Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 12:20 AM EST

PDB ID	:	1G64
Title	:	THE THREE-DIMENSIONAL STRUCTURE OF ATP:CORRINOID ADENOSYLTRANSFERASE FROM SALMONELLA TYPHIMURIUM. COBALAMIN/ATP TERNARY COMPLEX
Authors	:	Rayment, I.; Escalante-Semerena, J.C.; Bauer, C.B.
Deposited on	:	2000-11-03
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

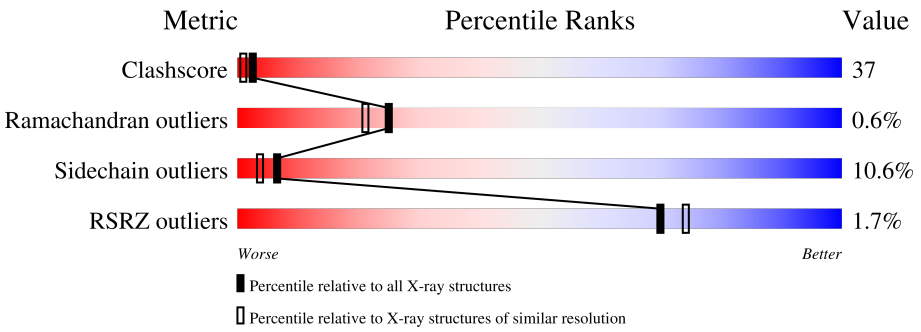
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

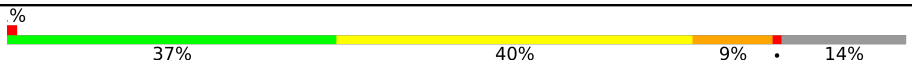
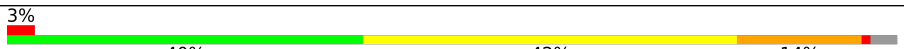
The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 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	196	
1	B	196	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3221 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.

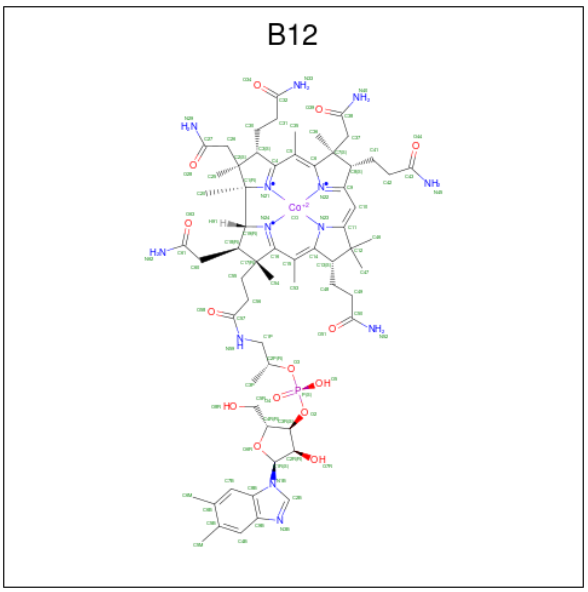
- Molecule 1 is a protein called COB(I)ALAMIN ADENOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	169	1302	823	230	241	8	0	1	0
1	B	190	1472	922	268	274	8	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

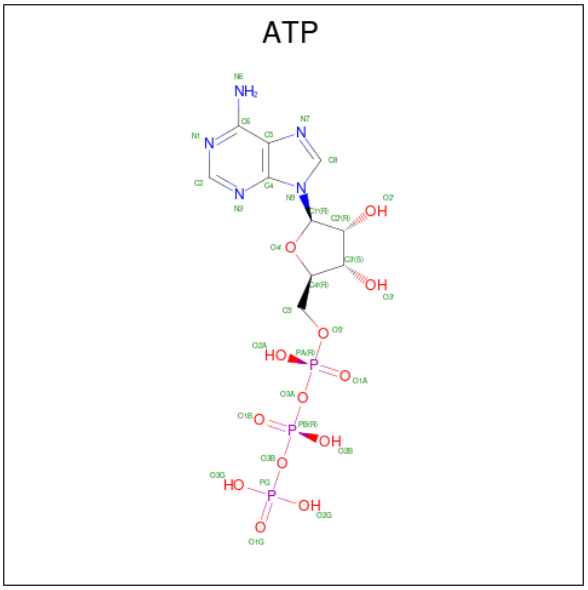
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	A	1	91	62	1	13	14	1	0	0

- Molecule 4 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			
4	A	1	31	10	5	13	3		0	0
4	B	1	31	10	5	13	3		0	0

- Molecule 5 is water.

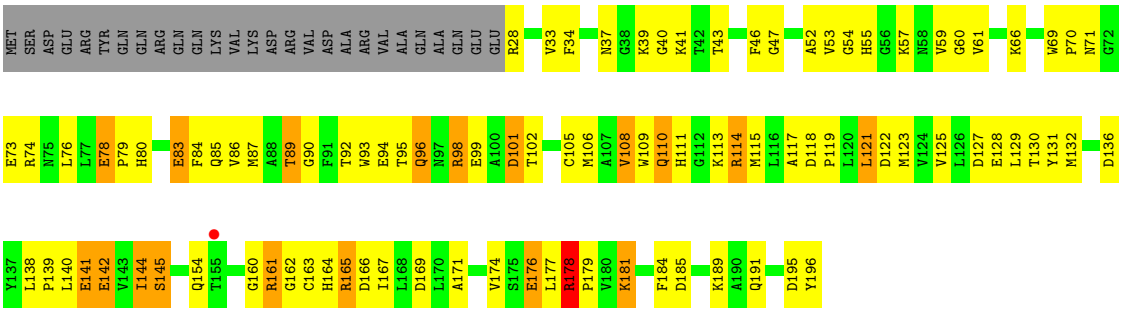
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	141	141	141	0	0
5	B	151	151	151	0	0

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 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.

