Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 02:24 am GMT

PDB ID	:	1O9T
Title	:	Methionine adenosyltransferase complexed with both substrates ATP and methionine
Authors	:	Gonzalez, B.; Pajares, M.A.; Hermoso, J.A.; Sanz-Aparicio, J.
Deposited on	:	2002-12-18
Resolution	:	2.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

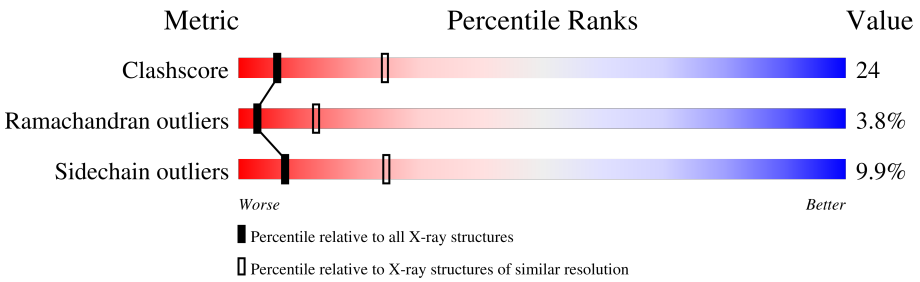
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 of 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	55% 31% 6% • 7%
1	B	396	54% 31% 8% • 7%

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	PO4	A	1398	-	X	-	-
3	PO4	B	1398	-	X	X	-
6	ATP	B	1397	-	-	X	-

2 Entry composition (i)

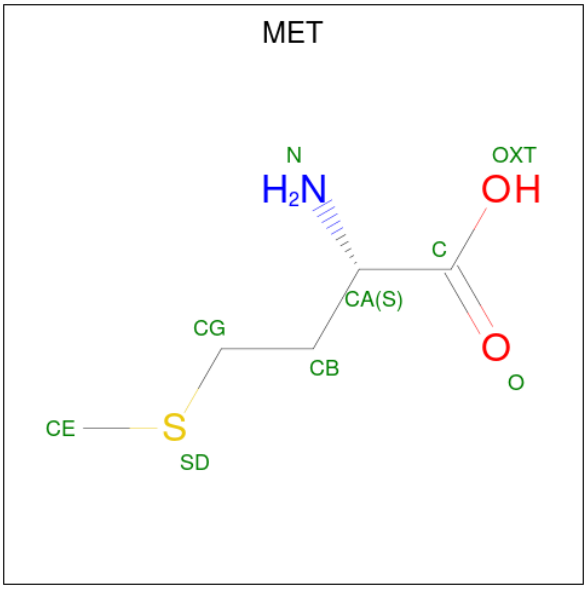
There are 7 unique types of molecules in this entry. The entry contains 5923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-ADENOSYLMETHIONINE SYNTHETASE.

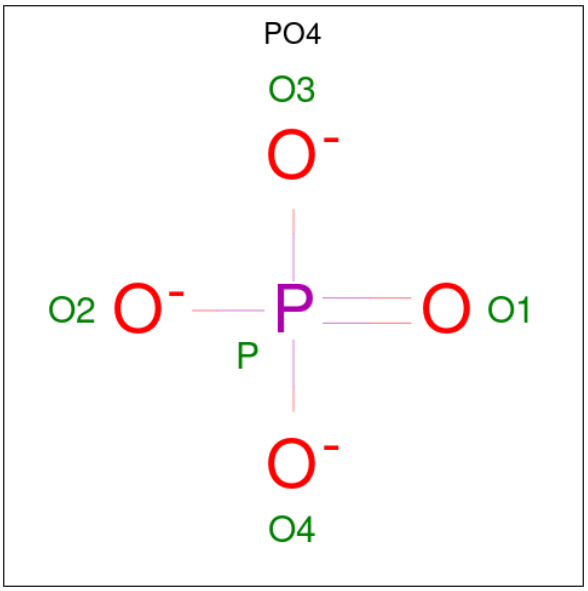
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2846	1803	491	536	16	0	0	0
1	B	368	2846	1803	491	536	16	0	0	0

- Molecule 2 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

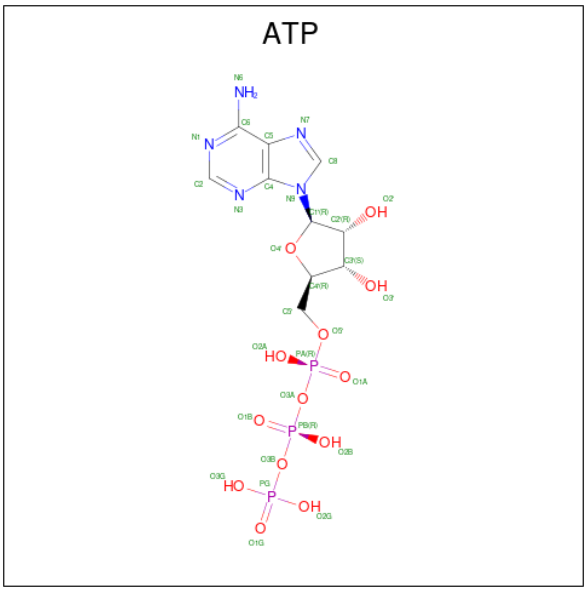
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	B	1	Total K 1 1	0	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	31	10	5	13	3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	94	94	94	0	0
			Total	O		
7	B	82	82	82	0	0

