Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:01 PM GMT

PDB ID	:	1W7A
Title	:	ATP BOUND MUTS
Authors	:	Lamers, M.H.; Georgijevic, D.; Lebbink, J.; Winterwerp, H.H.K.; Agianian, B.; De Wind, N.; Sixma, T.K.
Deposited on	:	2004-08-31
Resolution	:	2.27 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:

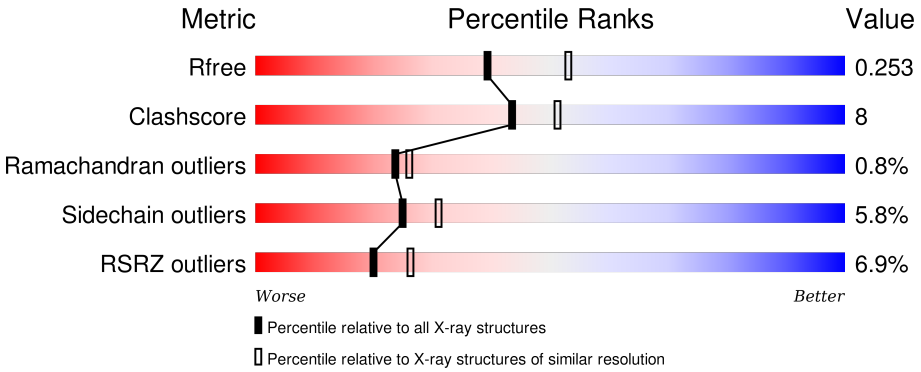
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.27 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	800	6% 80% 16%
1	B	800	7% 75% 17% 5%
2	E	30	13% 33% 23% 40%
3	F	30	3% 30% 23% 43%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13285 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6225	3915	1106	1175	29			
1	B	762	Total	C	N	O	S	0	0	0
			6017	3784	1071	1134	28			

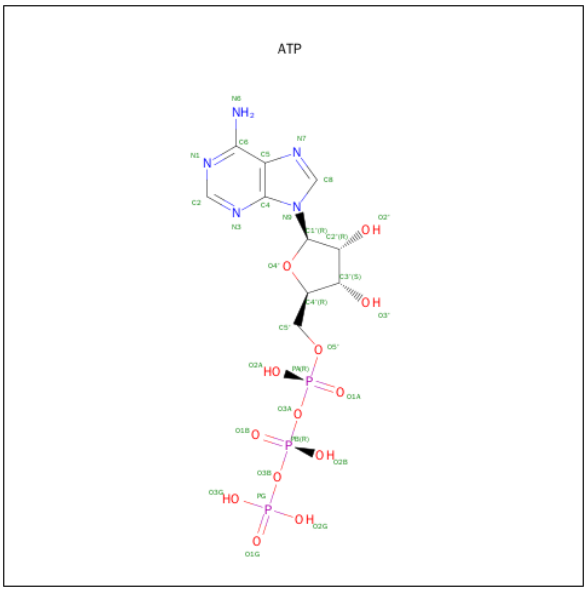
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP* AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			

- Molecule 3 is a DNA chain called 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP *GP*AP*CP*AP*CP*TP*GP*GP*TP*GP*CP*TP*TP*GP*GP*CP*AP*GP* CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			347	166	62	103	16			

- 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
4	A	1	Total C N O P 31 10 5 13 3	0	0
4	B	1	Total C N O P 31 10 5 13 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is water.

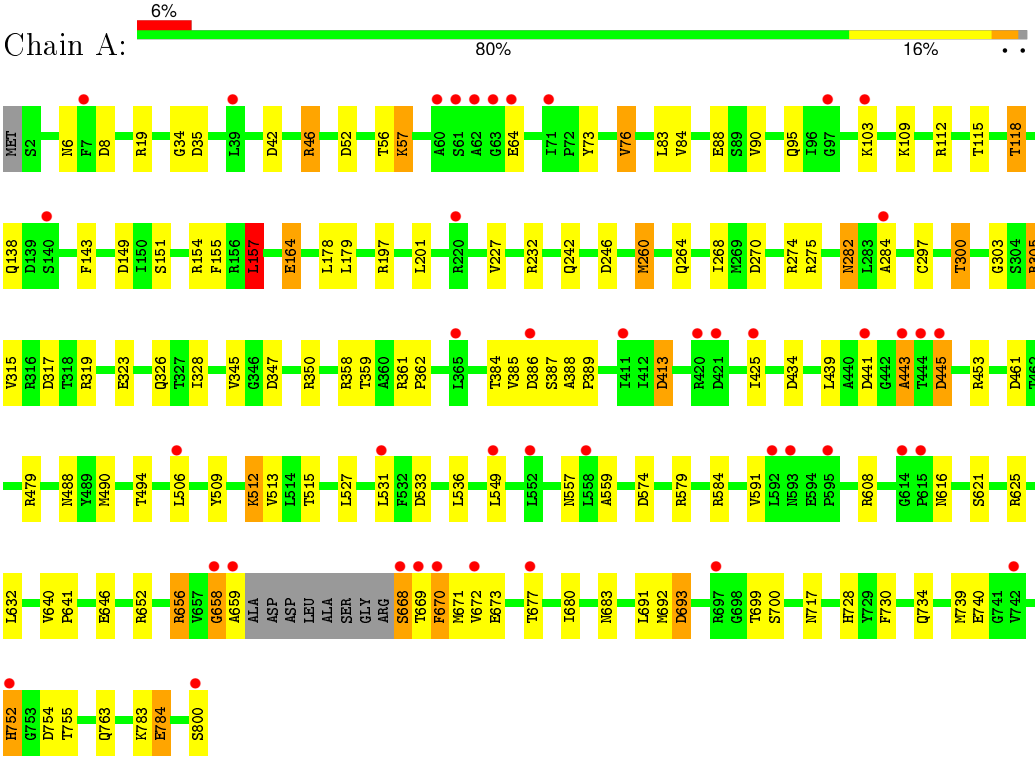
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	132	Total O 132 132	0	0
6	B	124	Total O 124 124	0	0
6	E	5	Total O 5 5	0	0
6	F	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