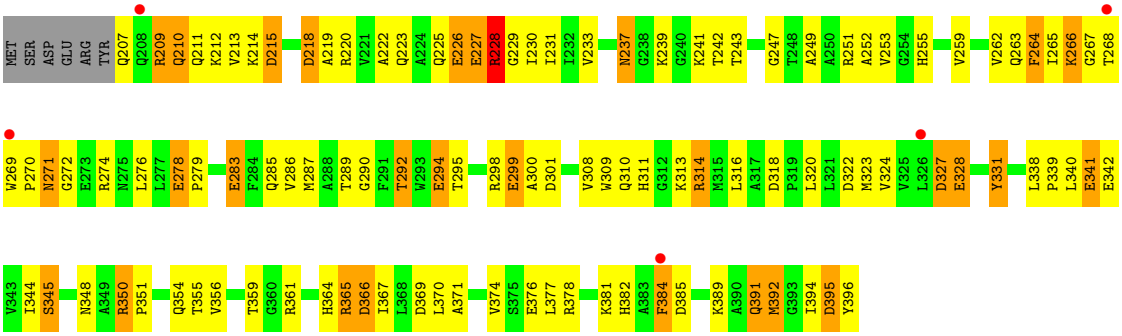
• Molecule 1: COB(I)ALAMIN ADENOSYLTRANSFERASE

Chain A:



• Molecule 1: COB(I)ALAMIN ADENOSYLTRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	80.00Å 80.00Å 142.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 22.24 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.10) 98.3 (22.24-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.06Å)	Xtriage
Refinement program	TNT, CNS	Depositor
R, R_{free}	0.206 , 0.288 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 128.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3221	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B12, ATP, MG

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	1.09	9/1333 (0.7%)	1.59	16/1807 (0.9%)
1	B	1.09	11/1499 (0.7%)	1.61	24/2028 (1.2%)
All	All	1.09	20/2832 (0.7%)	1.60	40/3835 (1.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	GLU	CD-OE2	8.43	1.34	1.25
1	B	278	GLU	CD-OE2	6.89	1.33	1.25
1	B	227	GLU	CD-OE2	6.75	1.33	1.25
1	A	141[A]	GLU	CD-OE2	6.67	1.32	1.25
1	A	141[B]	GLU	CD-OE2	6.67	1.32	1.25
1	B	299	GLU	CD-OE2	6.43	1.32	1.25
1	A	83	GLU	CD-OE2	6.41	1.32	1.25
1	B	341	GLU	CD-OE2	6.18	1.32	1.25
1	A	176	GLU	CD-OE2	5.92	1.32	1.25
1	A	94	GLU	CD-OE2	5.86	1.32	1.25
1	B	328	GLU	CD-OE2	5.83	1.32	1.25
1	B	342	GLU	CD-OE2	5.82	1.32	1.25
1	B	213	VAL	CB-CG2	-5.64	1.41	1.52
1	B	376	GLU	CD-OE2	5.62	1.31	1.25
1	B	294	GLU	CD-OE2	5.51	1.31	1.25
1	A	99	GLU	CD-OE2	5.47	1.31	1.25
1	A	128	GLU	CD-OE2	5.25	1.31	1.25
1	A	142	GLU	CD-OE2	5.10	1.31	1.25
1	A	78	GLU	CD-OE2	5.09	1.31	1.25
1	B	226	GLU	CD-OE2	5.05	1.31	1.25

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	161	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	B	251	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	B	385	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	A	101	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	A	98	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	385	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	209	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	122	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	195	ASP	CB-CG-OD1	7.03	124.62	118.30
1	B	218	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	384	PHE	CB-CG-CD1	-6.75	116.07	120.80
1	B	327	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	169	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	264	PHE	N-CA-CB	6.60	122.48	110.60
1	A	114	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	228	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	80	HIS	C-N-CA	-6.43	108.79	122.30
1	A	101	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	391	GLN	CB-CA-C	6.28	122.95	110.40
1	B	318	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	228	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	185	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	318	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	161	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	178	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	292	THR	C-N-CA	-5.76	107.29	121.70
1	B	251	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	327	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	B	322	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	144	ILE	CA-CB-CG1	-5.62	100.32	111.00
1	B	215	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	220	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	366	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	136	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	A	127	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	218	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	395	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	209	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	314	ARG	CD-NE-CZ	-5.12	116.44	123.60

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	1302	0	1285	101	0
1	B	1472	0	1458	121	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	91	0	88	10	0
4	A	31	0	12	4	0
4	B	31	0	12	3	0
5	A	141	0	0	11	2
5	B	151	0	0	15	3
All	All	3221	0	2855	214	5

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 37.

