG11	1:E:200:CYS:SG	2.15	0.87
1:B:131[B]:VAL:HG11	1:B:200:CYS:SG	2.14	0.86
1:F:131[B]:VAL:HG11	1:F:200:CYS:SG	2.15	0.86
1:E:117[B]:ASN:HB3	1:F:117[B]:ASN:HA	1.59	0.83
1:C:131[B]:VAL:HG11	1:C:200:CYS:SG	2.19	0.83
1:B:117[B]:ASN:HB3	1:C:117[B]:ASN:HA	1.58	0.83
1:D:117[B]:ASN:HA	1:F:117[B]:ASN:HB3	1.60	0.82
1:D:131[B]:VAL:HG11	1:D:200:CYS:SG	2.19	0.82
1:C:12[B]:ILE:HD11	1:C:247:ILE:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12[B]:ILE:HD11	1:D:247:ILE:HD11	1.64	0.80
1:A:117[B]:ASN:HA	1:C:117[B]:ASN:HD22	1.51	0.76
1:E:12[B]:ILE:HD11	1:E:247:ILE:HD11	1.67	0.76
1:A:117[B]:ASN:HB3	1:B:117[B]:ASN:HA	1.68	0.74
1:A:117[B]:ASN:HA	1:C:117[B]:ASN:HB3	1.69	0.74
1:B:2:ILE:HD11	4:B:423:HOH:O	1.87	0.74
1:D:182[B]:VAL:HG13	1:F:182:VAL:HG11	1.68	0.73
1:D:117[B]:ASN:HB3	1:E:117[B]:ASN:HA	1.71	0.71
1:A:117[B]:ASN:HD22	1:B:117[B]:ASN:HA	1.54	0.71
1:B:117[B]:ASN:HD22	1:C:117[B]:ASN:HA	1.58	0.68
1:E:236[A]:THR:HG22	1:E:240:LYS:HE3	1.76	0.65
1:B:105:PHE:HE2	1:B:238:LYS:HE3	1.61	0.65
1:B:138:CYS:SG	1:B:205[B]:CYS:HB3	2.36	0.65
1:D:138:CYS:SG	1:D:205[B]:CYS:HB3	2.36	0.65
1:E:23:ILE:HD12	1:E:48[B]:ILE:HD13	1.80	0.64
1:E:222:PRO:HB2	4:F:397:HOH:O	1.99	0.63
1:D:4:GLN:NE2	4:D:1209:HOH:O	2.28	0.62
1:B:105:PHE:CE2	1:B:238:LYS:HE3	2.34	0.61
1:A:213:THR:HG21	1:A:232[B]:MET:HG2	1.80	0.61
1:E:48[A]:ILE:HG22	1:E:248[A]:GLN:OE1	2.01	0.60
1:E:244:TYR:O	1:E:248[A]:GLN:HG2	2.01	0.60
1:A:138:CYS:SG	1:A:205[B]:CYS:HB3	2.42	0.60
1:D:117[B]:ASN:HD22	1:E:117[B]:ASN:HA	1.67	0.59
1:E:117[B]:ASN:HD22	1:F:117[B]:ASN:HA	1.67	0.59
1:E:48[B]:ILE:HD12	1:E:53[B]:VAL:HG21	1.83	0.59
1:D:182[B]:VAL:HG12	1:D:183[B]:TYR:CD2	2.37	0.59
1:E:211[A]:MET:SD	1:E:235:ASN:CB	2.91	0.58
1:D:114:MET:SD	1:D:183[B]:TYR:HE1	2.27	0.58
1:E:138:CYS:SG	1:E:205[B]:CYS:HB3	2.44	0.58
1:A:244:TYR:CE2	1:A:248:GLN:NE2	2.72	0.58
1:C:103:GLY:HA2	1:C:211[B]:MET:SD	2.44	0.58
1:C:32:VAL:HG21	1:C:43[B]:ILE:HD12	1.85	0.58
1:E:116[B]:LYS:O	1:E:117[B]:ASN:OD1	2.22	0.57
1:D:32:VAL:HG21	1:D:43[B]:ILE:HD12	1.87	0.57
1:A:103:GLY:HA2	1:A:211[B]:MET:SD	2.45	0.57
1:B:211[A]:MET:SD	1:B:235:ASN:CB	2.93	0.56
1:D:163:ILE:CD1	1:D:183[B]:TYR:HD1	2.18	0.56
1:C:112:ILE:HD13	1:C:183[B]:TYR:HB3	1.87	0.56
1:E:211[A]:MET:SD	1:E:235:ASN:HB2	2.46	0.56
4:A:1122:HOH:O	1:C:222:PRO:HB2	2.04	0.56
1:A:4:GLN:NE2	4:A:402:HOH:O	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:THR:HG21	1:C:232[B]:MET:HG2	1.88	0.55
