



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:50 PM UTC

PDB ID : 1W7A / pdb_00001w7a
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

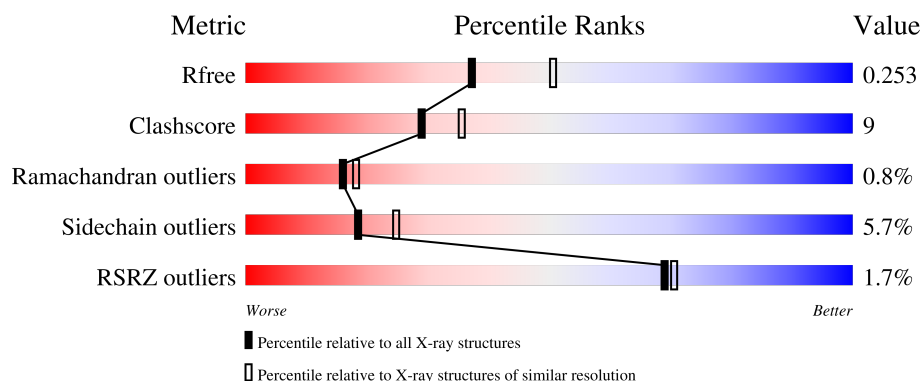
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	800	 81% 15% ..
1	B	800	 76% 16% 5%
2	E	30	 33% 27% 40%
3	F	30	 37% 20% 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			

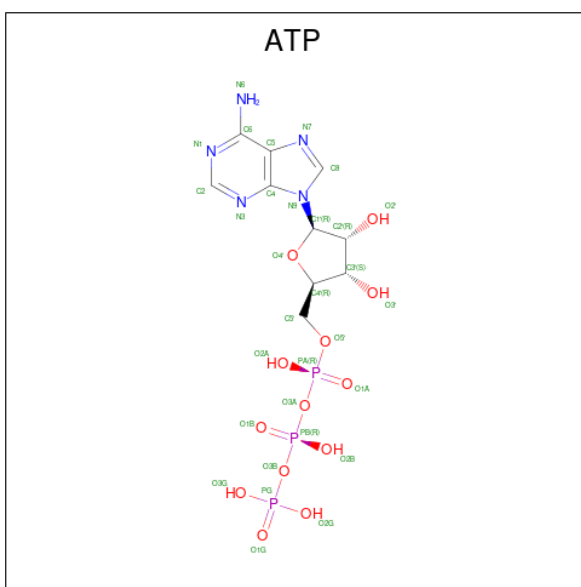
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*A P*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP* AP*T)-3'.

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*A P*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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

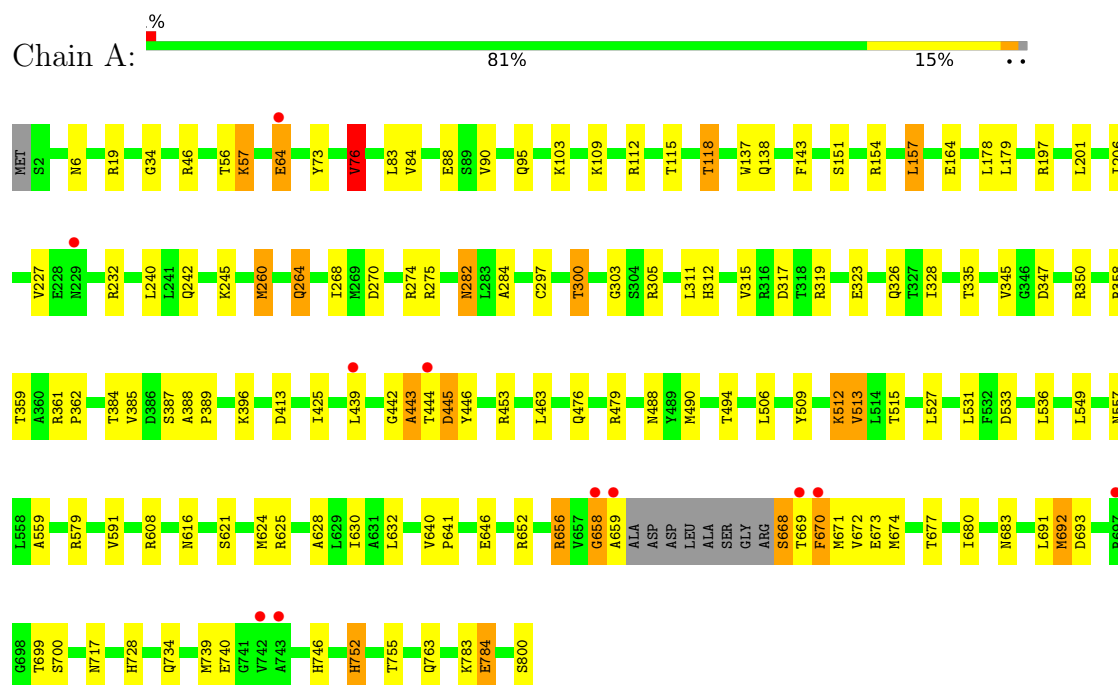
- Molecule 6 is water.

