Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:44 AM GMT

PDB ID	:	3FVQ
Title	:	Crystal structure of the nucleotide binding domain FbpC complexed with ATP
Authors	:	Newstead, S.; Bilton, P.; Carpenter, E.P.; Campopiano, D.; Iwata, S.
Deposited on	:	2009-01-16
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

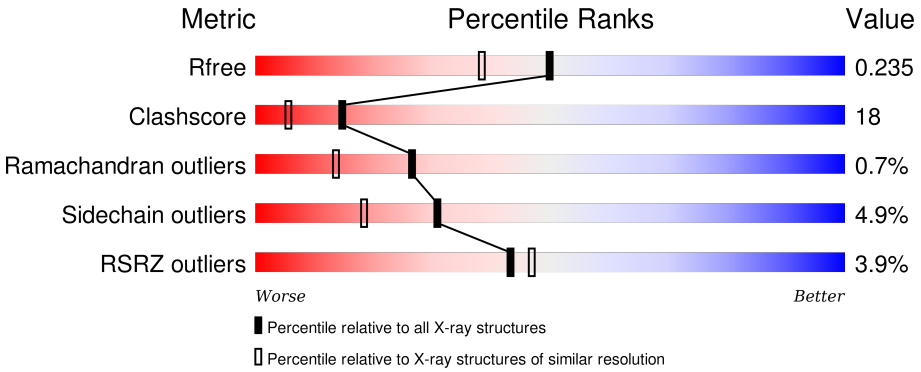
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	5% 70% 23%
1	B	359	3% 70% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5963 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.

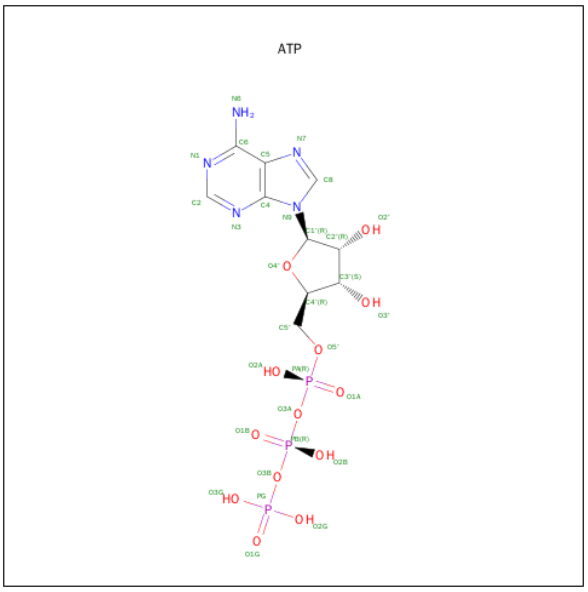
- Molecule 1 is a protein called Fe(3+) ions import ATP-binding protein fbpC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	10	0
			2653	1677	477	492	7			
1	B	350	Total	C	N	O	S	0	13	0
			2723	1719	494	504	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	VAL	SEE REMARK 999	UNP Q5FA19
A	283	TYR	PHE	SEE REMARK 999	UNP Q5FA19
A	353	GLU	-	EXPRESSION TAG	UNP Q5FA19
A	354	HIS	-	EXPRESSION TAG	UNP Q5FA19
A	355	HIS	-	EXPRESSION TAG	UNP Q5FA19
A	356	HIS	-	EXPRESSION TAG	UNP Q5FA19
A	357	HIS	-	EXPRESSION TAG	UNP Q5FA19
A	358	HIS	-	EXPRESSION TAG	UNP Q5FA19
A	359	HIS	-	EXPRESSION TAG	UNP Q5FA19
B	147	ALA	VAL	SEE REMARK 999	UNP Q5FA19
B	283	TYR	PHE	SEE REMARK 999	UNP Q5FA19
B	353	GLU	-	EXPRESSION TAG	UNP Q5FA19
B	354	HIS	-	EXPRESSION TAG	UNP Q5FA19
B	355	HIS	-	EXPRESSION TAG	UNP Q5FA19
B	356	HIS	-	EXPRESSION TAG	UNP Q5FA19
B	357	HIS	-	EXPRESSION TAG	UNP Q5FA19
B	358	HIS	-	EXPRESSION TAG	UNP Q5FA19
B	359	HIS	-	EXPRESSION TAG	UNP Q5FA19

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

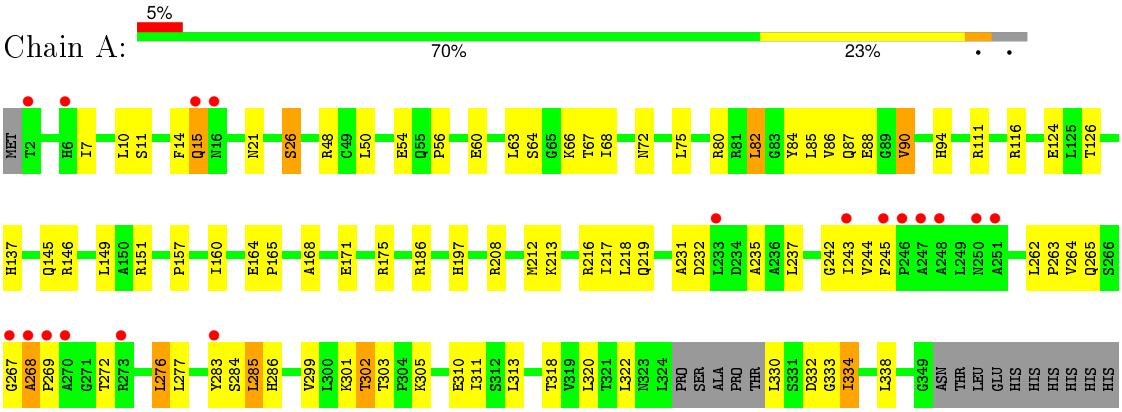
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	243	Total	O	0	0
			243	243		
4	B	279	Total	O	0	0
			279	279		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

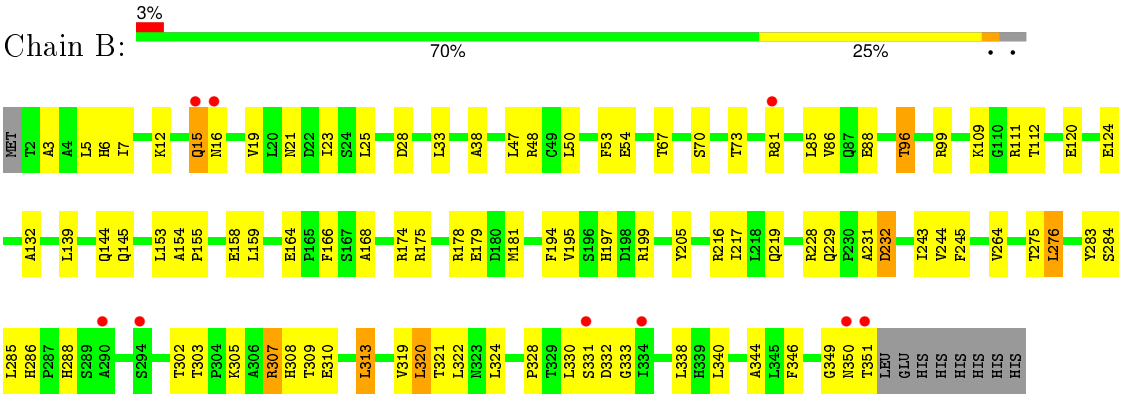
- Molecule 1: Fe(3+) ions import ATP-binding protein fbpC

Chain A:



- Molecule 1: Fe(3+) ions import ATP-binding protein fbpC