1:D:19:TYR:CE1	1:D:61:ARG:HA	2.41	0.55
1:E:105:PHE:CE2	1:E:238:LYS:HE3	2.41	0.55
1:D:163:ILE:HD12	1:D:183[B]:TYR:HD1	1.71	0.55
1:A:105:PHE:HE2	1:A:238:LYS:HE3	1.70	0.55
1:F:213:THR:HG21	1:F:232[B]:MET:HG2	1.89	0.55
1:B:232[A]:MET:O	1:B:236:THR:HG23	2.07	0.55
1:D:112:ILE:CD1	1:D:183[B]:TYR:HB3	2.38	0.54
1:B:222:PRO:HB2	4:C:386:HOH:O	2.08	0.54
1:B:213:THR:HG21	1:B:232[B]:MET:HG2	1.89	0.54
1:D:178:THR:HG23	1:D:182[B]:VAL:HG21	1.90	0.54
1:E:105:PHE:HE2	1:E:238:LYS:HE3	1.71	0.54
1:B:117[B]:ASN:HB3	1:C:117[B]:ASN:CA	2.34	0.54
1:C:138:CYS:SG	1:C:205[B]:CYS:HB3	2.47	0.53
1:A:105:PHE:CE2	1:A:238:LYS:HE3	2.43	0.53
1:B:211[A]:MET:SD	1:B:235:ASN:HB2	2.49	0.53
1:C:112:ILE:CD1	1:C:183[B]:TYR:HB3	2.39	0.53
1:F:103:GLY:HA2	1:F:211[B]:MET:SD	2.49	0.53
1:A:31:LYS:HG2	1:A:42[B]:PHE:CE1	2.44	0.52
1:B:4:GLN:NE2	4:B:423:HOH:O	2.42	0.52
1:F:18:LEU:HD11	1:F:21:PRO:HA	1.91	0.52
1:D:103:GLY:HA2	1:D:211[B]:MET:SD	2.49	0.52
1:F:116[B]:LYS:O	1:F:117[B]:ASN:OD1	2.27	0.52
1:B:103:GLY:HA2	1:B:211[B]:MET:SD	2.49	0.52
1:F:131[B]:VAL:CG1	1:F:200:CYS:SG	2.94	0.52
1:C:31:LYS:HG2	1:C:42[A]:PHE:CE2	2.44	0.52
1:D:140:SER:HB3	1:D:258:SER:CB	2.40	0.52
1:F:138:CYS:SG	1:F:205[B]:CYS:HB3	2.49	0.52
1:A:232[A]:MET:O	1:A:236:THR:HG23	2.10	0.52
1:D:116[B]:LYS:O	1:D:117[B]:ASN:OD1	2.27	0.52
1:E:117[B]:ASN:CB	1:F:117[B]:ASN:HA	2.38	0.52
1:A:222:PRO:HB2	4:B:509:HOH:O	2.10	0.51
1:B:117[B]:ASN:CB	1:C:117[B]:ASN:HA	2.36	0.51
1:D:112:ILE:HD13	1:D:183[B]:TYR:HB3	1.92	0.51
1:E:32:VAL:HG21	1:E:43[B]:ILE:HD12	1.91	0.51
1:D:211[A]:MET:SD	1:D:235:ASN:CB	3.00	0.50
1:D:211[A]:MET:SD	1:D:235:ASN:HB2	2.50	0.50
1:E:131[B]:VAL:CG1	1:E:200:CYS:SG	2.96	0.50
1:F:31:LYS:HG2	1:F:42[A]:PHE:CE1	2.46	0.50
1:F:140:SER:HB3	1:F:258:SER:CB	2.42	0.50
1:D:117[B]:ASN:HA	1:F:117[B]:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131[B]:VAL:HG12	1:E:133[B]:MET:HG3	1.93	0.49
1:D:178:THR:HG23	1:D:182[B]:VAL:CG2	2.43	0.49
1:B:140:SER:HB3	1:B:258:SER:CB	2.42	0.49
1:B:2:ILE:C	1:B:2:ILE:HD12	2.33	0.49
1:F:211[A]:MET:HE2	1:F:232[A]:MET:SD	2.52	0.49
1:A:211[A]:MET:SD	1:A:235:ASN:HB2	2.53	0.48
1:C:178:THR:HG23	1:C:182[B]:VAL:HG21	1.93	0.48
1:B:31:LYS:HG2	1:B:42[A]:PHE:CE2	2.48	0.48
1:E:150:LYS:HE3	1:E:158:GLU:OE2	2.13	0.48
1:E:31:LYS:HG2	1:E:42[A]:PHE:CE2	2.47	0.48
1:C:19:TYR:CE1	1:C:61:ARG:HA	2.48	0.48
1:A:117[B]:ASN:HA	1:C:117[B]:ASN:ND2	2.26	0.48