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

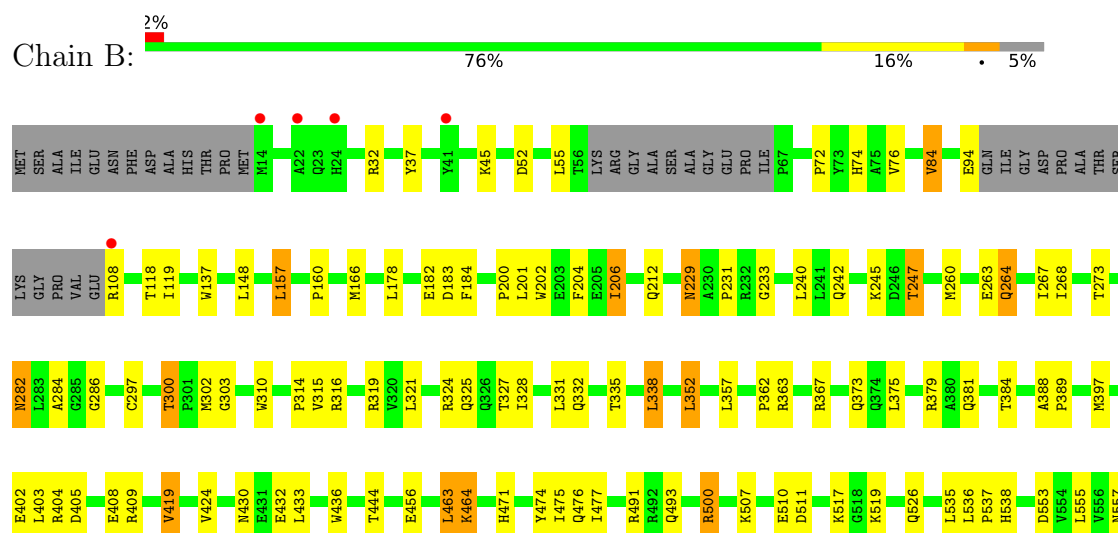
3 Residue-property plots

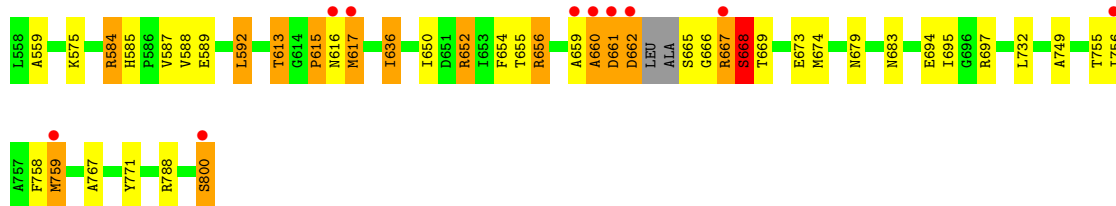
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA MISMATCH REPAIR PROTEIN MUTS