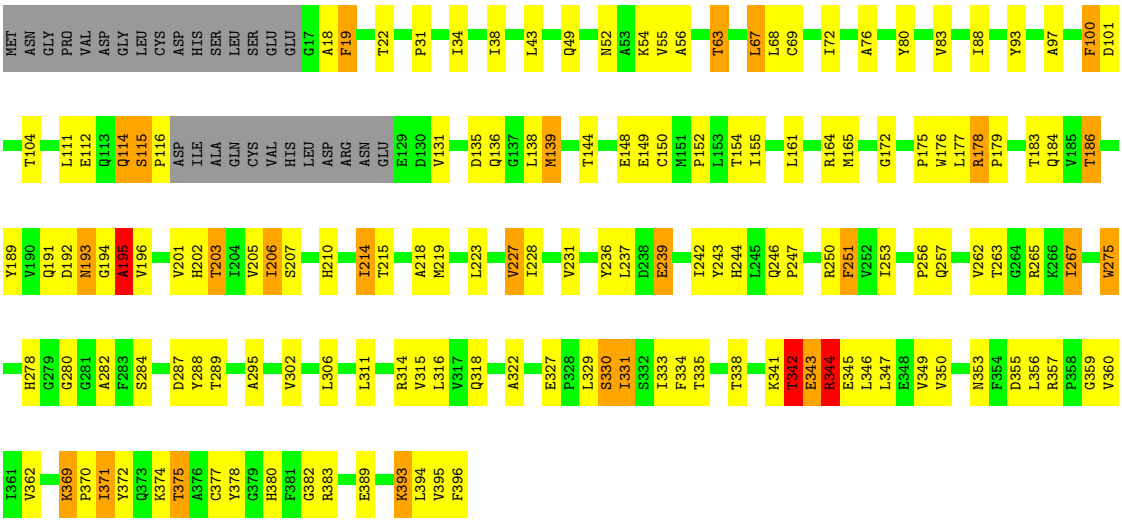
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

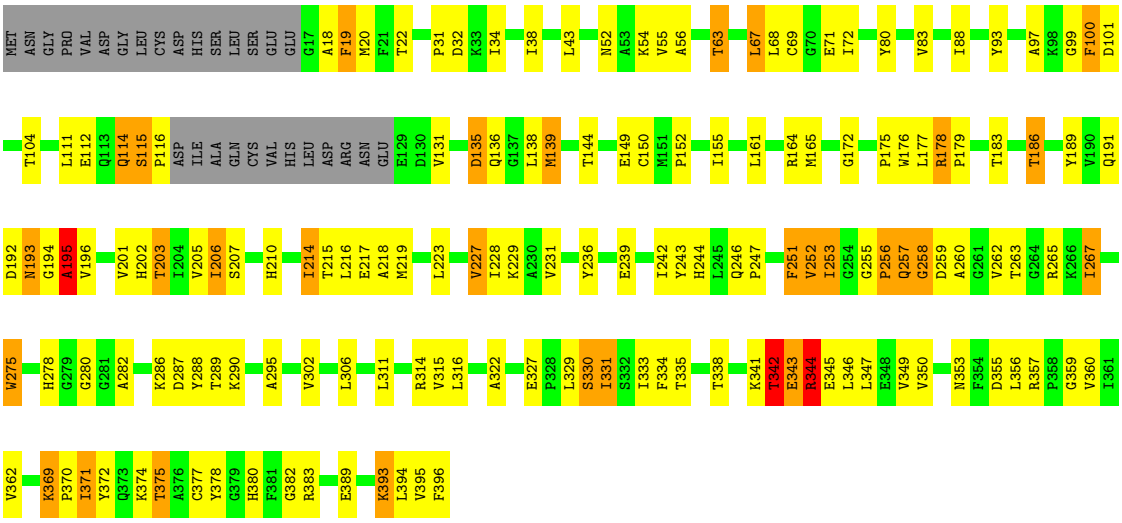
• Molecule 1: S-ADENOSYLMETHIONINE SYNTHETASE

Chain A: 55% 31% 6% • 7%



• Molecule 1: S-ADENOSYLMETHIONINE SYNTHETASE

Chain B: 54% 31% 8% • 7%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	114.99Å 114.99Å 160.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.5 (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.265 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5923	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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, ATP, MG, K

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	0.38	0/2901	0.71	4/3926 (0.1%)
1	B	0.39	0/2901	0.69	2/3926 (0.1%)
All	All	0.38	0/5802	0.70	6/7852 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	ARG	NE-CZ-NH2	6.53	123.57	120.30
1	A	250	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	B	178	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	178	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	B	195	ALA	O-C-N	6.09	132.45	122.70
1	A	195	ALA	O-C-N	5.86	132.08	122.70

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	2846	0	2852	131	0
1	B	2846	0	2852	150	0
2	A	9	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	3	0
4	A	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	31	0	12	12	0
7	A	94	0	0	3	0
7	B	82	0	0	14	0
All	All	5923	0	5724	276	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 24.