1:C:244:TYR:CE2	1:C:248:GLN:NE2	2.82	0.48
1:D:112:ILE:HD13	1:D:183[A]:TYR:HD1	1.79	0.48
1:A:19:TYR:CE1	1:A:61:ARG:HA	2.48	0.48
1:A:116[B]:LYS:O	1:A:117[B]:ASN:OD1	2.31	0.47
1:A:117[B]:ASN:CA	1:C:117[B]:ASN:HB3	2.43	0.47
1:A:211[A]:MET:SD	1:A:235:ASN:CB	3.02	0.47
1:A:116[A]:LYS:HE3	1:B:113:ASP:OD2	2.13	0.47
1:C:131[B]:VAL:CG1	1:C:200:CYS:SG	3.00	0.47
1:E:19:TYR:CE1	1:E:61:ARG:HA	2.49	0.47
1:C:211[A]:MET:SD	1:C:235:ASN:CB	3.03	0.47
1:B:182:VAL:HG11	1:C:182[B]:VAL:HG13	1.96	0.47
1:D:182[A]:VAL:HG11	1:E:182:VAL:HG13	1.96	0.47
1:C:116[B]:LYS:O	1:C:117[B]:ASN:OD1	2.33	0.47
1:E:232[B]:MET:O	1:E:236[B]:THR:HG23	2.15	0.47
1:D:182[B]:VAL:HG12	1:D:183[B]:TYR:HD2	1.79	0.46
1:D:116[A]:LYS:HE3	1:E:113:ASP:OD2	2.14	0.46
1:D:117[B]:ASN:HA	1:F:117[B]:ASN:CB	2.37	0.46
1:E:103:GLY:HA2	1:E:211[B]:MET:SD	2.55	0.46
1:D:113:ASP:OD2	1:F:116[A]:LYS:HE3	2.14	0.46
1:D:31:LYS:HG2	1:D:42[B]:PHE:CE1	2.50	0.46
1:E:12[B]:ILE:HD11	1:E:247:ILE:CD1	2.43	0.46
1:B:100[A]:TYR:O	1:B:101[A]:LYS:HD3	2.16	0.46
1:B:211[A]:MET:HE1	1:B:232[A]:MET:HA	1.96	0.46
1:B:19:TYR:CE1	1:B:61:ARG:HA	2.50	0.46
1:F:19:TYR:CE1	1:F:61:ARG:HA	2.51	0.45
1:B:129:ALA:HB2	1:B:269:LEU:HD23	1.99	0.45
1:F:211[A]:MET:SD	1:F:235:ASN:CB	3.05	0.45
1:B:116[B]:LYS:O	1:B:117[B]:ASN:OD1	2.34	0.45
1:E:140:SER:HB3	1:E:258:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:CZ	1:B:211[B]:MET:HE2	2.51	0.45
1:E:236[A]:THR:CG2	1:E:240:LYS:HE3	2.44	0.45
1:A:211[A]:MET:HE2	1:A:232[A]:MET:SD	2.56	0.45
1:D:114:MET:SD	1:D:183[B]:TYR:CE1	3.09	0.45
1:C:230:ARG:NH1	4:C:1204:HOH:O	2.38	0.45
1:F:211[A]:MET:SD	1:F:235:ASN:HB2	2.57	0.45
1:B:117[B]:ASN:ND2	1:C:117[B]:ASN:HA	2.30	0.44
1:E:23:ILE:HD12	1:E:48[B]:ILE:CD1	2.46	0.44
1:D:117[B]:ASN:CA	1:F:117[B]:ASN:HB3	2.38	0.44
1:A:116[B]:LYS:HD3	1:B:115:THR:O	2.17	0.44
1:F:244:TYR:CE2	1:F:248:GLN:NE2	2.86	0.44
1:A:101:LYS:NZ	1:A:101:LYS:HB3	2.32	0.43
1:A:150:LYS:HE3	1:A:158:GLU:OE2	2.17	0.43
1:D:131[B]:VAL:CG1	1:D:200:CYS:SG	2.99	0.43
2:A:901:MTA:H2'	2:A:901:MTA:N3	2.34	0.43
1:D:12[B]:ILE:HD11	1:D:247:ILE:CD1	2.42	0.43
1:D:105:PHE:HE2	1:D:238:LYS:HE2	1.84	0.43
1:A:113:ASP:OD2	1:C:116[A]:LYS:HE3	2.19	0.43
1:E:21:PRO:HB2	1:E:23:ILE:CD1	2.48	0.43
1:B:131[B]:VAL:CG1	1:B:200:CYS:SG	2.97	0.43
1:C:12[B]:ILE:HD11	1:C:247:ILE:CD1	2.41	0.43
1:D:232[A]:MET:O	1:D:236:THR:HG23	2.19	0.43
1:C:179:TRP:O	1:C:183[A]:TYR:HB2	2.19	0.43
1:C:178:THR:HG23	1:C:182[B]:VAL:CG2	2.49	0.43