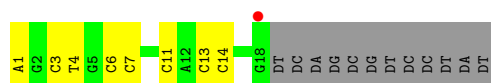
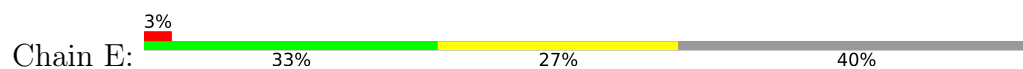


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

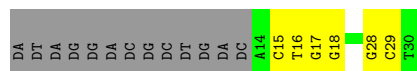
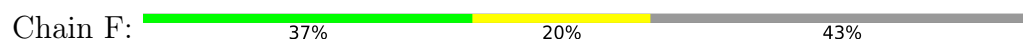




● Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP *CP*AP*CP*CP*AP*GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP* AP*T)-3'



● 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

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 20.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.27) 98.2 (20.00-2.27)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (1.97%)	wwPDB-VP
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 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	0.78	2/6331 (0.0%)	0.89	5/8569 (0.1%)
1	B	0.80	2/6115 (0.0%)	0.87	5/8270 (0.1%)
2	E	0.47	0/412	1.01	1/634 (0.2%)
3	F	0.49	0/388	0.99	0/598
All	All	0.77	4/13246 (0.0%)	0.89	11/18071 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	660	ALA	CA-CB	-6.85	1.41	1.53
1	A	692	MET	SD-CE	-6.37	1.63	1.79
1	A	624	MET	SD-CE	-5.77	1.65	1.79
1	B	260	MET	SD-CE	5.63	1.93	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	636	ILE	N-CA-C	-8.03	105.66	113.53
2	E	11	DC	C5'-C4'-O4'	-7.99	97.41	109.40
1	A	445	ASP	N-CA-C	-7.43	94.97	110.80
1	A	442	GLY	N-CA-C	-6.64	106.13	114.16
1	A	444	THR	N-CA-C	6.53	120.07	108.24
1	A	76	VAL	CB-CA-C	-6.34	103.58	112.14
1	B	206	ILE	N-CA-C	5.88	116.66	110.72
1	A	206	ILE	N-CA-C	5.26	115.99	110.62
1	B	656	ARG	N-CA-C	-5.19	104.12	110.65
1	B	615	PRO	N-CA-C	5.16	123.09	112.47
1	B	659	ALA	N-CA-C	5.11	117.43	109.52

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	6225	0	6268	102	0
1	B	6017	0	6062	115	0
2	E	367	0	202	5	0
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	21	0
6	B	124	0	0	12	0
6	E	5	0	0	1	0
6	F	5	0	0	1	0
All	All	13285	0	12750	224	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 9.