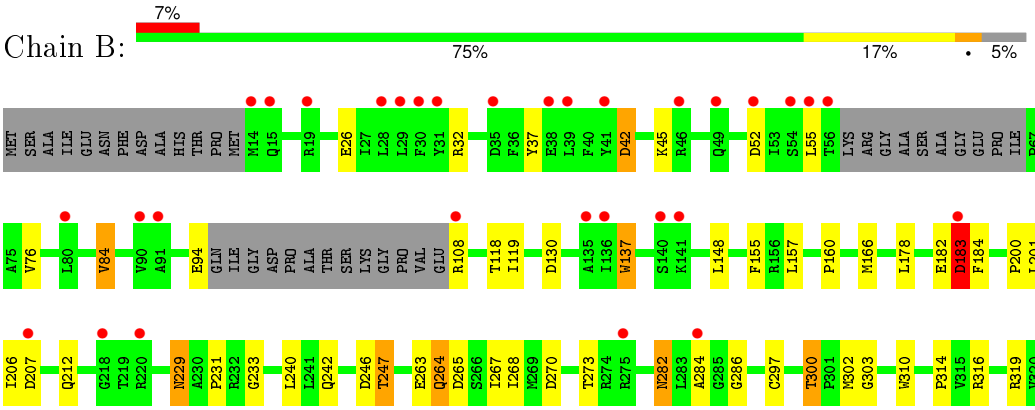
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

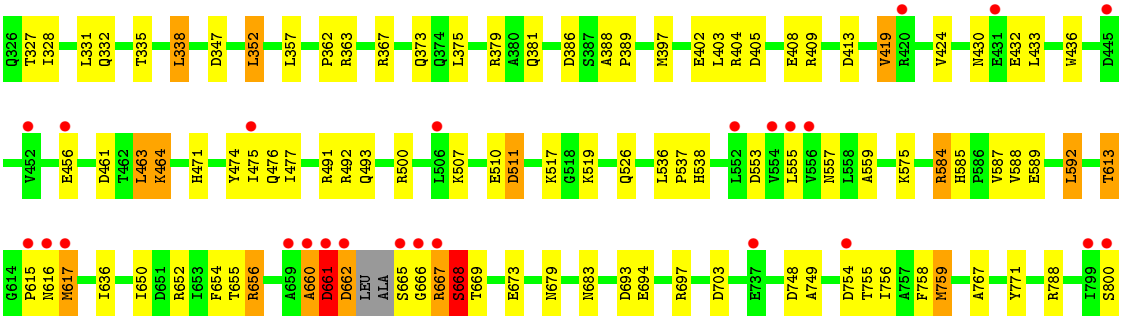
Chain A:



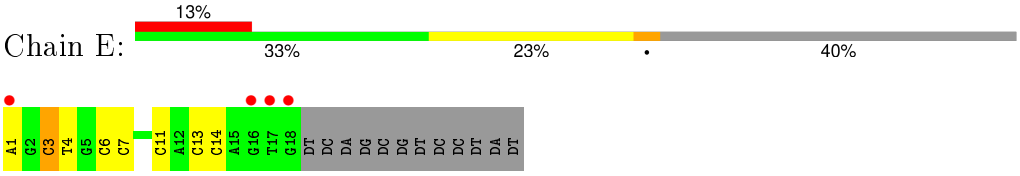
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

Chain B:

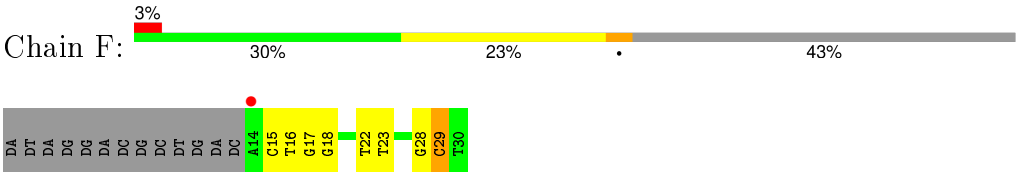




• Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP* GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP* AP*T)-3'