2:C:901:MTA:H2'	2:C:901:MTA:N3	2.34	0.43
1:D:265:LEU:HD23	1:D:265:LEU:HA	1.88	0.43
1:F:232[A]:MET:O	1:F:236:THR:HG23	2.19	0.43
1:D:229[B]:THR:HG21	4:E:1227:HOH:O	2.18	0.42
1:C:105:PHE:CZ	1:C:211[B]:MET:CE	3.03	0.42
1:D:249:LYS:HB2	1:D:249:LYS:NZ	2.35	0.42
1:B:2:ILE:O	1:B:2:ILE:HD12	2.20	0.42
1:F:105:PHE:CZ	1:F:211[B]:MET:CE	3.03	0.42
1:A:117[B]:ASN:CB	1:B:117[B]:ASN:HA	2.45	0.42
1:C:232[A]:MET:O	1:C:236:THR:HG23	2.20	0.42
2:D:901:MTA:N3	2:D:901:MTA:H2'	2.35	0.42
1:C:249:LYS:HB2	1:C:249:LYS:NZ	2.35	0.41
1:D:150:LYS:HE3	1:D:158:GLU:OE1	2.19	0.41
1:E:211[A]:MET:SD	1:E:235:ASN:HB3	2.59	0.41
1:B:76:ILE:HG23	1:B:204[B]:MET:HE1	2.02	0.41
1:C:140:SER:HB3	1:C:258:SER:CB	2.50	0.41
1:A:115:THR:O	1:C:116[B]:LYS:HD3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LYS:HE3	1:B:158:GLU:OE2	2.20	0.41
1:D:105:PHE:CZ	1:D:211[B]:MET:CE	3.03	0.41
1:D:232[B]:MET:O	1:D:236:THR:HG23	2.19	0.41
1:D:129:ALA:HB2	1:D:269:LEU:HD23	2.03	0.41
1:B:105:PHE:CE1	1:B:211[B]:MET:HE2	2.55	0.41
1:D:238:LYS:HB3	1:D:238:LYS:HE2	1.89	0.41
1:E:80:LYS:HD2	4:E:881:HOH:O	2.21	0.41
1:E:105:PHE:CZ	1:E:211[B]:MET:CE	3.04	0.41
1:F:265:LEU:HA	1:F:265:LEU:HD23	1.85	0.41
1:A:32:VAL:HG21	1:A:43:ILE:HD12	2.02	0.40
1:F:105:PHE:CZ	1:F:211[B]:MET:HE2	2.56	0.40
1:B:211[A]:MET:SD	1:B:235:ASN:HB3	2.60	0.40
1:B:249:LYS:HB2	1:B:249:LYS:NZ	2.36	0.40
1:B:116[A]:LYS:HE3	1:C:113:ASP:OD2	2.21	0.40
1:D:177:ARG:O	1:D:181[B]:GLU:HB2	2.21	0.40
2:E:901:MTA:N3	2:E:901:MTA:H2'	2.37	0.40
2:F:901:MTA:N3	2:F:901:MTA:H2'	2.36	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	281/270 (104%)	278 (99%)	3 (1%)	0	100	100
1	B	291/270 (108%)	289 (99%)	2 (1%)	0	100	100
1	C	291/270 (108%)	289 (99%)	2 (1%)	0	100	100
1	D	290/270 (107%)	289 (100%)	1 (0%)	0	100	100
1	E	299/270 (111%)	298 (100%)	1 (0%)	0	100	100
1	F	285/270 (106%)	280 (98%)	5 (2%)	0	100	100
All	All	1737/1620 (107%)	1723 (99%)	14 (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	222/231 (96%)	218 (98%)	4 (2%)	64	27
1	B	234/231 (101%)	231 (99%)	3 (1%)	73	40
1	C	234/231 (101%)	231 (99%)	3 (1%)	73	40
1	D	232/231 (100%)	228 (98%)	4 (2%)	66	29
1	E	239/231 (104%)	236 (99%)	3 (1%)	73	40
1	F	229/231 (99%)	226 (99%)	3 (1%)	73	40
All	All	1390/1386 (100%)	1370 (99%)	20 (1%)	68	38

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	162	TYR
1	A	197	ASN
1	A	265	LEU
1	B	34	THR
1	B	162	TYR
1	B	197	ASN