All (276) 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:B:19:PHE:CE1	1:B:189:TYR:HB2	1.89	1.08
1:A:19:PHE:CE1	1:A:189:TYR:HB2	1.98	0.99
1:A:267:ILE:HD11	1:A:282:ALA:HA	1.47	0.96
1:B:267:ILE:HD11	1:B:282:ALA:HA	1.45	0.95
1:A:100:PHE:HD2	1:A:256:PRO:HG2	1.33	0.93
1:A:100:PHE:CD2	1:A:256:PRO:HG2	2.04	0.92
1:B:215:THR:HG21	7:B:2041:HOH:O	1.71	0.90
1:B:19:PHE:HE1	1:B:189:TYR:CB	1.84	0.89
1:B:290:LYS:HE2	6:B:1397:ATP:H2'	1.53	0.88
1:B:216:LEU:HD23	7:B:2045:HOH:O	1.73	0.86
1:B:19:PHE:CE1	1:B:189:TYR:CB	2.56	0.85
1:A:262:VAL:HG11	1:B:262:VAL:HG11	1.60	0.84
1:B:278:HIS:HD2	1:B:280:GLY:H	1.28	0.82
1:B:290:LYS:HG2	6:B:1397:ATP:H3'	1.62	0.82
1:A:19:PHE:HD1	1:A:19:PHE:C	1.83	0.82
2:A:1397:MET:N	6:B:1397:ATP:O2B	2.15	0.80
1:A:138:LEU:HD22	1:B:22:THR:H	1.47	0.79
1:B:203:THR:HB	1:B:242:ILE:HB	1.65	0.79
1:A:203:THR:HB	1:A:242:ILE:HB	1.65	0.79
1:B:205:VAL:HG22	1:B:244:HIS:HB2	1.64	0.78
1:A:278:HIS:HD2	1:A:280:GLY:H	1.28	0.78
1:A:205:VAL:HG22	1:A:244:HIS:HB2	1.66	0.78
1:B:72:ILE:HG12	1:B:111:LEU:HD11	1.66	0.77
1:B:210:HIS:CE1	1:B:251:PHE:H	2.03	0.77
1:A:19:PHE:C	1:A:19:PHE:CD1	2.58	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLY:O	1:B:195:ALA:HB2	1.89	0.72
1:B:223:LEU:O	1:B:227:VAL:HG22	1.89	0.72
1:B:19:PHE:HE1	1:B:189:TYR:HB3	1.55	0.71
1:B:100:PHE:HD2	1:B:256:PRO:HG2	1.54	0.71
1:B:262:VAL:HG13	7:B:2010:HOH:O	1.90	0.71
1:A:194:GLY:O	1:A:195:ALA:HB2	1.90	0.71
1:B:100:PHE:CD2	1:B:256:PRO:HG2	2.25	0.71
1:A:19:PHE:HD1	1:A:19:PHE:O	1.73	0.70
1:B:55:VAL:HA	1:B:72:ILE:HG22	1.73	0.70
1:A:322:ALA:HB2	1:A:329:LEU:HD22	1.74	0.70
1:A:72:ILE:HG12	1:A:111:LEU:HD11	1.74	0.70
1:A:148:GLU:HB2	7:A:2030:HOH:O	1.92	0.69
1:B:322:ALA:HB2	1:B:329:LEU:HD22	1.73	0.69
1:A:186:THR:CG2	1:A:203:THR:HG23	2.23	0.69
1:A:55:VAL:HA	1:A:72:ILE:HG22	1.73	0.69
1:B:286:LYS:NZ	3:B:1398:PO4:O2	2.26	0.69
1:A:353:ASN:HD22	1:A:394:LEU:HD22	1.58	0.69
1:B:186:THR:CG2	1:B:203:THR:HG23	2.23	0.68
1:B:71:GLU:HB3	6:B:1397:ATP:N6	2.09	0.68
1:B:19:PHE:CD1	1:B:189:TYR:HB2	2.30	0.67
1:B:353:ASN:HD22	1:B:394:LEU:HD22	1.58	0.67
1:B:286:LYS:HD3	6:B:1397:ATP:O3'	1.94	0.67
1:A:342:THR:O	1:A:345:GLU:HB2	1.94	0.66
1:B:31:PRO:HG3	1:B:256:PRO:HA	1.77	0.66
1:A:19:PHE:CE1	1:A:189:TYR:CB	2.77	0.66
1:A:267:ILE:HG23	1:A:278:HIS:CE1	2.30	0.66
1:B:267:ILE:HG23	1:B:278:HIS:CE1	2.30	0.65
1:A:333:ILE:O	1:A:343:GLU:HG2	1.97	0.65
1:B:286:LYS:HE2	6:B:1397:ATP:O3'	1.97	0.65
1:A:329:LEU:O	1:A:330:SER:HB3	1.97	0.65
1:A:22:THR:H	1:B:138:LEU:HD22	1.61	0.64
1:A:31:PRO:HG3	1:A:256:PRO:HA	1.79	0.64
1:B:286:LYS:CD	6:B:1397:ATP:O3'	2.45	0.64
1:B:186:THR:HG23	1:B:203:THR:HG23	1.79	0.64
1:B:333:ILE:O	1:B:343:GLU:HG2	1.97	0.63
1:A:186:THR:HG23	1:A:203:THR:HG23	1.80	0.63
1:A:210:HIS:CE1	1:A:251:PHE:H	2.18	0.62
1:A:19:PHE:CD1	1:A:189:TYR:HB2	2.36	0.61
1:B:99:GLY:HA3	1:B:255:GLY:HA3	1.81	0.61
1:B:329:LEU:O	1:B:330:SER:HB3	2.00	0.61
1:A:223:LEU:O	1:A:227:VAL:HG22	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:CE	6:B:1397:ATP:O3'	2.50	0.59
1:B:335:THR:HG22	1:B:338:THR:H	1.67	0.59