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.86Å 89.09Å 149.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.27 – 1.90 47.33 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.4 (52.27-1.90) 87.4 (47.33-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.195 , 0.256 0.185 , 0.235	Depositor DCC
R_{free} test set	2624 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	17.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 51946 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/2731	0.78	1/3702 (0.0%)
1	B	0.78	2/2813 (0.1%)	0.81	2/3819 (0.1%)
All	All	0.74	2/5544 (0.0%)	0.79	3/7521 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	ALA	CA-CB	5.72	1.64	1.52
1	B	195	VAL	CB-CG1	5.31	1.64	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	232	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	B	232	ASP	CB-CA-C	-5.19	100.02	110.40
1	A	48	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2653	0	2711	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2723	0	2796	110	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	243	0	0	21	0
4	B	279	0	0	13	0
All	All	5963	0	5531	195	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 18.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HB3	4:A:448:HOH:O	1.39	1.22
1:A:242:GLY:HA3	1:A:277:LEU:HD11	1.30	1.07
1:B:178:ARG:HD2	4:B:448:HOH:O	1.58	1.03
1:B:5:LEU:HD11	1:B:50[B]:LEU:HD11	1.38	1.01
1:B:145:GLN:HE22	1:B:168:ALA:H	1.10	0.98
1:A:116:ARG:HB2	4:A:545:HOH:O	1.61	0.98
1:B:228:ARG:C	1:B:229[B]:GLN:HE21	1.69	0.96
1:B:21:ASN:HB3	4:B:557:HOH:O	1.64	0.96
1:B:112[A]:THR:HG22	4:B:451:HOH:O	1.68	0.94
1:B:5:LEU:HD11	1:B:50[B]:LEU:CD1	1.98	0.93
1:B:303[A]:THR:CG2	1:B:310:GLU:HB3	1.98	0.93
1:A:303:THR:HG22	1:A:305:LYS:HE3	1.52	0.91
1:A:145:GLN:HE22	1:A:168:ALA:H	1.19	0.90
1:A:151:ARG:HD2	4:A:410:HOH:O	1.71	0.89
1:B:7:ILE:HD11	1:B:50[A]:LEU:HD21	1.55	0.88
1:B:228:ARG:C	1:B:229[B]:GLN:NE2	2.27	0.88
1:A:276:LEU:CD2	1:B:344:ALA:HB3	2.04	0.87
1:B:5:LEU:CD1	1:B:50[B]:LEU:HD11	2.05	0.86
1:A:243:ILE:HD12	1:A:283:TYR:HE2	1.37	0.86
1:A:243:ILE:HD12	1:A:283:TYR:CE2	2.11	0.85
1:A:232:ASP:HB3	1:A:235:ALA:H	1.41	0.83