1	C	34	THR
1	C	162	TYR
1	C	197	ASN
1	D	34	THR
1	D	162	TYR
1	D	197	ASN
1	D	265	LEU
1	E	34	THR
1	E	162	TYR
1	E	197	ASN
1	F	34	THR
1	F	162	TYR

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Mol	Chain	Res	Type
1	F	197	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 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 ⓘ

19 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	$\# Z > 2$
3	SO4	A	271[A]	-	4,4,4	0.20	0	6,6,6	0.11	0
3	SO4	A	271[B]	-	4,4,4	0.13	0	6,6,6	0.11	0
2	MTA	A	901	-	19,22,22	1.19	2 (10%)	18,32,32	1.92	4 (22%)
3	SO4	A	902	-	4,4,4	0.11	0	6,6,6	0.42	0
3	SO4	B	271	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	B	272	-	4,4,4	0.21	0	6,6,6	0.14	0
2	MTA	B	901	-	19,22,22	1.30	2 (10%)	18,32,32	2.00	6 (33%)
3	SO4	B	902	-	4,4,4	0.16	0	6,6,6	0.53	0
2	MTA	C	901	-	19,22,22	1.17	2 (10%)	18,32,32	2.12	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	902	-	4,4,4	0.16	0	6,6,6	0.49	0
3	SO4	D	271[A]	-	4,4,4	0.15	0	6,6,6	0.15	0
3	SO4	D	271[B]	-	4,4,4	0.19	0	6,6,6	0.14	0
2	MTA	D	901	-	19,22,22	1.15	3 (15%)	18,32,32	2.12	5 (27%)
3	SO4	D	902	-	4,4,4	0.19	0	6,6,6	0.51	0
3	SO4	E	271	-	4,4,4	0.18	0	6,6,6	0.15	0
2	MTA	E	901	-	19,22,22	1.19	2 (10%)	18,32,32	2.06	4 (22%)
3	SO4	E	902	-	4,4,4	0.11	0	6,6,6	0.44	0
2	MTA	F	901	-	19,22,22	1.27	3 (15%)	18,32,32	1.88	5 (27%)
3	SO4	F	902	-	4,4,4	0.18	0	6,6,6	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
3	SO4	A	271[A]	-	-	0/0/0/0	0/0/0/0
3	SO4	A	271[B]	-	-	0/0/0/0	0/0/0/0
2	MTA	A	901	-	-	0/3/23/23	0/3/3/3
3	SO4	A	902	-	-	0/0/0/0	0/0/0/0
3	SO4	B	271	-	-	0/0/0/0	0/0/0/0
3	SO4	B	272	-	-	0/0/0/0	0/0/0/0
2	MTA	B	901	-	-	0/3/23/23	0/3/3/3
3	SO4	B	902	-	-	0/0/0/0	0/0/0/0
2	MTA	C	901	-	-	0/3/23/23	0/3/3/3
3	SO4	C	902	-	-	0/0/0/0	0/0/0/0
3	SO4	D	271[A]	-	-	0/0/0/0	0/0/0/0
3	SO4	D	271[B]	-	-	0/0/0/0	0/0/0/0
2	MTA	D	901	-	-	0/3/23/23	0/3/3/3
3	SO4	D	902	-	-	0/0/0/0	0/0/0/0
3	SO4	E	271	-	-	0/0/0/0	0/0/0/0
2	MTA	E	901	-	-	0/3/23/23	0/3/3/3
3	SO4	E	902	-	-	0/0/0/0	0/0/0/0
2	MTA	F	901	-	-	0/3/23/23	0/3/3/3
3	SO4	F	902	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	MTA	C5'-S5'	-2.08	1.78	1.80
2	D	901	MTA	C5'-S5'	-2.06	1.78	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	MTA	O4'-C1'	2.44	1.44	1.41
2	C	901	MTA	O4'-C1'	2.58	1.44	1.41
2	D	901	MTA	C5-C4	2.68	1.46	1.40
2	E	901	MTA	O4'-C1'	2.75	1.45	1.41
2	F	901	MTA	O4'-C1'	2.79	1.45	1.41