1:A:335:THR:HG22	1:A:338:THR:H	1.67	0.59
1:B:369:LYS:O	1:B:371:ILE:HD13	2.02	0.59
1:B:217:GLU:CG	7:B:2044:HOH:O	2.50	0.59
1:A:239:GLU:HB2	7:A:2055:HOH:O	2.03	0.59
1:A:345:GLU:O	1:A:349:VAL:HG23	2.03	0.59
1:B:56:ALA:H	1:B:72:ILE:HG22	1.68	0.58
1:B:290:LYS:CG	6:B:1397:ATP:H3'	2.32	0.58
1:B:393:LYS:HG2	7:B:2080:HOH:O	2.02	0.58
1:A:172:GLY:O	1:A:175:PRO:HD3	2.04	0.58
1:A:19:PHE:CD1	1:A:19:PHE:O	2.56	0.58
1:A:369:LYS:O	1:A:371:ILE:HD13	2.03	0.58
1:A:56:ALA:H	1:A:72:ILE:HG22	1.69	0.57
1:B:72:ILE:CG1	1:B:111:LEU:HD11	2.34	0.57
1:B:172:GLY:O	1:B:175:PRO:HD3	2.02	0.57
1:B:393:LYS:H	1:B:393:LYS:HD2	1.69	0.57
1:B:93:TYR:OH	1:B:256:PRO:HD3	2.04	0.57
1:A:393:LYS:H	1:A:393:LYS:HD2	1.69	0.56
1:A:344:ARG:NE	1:A:347:LEU:HD23	2.20	0.56
1:A:97:ALA:O	1:A:253:ILE:HG23	2.05	0.56
1:B:97:ALA:O	1:B:253:ILE:HG23	2.05	0.56
1:A:22:THR:OG1	1:A:186:THR:HB	2.06	0.56
1:A:184:GLN:OE1	1:B:136:GLN:HB2	2.06	0.56
1:B:246:GLN:N	1:B:247:PRO:HD3	2.21	0.56
1:B:228:ILE:HG21	1:B:243:TYR:HE2	1.71	0.55
1:B:259:ASP:HB3	7:B:2057:HOH:O	2.06	0.55
1:A:246:GLN:N	1:A:247:PRO:HD3	2.21	0.55
1:B:344:ARG:NE	1:B:347:LEU:HD23	2.22	0.55
1:B:114:GLN:HE21	1:B:114:GLN:N	2.05	0.55
1:A:186:THR:HG21	1:A:203:THR:HG23	1.89	0.55
1:A:228:ILE:HG21	1:A:243:TYR:HE2	1.70	0.55
1:A:207:SER:HA	1:A:246:GLN:OE1	2.07	0.54
1:A:67:LEU:HD22	1:A:69:CYS:SG	2.47	0.54
3:B:1398:PO4:P	7:B:2082:HOH:O	2.66	0.54
1:B:194:GLY:O	1:B:195:ALA:CB	2.56	0.54
1:B:257:GLN:HB3	7:B:2055:HOH:O	2.08	0.54
1:B:22:THR:OG1	1:B:186:THR:HB	2.07	0.54
1:B:229:LYS:HE3	7:B:2047:HOH:O	2.08	0.54
1:B:43:LEU:HD13	1:B:55:VAL:HB	1.90	0.54
1:A:114:GLN:HE21	1:A:114:GLN:N	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HD22	1:B:69:CYS:SG	2.49	0.53
1:B:72:ILE:HD11	1:B:80:TYR:OH	2.08	0.53
1:B:207:SER:HA	1:B:246:GLN:OE1	2.08	0.53
1:A:136:GLN:NE2	1:A:322:ALA:HA	2.23	0.53
1:B:186:THR:HG21	1:B:203:THR:HG23	1.90	0.53
1:B:71:GLU:HB3	6:B:1397:ATP:HN61	1.71	0.53
1:A:144:THR:O	1:A:150:CYS:HA	2.09	0.52
1:A:395:VAL:HG12	1:A:395:VAL:O	2.10	0.52
1:A:72:ILE:CG1	1:A:111:LEU:HD11	2.39	0.52
1:B:52:ASN:HA	1:B:288:TYR:OH	2.10	0.52
1:B:275:TRP:HE1	1:B:314:ARG:HH21	1.57	0.52
1:A:43:LEU:HD13	1:A:55:VAL:HB	1.90	0.52
1:A:72:ILE:HD11	1:A:80:TYR:OH	2.08	0.52
1:B:302:VAL:O	1:B:306:LEU:HD13	2.09	0.52
1:B:259:ASP:CB	7:B:2057:HOH:O	2.58	0.52
1:A:275:TRP:HE1	1:A:314:ARG:HH21	1.56	0.52
1:B:144:THR:O	1:B:150:CYS:HA	2.09	0.52
1:B:383:ARG:O	1:B:389:GLU:HG3	2.09	0.52
1:B:201:VAL:HG23	1:B:236:TYR:HB3	1.92	0.52
1:A:346:LEU:O	1:A:350:VAL:HG23	2.10	0.51
1:B:345:GLU:O	1:B:349:VAL:HG23	2.09	0.51
1:A:311:LEU:HD22	1:A:341:LYS:HD2	1.91	0.51
1:A:383:ARG:O	1:A:389:GLU:HG3	2.10	0.51
1:A:52:ASN:HA	1:A:288:TYR:OH	2.11	0.51
1:A:201:VAL:HG23	1:A:236:TYR:HB3	1.92	0.51
1:A:202:HIS:ND1	1:A:203:THR:HG22	2.26	0.51
1:B:219:MET:HE1	1:B:246:GLN:HE21	1.74	0.51
1:B:346:LEU:O	1:B:350:VAL:HG23	2.10	0.51
1:A:302:VAL:O	1:A:306:LEU:HD13	2.09	0.51
1:A:371:ILE:HB	1:A:374:LYS:HE2	1.93	0.51
1:B:395:VAL:O	1:B:395:VAL:HG12	2.10	0.51
1:B:52:ASN:HA	1:B:288:TYR:HH	1.76	0.51
1:B:371:ILE:HD13	1:B:371:ILE:H	1.76	0.51