1:A:299:VAL:HG21	1:A:330:LEU:HD21	1.62	0.82
1:B:228:ARG:O	1:B:229[B]:GLN:NE2	2.13	0.82
1:A:264:VAL:HG21	1:B:346:PHE:HB2	1.63	0.81
1:A:242:GLY:CA	1:A:277:LEU:HD11	2.09	0.81
1:A:320:LEU:HG	1:A:322:LEU:HD21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:HB1	1:A:269:PRO:HD2	1.60	0.81
1:B:70:SER:OG	1:B:73:THR:HG22	1.81	0.81
1:A:276:LEU:HD22	4:A:448:HOH:O	1.81	0.79
1:A:171:GLU:HG3	1:A:175:ARG:HE	1.48	0.78
1:B:85:LEU:HD21	4:B:459:HOH:O	1.84	0.76
1:A:164:GLU:OE1	1:A:197:HIS:HD2	1.69	0.75
1:B:48[B]:ARG:HG2	1:B:53:PHE:HB2	1.69	0.75
1:B:109:LYS:HD3	1:B:111:ARG:NH1	2.02	0.74
1:A:26:SER:O	1:A:208:ARG:NH2	2.20	0.73
1:A:7:ILE:HD11	1:A:50:LEU:HD21	1.69	0.73
1:B:7:ILE:CD1	1:B:50[A]:LEU:HD21	2.18	0.72
1:A:276:LEU:CD2	1:B:344:ALA:CB	2.68	0.71
1:B:349:GLY:O	1:B:351:THR:N	2.24	0.71
1:B:178:ARG:HD3	1:B:205:TYR:CE2	2.25	0.71
1:B:164:GLU:OE1	1:B:197:HIS:HD2	1.73	0.70
1:B:303[A]:THR:HG22	1:B:310:GLU:HB3	1.74	0.70
1:A:116:ARG:CG	4:A:545:HOH:O	2.39	0.69
1:B:67:THR:HG22	1:B:73:THR:HG21	1.75	0.69
1:B:351:THR:O	1:B:351:THR:HG23	1.93	0.68
1:B:216:ARG:NE	4:B:410:HOH:O	2.25	0.68
1:A:334:ILE:HD12	4:A:519:HOH:O	1.91	0.68
1:A:94:HIS:HE1	4:A:387:HOH:O	1.76	0.67
1:A:301:LYS:HA	1:A:332:ASP:OD2	1.94	0.67
1:A:268:ALA:HB1	1:A:269:PRO:CD	2.25	0.67
1:B:284:SER:OG	1:B:286:HIS:HE1	1.76	0.67
1:B:219:GLN:NE2	1:B:231:ALA:H	1.92	0.67
1:B:313:LEU:O	1:B:319:VAL:HG13	1.95	0.66
1:B:96:THR:HG21	4:B:477:HOH:O	1.96	0.65
1:B:303[A]:THR:HG23	1:B:310:GLU:HB3	1.74	0.65
1:B:67:THR:CG2	1:B:73:THR:HG21	2.26	0.64
1:B:48[B]:ARG:HH11	1:B:48[B]:ARG:HG3	1.63	0.64
1:A:14:PHE:O	1:A:15:GLN:C	2.34	0.63
4:A:590:HOH:O	1:B:275:THR:HG23	1.97	0.63
1:A:245:PHE:HZ	1:B:320:LEU:HD22	1.64	0.63
1:B:124:GLU:HG3	4:B:580:HOH:O	1.98	0.62
1:A:171:GLU:CG	1:A:175:ARG:HE	2.12	0.62
1:A:82:LEU:O	1:A:82:LEU:HD23	2.00	0.62
1:B:228:ARG:HB3	1:B:229[B]:GLN:HE22	1.64	0.61
1:A:7:ILE:CD1	1:A:50:LEU:HD21	2.29	0.61
1:A:186:ARG:NH1	4:A:599:HOH:O	2.33	0.61
1:B:219:GLN:HE22	1:B:231:ALA:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:HG22	1:B:99:ARG:H	1.66	0.61
1:A:171:GLU:HG3	1:A:175:ARG:NE	2.16	0.61