• Molecule 3: 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP *GP*AP*CP*AP*CP*TP*GP* GP*TP*GP*CP*TP*TP*GP*GP*CP*AP*GP* CP*T)-3'



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.64Å 93.04Å 262.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.27 19.80 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.27) 98.1 (19.80-2.27)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.216 , 0.253 0.217 , 0.253	Depositor DCC
R_{free} test set	2002 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.4	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 101609 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13285	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: MG, 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	0.58	0/6331	0.77	19/8569 (0.2%)
1	B	0.59	1/6115 (0.0%)	0.75	17/8270 (0.2%)
2	E	0.88	0/412	1.33	2/634 (0.3%)
3	F	1.01	1/388 (0.3%)	1.39	3/598 (0.5%)
All	All	0.61	2/13246 (0.0%)	0.82	41/18071 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	23	DT	C3'-O3'	-5.58	1.36	1.44
1	B	660	ALA	CA-CB	-5.02	1.41	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	22	DT	O4'-C1'-N1	-6.79	103.25	108.00
1	A	246	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	149	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	703	ASP	CB-CG-OD2	6.31	123.98	118.30
2	E	11	DC	C5'-C4'-O4'	-6.26	97.41	109.30
1	B	42	ASP	CB-CG-OD2	6.12	123.80	118.30
1	A	121	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	693	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	270	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	434	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	445	ASP	N-CA-C	-5.93	94.97	111.00
1	A	52	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	441	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	305	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	E	3	DC	O4'-C1'-N1	5.83	112.08	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	23	DT	O4'-C1'-N1	-5.68	104.02	108.00
1	A	157	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	413	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	754	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	461	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	461	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	693	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	265	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	35	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	183	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	413	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	511	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	305	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	574	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	347	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	207	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	386	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	386	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	8	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	661	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	130	ASP	CB-CG-OD2	5.13	122.92	118.30
3	F	29	DC	O4'-C1'-N1	5.12	111.59	108.00
1	B	748	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	754	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	42	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	246	ASP	CB-CG-OD2	5.03	122.82	118.30

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	6225	0	6268	93	0
1	B	6017	0	6062	108	0
2	E	367	0	202	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	347	0	194	4	0
4	A	31	0	12	0	0
4	B	31	0	12	2	0
5	A	1	0	0	0	0
6	A	132	0	0	18	0
6	B	124	0	0	11	0
6	E	5	0	0	1	0
6	F	5	0	0	1	0
All	All	13285	0	12750	208	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 8.