1:B:227:VAL:O	1:B:231:VAL:HG22	2.11	0.50
1:B:202:HIS:ND1	1:B:203:THR:HG22	2.26	0.50
1:B:210:HIS:HE1	1:B:251:PHE:H	1.55	0.50
1:B:311:LEU:HD22	1:B:341:LYS:HD2	1.91	0.50
1:A:371:ILE:HD13	1:A:371:ILE:H	1.77	0.50
1:A:375:THR:HG23	1:A:380:HIS:NE2	2.27	0.50
2:A:1397:MET:N	6:B:1397:ATP:PB	2.85	0.49
1:B:161:LEU:HD23	1:B:183:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:TYR:O	1:A:375:THR:HG22	2.12	0.49
1:B:227:VAL:CG2	1:B:228:ILE:N	2.74	0.49
1:A:284:SER:HB2	7:A:2004:HOH:O	2.12	0.49
1:A:227:VAL:O	1:A:231:VAL:HG22	2.12	0.49
1:B:375:THR:HG23	1:B:380:HIS:NE2	2.27	0.49
1:A:161:LEU:HD23	1:A:183:THR:HG23	1.95	0.49
1:B:161:LEU:O	1:B:165:MET:HG3	2.12	0.49
1:A:318:GLN:NE2	1:B:20:MET:O	2.46	0.49
1:B:372:TYR:O	1:B:375:THR:HG22	2.12	0.49
1:A:214:ILE:HD12	1:A:219:MET:CG	2.43	0.48
1:B:214:ILE:HD12	1:B:219:MET:CG	2.43	0.48
1:A:219:MET:O	1:A:223:LEU:HD13	2.14	0.48
1:A:93:TYR:CZ	1:A:256:PRO:HG3	2.48	0.48
1:B:371:ILE:HB	1:B:374:LYS:HE2	1.94	0.48
1:B:331:ILE:HG23	1:B:347:LEU:HD11	1.95	0.48
1:B:165:MET:SD	1:B:206:ILE:HD11	2.54	0.48
1:B:176:TRP:CZ3	1:B:177:LEU:HD13	2.49	0.47
3:B:1398:PO4:O4	7:B:2082:HOH:O	2.20	0.47
1:B:219:MET:O	1:B:223:LEU:HD13	2.14	0.47
1:A:331:ILE:HG23	1:A:347:LEU:HD11	1.96	0.47
1:A:93:TYR:CE1	1:A:256:PRO:HD3	2.50	0.47
1:A:161:LEU:O	1:A:165:MET:HG3	2.13	0.47
1:A:176:TRP:CZ3	1:A:177:LEU:HD13	2.49	0.47
1:B:136:GLN:NE2	1:B:322:ALA:HA	2.29	0.47
1:B:217:GLU:CD	7:B:2044:HOH:O	2.53	0.47
1:A:19:PHE:HE1	1:A:189:TYR:HB2	1.72	0.47
1:B:165:MET:CE	1:B:206:ILE:HD11	2.45	0.47
1:B:316:LEU:HB3	1:B:334:PHE:HB2	1.97	0.47
1:A:152:PRO:HB2	1:A:155:ILE:HG22	1.97	0.47
1:A:165:MET:SD	1:A:206:ILE:HD11	2.55	0.46
1:A:316:LEU:HB3	1:A:334:PHE:HB2	1.97	0.46
1:B:152:PRO:HB2	1:B:155:ILE:HG22	1.96	0.46
1:A:219:MET:HE1	1:A:246:GLN:HE21	1.81	0.46
1:A:115:SER:H	1:A:116:PRO:HD2	1.80	0.46
1:A:215:THR:HG23	1:A:218:ALA:H	1.81	0.46
1:B:32:ASP:OD2	7:B:2006:HOH:O	2.21	0.46
1:B:344:ARG:HD2	1:B:344:ARG:HA	1.64	0.46
1:B:34:ILE:O	1:B:38:ILE:HG13	2.16	0.45
1:B:259:ASP:O	1:B:260:ALA:HB3	2.16	0.45
1:A:334:PHE:HZ	1:B:19:PHE:CD2	2.33	0.45
1:B:115:SER:H	1:B:116:PRO:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLY:O	1:A:195:ALA:CB	2.57	0.45
1:B:165:MET:HE2	1:B:177:LEU:HD11	1.98	0.45
1:B:215:THR:HG23	1:B:218:ALA:H	1.82	0.45
1:A:34:ILE:O	1:A:38:ILE:HG13	2.16	0.45
1:A:165:MET:CE	1:A:206:ILE:HD11	2.46	0.45
1:A:205:VAL:HG21	1:B:136:GLN:HG3	1.99	0.45
1:B:257:GLN:O	1:B:259:ASP:N	2.49	0.45
1:A:344:ARG:HD2	1:A:344:ARG:HA	1.62	0.45
1:A:353:ASN:ND2	1:A:394:LEU:HA	2.32	0.45
1:A:19:PHE:HE1	1:A:189:TYR:CG	2.34	0.45
1:A:227:VAL:CG2	1:A:228:ILE:N	2.80	0.44
1:B:217:GLU:HA	7:B:2043:HOH:O	2.17	0.44
1:A:139:MET:HG2	1:A:295:ALA:HB3	1.99	0.44
1:B:111:LEU:HD13	1:B:112:GLU:N	2.32	0.44
1:A:111:LEU:HD13	1:A:112:GLU:N	2.32	0.44
1:A:355:ASP:OD2	1:A:360:VAL:HG21	2.18	0.44
1:B:257:GLN:O	1:B:260:ALA:N	2.48	0.44
1:B:257:GLN:C	1:B:259:ASP:N	2.69	0.44
1:A:165:MET:HE2	1:A:177:LEU:HD11	2.00	0.44
1:B:353:ASN:ND2	1:B:394:LEU:HA	2.33	0.44
1:B:252:VAL:HG12	1:B:253:ILE:HD13	1.99	0.43