1:B:145:GLN:NE2	1:B:168:ALA:H	1.91	0.61
1:A:299:VAL:CG2	1:A:330:LEU:HD21	2.30	0.61
1:A:68:ILE:HD12	1:A:80:ARG:HD3	1.82	0.61
1:A:84:TYR:CE2	1:A:86[B]:VAL:HG12	2.36	0.60
1:A:286:HIS:HD2	4:A:532:HOH:O	1.85	0.60
1:B:88:GLU:CD	1:B:88:GLU:H	2.04	0.60
1:A:219:GLN:HE22	1:A:231:ALA:H	1.49	0.60
1:A:276:LEU:HD21	1:B:344:ALA:HB3	1.83	0.59
1:B:154:ALA:HB3	1:B:155:PRO:HD3	1.85	0.59
1:B:70:SER:OG	1:B:73:THR:CG2	2.50	0.59
1:A:284:SER:OG	1:A:286:HIS:HE1	1.84	0.59
1:A:219:GLN:NE2	1:A:231:ALA:H	2.00	0.59
1:B:275:THR:HG22	4:B:489:HOH:O	2.02	0.58
1:A:303:THR:HG21	4:A:483:HOH:O	2.03	0.58
1:B:313:LEU:O	1:B:319:VAL:HA	2.04	0.58
1:B:174:ARG:O	1:B:178:ARG:HG2	2.05	0.57
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.69	0.57
1:A:302:THR:O	1:A:302:THR:HG22	2.03	0.56
1:A:213:LYS:HB3	1:A:218:LEU:HD13	1.86	0.56
1:B:232:ASP:OD1	4:B:543:HOH:O	2.17	0.56
1:A:276:LEU:CD2	4:A:448:HOH:O	2.48	0.56
1:B:175:ARG:HA	1:B:178:ARG:HG2	1.88	0.55
1:A:116:ARG:CB	4:A:545:HOH:O	2.30	0.55
1:A:84:TYR:CZ	1:A:86[B]:VAL:HG12	2.41	0.55
1:A:88:GLU:CD	1:A:88:GLU:N	2.60	0.55
1:B:330:LEU:C	1:B:332:ASP:H	2.09	0.55
1:A:88:GLU:H	1:A:88:GLU:CD	2.10	0.54
1:B:285:LEU:O	1:B:288:HIS:CD2	2.61	0.54
1:A:171:GLU:HG2	1:B:199:ARG:NH1	2.22	0.54
1:A:164:GLU:OE1	1:A:197:HIS:CD2	2.55	0.54
1:A:269:PRO:HG2	1:A:272:THR:OG1	2.08	0.53
1:B:109:LYS:HD3	1:B:111:ARG:CZ	2.38	0.53
1:A:311:ILE:HG22	1:A:313:LEU:HG	1.90	0.53
1:A:87:GLN:O	4:A:565:HOH:O	2.19	0.53
1:A:320:LEU:CG	1:A:322:LEU:HD21	2.37	0.53
1:A:320:LEU:HG	1:A:322:LEU:CD2	2.37	0.53
1:A:66:LYS:HE2	1:A:75:LEU:HD11	1.90	0.52
1:B:48[B]:ARG:HH11	1:B:48[B]:ARG:CG	2.21	0.52
1:B:5:LEU:HD11	1:B:50[B]:LEU:HD13	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ILE:CD1	4:A:519:HOH:O	2.54	0.52
1:B:330:LEU:C	1:B:332:ASP:N	2.61	0.52
1:A:299:VAL:HG21	1:A:330:LEU:CD2	2.39	0.51
1:A:269:PRO:HD2	1:A:272:THR:OG1	2.10	0.51
1:B:351:THR:O	1:B:351:THR:CG2	2.58	0.51
1:B:330:LEU:O	1:B:332:ASP:N	2.44	0.51
1:A:276:LEU:CG	4:A:448:HOH:O	2.56	0.50
1:A:145:GLN:NE2	1:A:168:ALA:H	1.99	0.49
1:B:6[A]:HIS:HD2	4:B:369:HOH:O	1.95	0.49
1:A:244:VAL:HG22	4:A:486:HOH:O	2.11	0.49