All (224) 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:784:GLU:H	1:A:784:GLU:CD	1.89	0.81
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
2:E:3:DC:H2''	2:E:4:DT:H5'	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:326:GLN:HB3	6:A:2073:HOH:O	1.94	0.67
1:B:282:ASN:HD22	1:B:284:ALA:H	1.41	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
1:B:617:MET:HE3	1:B:758:PHE:CD2	2.31	0.66
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:46:ARG:NH2	1:A:88:GLU:CD	2.54	0.65
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: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:B:617:MET:HE3	1:B:758:PHE:HD2	1.65	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
2:E:1:DA:H3'	6:E:2001:HOH:O	2.01	0.60
1:B:245:LYS:NZ	6:B:2033:HOH:O	2.26	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:282:ASN:HD22	1:A:282:ASN:C	2.10	0.60
1:A:674:MET:HA	1:A:674:MET:HE2	1.82	0.59
1:A:270:ASP:O	1:A:274:ARG:HG3	2.03	0.59
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: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:A:652:ARG:HD3	6:A:2106:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LYS:NZ	6:B:2071:HOH:O	2.37	0.57
1:A:396:LYS:NZ	6:A:2074:HOH:O	2.38	0.56
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: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:B:55:LEU:HG	1:B:55:LEU:O	2.05	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:717:ASN:HB2	1:A:739:MET:HE1	1.87	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
1:A:512:LYS:HB2	1:A:512:LYS:HZ2	1.70	0.55
1:A:752:HIS:O	1:A:755:THR:HG22	2.07	0.55
1:A:157:LEU:HD23	1:A:157:LEU:C	2.31	0.55
1:A:143:PHE:C	1:A:232:ARG:HD3	2.32	0.54
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:A:717:ASN:HB2	1:A:739:MET:CE	2.38	0.53
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:632:LEU:HD23	1:A:632:LEU:C	2.33	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:A:656:ARG:HB2	1:A:692:MET:HE1	1.91	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:A:680:ILE:HD13	1:A:692:MET:HE1	1.91	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:A:328:ILE:HG23	1:A:559:ALA:HA	1.92	0.51
1:B:84:VAL:HG11	1:B:119:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.46	0.51
1:B:759:MET:HA	1:B:759:MET:HE3	1.93	0.51
1:A:115:THR:OG1	1:A:118:THR:HB	2.11	0.51
1:A:494:THR:OG1	1:B:491:ARG:HD2	2.11	0.50
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.92	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:B:373:GLN:HG2	1:B:404:ARG:HE	1.77	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:405:ASP:OD2	1:B:409:ARG:NH1	2.40	0.49
1:B:430:ASN:HD21	1:B:432:GLU:HB2	1.77	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:692:MET:HE2	1:A:692:MET:HA	1.95	0.48
1:A:359:THR:HG22	1:A:359:THR:O	2.14	0.48
1:A:752:HIS:HD2	1:A:755:THR:CG2	2.27	0.48
1:B:616:ASN:O	1:B:617:MET:CB	2.61	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:A:245:LYS:NZ	6:A:2060:HOH:O	2.46	0.47
1:A:579:ARG:HH21	1:A:646:GLU:CD	2.22	0.47
1:B:588:VAL:O	1:B:592:LEU:HD22	2.13	0.47
1:B:662:ASP:CB	1:B:666:GLY:HA3	2.20	0.47
1:B:229:ASN:H	1:B:229:ASN:HD22	1.61	0.47
1:B:526:GLN:HG2	6:B:2074:HOH:O	2.15	0.47
3:F:28:DG:H2''	3:F:29:DC:H5''	1.95	0.47
1:B:182:GLU:C	1:B:184:PHE:H	2.23	0.47
1:B:300:THR:CG2	1:B:302:MET:HG2	2.44	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:585:HIS:HD2	1:B:587:VAL:H	1.63	0.47