All (208) 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:662:ASP:HB3	1:B:666:GLY:HA3	1.28	1.13
1:A:784:GLU:OE1	1:A:784:GLU:N	1.82	1.10
1:A:46:ARG:NH2	1:A:88:GLU:OE1	2.08	0.87
1:B:660:ALA:HB3	1:B:669:THR:HG23	1.56	0.87
1:B:662:ASP:HB3	1:B:666:GLY:CA	2.07	0.83
1:A:154:ARG:NH1	6:A:2038:HOH:O	2.13	0.82
1:B:660:ALA:CB	1:B:669:THR:HG23	2.10	0.82
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.63	0.79
1:A:668:SER:OG	1:A:669:THR:N	2.12	0.79
1:A:118:THR:HG22	6:A:2024:HOH:O	1.83	0.79
1:A:34:GLY:H	1:A:95:GLN:HE22	1.30	0.78
1:A:784:GLU:H	1:A:784:GLU:CD	1.89	0.76
2:E:3:DC:H2"	2:E:4:DT:H5'	1.69	0.75
1:A:680:ILE:HD13	1:A:692:MET:HE1	1.69	0.75
1:B:616:ASN:HA	4:B:1801:ATP:O1B	1.90	0.72
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.70	0.72
1:A:109:LYS:HE2	6:A:2022:HOH:O	1.90	0.72
1:B:616:ASN:O	1:B:617:MET:HB2	1.90	0.71
1:B:507:LYS:NZ	1:B:510:GLU:OE1	2.25	0.69
1:B:660:ALA:HB1	1:B:669:THR:HA	1.74	0.69
1:B:662:ASP:N	1:B:662:ASP:OD1	2.27	0.68
1:B:282:ASN:HD22	1:B:284:ALA:H	1.41	0.67
1:A:326:GLN:HB3	6:A:2073:HOH:O	1.94	0.67
1:B:463:LEU:HD12	1:B:464:LYS:N	2.09	0.67
1:A:34:GLY:H	1:A:95:GLN:NE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:THR:HA	6:A:2108:HOH:O	1.94	0.66
1:A:300:THR:HG22	1:A:303:GLY:H	1.61	0.66
1:A:358:ARG:NH2	1:A:533:ASP:OD1	2.27	0.64
1:B:212:GLN:HG2	6:B:2003:HOH:O	1.96	0.64
1:A:656:ARG:HB2	1:A:692:MET:HE2	1.80	0.63
1:B:430:ASN:HD22	1:B:433:LEU:H	1.44	0.63
1:A:282:ASN:HD22	1:A:284:ALA:H	1.45	0.63
1:A:672:VAL:N	6:A:2108:HOH:O	2.28	0.63
1:A:305:ARG:NH2	1:A:347:ASP:OD2	2.32	0.62
1:A:717:ASN:HB2	1:A:739:MET:HE1	1.80	0.62
1:A:509:TYR:CZ	1:A:513:VAL:HG21	2.34	0.61
1:B:267:ILE:HB	1:B:314:PRO:HG2	1.82	0.61
1:B:300:THR:HG22	1:B:303:GLY:H	1.66	0.61
1:A:46:ARG:NH2	1:A:88:GLU:CD	2.54	0.61
2:E:1:DA:H3'	6:E:2001:HOH:O	2.01	0.60
1:A:673:GLU:O	1:A:677:THR:HG23	2.01	0.60
1:A:752:HIS:CD2	1:A:755:THR:HG23	2.36	0.60
1:A:752:HIS:CD2	1:A:755:THR:CG2	2.85	0.59
1:B:404:ARG:O	1:B:408:GLU:HG3	2.02	0.59
1:A:270:ASP:O	1:A:274:ARG:HG3	2.03	0.59
1:A:73:TYR:O	1:A:76:VAL:HG22	2.02	0.59
1:B:667:ARG:O	1:B:668:SER:HB3	2.03	0.59
1:A:345:VAL:HG11	1:A:549:LEU:HD13	1.84	0.59
2:E:6:DC:H2"	2:E:7:DC:H5'	1.84	0.58
1:A:300:THR:CG2	1:A:303:GLY:H	2.17	0.57
1:A:315:VAL:HG12	1:A:317:ASP:H	1.69	0.57
1:B:517:LYS:NZ	6:B:2071:HOH:O	2.37	0.57
1:A:652:ARG:HD3	6:A:2106:HOH:O	2.04	0.57
1:A:443:ALA:HA	1:A:509:TYR:OH	2.06	0.56
1:A:616:ASN:HB3	6:A:2131:HOH:O	2.04	0.56
1:B:660:ALA:O	1:B:661:ASP:HB2	2.06	0.56
1:B:476:GLN:OE1	1:B:500:ARG:HD3	2.06	0.56
1:B:55:LEU:O	1:B:55:LEU:HG	2.05	0.56
1:B:363:ARG:O	1:B:367:ARG:HG3	2.05	0.56
1:B:613:THR:CG2	1:B:767:ALA:H	2.18	0.56
1:A:46:ARG:NH2	1:A:88:GLU:OE2	2.39	0.56
1:A:800:SER:HA	6:A:2130:HOH:O	2.05	0.56
1:B:263:GLU:HG2	1:B:268:ILE:HD11	1.88	0.55
1:A:282:ASN:C	1:A:282:ASN:HD22	2.10	0.55
1:B:160:PRO:HG2	1:B:166:MET:SD	2.46	0.55
3:F:15:DC:H2"	3:F:16:DT:H5'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:HZ3	1:A:512:LYS:HB2	1.70	0.55
1:A:752:HIS:O	1:A:755:THR:HG22	2.07	0.55
1:A:728:HIS:HB2	6:A:2117:HOH:O	2.06	0.54
1:A:282:ASN:ND2	1:A:284:ALA:H	2.06	0.54
1:B:327:THR:HG22	1:B:331:LEU:HD12	1.90	0.54
1:B:300:THR:HB	1:B:553:ASP:OD2	2.08	0.54
1:B:324:ARG:O	1:B:328:ILE:HG12	2.08	0.53
1:B:282:ASN:HD21	1:B:286:GLY:H	1.57	0.53