All (214) 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:301:ASP:OD1	5:B:1277:HOH:O	1.67	1.08
1:A:179:PRO:HD2	5:A:1432:HOH:O	1.56	1.04
1:A:140:LEU:HG	1:A:144:ILE:HD12	1.45	0.97
3:A:800:B12:H362	3:A:800:B12:H351	1.45	0.97
1:A:178:ARG:HG2	1:A:179:PRO:HD2	1.46	0.96
1:B:382:HIS:CD2	1:B:384:PHE:H	1.85	0.93
1:B:382:HIS:HD2	1:B:384:PHE:H	1.03	0.92
1:B:265:ILE:HD12	1:B:328:GLU:HB3	1.53	0.88
1:B:271:ASN:ND2	1:B:274:ARG:H	1.72	0.86
1:B:265:ILE:HD12	1:B:328:GLU:CB	2.06	0.84
1:A:53:VAL:HG12	1:B:276:LEU:HD13	1.62	0.81
1:B:285:GLN:HG3	1:B:311:HIS:CG	2.17	0.80
1:A:179:PRO:CD	5:A:1432:HOH:O	2.22	0.79
1:B:271:ASN:HD22	1:B:274:ARG:H	1.28	0.77
1:A:76:LEU:HD23	1:B:253:VAL:HG12	1.66	0.77
1:B:233:VAL:HB	1:B:374:VAL:HG22	1.68	0.75
1:B:219:ALA:O	1:B:223:GLN:HG3	1.85	0.75
1:B:269:TRP:HB3	1:B:270:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD12	1:A:139:PRO:HD2	1.69	0.75
3:A:800:B12:H552	3:A:800:B12:H531	1.68	0.75
1:B:228:ARG:N	1:B:228:ARG:HD3	1.99	0.74
1:B:382:HIS:HD2	1:B:384:PHE:N	1.82	0.74
1:A:140:LEU:O	1:A:144:ILE:HD12	1.88	0.73
1:B:340:LEU:HD11	1:B:344:ILE:HD11	1.71	0.73
1:A:140:LEU:HG	1:A:144:ILE:CD1	2.16	0.73
1:B:285:GLN:HG3	1:B:311:HIS:CD2	2.24	0.72
1:B:301:ASP:HA	5:B:1277:HOH:O	1.89	0.71
1:B:237:ASN:HD22	1:B:237:ASN:N	1.88	0.70
1:A:121:LEU:O	1:A:154:GLN:HG3	1.91	0.69
1:A:189:LYS:O	1:A:191:GLN:HG3	1.92	0.69
1:A:53:VAL:CG1	1:B:276:LEU:HD13	2.23	0.68
1:B:211:GLN:NE2	1:B:215:ASP:OD1	2.27	0.68
1:A:165:ARG:NH2	5:A:1225:HOH:O	2.27	0.67
1:B:278:GLU:HB3	1:B:279:PRO:HD3	1.77	0.66
1:A:66:LYS:HD3	1:A:89:THR:HA	1.78	0.65
3:A:800:B12:H351	3:A:800:B12:C36	2.23	0.65
1:B:211:GLN:HG3	1:B:215:ASP:OD2	1.96	0.65
1:A:41:LYS:HE3	4:A:999:ATP:O1B	1.97	0.64
1:A:37:ASN:ND2	5:A:1321:HOH:O	2.30	0.64
1:B:209:ARG:O	1:B:212:LYS:HB3	1.98	0.64
1:B:310:GLN:HG3	5:B:1386:HOH:O	1.97	0.63
1:B:340:LEU:O	1:B:344:ILE:HG12	1.98	0.63
1:A:83:GLU:OE1	1:A:114:ARG:NH2	2.31	0.63
1:B:364:HIS:ND1	1:B:366:ASP:HB2	2.14	0.62
1:A:111:HIS:O	1:A:114:ARG:HB3	1.98	0.62
1:A:57:LYS:CE	1:B:392:MET:HE3	2.30	0.61
1:A:83:GLU:CD	1:A:114:ARG:HH22	2.04	0.61
1:B:365:ARG:HB3	5:B:1416:HOH:O	1.99	0.61
1:A:41:LYS:NZ	5:A:1247:HOH:O	2.30	0.61
1:A:76:LEU:HD23	1:B:253:VAL:CG1	2.31	0.60
1:A:55:HIS:HE1	1:B:396:TYR:OXT	1.85	0.60
1:A:87:MET:HE1	1:A:108:VAL:CG2	2.32	0.60
1:B:265:ILE:CD1	1:B:328:GLU:HB3	2.30	0.60
1:B:370:LEU:HA	5:B:1221:HOH:O	2.02	0.60
1:B:309:TRP:NE1	1:B:313:LYS:HD2	2.17	0.59
1:B:287:MET:HE1	1:B:308:VAL:HG23	1.83	0.59
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.16	0.59
3:A:800:B12:H601	3:A:800:B12:H262	1.85	0.59
1:A:129:LEU:HD11	1:A:138:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:TRP:O	1:B:313:LYS:HG3	2.01	0.59
1:B:239:LYS:O	1:B:377:LEU:HD23	2.04	0.58
1:A:102:THR:O	1:A:106:MET:HG2	2.04	0.58
1:B:287:MET:HE1	1:B:308:VAL:CG2	2.34	0.58
1:B:311:HIS:O	1:B:314:ARG:HB3	2.03	0.58
1:A:178:ARG:HG2	5:A:1432:HOH:O	2.03	0.57
1:A:87:MET:CE	1:A:108:VAL:HG21	2.35	0.57
1:A:129:LEU:O	1:A:132:MET:N	2.36	0.56
1:B:300:ALA:HA	5:B:1211:HOH:O	2.04	0.56
1:B:345:SER:O	1:B:348:ASN:HB2	2.04	0.56
1:B:283:GLU:OE2	1:B:314:ARG:NH2	2.38	0.56
1:A:86:VAL:HG12	1:A:87:MET:N	2.20	0.56
1:B:249:ALA:O	1:B:252:ALA:HB3	2.06	0.56
1:B:271:ASN:ND2	1:B:274:ARG:N	2.50	0.56
4:B:1000:ATP:H5'2	5:B:1380:HOH:O	2.05	0.55
1:B:226:GLU:HG2	1:B:228:ARG:HD2	1.89	0.55
1:A:69:TRP:HB3	1:A:70:PRO:HD2	1.88	0.55
3:A:800:B12:H552	3:A:800:B12:C53	2.37	0.55
1:A:178:ARG:HG2	1:A:179:PRO:CD	2.30	0.54
1:A:78:GLU:O	5:A:1257:HOH:O	2.18	0.54
1:B:211:GLN:HA	1:B:214:LYS:HE3	1.90	0.54
1:A:178:ARG:HH11	1:A:178:ARG:CB	2.20	0.54
1:A:89:THR:HG23	1:A:90:GLY:N	2.21	0.54
1:A:177:LEU:HD13	1:B:377:LEU:HD11	1.88	0.53
1:B:269:TRP:HB3	1:B:270:PRO:CD	2.37	0.53
1:B:310:GLN:O	1:B:313:LYS:HB2	2.08	0.53
1:A:95:THR:HG23	5:A:1350:HOH:O	2.08	0.53
1:A:69:TRP:HB3	1:A:70:PRO:CD	2.39	0.53
1:B:292:THR:O	1:B:301:ASP:OD2	2.26	0.53
1:A:78:GLU:HB3	1:A:79:PRO:HD3	1.90	0.53
1:A:111:HIS:O	1:A:115:MET:HG3	2.10	0.52
1:A:57:LYS:HE2	1:B:392:MET:HE3	1.91	0.52
1:A:40:GLY:N	4:A:999:ATP:O1B	2.43	0.52
1:A:46:PHE:CD1	1:A:73:GLU:HG2	2.45	0.52
1:A:109:TRP:NE1	1:A:113:LYS:HD2	2.25	0.52
3:A:800:B12:H353	3:A:800:B12:H302	1.92	0.51
1:A:85:GLN:HG3	1:A:111:HIS:CG	2.45	0.51
1:B:269:TRP:CE3	1:B:396:TYR:CD2	2.99	0.51
1:B:237:ASN:N	1:B:237:ASN:ND2	2.59	0.51
1:A:164:HIS:HB3	1:A:167:ILE:HD12	1.92	0.51
1:B:382:HIS:CD2	1:B:384:PHE:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:THR:O	1:B:298:ARG:HG3	2.12	0.50
1:B:351:PRO:HG2	1:B:354:GLN:NE2	2.26	0.50
1:A:177:LEU:HD13	1:B:377:LEU:CD1	2.41	0.50
1:B:300:ALA:CA	5:B:1211:HOH:O	2.59	0.50
1:A:164:HIS:ND1	1:A:166:ASP:HB2	2.27	0.50
1:B:365:ARG:O	1:B:369:ASP:N	2.36	0.50
1:B:269:TRP:CZ3	1:B:396:TYR:CE2	3.00	0.49
1:A:87:MET:HE2	1:A:108:VAL:HG21	1.95	0.49
1:A:164:HIS:N	5:A:1356:HOH:O	2.34	0.49