1:B:72:ILE:CD1	1:B:111:LEU:HD11	2.49	0.43
1:B:219:MET:CE	1:B:246:GLN:HE21	2.30	0.43
1:A:214:ILE:HD12	1:A:219:MET:HG2	2.01	0.43
1:B:214:ILE:HD12	1:B:219:MET:HG3	2.01	0.43
1:B:342:THR:O	1:B:345:GLU:HB2	2.18	0.43
1:A:52:ASN:HA	1:A:288:TYR:HH	1.82	0.43
1:A:395:VAL:O	1:A:396:PHE:HB2	2.18	0.43
1:B:101:ASP:HB3	1:B:104:THR:OG1	2.18	0.43
1:B:149:GLU:O	1:B:150:CYS:HB2	2.19	0.43
1:A:88:ILE:HG22	1:A:93:TYR:HB2	2.00	0.43
1:A:101:ASP:HB3	1:A:104:THR:OG1	2.18	0.43
1:A:219:MET:CE	1:A:246:GLN:HE21	2.32	0.43
1:A:393:LYS:O	1:A:394:LEU:HB2	2.18	0.43
1:B:80:TYR:HA	1:B:83:VAL:HG22	2.00	0.43
1:B:139:MET:HG2	1:B:295:ALA:HB3	2.00	0.43
1:B:395:VAL:O	1:B:396:PHE:HB2	2.19	0.42
1:A:72:ILE:CD1	1:A:111:LEU:HD11	2.48	0.42
1:A:80:TYR:HA	1:A:83:VAL:HG22	2.00	0.42
1:A:253:ILE:O	1:A:253:ILE:HG22	2.18	0.42
1:B:88:ILE:HG22	1:B:93:TYR:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:CG1	1:B:263:THR:N	2.82	0.42
1:A:93:TYR:CE2	1:A:256:PRO:HG3	2.54	0.42
1:A:341:LYS:O	1:A:342:THR:HG22	2.20	0.42
1:B:267:ILE:HD13	1:B:267:ILE:HA	1.77	0.42
1:B:393:LYS:O	1:B:394:LEU:HB2	2.18	0.42
1:B:359:GLY:O	1:B:362:VAL:HG22	2.19	0.42
1:A:136:GLN:CG	1:B:205:VAL:HG21	2.49	0.42
1:A:149:GLU:O	1:A:150:CYS:HB2	2.19	0.42
1:A:262:VAL:CG1	1:A:263:THR:N	2.82	0.42
1:A:377:CYS:O	1:A:378:TYR:HB2	2.20	0.42
1:B:161:LEU:HD23	1:B:183:THR:CG2	2.50	0.42
1:A:139:MET:SD	1:A:139:MET:N	2.93	0.42
1:B:355:ASP:OD2	1:B:360:VAL:HG21	2.19	0.42
1:A:334:PHE:HZ	1:B:19:PHE:HD2	1.68	0.42
1:B:135:ASP:O	1:B:136:GLN:C	2.59	0.42
1:A:214:ILE:HD12	1:A:219:MET:HG3	2.01	0.41
1:B:192:ASP:O	1:B:194:GLY:N	2.54	0.41
1:B:257:GLN:O	1:B:258:GLY:C	2.59	0.41
1:A:49:GLN:HB2	1:A:76:ALA:HB1	2.02	0.41
1:B:214:ILE:HD12	1:B:219:MET:HG2	2.01	0.41
1:B:343:GLU:OE2	1:B:346:LEU:HD12	2.20	0.41
1:B:290:LYS:NZ	6:B:1397:ATP:C2	2.89	0.41
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.84	0.41
1:B:219:MET:HE1	1:B:246:GLN:NE2	2.35	0.41
1:A:327:GLU:HA	1:A:357:ARG:HG2	2.03	0.41
1:B:377:CYS:O	1:B:378:TYR:HB2	2.21	0.41
1:A:369:LYS:HG3	1:A:370:PRO:HD2	2.02	0.41
1:B:369:LYS:HG3	1:B:370:PRO:HD2	2.02	0.41
1:A:382:GLY:H	1:A:389:GLU:CD	2.23	0.41
1:B:192:ASP:O	1:B:193:ASN:C	2.59	0.41
1:A:54:LYS:HA	1:A:287:ASP:OD2	2.21	0.41
1:A:154:THR:HG23	1:A:155:ILE:N	2.36	0.41
1:A:178:ARG:HB3	1:A:179:PRO:HD2	2.02	0.41
1:A:192:ASP:O	1:A:194:GLY:N	2.54	0.41
1:B:178:ARG:HB3	1:B:179:PRO:HD2	2.02	0.41
1:A:161:LEU:HD23	1:A:183:THR:CG2	2.51	0.41
1:A:251:PHE:CE2	2:A:1397:MET:HA	2.56	0.41
1:A:344:ARG:CD	1:A:347:LEU:HD23	2.51	0.41
1:B:382:GLY:H	1:B:389:GLU:CD	2.24	0.41
1:B:54:LYS:HA	1:B:287:ASP:OD2	2.21	0.40
1:B:327:GLU:HA	1:B:357:ARG:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:O	1:A:193:ASN:C	2.59	0.40
1:A:359:GLY:O	1:A:362:VAL:HG22	2.20	0.40
1:A:93:TYR:CZ	1:A:256:PRO:HD3	2.56	0.40
1:B:161:LEU:HD12	1:B:161:LEU:HA	1.95	0.40
1:B:262:VAL:HG12	1:B:263:THR:N	2.35	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	364/396 (92%)	311 (85%)	41 (11%)	12 (3%)	4 15
1	B	364/396 (92%)	312 (86%)	36 (10%)	16 (4%)	2 10
All	All	728/792 (92%)	623 (86%)	77 (11%)	28 (4%)	3 13