1:A:282:ASN:HD22	1:A:284:ALA:N	2.06	0.53
1:A:717:ASN:HB2	1:A:739:MET:CE	2.38	0.53
1:B:37:TYR:CD2	1:B:76:VAL:HG21	2.44	0.53
1:B:310:TRP:O	1:B:636:ILE:CD1	2.57	0.53
1:B:264:GLN:H	1:B:264:GLN:HE21	1.55	0.52
1:B:471:HIS:CE1	1:B:493:GLN:HB2	2.43	0.52
1:B:617:MET:N	4:B:1801:ATP:O1B	2.39	0.52
1:B:157:LEU:HD13	1:B:233:GLY:HA3	1.91	0.52
1:B:297:CYS:H	1:B:557:ASN:HD21	1.58	0.52
1:B:37:TYR:CE2	1:B:76:VAL:HG21	2.44	0.51
1:B:108:ARG:N	6:B:2009:HOH:O	2.43	0.51
1:B:84:VAL:HG11	1:B:119:ILE:HD13	1.93	0.51
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.92	0.51
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.46	0.51
1:A:115:THR:OG1	1:A:118:THR:HB	2.11	0.51
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.92	0.50
1:A:494:THR:OG1	1:B:491:ARG:HD2	2.11	0.50
1:B:338:LEU:HD13	1:B:381:GLN:OE1	2.11	0.50
1:B:316:ARG:HD3	1:B:650:ILE:O	2.12	0.50
1:A:6:ASN:HD22	1:A:6:ASN:H	1.60	0.50
1:B:679:ASN:ND2	1:B:683:ASN:HD22	2.10	0.50
1:A:157:LEU:C	1:A:157:LEU:HD23	2.31	0.50
1:B:373:GLN:HG2	1:B:404:ARG:HE	1.77	0.49
1:A:143:PHE:C	1:A:232:ARG:HD3	2.32	0.49
1:A:640:VAL:HG13	1:A:641:PRO:HD2	1.93	0.49
1:B:32:ARG:NH1	1:B:94:GLU:OE1	2.45	0.49
3:F:28:DG:H5"	6:F:2004:HOH:O	2.12	0.49
1:B:430:ASN:HD21	1:B:432:GLU:HB2	1.77	0.49
1:B:405:ASP:OD2	1:B:409:ARG:NH1	2.40	0.49
1:A:672:VAL:HB	6:A:2108:HOH:O	2.13	0.49
1:B:264:GLN:H	1:B:264:GLN:NE2	2.10	0.49
1:A:359:THR:O	1:A:359:THR:HG22	2.14	0.48
1:A:632:LEU:C	1:A:632:LEU:HD23	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:ASN:O	1:B:617:MET:CB	2.61	0.48
1:A:752:HIS:HD2	1:A:755:THR:CG2	2.27	0.48
1:A:652:ARG:NH1	1:A:683:ASN:O	2.47	0.48
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.96	0.48
1:A:274:ARG:NH2	1:A:312:HIS:O	2.47	0.48
1:A:670:PHE:N	6:A:2108:HOH:O	2.46	0.48
1:B:72:PRO:HB2	1:B:74:HIS:CE1	2.49	0.48
1:B:662:ASP:CB	1:B:666:GLY:HA3	2.20	0.47
1:B:588:VAL:O	1:B:592:LEU:HD22	2.13	0.47
1:B:229:ASN:HD22	1:B:229:ASN:H	1.61	0.47
3:F:28:DG:H2"	3:F:29:DC:H5"	1.95	0.47
1:B:526:GLN:HG2	6:B:2074:HOH:O	2.15	0.47
1:B:300:THR:CG2	1:B:302:MET:HG2	2.44	0.47
1:B:585:HIS:HD2	1:B:587:VAL:H	1.63	0.47
1:B:319:ARG:NE	6:B:2050:HOH:O	2.45	0.47
1:B:332:GLN:HB2	6:B:2080:HOH:O	2.15	0.47
1:B:584:ARG:HD2	1:B:589:GLU:OE1	2.14	0.47
1:A:453:ARG:NE	6:A:2081:HOH:O	2.45	0.47
1:A:699:THR:HA	1:B:616:ASN:ND2	2.29	0.47
1:B:788:ARG:NE	6:B:2121:HOH:O	2.47	0.47
1:B:656:ARG:NH1	1:B:673:GLU:HG3	2.30	0.46
1:A:608:ARG:NH2	1:A:740:GLU:OE1	2.39	0.46
1:A:118:THR:CG2	6:A:2024:HOH:O	2.49	0.46
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.97	0.46
1:A:425:ILE:CD1	1:A:527:LEU:HB2	2.45	0.46
1:B:617:MET:HB3	1:B:758:PHE:CD2	2.50	0.46
1:A:179:LEU:HD23	1:A:197:ARG:HB2	1.98	0.46
1:B:652:ARG:HD2	1:B:654:PHE:CZ	2.51	0.46
1:B:759:MET:CE	1:B:759:MET:HA	2.46	0.46
1:A:138:GLN:HB3	1:A:143:PHE:CD1	2.51	0.46
3:F:17:DG:H1'	3:F:18:DG:C8	2.51	0.46
1:A:621:SER:OG	1:A:693:ASP:OD2	2.34	0.45
1:A:746:HIS:CE1	1:A:763:GLN:HB2	2.51	0.45
1:B:206:ILE:HD12	1:B:231:PRO:HB3	1.97	0.45
1:A:64:GLU:HG3	6:A:2014:HOH:O	2.16	0.45
1:A:56:THR:OG1	1:A:57:LYS:N	2.50	0.45
1:A:268:ILE:HB	1:A:652:ARG:HG2	1.98	0.44
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.99	0.44
1:A:783:LYS:N	1:A:784:GLU:OE1	2.50	0.44
1:A:6:ASN:H	1:A:6:ASN:ND2	2.16	0.44