1:B:266:LYS:HE2	1:B:267:GLY:O	2.12	0.49
1:B:278:GLU:HB3	1:B:279:PRO:CD	2.42	0.49
1:B:265:ILE:HD12	1:B:328:GLU:CG	2.43	0.49
1:B:309:TRP:CD1	1:B:313:LYS:HD2	2.47	0.49
3:A:800:B12:C7B	3:A:800:B12:N45	2.76	0.49
1:B:239:LYS:NZ	4:B:1000:ATP:O3G	2.46	0.49
1:A:66:LYS:HD2	5:A:1395:HOH:O	2.12	0.49
3:A:800:B12:H531	3:A:800:B12:H543	1.94	0.49
1:A:139:PRO:O	1:A:142:GLU:HB2	2.13	0.48
1:A:184:PHE:HB2	5:A:1330:HOH:O	2.11	0.48
1:B:364:HIS:O	1:B:367:ILE:HB	2.12	0.48
1:A:57:LYS:HE2	1:B:392:MET:CE	2.43	0.48
1:A:33:VAL:HG12	1:A:34:PHE:N	2.28	0.48
1:A:177:LEU:CD1	1:B:377:LEU:HD11	2.43	0.48
1:A:39:LYS:NZ	4:A:999:ATP:O3G	2.41	0.47
1:B:286:VAL:HG12	1:B:287:MET:N	2.28	0.47
1:B:382:HIS:CD2	1:B:384:PHE:CB	2.98	0.47
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.79	0.47
1:A:95:THR:O	1:A:98:ARG:HG3	2.15	0.47
1:B:345:SER:O	1:B:348:ASN:N	2.46	0.47
1:A:71:ASN:CG	1:A:74:ARG:HB2	2.35	0.47
1:A:110:GLN:OE1	1:A:113:LYS:NZ	2.43	0.47
1:B:279:PRO:HG2	5:B:1232:HOH:O	2.15	0.47
1:A:87:MET:HE1	1:A:105:CYS:HA	1.96	0.47
1:A:130:THR:HG21	1:A:160:GLY:O	2.15	0.47
1:A:138:LEU:HD12	1:A:139:PRO:CD	2.42	0.47
1:A:196:TYR:OXT	1:B:255:HIS:HE1	1.98	0.46
1:B:331:TYR:CD1	1:B:331:TYR:N	2.80	0.46
1:A:109:TRP:NE1	1:A:113:LYS:CD	2.78	0.46
1:A:37:ASN:HB2	1:A:179:PRO:HG3	1.97	0.46
3:A:800:B12:H541	3:A:800:B12:H602	1.77	0.46
1:A:92:THR:O	1:A:93:TRP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:CG1	1:A:87:MET:N	2.79	0.46
1:A:178:ARG:CG	1:A:178:ARG:NH1	2.79	0.46
1:B:230:ILE:O	1:B:355:THR:HG23	2.16	0.46
1:B:300:ALA:N	5:B:1211:HOH:O	2.47	0.46
1:B:341:GLU:O	1:B:345:SER:N	2.44	0.46
1:A:178:ARG:HG3	1:A:178:ARG:NH1	2.31	0.46
1:A:131:TYR:OH	1:A:161:ARG:HB2	2.16	0.45
1:A:78:GLU:N	1:A:79:PRO:CD	2.80	0.45
1:B:289:THR:HG22	1:B:290:GLY:N	2.31	0.45
1:A:54:GLY:HA3	1:B:272:GLY:O	2.16	0.45
1:A:171:ALA:O	1:B:381:LYS:NZ	2.43	0.45
1:B:228:ARG:HD3	1:B:228:ARG:H	1.80	0.45
1:B:289:THR:CG2	1:B:290:GLY:N	2.79	0.45
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.71	0.45
1:B:241:LYS:N	4:B:1000:ATP:O1B	2.41	0.45
1:A:43:THR:O	1:B:247:GLY:HA3	2.17	0.45
1:B:271:ASN:CG	1:B:274:ARG:HB2	2.38	0.44
1:B:392:MET:HE3	1:B:392:MET:HB3	1.80	0.44
1:A:59:VAL:HA	1:A:123:MET:O	2.18	0.44
1:B:269:TRP:CE3	1:B:396:TYR:CE2	3.06	0.44
1:B:314:ARG:HH11	1:B:314:ARG:HD3	1.55	0.44
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.74	0.44
1:A:59:VAL:HG12	1:A:60:GLY:N	2.33	0.43
1:A:181:LYS:HB2	1:B:374:VAL:HB	2.00	0.43
1:A:74:ARG:HG3	1:A:84:PHE:CG	2.54	0.43
1:A:87:MET:HE2	1:A:87:MET:HB2	1.83	0.43
1:B:218:ASP:O	1:B:222:ALA:HB2	2.19	0.43
1:B:263:GLN:NE2	1:B:271:ASN:OD1	2.38	0.43
1:B:295:THR:HA	1:B:298:ARG:HG3	1.99	0.43
1:B:231:ILE:HB	1:B:371:ALA:HA	2.00	0.43
1:B:241:LYS:HE3	1:B:361:ARG:HG3	2.01	0.43
1:A:61:VAL:HG22	1:A:125:VAL:HB	2.00	0.43
1:A:92:THR:OG1	1:A:101:ASP:OD2	2.28	0.43
3:A:800:B12:H353	3:A:800:B12:C30	2.48	0.43
1:B:324:VAL:O	1:B:356:VAL:HA	2.19	0.43
1:B:394:ILE:HG22	1:B:395:ASP:OD2	2.18	0.43
1:A:109:TRP:CD1	1:A:113:LYS:HD3	2.54	0.43
1:B:259:VAL:HA	1:B:323:MET:O	2.19	0.43
1:B:242:THR:OG1	1:B:327:ASP:OD1	2.37	0.42
1:B:299:GLU:C	5:B:1211:HOH:O	2.57	0.42
1:B:348:ASN:ND2	5:B:1511:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ARG:HA	1:B:365:ARG:HD3	1.88	0.42
1:B:278:GLU:N	1:B:279:PRO:HD2	2.34	0.42
1:B:283:GLU:OE2	1:B:285:GLN:NE2	2.39	0.42
1:A:117:ALA:O	1:A:119:PRO:HD3	2.20	0.42
4:A:999:ATP:H2'	4:A:999:ATP:O5'	2.20	0.42
1:B:242:THR:HG21	5:B:1379:HOH:O	2.18	0.42
1:B:364:HIS:CE1	1:B:366:ASP:HB2	2.54	0.42
1:A:66:LYS:HD3	1:A:89:THR:CA	2.47	0.42
1:A:52:ALA:O	1:A:57:LYS:HB2	2.20	0.41
1:A:57:LYS:CE	1:B:392:MET:CE	2.96	0.41
1:A:87:MET:HE1	1:A:108:VAL:HG23	2.01	0.41
1:A:118:ASP:HA	1:A:119:PRO:HD3	1.59	0.41
1:A:57:LYS:HE3	1:B:392:MET:HE3	2.01	0.41
1:B:211:GLN:HE21	1:B:215:ASP:CG	2.18	0.41
1:A:47:GLY:HA3	1:B:243:THR:O	2.20	0.41
1:B:210:GLN:HB3	5:B:1362:HOH:O	2.20	0.41
1:B:229:GLY:HA3	1:B:354:GLN:O	2.20	0.41
1:B:229:GLY:O	1:B:350:ARG:NH2	2.53	0.41
1:A:174:VAL:HB	1:B:381:LYS:HB2	2.02	0.41
1:B:286:VAL:CG1	1:B:287:MET:N	2.84	0.41
1:A:96:GLN:H	1:A:96:GLN:HG3	1.34	0.41
1:A:111:HIS:ND1	1:A:114:ARG:NH1	2.69	0.41
1:A:163:CYS:SG	1:A:167:ILE:CG2	3.09	0.41
1:B:338:LEU:HA	1:B:339:PRO:HD2	1.70	0.41
1:B:344:ILE:O	1:B:348:ASN:ND2	2.54	0.41
1:A:69:TRP:CB	1:A:70:PRO:CD	2.98	0.41
1:A:140:LEU:HD21	1:A:166:ASP:OD2	2.21	0.40
1:A:178:ARG:HH11	1:A:178:ARG:HB2	1.85	0.40
1:B:226:GLU:HG2	1:B:227:GLU:N	2.36	0.40
1:B:207:GLN:O	5:B:1362:HOH:O	2.22	0.40
1:B:316:LEU:O	1:B:351:PRO:HD2	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:GLU:OE1	5:B:1275:HOH:O[6_455]	0.94	1.26
1:B:227:GLU:CD	5:B:1275:HOH:O[6_455]	1.15	1.05
1:B:227:GLU:OE2	5:B:1275:HOH:O[6_455]	1.59	0.61
5:A:1338:HOH:O	5:A:1393:HOH:O[3_555]	1.96	0.24
5:A:1245:HOH:O	5:A:1319:HOH:O[4_454]	2.00	0.20