2	A	901	MTA	O4'-C1'	2.90	1.45	1.41
2	E	901	MTA	C5-C4	2.93	1.47	1.40
2	C	901	MTA	C5-C4	2.97	1.47	1.40
2	A	901	MTA	C5-C4	2.99	1.47	1.40
2	F	901	MTA	C5-C4	3.04	1.47	1.40
2	B	901	MTA	C5-C4	3.05	1.47	1.40
2	B	901	MTA	O4'-C1'	3.16	1.45	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	MTA	N3-C2-N1	-6.16	123.50	128.86
2	B	901	MTA	N3-C2-N1	-6.10	123.55	128.86
2	D	901	MTA	N3-C2-N1	-5.60	123.98	128.86
2	C	901	MTA	N3-C2-N1	-5.06	124.45	128.86
2	A	901	MTA	N3-C2-N1	-4.87	124.61	128.86
2	F	901	MTA	N3-C2-N1	-4.61	124.84	128.86
2	F	901	MTA	C4-C5-N7	-2.55	106.94	109.41
2	D	901	MTA	C4-C5-N7	-2.27	107.22	109.41
2	C	901	MTA	C4-C5-N7	-2.14	107.34	109.41
2	B	901	MTA	C4-C5-N7	-2.07	107.41	109.41
2	B	901	MTA	C4'-O4'-C1'	2.04	111.94	109.77
2	F	901	MTA	C4'-O4'-C1'	2.08	111.98	109.77
2	C	901	MTA	C1'-N9-C4	2.11	130.28	126.64
2	B	901	MTA	C1'-N9-C4	2.12	130.31	126.64
2	D	901	MTA	C1'-N9-C4	2.13	130.31	126.64
2	A	901	MTA	C1'-N9-C4	2.14	130.33	126.64
2	E	901	MTA	N6-C6-N1	2.19	123.12	118.77
2	F	901	MTA	C1'-N9-C4	2.23	130.48	126.64
2	B	901	MTA	C2-N1-C6	2.25	122.70	118.77
2	C	901	MTA	C2'-C3'-C4'	2.44	107.37	102.62
2	A	901	MTA	C4'-O4'-C1'	2.61	112.55	109.77
2	B	901	MTA	CS-S5'-C5'	2.61	105.39	101.19
2	E	901	MTA	C2-N1-C6	2.73	123.55	118.77
2	D	901	MTA	C4'-O4'-C1'	2.97	112.93	109.77
2	E	901	MTA	CS-S5'-C5'	3.08	106.14	101.19
2	C	901	MTA	C4'-O4'-C1'	3.41	113.40	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	MTA	CS-S5'-C5'	3.70	107.13	101.19
2	A	901	MTA	CS-S5'-C5'	3.80	107.30	101.19
2	C	901	MTA	CS-S5'-C5'	4.13	107.82	101.19
2	D	901	MTA	CS-S5'-C5'	4.13	107.83	101.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	MTA	1	0
2	C	901	MTA	1	0
2	D	901	MTA	1	0
2	E	901	MTA	1	0
2	F	901	MTA	1	0

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	270/270 (100%)	1.05	38 (14%) 3 3	17, 25, 48, 88	0
1	B	270/270 (100%)	1.13	37 (13%) 3 4	17, 24, 49, 90	0
1	C	270/270 (100%)	1.12	36 (13%) 4 4	17, 25, 49, 91	0
1	D	270/270 (100%)	1.12	42 (15%) 2 3	17, 26, 50, 88	0
1	E	270/270 (100%)	1.08	35 (12%) 4 4	17, 24, 45, 90	0
1	F	270/270 (100%)	1.16	40 (14%) 3 3	18, 26, 49, 98	0
All	All	1620/1620 (100%)	1.11	228 (14%) 3 3	17, 25, 49, 98	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	CYS	12.9
1	C	259	CYS	12.7
1	F	256	GLU	11.4
1	F	259	CYS	11.0
1	E	257	GLY	10.6
1	D	259	CYS	10.3
1	F	257	GLY	9.9
1	A	259	CYS	9.2
1	E	259	CYS	8.9
1	B	262	CYS	8.5
1	B	257	GLY	8.3