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	196	VAL
1	B	18	ALA
1	B	196	VAL
1	A	131	VAL
1	A	193	ASN
1	A	344	ARG
1	B	135	ASP
1	B	193	ASN
1	B	256	PRO
1	B	344	ARG
1	A	63	THR
1	A	115	SER

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Mol	Chain	Res	Type
1	A	135	ASP
1	A	342	THR
1	B	63	THR
1	B	115	SER
1	B	131	VAL
1	B	258	GLY
1	B	342	THR
1	A	195	ALA
1	A	330	SER
1	B	195	ALA
1	B	356	LEU
1	A	356	LEU
1	B	330	SER
1	B	253	ILE
1	B	252	VAL

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	307/332 (92%)	277 (90%)	30 (10%)	8 24
1	B	307/332 (92%)	277 (90%)	30 (10%)	8 24
All	All	614/664 (92%)	554 (90%)	60 (10%)	8 24

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	PHE
1	A	63	THR
1	A	67	LEU
1	A	68	LEU
1	A	100	PHE
1	A	114	GLN
1	A	139	MET
1	A	164	ARG

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Mol	Chain	Res	Type
1	A	186	THR
1	A	191	GLN
1	A	203	THR
1	A	206	ILE
1	A	214	ILE
1	A	227	VAL
1	A	239	GLU
1	A	251	PHE
1	A	257	GLN
1	A	265	ARG
1	A	267	ILE
1	A	275	TRP
1	A	289	THR
1	A	315	VAL
1	A	331	ILE
1	A	342	THR
1	A	343	GLU
1	A	344	ARG
1	A	369	LYS
1	A	371	ILE
1	A	375	THR
1	A	393	LYS
1	B	19	PHE
1	B	63	THR
1	B	67	LEU
1	B	68	LEU
1	B	100	PHE
1	B	114	GLN
1	B	139	MET
1	B	164	ARG
1	B	186	THR
1	B	191	GLN
1	B	203	THR
1	B	206	ILE
1	B	214	ILE
1	B	227	VAL
1	B	239	GLU
1	B	251	PHE
1	B	257	GLN
1	B	265	ARG
1	B	267	ILE
1	B	275	TRP

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Mol	Chain	Res	Type
1	B	289	THR
1	B	315	VAL
1	B	331	ILE
1	B	342	THR
1	B	343	GLU
1	B	344	ARG
1	B	369	LYS
1	B	371	ILE
1	B	375	THR
1	B	393	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	113	GLN
1	A	114	GLN
1	A	136	GLN
1	A	159	HIS
1	A	162	ASN
1	A	191	GLN
1	A	209	GLN
1	A	210	HIS
1	A	278	HIS
1	A	318	GLN
1	A	353	ASN
1	A	380	HIS
1	B	52	ASN
1	B	113	GLN
1	B	114	GLN
1	B	136	GLN
1	B	159	HIS
1	B	162	ASN
1	B	184	GLN
1	B	191	GLN
1	B	209	GLN
1	B	210	HIS
1	B	278	HIS
1	B	318	GLN
1	B	353	ASN
1	B	380	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
6	ATP	B	1397	4	26,33,33	2.06	10 (38%)	31,52,52	2.67	15 (48%)
3	PO4	A	1398	-	4,4,4	4.04	3 (75%)	6,6,6	1.71	2 (33%)
2	MET	A	1397	4	7,8,8	0.62	0	7,9,9	0.84	0
3	PO4	B	1398	-	4,4,4	3.30	3 (75%)	6,6,6	1.63	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	B	1397	4	-	6/18/38/38	0/3/3/3
2	MET	A	1397	4	-	6/8/8/8	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1398	PO4	P-O1	5.65	1.64	1.50
3	B	1398	PO4	P-O1	4.76	1.62	1.50
6	B	1397	ATP	PG-O1G	4.26	1.64	1.50
3	A	1398	PO4	P-O4	4.26	1.67	1.54
6	B	1397	ATP	O4'-C1'	4.04	1.46	1.41
3	B	1398	PO4	P-O3	3.82	1.66	1.54
6	B	1397	ATP	PG-O2G	-3.68	1.40	1.54
3	A	1398	PO4	P-O3	3.49	1.65	1.54
6	B	1397	ATP	PB-O2B	-3.47	1.39	1.55
6	B	1397	ATP	PB-O1B	3.03	1.61	1.50
6	B	1397	ATP	C2-N3	2.89	1.36	1.32
6	B	1397	ATP	O3'-C3'	-2.28	1.37	1.43
6	B	1397	ATP	O4'-C4'	2.24	1.50	1.45
6	B	1397	ATP	C2'-C1'	-2.10	1.50	1.53
3	B	1398	PO4	P-O4	2.10	1.60	1.54
6	B	1397	ATP	PA-O5'	2.05	1.67	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1397	ATP	N3-C2-N1	-6.33	118.79	128.68
6	B	1397	ATP	O2G-PG-O3B	5.69	123.72	104.64
6	B	1397	ATP	PB-O3B-PG	-5.31	114.59	132.83
6	B	1397	ATP	O3B-PG-O1G	-4.64	85.46	111.19
6	B	1397	ATP	C3'-C2'-C1'	4.28	107.42	100.98
6	B	1397	ATP	C4-C5-N7	3.37	112.91	109.40
6	B	1397	ATP	O5'-C5'-C4'	2.98	119.25	108.99
6	B	1397	ATP	C2'-C3'-C4'	2.94	108.35	102.64
6	B	1397	ATP	PA-O3A-PB	-2.62	123.84	132.83
3	A	1398	PO4	O4-P-O2	2.46	115.86	107.97
3	B	1398	PO4	O4-P-O1	-2.40	102.12	110.89
6	B	1397	ATP	C2-N1-C6	2.37	122.81	118.75
6	B	1397	ATP	O2A-PA-O1A	2.30	123.62	112.24
6	B	1397	ATP	O3G-PG-O2G	2.14	115.80	107.64
6	B	1397	ATP	O3G-PG-O1G	-2.07	102.57	110.68
6	B	1397	ATP	O5'-PA-O1A	-2.06	101.00	109.07
3	A	1398	PO4	O3-P-O2	2.04	114.51	107.97
6	B	1397	ATP	O2A-PA-O5'	-2.00	98.44	107.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1397	ATP	C4'-C5'-O5'-PA
6	B	1397	ATP	C3'-C4'-C5'-O5'
2	A	1397	MET	OXT-C-CA-N
6	B	1397	ATP	O4'-C4'-C5'-O5'
2	A	1397	MET	CA-CB-CG-SD
2	A	1397	MET	O-C-CA-CB
2	A	1397	MET	OXT-C-CA-CB
6	B	1397	ATP	PA-O3A-PB-O1B
2	A	1397	MET	CB-CG-SD-CE
2	A	1397	MET	O-C-CA-N
6	B	1397	ATP	PG-O3B-PB-O1B
6	B	1397	ATP	PA-O3A-PB-O2B