1:B:124:GLU:OE2	4:B:566:HOH:O	2.19	0.49
1:A:276:LEU:HD22	1:B:344:ALA:CB	2.42	0.49
1:B:139:LEU:HB2	1:B:144:GLN:HG3	1.95	0.49
1:B:86:VAL:CG1	1:B:88:GLU:OE1	2.61	0.48
1:A:126:THR:O	1:A:146:ARG:HD2	2.13	0.48
1:B:96:THR:HG23	1:B:132:ALA:O	2.14	0.48
1:B:81[B]:ARG:HH22	1:B:158:GLU:H	1.61	0.48
1:B:228:ARG:CB	1:B:229[B]:GLN:HE22	2.26	0.48
1:A:243:ILE:CD1	1:A:283:TYR:HE2	2.16	0.48
1:B:228:ARG:CB	1:B:229[B]:GLN:NE2	2.77	0.48
1:B:120:GLU:O	1:B:124:GLU:HG3	2.14	0.47
1:A:283:TYR:CD2	1:B:322:LEU:HD22	2.49	0.47
1:B:164:GLU:OE1	1:B:197:HIS:CD2	2.63	0.47
1:B:328:PRO:HB2	1:B:330:LEU:HD21	1.95	0.47
1:A:285:LEU:HB2	1:B:324:LEU:CD1	2.43	0.47
1:A:264:VAL:CG2	1:B:346:PHE:HB2	2.39	0.47
1:B:12:LYS:O	1:B:19[B]:VAL:HG22	2.15	0.47
1:A:116:ARG:HG3	4:A:545:HOH:O	2.12	0.46
1:B:86:VAL:HG13	1:B:88:GLU:OE1	2.16	0.46
1:A:212:MET:HG2	1:A:217:ILE:HD13	1.98	0.46
1:B:88:GLU:OE1	1:B:88:GLU:N	2.31	0.46
1:B:15:GLN:HB2	1:B:16:ASN:H	1.45	0.46
1:A:149:LEU:HB2	4:A:480:HOH:O	2.15	0.46
1:B:48[B]:ARG:CG	1:B:48[B]:ARG:NH1	2.78	0.46
1:A:303:THR:CG2	1:A:305:LYS:HE3	2.37	0.45
1:A:82:LEU:C	1:A:82:LEU:HD23	2.37	0.45
1:A:305:LYS:HD3	1:A:305:LYS:HA	1.71	0.45
1:B:308:HIS:CD2	4:B:441:HOH:O	2.69	0.45
1:B:3:ALA:HB3	1:B:159:LEU:HB2	1.99	0.45
1:B:88:GLU:CD	1:B:88:GLU:N	2.69	0.45
1:A:137:HIS:HD2	4:A:381:HOH:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ILE:HD13	1:B:283:TYR:HE2	1.81	0.44
1:B:307:ARG:HG3	1:B:307:ARG:O	2.18	0.44
1:A:86[A]:VAL:HG12	1:A:88:GLU:OE2	2.17	0.44
1:A:21[B]:ASN:HB2	1:A:216:ARG:HG2	1.99	0.44
1:A:285:LEU:HD13	1:B:328:PRO:HG3	1.99	0.44
1:A:10[A]:LEU:HD11	1:A:56:PRO:HG2	2.00	0.44
1:B:7:ILE:HD11	1:B:50[A]:LEU:CD2	2.37	0.44
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.32	0.44
1:B:181:MET:HE3	1:B:194:PHE:HZ	1.83	0.44
1:B:302:THR:HG23	1:B:309:THR:HG21	1.99	0.43
1:A:265:GLN:OE1	4:A:531:HOH:O	2.21	0.43
1:B:276:LEU:C	1:B:276:LEU:HD12	2.38	0.43
1:B:166:PHE:HZ	1:B:181:MET:CE	2.31	0.43
1:B:25:LEU:HD21	1:B:33:LEU:HD21	2.01	0.43
1:B:178:ARG:HG3	1:B:179[B]:GLU:H	1.83	0.43
1:A:305:LYS:NZ	1:A:310:GLU:OE1	2.52	0.43
1:B:244:VAL:HG12	1:B:245:PHE:N	2.33	0.43