1:A:453:ARG:NE	6:A:2081:HOH:O	2.45	0.47
1:B:584:ARG:HD2	1:B:589:GLU:OE1	2.14	0.47
1:A:699:THR:HA	1:B:616:ASN:ND2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ARG:NE	6:B:2121:HOH:O	2.47	0.47
1:A:608:ARG:NH2	1:A:740:GLU:OE1	2.39	0.46
1:B:656:ARG:NH1	1:B:673:GLU:HG3	2.30	0.46
1:A:118:THR:CG2	6:A:2024:HOH:O	2.49	0.46
1:A:425:ILE:CD1	1:A:527:LEU:HB2	2.45	0.46
1:B:375:LEU:HD22	1:B:397:MET:HG2	1.97	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:A:669:THR:C	1:A:671:MET:H	2.23	0.46
1:B:652:ARG:HD2	1:B:654:PHE:CZ	2.51	0.46
1:B:759:MET:HA	1:B:759:MET:CE	2.46	0.46
1:A:138:GLN:HB3	1:A:143:PHE:CD1	2.51	0.46
1:B:282:ASN:HD22	1:B:282:ASN:C	2.24	0.46
3:F:17:DG:HI'	3:F:18:DG:C8	2.51	0.46
1:A:305:ARG:HH22	1:A:347:ASP:CG	2.21	0.45
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:B:463:LEU:HD12	1:B:463:LEU:C	2.41	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:B:674:MET:HE1	1:B:695:ILE:HG23	1.99	0.44
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.99	0.44
1:A:6:ASN:H	1:A:6:ASN:ND2	2.16	0.44
1:A:783:LYS:N	1:A:784:GLU:OE1	2.50	0.44
1:A:151:SER:HB3	1:A:350:ARG:HG2	1.98	0.44
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:240:LEU:C	1:A:240:LEU:HD23	2.42	0.44
1:A:656:ARG:HG3	1:A:677:THR:HG22	1.99	0.44
1:A:680:ILE:CD1	1:A:692:MET:HE1	2.48	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:A:264:GLN:CD	1:A:264:GLN:H	2.26	0.43
1:A:658:GLY:O	1:A:659:ALA:CB	2.67	0.43
1:B:403:LEU:HD21	1:B:538:HIS:CD2	2.54	0.43
1:B:463:LEU:HD22	1:B:477:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:HIS:HE1	6:B:2089:HOH:O	2.01	0.43
1:B:613:THR:HG23	1:B:767:ALA:CB	2.49	0.43
1:A:656:ARG:HB2	1:A:692:MET:CE	2.48	0.43
1:B:118:THR:OG1	1:B:247:THR:HG21	2.18	0.43
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:83:LEU:HD13	1:A:90:VAL:HG21	2.02	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:B:666:GLY:O	1:B:667:ARG:C	2.62	0.42
1:B:118:THR:CB	1:B:247:THR:HG21	2.49	0.42
1:B:310:TRP:O	1:B:636:ILE:HD11	2.19	0.42
1:A:621:SER:O	1:A:625:ARG:HG3	2.20	0.42
1:B:656:ARG:O	1:B:656:ARG:HG3	2.19	0.42
1:A:297:CYS:H	1:A:557:ASN:ND2	2.18	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:338:LEU:CD1	1:B:381:GLN:OE1	2.67	0.41
1:B:402:GLU:HG2	6:B:2061:HOH:O	2.19	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:A:439:LEU:HD12	1:A:512:LYS:HZ3	1.85	0.41
1:A:446:TYR:CD1	1:A:446:TYR:C	2.98	0.41
1:A:669:THR:C	6:A:2108:HOH:O	2.63	0.41
1:B:268:ILE:HB	1:B:652:ARG:HB3	2.01	0.41
1:B:212:GLN:NE2	1:B:242:GLN:NE2	2.69	0.41
1:B:436:TRP:CZ2	1:B:519:LYS:HD3	2.56	0.41
1:B:755:THR:OG1	1:B:756:ILE:N	2.53	0.41
2:E:13:DC:H2''	2:E:14:DC:H5'	2.02	0.41
1:A:282:ASN:C	1:A:282:ASN:ND2	2.77	0.41
1:B:148:LEU:HB3	1:B:240:LEU:HD21	2.01	0.41
1:B:157:LEU:C	1:B:157:LEU:HD12	2.45	0.41
1:B:352:LEU:HD12	1:B:352:LEU:HA	1.92	0.41
1:B:273:THR:HG23	1:B:655:THR:HG23	2.03	0.40
1:B:660:ALA:HB3	1:B:669:THR:CG2	2.38	0.40
1:B:694:GLU:OE1	1:B:697:ARG:NE	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:CYS:H	1:A:557:ASN:HD21	1.70	0.40
1:B:660:ALA:HB2	1:B:669:THR:HG23	1.96	0.40
1:A:19:ARG:NH2	6:A:2006:HOH:O	2.54	0.40
1:A:164:GLU:OE2	6:A:2043:HOH:O	2.22	0.40
1:A:227:VAL:HG12	1:A:260:MET:HB2	2.02	0.40
1:B:463:LEU:CD1	1:B:475:ILE:HG23	2.51	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%)	16	18
1	B	754/800 (94%)	724 (96%)	23 (3%)	7 (1%)	14	15
All	All	1541/1600 (96%)	1480 (96%)	48 (3%)	13 (1%)	16	18