1:A:151:SER:HB3	1:A:350:ARG:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:DC:C2'	2:E:7:DC:H5'	2.48	0.44
1:A:319:ARG:O	1:A:323:GLU:HG3	2.17	0.44
1:A:656:ARG:HG3	1:A:677:THR:HG22	1.99	0.44
1:B:362:PRO:HG3	1:B:419:VAL:HG13	1.98	0.44
1:B:660:ALA:CB	1:B:669:THR:HA	2.45	0.43
1:B:182:GLU:O	1:B:184:PHE:N	2.51	0.43
1:B:585:HIS:CE1	6:B:2089:HOH:O	2.71	0.43
1:B:388:ALA:N	1:B:389:PRO:CD	2.82	0.43
1:B:463:LEU:HD22	1:B:477:ILE:HD11	2.01	0.43
1:B:403:LEU:HD21	1:B:538:HIS:CD2	2.54	0.43
1:A:658:GLY:O	1:A:659:ALA:CB	2.67	0.43
1:B:613:THR:HG23	1:B:767:ALA:CB	2.49	0.43
1:B:585:HIS:HE1	6:B:2089:HOH:O	2.01	0.43
1:A:579:ARG:HH21	1:A:646:GLU:CD	2.22	0.43
1:B:118:THR:OG1	1:B:247:THR:HG21	2.18	0.43
1:A:656:ARG:HB2	1:A:692:MET:CE	2.48	0.42
1:B:200:PRO:HB2	1:B:202:TRP:CD1	2.53	0.42
1:B:749:ALA:HB3	1:B:771:TYR:CE2	2.54	0.42
1:B:800:SER:HA	6:B:2123:HOH:O	2.17	0.42
1:B:430:ASN:ND2	1:B:433:LEU:H	2.16	0.42
1:A:512:LYS:HB2	1:A:512:LYS:NZ	2.33	0.42
1:B:321:LEU:O	1:B:325:GLN:HG3	2.20	0.42
1:B:137:TRP:HB3	1:B:204:PHE:CE2	2.54	0.42
1:A:669:THR:CA	6:A:2108:HOH:O	2.62	0.42
1:B:310:TRP:O	1:B:636:ILE:HD12	2.19	0.42
1:A:83:LEU:HD13	1:A:90:VAL:HG21	2.02	0.42
1:B:310:TRP:O	1:B:636:ILE:HD11	2.19	0.42
1:B:118:THR:CB	1:B:247:THR:HG21	2.49	0.42
1:B:656:ARG:O	1:B:656:ARG:HG3	2.19	0.42
1:A:621:SER:O	1:A:625:ARG:HG3	2.20	0.42
1:B:338:LEU:CD1	1:B:381:GLN:OE1	2.67	0.41
1:B:182:GLU:C	1:B:184:PHE:H	2.23	0.41
1:A:297:CYS:H	1:A:557:ASN:ND2	2.18	0.41
1:B:402:GLU:HG2	6:B:2061:HOH:O	2.19	0.41
1:A:361:ARG:HB3	1:A:362:PRO:HD2	2.02	0.41
1:A:463:LEU:HA	1:A:476:GLN:O	2.20	0.41
1:B:463:LEU:HB2	1:B:477:ILE:HD13	2.02	0.41
1:B:536:LEU:N	1:B:537:PRO:CD	2.83	0.41
1:B:268:ILE:HB	1:B:652:ARG:HB3	2.01	0.41
1:A:439:LEU:HD12	1:A:512:LYS:HZ1	1.85	0.41
1:A:680:ILE:CD1	1:A:692:MET:HE1	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLN:NE2	1:B:242:GLN:NE2	2.69	0.41
2:E:13:DC:H2"	2:E:14:DC:H5'	2.02	0.41
1:B:755:THR:OG1	1:B:756:ILE:N	2.53	0.41
1:B:436:TRP:CZ2	1:B:519:LYS:HD3	2.56	0.41
1:A:669:THR:C	1:A:671:MET:H	2.23	0.41
1:B:148:LEU:HB3	1:B:240:LEU:HD21	2.01	0.41
1:A:305:ARG:HH22	1:A:347:ASP:CG	2.21	0.41
1:B:352:LEU:HA	1:B:352:LEU:HD12	1.92	0.41
1:B:463:LEU:HD12	1:B:463:LEU:C	2.41	0.41
1:B:660:ALA:HB3	1:B:669:THR:CG2	2.38	0.40
1:B:273:THR:HG23	1:B:655:THR:HG23	2.03	0.40
1:B:694:GLU:OE1	1:B:697:ARG:NE	2.47	0.40
1:B:660:ALA:HB2	1:B:669:THR:HG23	1.96	0.40
1:A:297:CYS:H	1:A:557:ASN:HD21	1.70	0.40
1:A:19:ARG:NH2	6:A:2006:HOH:O	2.54	0.40
1:B:282:ASN:C	1:B:282:ASN:HD22	2.24	0.40
1:A:164:GLU:OE2	6:A:2043:HOH:O	2.22	0.40
1:B:463:LEU:CD1	1:B:475:ILE:HG23	2.51	0.40
1:A:227:VAL:HG12	1:A:260:MET:HB2	2.02	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	787/800 (98%)	756 (96%)	25 (3%)	6 (1%)	24	26
1	B	754/800 (94%)	724 (96%)	23 (3%)	7 (1%)	21	22
All	All	1541/1600 (96%)	1480 (96%)	48 (3%)	13 (1%)	24	26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	667	ARG
1	B	668	SER
1	B	183	ASP
1	B	617	MET
1	A	103	LYS
1	A	443	ALA
1	B	661	ASP
1	B	45	LYS
1	A	387	SER
1	A	670	PHE
1	B	615	PRO
1	A	385	VAL
1	A	658	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	658/664 (99%)	618 (94%)	40 (6%)	23	29
1	B	636/664 (96%)	601 (94%)	35 (6%)	27	34
All	All	1294/1328 (97%)	1219 (94%)	75 (6%)	25	31