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	168/196 (86%)	163 (97%)	4 (2%)	1 (1%)	25	21
1	B	188/196 (96%)	173 (92%)	14 (7%)	1 (0%)	29	26
All	All	356/392 (91%)	336 (94%)	18 (5%)	2 (1%)	25	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ARG
1	A	162	GLY

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	134/157 (85%)	121 (90%)	13 (10%)	8	5
1	B	151/157 (96%)	133 (88%)	18 (12%)	5	2
All	All	285/314 (91%)	254 (89%)	31 (11%)	6	3

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	89	THR
1	A	96	GLN
1	A	108	VAL

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Mol	Chain	Res	Type
1	A	110	GLN
1	A	121	LEU
1	A	141[A]	GLU
1	A	141[B]	GLU
1	A	145	SER
1	A	165	ARG
1	A	176	GLU
1	A	178	ARG
1	A	181	LYS
1	B	210	GLN
1	B	225	GLN
1	B	228	ARG
1	B	237	ASN
1	B	262	VAL
1	B	264	PHE
1	B	266	LYS
1	B	268	THR
1	B	271	ASN
1	B	294	GLU
1	B	331	TYR
1	B	345	SER
1	B	359	THR
1	B	365	ARG
1	B	378	ARG
1	B	389	LYS
1	B	391	GLN
1	B	392	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	55	HIS
1	A	191	GLN
1	B	210	GLN
1	B	225	GLN
1	B	237	ASN
1	B	255	HIS
1	B	263	GLN
1	B	271	ASN
1	B	275	ASN
1	B	296	GLN

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Mol	Chain	Res	Type
1	B	353	HIS
1	B	382	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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	B12	A	800	-	90,101,101	1.05	7 (7%)	137,166,166	1.05	9 (6%)
4	ATP	A	999	2	26,33,33	1.89	4 (15%)	31,52,52	1.44	5 (16%)
4	ATP	B	1000	2	26,33,33	1.94	5 (19%)	31,52,52	1.65	7 (22%)

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	B12	A	800	-	-	6/52/223/223	0/3/11/11
4	ATP	A	999	2	-	0/18/38/38	0/3/3/3
4	ATP	B	1000	2	-	5/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	ATP	C2'-C3'	-7.84	1.31	1.53
4	B	1000	ATP	C2'-C3'	-7.70	1.32	1.53
3	A	800	B12	C2R-C1R	3.27	1.58	1.53
4	B	1000	ATP	C2'-C1'	-2.96	1.49	1.53
3	A	800	B12	C19-N24	-2.93	1.43	1.48
4	A	999	ATP	C2'-C1'	-2.85	1.49	1.53
3	A	800	B12	C17-C16	-2.63	1.48	1.54
3	A	800	B12	C12-C11	-2.62	1.47	1.52
4	A	999	ATP	C2-N1	2.54	1.38	1.33
4	B	1000	ATP	O4'-C1'	2.53	1.44	1.41
4	A	999	ATP	PG-O2G	-2.42	1.45	1.54
3	A	800	B12	C35-C5	2.34	1.55	1.50
4	B	1000	ATP	C2-N1	2.13	1.37	1.33
3	A	800	B12	C60-C18	-2.13	1.49	1.54
4	B	1000	ATP	PG-O2G	-2.05	1.46	1.54
3	A	800	B12	C1-C2	2.05	1.63	1.58

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1000	ATP	O4'-C1'-C2'	-5.75	98.53	106.93
3	A	800	B12	C7B-C8B-C9B	4.06	124.56	120.54
4	A	999	ATP	O3G-PG-O3B	3.31	115.73	104.64
4	A	999	ATP	O4'-C1'-C2'	-3.30	102.11	106.93
4	B	1000	ATP	C3'-C2'-C1'	3.06	105.59	100.98
4	B	1000	ATP	N6-C6-N1	2.80	124.39	118.57
4	A	999	ATP	N6-C6-N1	2.77	124.32	118.57
3	A	800	B12	C9-C10-C11	-2.76	121.98	125.97
3	A	800	B12	C5B-C4B-C9B	-2.69	117.41	121.22
4	B	1000	ATP	C4-C5-N7	2.62	112.13	109.40
4	A	999	ATP	C5-C6-N1	-2.56	114.55	120.35
3	A	800	B12	C12-C11-C10	-2.44	120.19	123.37
4	A	999	ATP	C3'-C2'-C1'	2.44	104.65	100.98
3	A	800	B12	O6R-C1R-C2R	-2.38	103.44	106.93
3	A	800	B12	O58-C57-C56	-2.29	117.82	122.02
3	A	800	B12	C12-C11-N23	-2.27	108.67	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	800	B12	C4B-C9B-C8B	-2.16	118.89	121.10
3	A	800	B12	C53-C15-C16	-2.10	116.78	120.38
4	B	1000	ATP	C5-C6-N1	-2.06	115.69	120.35
4	B	1000	ATP	O2G-PG-O3B	2.04	111.49	104.64
4	B	1000	ATP	O4'-C4'-C3'	-2.01	101.14	105.11