1:A:262:LEU:HA	1:A:263:PRO:HD3	1.85	0.43
1:B:23:ILE:HD13	1:B:217[A]:ILE:HG13	2.01	0.42
1:A:15:GLN:HB3	1:A:15:GLN:HE21	1.48	0.42
1:A:276:LEU:HD23	1:B:344:ALA:CB	2.47	0.42
1:B:284:SER:OG	1:B:286:HIS:CE1	2.65	0.42
1:A:338:LEU:HD12	1:B:284:SER:O	2.20	0.42
1:A:85:LEU:HD23	1:A:165:PRO:HB3	2.02	0.41
1:B:67:THR:HG21	1:B:73:THR:HG21	2.00	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.77	0.41
1:A:157:PRO:HG2	1:A:160:ILE:HB	2.02	0.41
1:B:166:PHE:HZ	1:B:181:MET:HE2	1.86	0.41
1:A:67:THR:O	1:A:67:THR:HG23	2.20	0.41
1:B:178:ARG:CD	1:B:205:TYR:CE2	3.01	0.41
1:A:301:LYS:HA	1:A:332:ASP:CG	2.40	0.41
1:A:284:SER:O	1:B:338:LEU:HD12	2.21	0.41
1:B:308:HIS:HE1	4:B:474:HOH:O	2.04	0.41
1:A:10[B]:LEU:HD23	1:A:11:SER:N	2.36	0.41
1:B:330:LEU:O	1:B:333:GLY:N	2.39	0.41
1:B:12:LYS:HE2	1:B:54:GLU:HG3	2.02	0.41
1:A:267:GLY:O	1:A:268:ALA:O	2.40	0.40
1:B:181:MET:HE1	1:B:194:PHE:CE2	2.56	0.40
1:B:313:LEU:HA	1:B:313:LEU:HD23	1.86	0.40
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.94	0.40
1:B:81[B]:ARG:NH2	1:B:158:GLU:H	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG13	1:A:90:VAL:O	2.22	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	349/359 (97%)	335 (96%)	11 (3%)	3 (1%)	21 9
1	B	361/359 (101%)	348 (96%)	11 (3%)	2 (1%)	30 17
All	All	710/718 (99%)	683 (96%)	22 (3%)	5 (1%)	26 14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ASN
1	A	90	VAL
1	A	268	ALA
1	A	333	GLY
1	B	331	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/288 (98%)	267 (95%)	15 (5%)	28	16
1	B	291/288 (101%)	278 (96%)	13 (4%)	34	21
All	All	573/576 (100%)	545 (95%)	28 (5%)	31	18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	SER
1	A	54[A]	GLU
1	A	54[B]	GLU
1	A	60	GLU
1	A	63	LEU
1	A	64	SER
1	A	72	ASN
1	A	82	LEU
1	A	111	ARG
1	A	276	LEU
1	A	285	LEU
1	A	302	THR
1	A	318	THR
1	A	334	ILE
1	B	15	GLN
1	B	28	ASP
1	B	47	LEU
1	B	96	THR
1	B	153	LEU
1	B	264	VAL
1	B	276	LEU
1	B	305	LYS
1	B	307	ARG
1	B	313	LEU
1	B	320	LEU
1	B	321	THR
1	B	340	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	72	ASN
1	A	94	HIS
1	A	137	HIS
1	A	145	GLN
1	A	188	ASN