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	57	LYS
1	A	76	VAL
1	A	84	VAL
1	A	112	ARG
1	A	118	THR
1	A	137	TRP
1	A	155	PHE
1	A	157	LEU
1	A	164	GLU
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	242	GLN
1	A	260	MET
1	A	264	GLN
1	A	275	ARG
1	A	282	ASN
1	A	300	THR
1	A	311	LEU
1	A	384	THR
1	A	413	ASP
1	A	445	ASP
1	A	479	ARG
1	A	488	ASN
1	A	490	MET
1	A	506	LEU
1	A	512	LYS
1	A	515	THR
1	A	531	LEU
1	A	536	LEU
1	A	584	ARG
1	A	591	VAL
1	A	656	ARG
1	A	668	SER
1	A	700	SER
1	A	730	PHE
1	A	734	GLN
1	A	748	ASP
1	A	752	HIS
1	A	784	GLU
1	B	26	GLU
1	B	42	ASP
1	B	52	ASP
1	B	84	VAL
1	B	137	TRP
1	B	155	PHE
1	B	178	LEU
1	B	183	ASP
1	B	201	LEU
1	B	229	ASN
1	B	247	THR
1	B	264	GLN
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	300	THR
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	379	ARG
1	B	419	VAL
1	B	424	VAL
1	B	456	GLU
1	B	463	LEU
1	B	464	LYS
1	B	492	ARG
1	B	511	ASP
1	B	575	LYS
1	B	584	ARG
1	B	592	LEU
1	B	613	THR
1	B	656	ARG
1	B	662	ASP
1	B	665	SER
1	B	668	SER
1	B	759	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	95	GLN
1	A	282	ASN
1	A	312	HIS
1	A	471	HIS
1	A	493	GLN
1	A	543	GLN
1	A	557	ASN
1	A	566	ASN
1	A	590	GLN
1	A	602	ASN
1	A	734	GLN
1	A	752	HIS
1	B	15	GLN
1	B	23	GLN
1	B	131	ASN