1	D	263	ASN	8.0
1	F	262	CYS	8.0
1	E	263	ASN	7.9
1	D	257	GLY	7.8
1	A	257	GLY	7.3
1	C	256	GLU	7.2
1	C	263	ASN	7.2
1	C	262	CYS	7.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	CYS	7.0
1	B	258	SER	7.0
1	C	221	ILE	6.8
1	D	262	CYS	6.8
1	B	48	ILE	6.7
1	B	256	GLU	6.3
1	F	258	SER	6.3
1	C	255	GLU	6.2
1	C	257	GLY	6.1
1	D	48	ILE	6.1
1	E	256	GLU	5.7
1	E	258	SER	5.7
1	F	18	LEU	5.4
1	C	264	SER	5.4
1	A	48	ILE	5.3
1	E	262	CYS	5.3
1	A	258	SER	5.3
1	C	18	LEU	5.2
1	B	255	GLU	5.2
1	F	255	GLU	5.2
1	D	50	ASN	5.1
1	A	256	GLU	5.1
1	A	221	ILE	5.0
1	B	270	VAL	4.9
1	F	270	VAL	4.7
1	A	254	PRO	4.7
1	A	2	ILE	4.6
1	D	255	GLU	4.6
1	A	263	ASN	4.5
1	A	270	VAL	4.4
1	A	21	PRO	4.4
1	F	263	ASN	4.4
1	F	221	ILE	4.2
1	B	100[A]	TYR	4.2
1	F	48	ILE	4.2
1	B	182	VAL	4.1
1	B	50	ASN	4.1
1	C	117[A]	ASN	4.1
1	C	183[A]	TYR	4.1
1	E	221	ILE	4.1
1	D	182[A]	VAL	4.1
1	D	183[A]	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	251	PRO	4.1
1	D	258	SER	4.1
1	F	183	TYR	4.0
1	C	48	ILE	4.0
1	E	270	VAL	4.0
1	E	236[A]	THR	4.0
1	E	255	GLU	3.9
1	C	182[A]	VAL	3.9
1	B	20	ASP	3.9
1	E	2	ILE	3.8
1	E	264	SER	3.8
1	D	256	GLU	3.8
1	B	263	ASN	3.8
1	D	5[A]	ASN	3.8
1	F	47	LYS	3.8
1	F	236	THR	3.8
1	A	261	CYS	3.8
1	E	23	ILE	3.8
1	F	182	VAL	3.8
1	F	22	GLY	3.8
1	E	18	LEU	3.7
1	F	264	SER	3.7
1	C	20	ASP	3.7
1	C	2	ILE	3.7
1	C	50	ASN	3.7
1	D	47	LYS	3.7
1	E	253	LYS	3.6
1	D	19	TYR	3.6
1	F	19	TYR	3.6
1	C	258	SER	3.6
1	D	253	LYS	3.6
1	B	254	PRO	3.6
1	B	18	LEU	3.5
1	B	2	ILE	3.5
1	F	260	SER	3.5
1	B	49	GLY	3.5
1	E	260	SER	3.5
1	F	50	ASN	3.4
1	C	5	ASN	3.4
1	F	20	ASP	3.4
1	C	270	VAL	3.4
1	D	22	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	19	TYR	3.3
1	A	260	SER	3.3
1	C	21	PRO	3.3
1	F	25[A]	SER	3.3
1	E	254	PRO	3.3
1	D	25	SER	3.3
1	A	255	GLU	3.3
1	A	22	GLY	3.3
1	C	261	CYS	3.3
1	E	5[A]	ASN	3.2
1	C	23	ILE	3.2
1	D	20	ASP	3.2
1	D	2	ILE	3.2
1	D	221	ILE	3.2
1	B	98[A]	MET	3.2
1	A	264	SER	3.2
1	D	265	LEU	3.2
1	F	234	GLU	3.2
1	D	254	PRO	3.1
1	A	117[A]	ASN	3.1
1	E	251	PRO	3.1
1	C	19	TYR	3.1
1	E	21	PRO	3.1
1	A	251	PRO	3.0
1	F	5	ASN	3.0
1	A	252	GLU	3.0
1	E	261	CYS	3.0
1	E	183	TYR	3.0
1	E	70	ILE	3.0
1	D	260	SER	3.0
1	D	42[A]	PHE	3.0
1	E	182	VAL	3.0
1	A	253	LYS	3.0
1	B	23	ILE	3.0
1	E	42[A]	PHE	2.9
1	B	264	SER	2.9
1	B	22	GLY	2.9
1	C	253	LYS	2.9
1	C	98[A]	MET	2.9
1	E	98	MET	2.9
1	B	221	ILE	2.9
1	B	253	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	25	SER	2.9
1	C	22	GLY	2.9