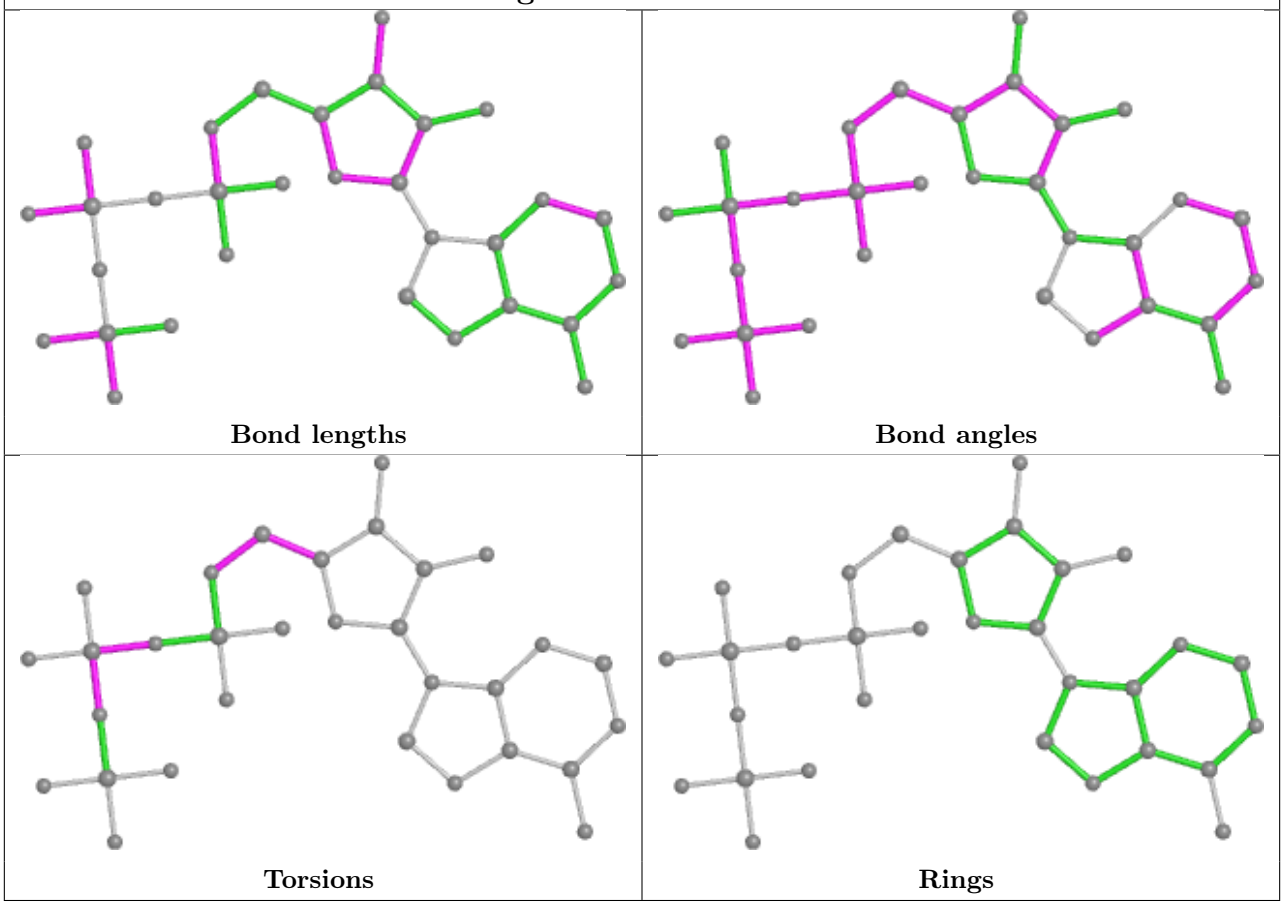
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1397	ATP	12	0
2	A	1397	MET	3	0
3	B	1398	PO4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP B 1397



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.