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1000	ATP	O4'-C4'-C5'-O5'
4	B	1000	ATP	C3'-C4'-C5'-O5'
3	A	800	B12	C38-C37-C7-C8
3	A	800	B12	C42-C41-C8-C9
3	A	800	B12	C48-C49-C50-O51
3	A	800	B12	C42-C41-C8-C7
3	A	800	B12	C38-C37-C7-C36
4	B	1000	ATP	C5'-O5'-PA-O1A
3	A	800	B12	C16-C17-C55-C56
4	B	1000	ATP	PB-O3A-PA-O1A
4	B	1000	ATP	C5'-O5'-PA-O3A

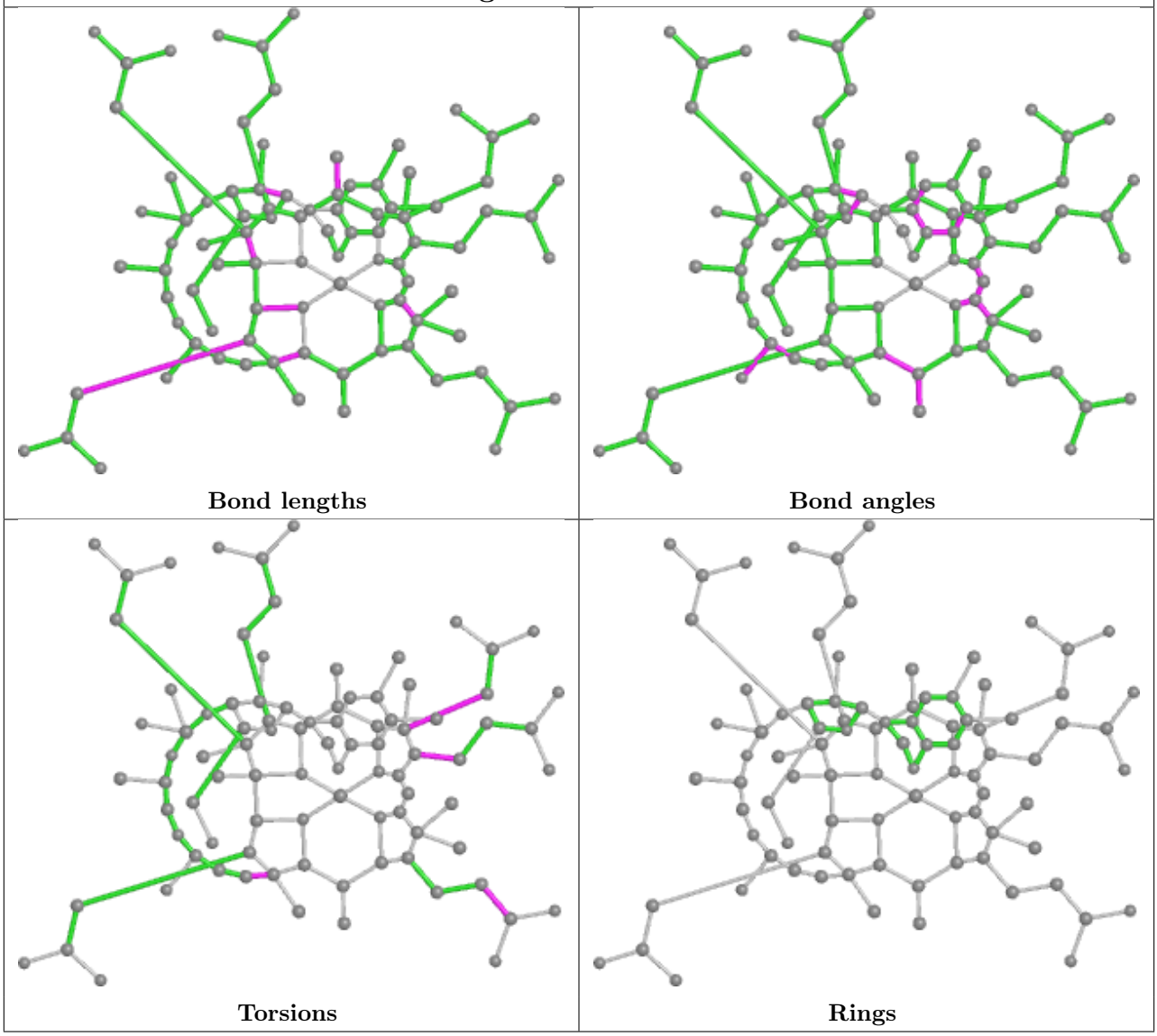
There are no ring outliers.

3 monomers are involved in 17 short contacts:

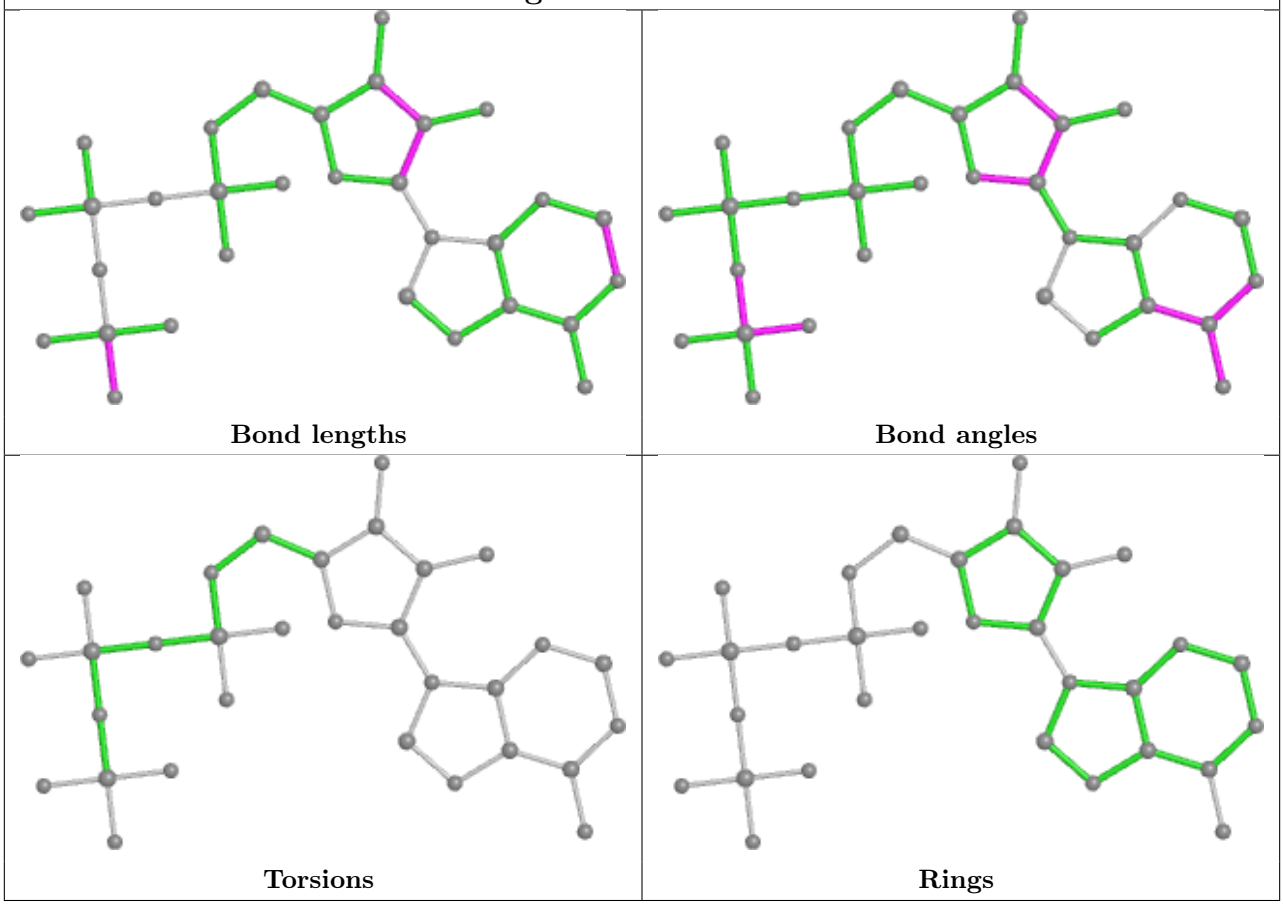
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	10	0
4	A	999	ATP	4	0
4	B	1000	ATP	3	0

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.

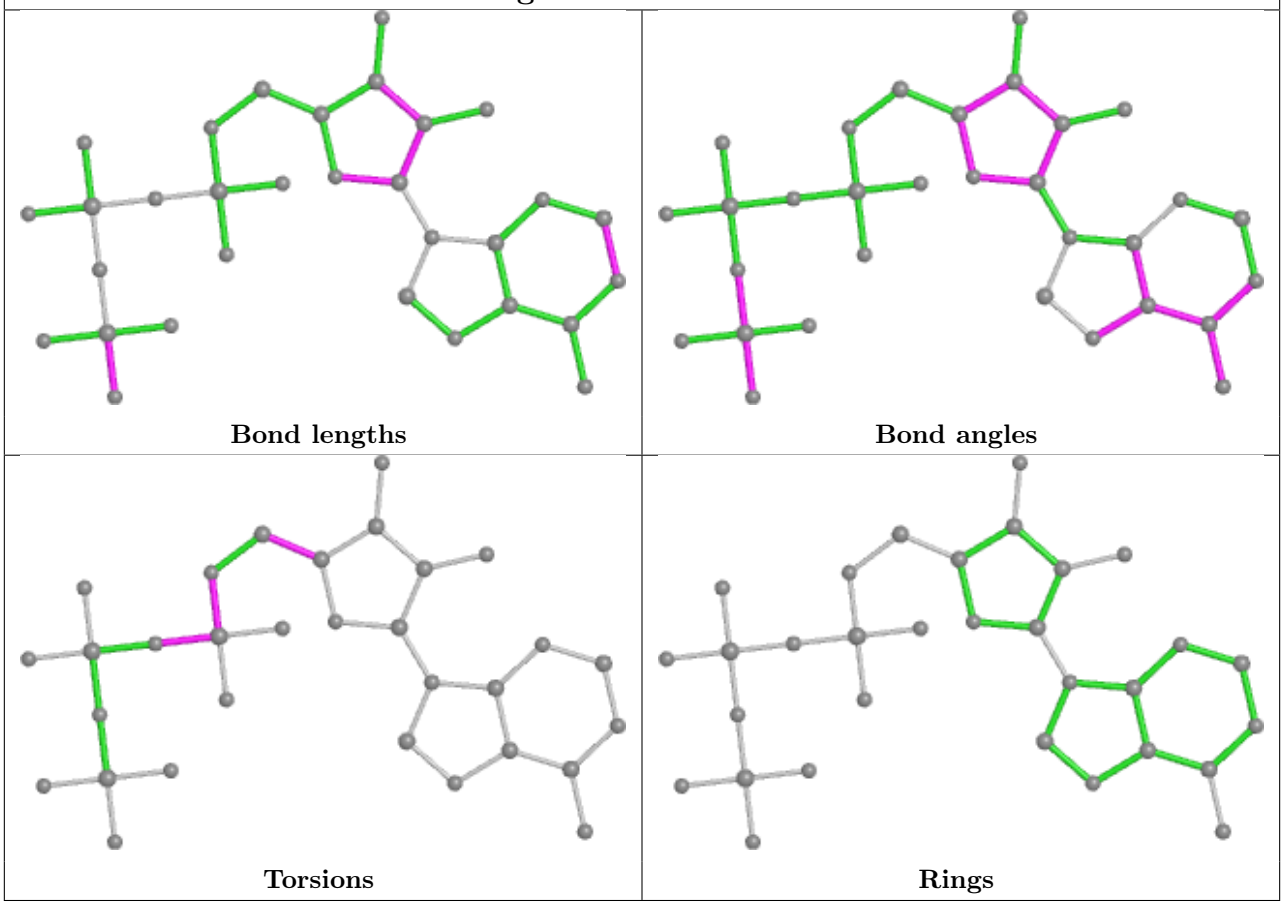
Ligand B12 A 800



Ligand ATP A 999



Ligand ATP B 1000



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)

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	169/196 (86%)	-0.21	1 (0%)	89	91	13, 34, 59, 78	0
1	B	190/196 (96%)	0.07	5 (2%)	56	61	19, 36, 66, 90	0
All	All	359/392 (91%)	-0.06	6 (1%)	70	74	13, 35, 62, 90	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	TRP	5.2
1	B	268	THR	4.0
1	B	384	PHE	3.3
1	B	208	GLN	2.8
1	B	326	LEU	2.2
1	A	155	THR	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