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Mol	Chain	Res	Type
1	B	138	GLN
1	B	212	GLN
1	B	229	ASN
1	B	242	GLN
1	B	264	GLN
1	B	282	ASN
1	B	430	ASN
1	B	471	HIS
1	B	538	HIS
1	B	543	GLN
1	B	557	ASN
1	B	585	HIS
1	B	590	GLN
1	B	616	ASN
1	B	679	ASN
1	B	714	ASN
1	B	717	ASN
1	B	791	GLN

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

Of 3 ligands modelled in this entry, 1 is 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	$\#\|Z\| > 2$
4	ATP	A	1801	5	24,33,33	1.08	2 (8%)	31,52,52	2.13	8 (25%)
4	ATP	B	1801	-	24,33,33	1.09	4 (16%)	31,52,52	1.98	6 (19%)

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
4	ATP	A	1801	5	-	0/18/38/38	0/3/3/3
4	ATP	B	1801	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	ATP	C4-N3	-2.44	1.31	1.35
4	B	1801	ATP	C5-N7	-2.23	1.31	1.39
4	A	1801	ATP	C5-N7	-2.04	1.32	1.39
4	B	1801	ATP	O4'-C1'	2.05	1.43	1.41
4	B	1801	ATP	C5-C4	2.10	1.45	1.40
4	A	1801	ATP	C5-C4	2.84	1.46	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1801	ATP	N3-C2-N1	-8.43	122.44	128.89
4	A	1801	ATP	N3-C2-N1	-8.19	122.62	128.89
4	A	1801	ATP	PA-O3A-PB	-3.35	123.32	132.73
4	A	1801	ATP	C2'-C1'-N9	-3.01	109.69	114.29
4	B	1801	ATP	C2'-C1'-N9	-2.97	109.76	114.29
4	B	1801	ATP	PB-O3B-PG	-2.88	123.00	132.67
4	A	1801	ATP	PB-O3B-PG	-2.82	123.21	132.67
4	B	1801	ATP	C4-C5-N7	-2.06	107.58	109.48
4	B	1801	ATP	C2-N1-C6	2.08	122.48	118.77
4	A	1801	ATP	O2B-PB-O1B	2.08	123.82	112.53
4	A	1801	ATP	C4'-O4'-C1'	2.09	112.02	109.72
4	A	1801	ATP	O3G-PG-O2G	2.13	115.48	107.38
4	B	1801	ATP	O2A-PA-O3A	2.32	115.59	105.09
4	A	1801	ATP	O2G-PG-O1G	2.98	120.17	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1801	ATP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	791/800 (98%)	0.31	47 (5%) 26 33	20, 31, 47, 64	0
1	B	762/800 (95%)	0.34	57 (7%) 17 23	17, 31, 50, 65	0
2	E	18/30 (60%)	0.46	4 (22%) 1 1	28, 37, 64, 64	0
3	F	17/30 (56%)	0.10	1 (5%) 26 33	25, 36, 63, 64	0
All	All	1588/1660 (95%)	0.33	109 (6%) 20 26	17, 31, 49, 65	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	ALA	8.0
1	B	660	ALA	7.1
1	B	667	ARG	7.0
1	A	444	THR	6.6
1	B	616	ASN	6.6
1	B	665	SER	6.0
1	B	661	ASP	5.7
1	B	30	PHE	5.6
1	A	62	ALA	5.4
1	A	658	GLY	5.3
1	A	669	THR	5.1
1	A	800	SER	5.0
1	B	617	MET	4.9
1	B	666	GLY	4.7
2	E	18	DG	4.6
1	A	475	ILE	4.6
1	B	29	LEU	4.6
3	F	14	DA	4.6
1	A	668	SER	4.2
1	B	19	ARG	4.1
1	B	39	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	799	ILE	3.9
2	E	1	DA	3.8
1	B	659	ALA	3.8
1	A	752	HIS	3.7
1	A	441	ASP	3.7
1	B	28	LEU	3.6
1	A	103	LYS	3.5
1	B	506	LEU	3.5
1	B	475	ILE	3.5
1	B	41	TYR	3.4
1	B	800	SER	3.4
1	B	456	GLU	3.4
1	B	91	ALA	3.3
1	B	136	ILE	3.3
1	A	593	ASN	3.2
1	B	55	LEU	3.2
1	A	97	GLY	3.2
1	B	662	ASP	3.1
1	A	592	LEU	3.1
1	B	90	VAL	3.1
1	A	365	LEU	3.0
1	B	74	HIS	3.0
1	A	443	ALA	3.0
1	B	108	ARG	3.0
1	B	552	LEU	3.0
1	B	52	ASP	3.0
1	A	552	LEU	3.0
1	B	218	GLY	2.9
1	A	63	GLY	2.9
1	B	54	SER	2.9
2	E	17	DT	2.8
1	B	555	LEU	2.8
1	B	183	ASP	2.8
1	A	595	PRO	2.8
1	B	141	LYS	2.7
1	A	670	PHE	2.7
1	A	64	GLU	2.7
1	A	220	ARG	2.6
1	B	754	ASP	2.6
1	A	140	SER	2.6
1	A	742	VAL	2.6
1	B	556	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	61	SER	2.6
1	B	452	VAL	2.6
1	A	421	ASP	2.6
1	B	35	ASP	2.6
1	A	411	ILE	2.5
1	A	672	VAL	2.5
1	B	140	SER	2.5
1	B	38	GLU	2.5
1	B	49	GLN	2.5
1	A	7	PHE	2.5
1	A	747	LEU	2.4
1	B	220	ARG	2.4
1	A	284	ALA	2.4
1	B	80	LEU	2.4
1	A	386	ASP	2.4
1	B	284	ALA	2.4
1	B	615	PRO	2.4
1	A	615	PRO	2.3
1	B	135	ALA	2.3
1	A	425	ILE	2.3
1	B	737	GLU	2.3
1	B	46	ARG	2.3
1	A	136	ILE	2.3
1	A	60	ALA	2.3
2	E	16	DG	2.3
1	A	445	ASP	2.3
1	A	677	THR	2.2
1	A	697	ARG	2.2
1	A	420	ARG	2.1
1	B	31	TYR	2.1
1	B	275	ARG	2.1
1	B	15	GLN	2.1
1	B	207	ASP	2.1
1	A	549	LEU	2.1
1	B	420	ARG	2.1
1	A	71	ILE	2.1
1	B	431	GLU	2.1
1	A	39	LEU	2.0
1	A	531	LEU	2.0
1	A	558	LEU	2.0
1	B	14	MET	2.0
1	A	614	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	506	LEU	2.0
1	B	445	ASP	2.0
1	B	56	THR	2.0
1	B	554	VAL	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
4	ATP	B	1801	31/31	0.84	0.23	0.62	41,52,58,65	0
4	ATP	A	1801	31/31	0.90	0.15	-0.33	52,55,63,64	0
5	MG	A	1802	1/1	0.87	0.07	-	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.