1	A	197	HIS
1	A	214	GLN
1	A	219	GLN
1	A	286	HIS
1	A	288	HIS
1	B	15	GLN
1	B	117	GLN
1	B	137	HIS
1	B	145	GLN
1	B	197	HIS
1	B	204	GLN
1	B	219	GLN
1	B	286	HIS
1	B	308	HIS
1	B	323	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	ATP	A	401	3	24,33,33	1.09	1 (4%)	31,52,52	2.23	6 (19%)
2	ATP	B	360	3	24,33,33	1.08	2 (8%)	31,52,52	2.16	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	401	3	-	0/18/38/38	0/3/3/3
2	ATP	B	360	3	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	ATP	O4'-C1'	2.41	1.44	1.41
2	B	360	ATP	C2-N3	2.58	1.36	1.32
2	A	401	ATP	C5-C4	2.82	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	360	ATP	N3-C2-N1	-9.17	121.87	128.89
2	A	401	ATP	N3-C2-N1	-9.05	121.96	128.89
2	B	360	ATP	C1'-N9-C4	-3.92	121.02	126.94
2	A	401	ATP	C1'-N9-C4	-3.86	121.12	126.94
2	B	360	ATP	C4-C5-N7	-3.31	106.44	109.48
2	A	401	ATP	C4-C5-N7	-2.84	106.86	109.48
2	A	401	ATP	O3G-PG-O1G	2.08	117.28	110.58
2	A	401	ATP	O2B-PB-O3B	2.61	116.93	105.09
2	B	360	ATP	C2-N1-C6	2.75	123.68	118.77
2	A	401	ATP	C2-N1-C6	3.14	124.38	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	343/359 (95%)	0.19	18 (5%) 31 34	3, 21, 39, 47	3 (0%)
1	B	350/359 (97%)	0.08	9 (2%) 59 63	4, 16, 34, 53	0
All	All	693/718 (96%)	0.14	27 (3%) 43 47	3, 18, 37, 53	3 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	9.1
1	B	350	ASN	4.8
1	A	15	GLN	4.5
1	A	16	ASN	3.8
1	A	273	ARG	3.7
1	A	268	ALA	3.6
1	A	267	GLY	3.4
1	A	245	PHE	3.3
1	A	2	THR	3.2
1	B	294	SER	3.1
1	A	270	ALA	3.0
1	B	290	ALA	2.9
1	A	243	ILE	2.7
1	A	247	ALA	2.7
1	A	251	ALA	2.6
1	A	246	PRO	2.6
1	A	283	TYR	2.4
1	A	233	LEU	2.3
1	B	331	SER	2.2
1	A	248	ALA	2.2
1	A	250	ASN	2.2
1	B	16	ASN	2.2
1	A	6[A]	HIS	2.2
1	B	334	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	15	GLN	2.1
1	B	81[A]	ARG	2.0
1	A	269	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ATP	A	401	31/31	0.99	0.09	-0.37	5,14,21,22	0
2	ATP	B	360	31/31	0.99	0.08	-0.44	2,9,13,16	0
3	CA	A	360	1/1	1.00	0.11	-	9,9,9,9	0
3	CA	B	361	1/1	1.00	0.09	-	5,5,5,5	0
3	CA	A	361	1/1	0.97	0.09	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.