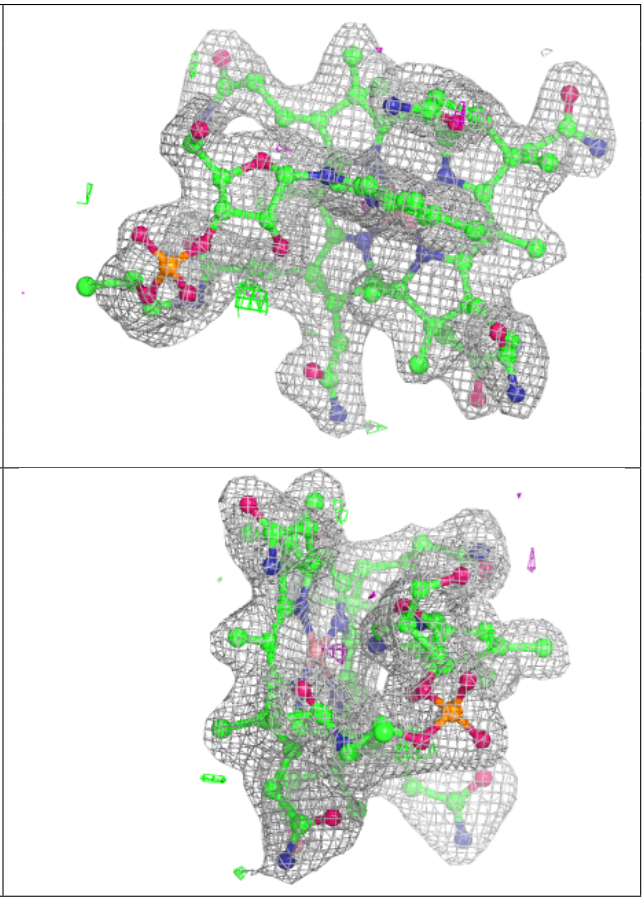
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	1001	1/1	0.95	0.05	28,28,28,28	0
3	B12	A	800	91/91	0.95	0.12	13,35,84,100	0
4	ATP	B	1000	31/31	0.97	0.10	15,38,100,100	0
4	ATP	A	999	31/31	0.98	0.07	12,23,47,54	0
2	MG	A	998	1/1	0.98	0.03	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

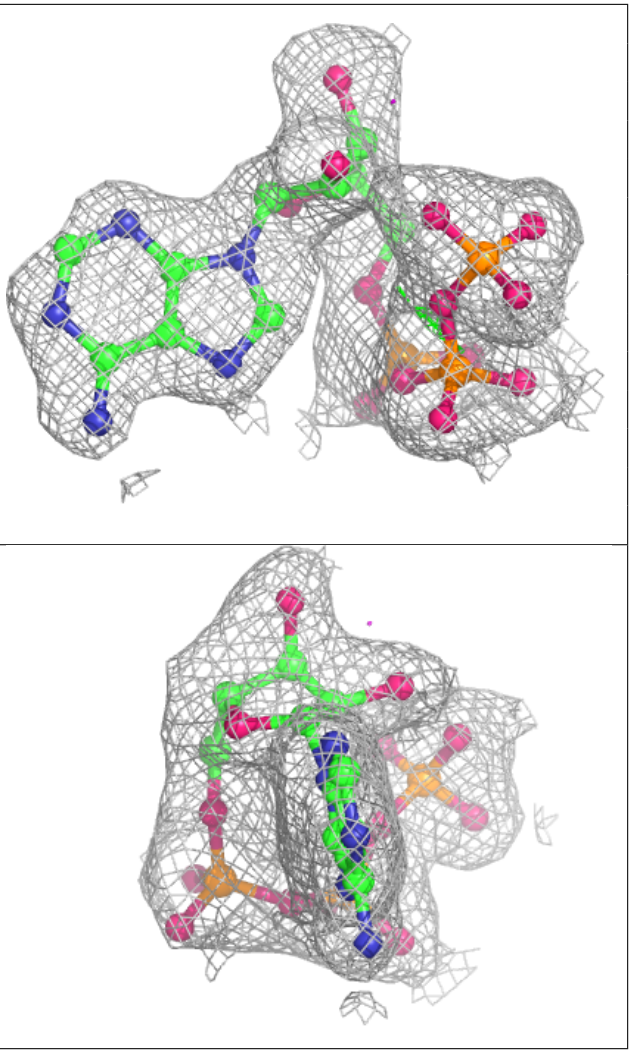
Electron density around B12 A 800:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



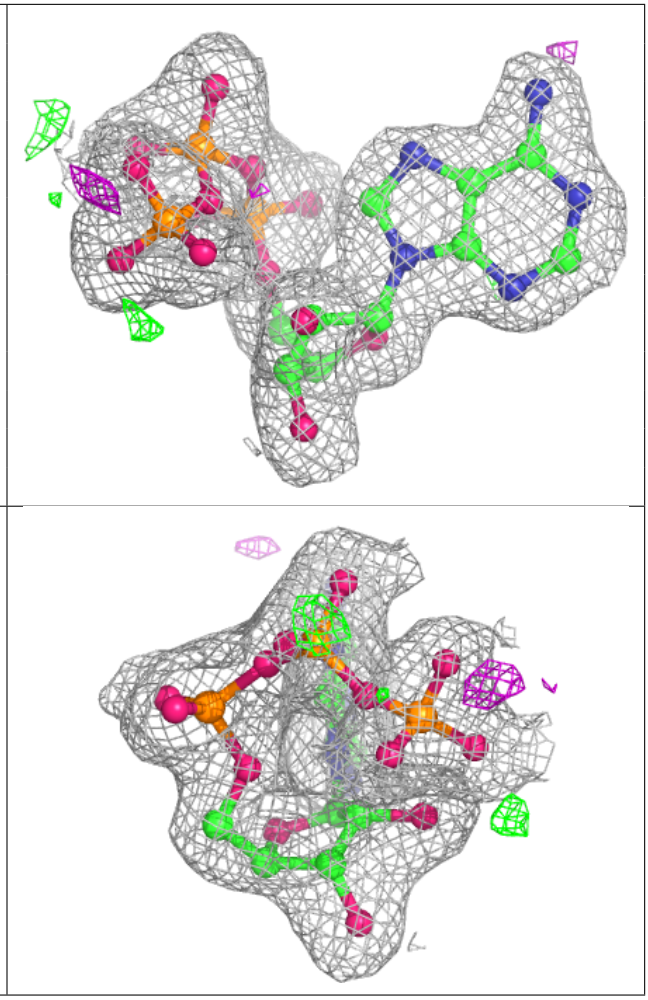
Electron density around ATP B 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 999:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.