1	D	18	LEU	2.9
1	D	267	THR	2.9
1	F	265	LEU	2.9
1	F	7	LYS	2.8
1	E	85	ARG	2.8
1	F	23	ILE	2.8
1	F	98	MET	2.8
1	A	6	GLU	2.8
1	E	265	LEU	2.8
1	E	48[A]	ILE	2.8
1	D	251	PRO	2.8
1	B	183	TYR	2.8
1	B	21	PRO	2.7
1	F	267	THR	2.7
1	A	182	VAL	2.7
1	D	177	ARG	2.7
1	B	42[A]	PHE	2.7
1	B	25	SER	2.7
1	A	100	TYR	2.6
1	E	47[A]	LYS	2.6
1	C	254	PRO	2.6
1	A	183	TYR	2.6
1	D	12[A]	ILE	2.6
1	A	50	ASN	2.6
1	B	117[A]	ASN	2.6
1	A	236	THR	2.6
1	B	5[A]	ASN	2.5
1	F	254	PRO	2.5
1	D	250	LEU	2.5
1	F	253	LYS	2.5
1	A	19	TYR	2.5
1	D	117[A]	ASN	2.5
1	D	270	VAL	2.5
1	B	251	PRO	2.5
1	A	23	ILE	2.5
1	A	5	ASN	2.5
1	B	177	ARG	2.5
1	D	184[A]	LYS	2.5
1	B	47	LYS	2.5
1	F	70	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	42[A]	PHE	2.4
1	F	261	CYS	2.4
1	A	85	ARG	2.4
1	E	117[A]	ASN	2.4
1	D	230	ARG	2.4
1	C	6	GLU	2.3
1	B	234	GLU	2.3
1	D	261	CYS	2.3
1	E	20	ASP	2.3
1	C	86	TRP	2.3
1	A	101	LYS	2.3
1	C	267	THR	2.3
1	C	265	LEU	2.3
1	E	25	SER	2.2
1	A	218	PHE	2.2
1	F	218	PHE	2.2
1	C	7	LYS	2.2
1	D	23	ILE	2.2
1	D	70	ILE	2.2
1	D	56	LEU	2.2
1	B	76	ILE	2.2
1	E	252	GLU	2.2
1	A	36	TYR	2.2
1	F	244	TYR	2.2
1	A	232[A]	MET	2.2
1	B	24	PHE	2.1
1	F	42[A]	PHE	2.1
1	D	231	VAL	2.1
1	C	260	SER	2.1
1	F	205[A]	CYS	2.1
1	C	198	LEU	2.1
1	F	117[A]	ASN	2.1
1	B	70	ILE	2.1
1	D	24	PHE	2.1
1	A	13	ILE	2.0
1	D	21	PRO	2.0
1	D	219	ALA	2.0
1	F	217	VAL	2.0
1	A	98	MET	2.0
1	B	236	THR	2.0
1	C	47	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	271[B]	5/5	0.87	0.23	14.51	28,28,34,36	5
3	SO4	A	271[A]	5/5	0.87	0.23	9.68	25,26,29,32	5
3	SO4	B	272	5/5	0.85	0.32	2.69	30,31,36,38	0
3	SO4	D	271[A]	5/5	0.88	0.17	2.69	28,31,34,35	5
3	SO4	D	271[B]	5/5	0.88	0.17	2.18	26,30,33,33	5
2	MTA	F	901	20/20	0.91	0.12	0.42	19,21,27,27	0
2	MTA	D	901	20/20	0.91	0.12	0.17	20,21,28,28	0
2	MTA	C	901	20/20	0.93	0.11	-0.30	19,21,27,30	0
2	MTA	B	901	20/20	0.94	0.11	-0.38	17,20,24,27	0
2	MTA	A	901	20/20	0.93	0.10	-0.38	18,20,26,29	0
2	MTA	E	901	20/20	0.95	0.10	-0.61	17,19,23,27	0
3	SO4	B	902	5/5	0.98	0.09	-2.01	20,20,25,26	0
3	SO4	D	902	5/5	0.97	0.08	-2.05	21,21,25,26	0
3	SO4	F	902	5/5	0.97	0.08	-2.43	21,22,25,26	0
3	SO4	A	902	5/5	0.97	0.08	-2.63	21,21,25,26	0
3	SO4	C	902	5/5	0.97	0.08	-2.63	20,21,24,25	0
3	SO4	E	902	5/5	0.98	0.07	-3.20	19,20,23,25	0
3	SO4	B	271	5/5	0.84	0.19	-	26,28,30,32	5
3	SO4	E	271	5/5	0.93	0.18	-	26,27,29,30	5

6.5 Other polymers [i](#)

There are no such residues in this entry.