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

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Mol	Chain	Res	Type
1	A	658	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	658/664 (99%)	621 (94%)	37 (6%)	19	25
1	B	636/664 (96%)	599 (94%)	37 (6%)	18	24
All	All	1294/1328 (97%)	1220 (94%)	74 (6%)	18	25

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	64	GLU
1	A	76	VAL
1	A	84	VAL
1	A	112	ARG
1	A	118	THR
1	A	137	TRP
1	A	157	LEU
1	A	178	LEU
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	335	THR
1	A	384	THR
1	A	413	ASP
1	A	445	ASP
1	A	479	ARG

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Mol	Chain	Res	Type
1	A	488	ASN
1	A	490	MET
1	A	506	LEU
1	A	512	LYS
1	A	513	VAL
1	A	515	THR
1	A	531	LEU
1	A	536	LEU
1	A	591	VAL
1	A	656	ARG
1	A	668	SER
1	A	700	SER
1	A	734	GLN
1	A	752	HIS
1	A	784	GLU
1	B	52	ASP
1	B	84	VAL
1	B	157	LEU
1	B	178	LEU
1	B	201	LEU
1	B	229	ASN
1	B	247	THR
1	B	264	GLN
1	B	282	ASN
1	B	300	THR
1	B	315	VAL
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	379	ARG
1	B	384	THR
1	B	419	VAL
1	B	424	VAL
1	B	444	THR
1	B	456	GLU
1	B	463	LEU
1	B	464	LYS
1	B	500	ARG
1	B	511	ASP
1	B	535	LEU
1	B	575	LYS

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Mol	Chain	Res	Type
1	B	584	ARG
1	B	592	LEU
1	B	613	THR
1	B	652	ARG
1	B	662	ASP
1	B	665	SER
1	B	668	SER
1	B	732	LEU
1	B	759	MET
1	B	800	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	86	GLN
1	A	95	GLN
1	A	276	ASN
1	A	282	ASN
1	A	312	HIS
1	A	374	GLN
1	A	493	GLN
1	A	557	ASN
1	A	566	ASN
1	A	590	GLN
1	A	602	ASN
1	A	714	ASN
1	A	734	GLN
1	A	746	HIS
1	A	752	HIS
1	B	15	GLN
1	B	23	GLN
1	B	24	HIS
1	B	138	GLN
1	B	171	GLN
1	B	212	GLN
1	B	229	ASN
1	B	242	GLN
1	B	264	GLN
1	B	282	ASN
1	B	332	GLN
1	B	344	GLN

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Mol	Chain	Res	Type
1	B	370	HIS
1	B	430	ASN
1	B	483	HIS
1	B	538	HIS
1	B	543	GLN
1	B	557	ASN
1	B	585	HIS
1	B	679	ASN
1	B	717	ASN
1	B	734	GLN
1	B	791	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	32,33,33	1.39	5 (15%)	48,52,52	1.93	14 (29%)
4	ATP	B	1801	-	32,33,33	1.61	7 (21%)	48,52,52	1.82	11 (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
4	ATP	A	1801	5	-	2/22/38/38	0/3/3/3
4	ATP	B	1801	-	-	4/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ATP	C5-C4	4.38	1.46	1.39
4	B	1801	ATP	PB-O3A	4.37	1.64	1.59
4	B	1801	ATP	C5-N7	-3.97	1.31	1.39
4	A	1801	ATP	C5-N7	-3.62	1.32	1.39
4	B	1801	ATP	C5-C4	3.44	1.45	1.39
4	B	1801	ATP	C4-N9	-2.62	1.32	1.37
4	A	1801	ATP	C8-N7	2.31	1.36	1.31
4	B	1801	ATP	PA-O3A	2.30	1.62	1.59
4	A	1801	ATP	PB-O3A	-2.26	1.57	1.59
4	B	1801	ATP	PB-O3B	2.16	1.61	1.59
4	B	1801	ATP	C8-N7	2.03	1.35	1.31
4	A	1801	ATP	C4-N9	-2.01	1.33	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1801	ATP	C5-C4-N3	-5.37	119.32	126.72
4	A	1801	ATP	C5-C4-N3	-5.25	119.49	126.72
4	A	1801	ATP	N3-C4-N9	4.44	134.72	127.17
4	B	1801	ATP	N3-C4-N9	4.33	134.54	127.17
4	B	1801	ATP	N3-C2-N1	-4.06	122.44	128.58
4	A	1801	ATP	N3-C2-N1	-3.94	122.62	128.58
4	A	1801	ATP	O3B-PB-O1B	-3.90	98.98	110.70
4	B	1801	ATP	C2-N3-C4	3.88	121.31	111.83
4	A	1801	ATP	C2-N3-C4	3.67	120.79	111.83
4	B	1801	ATP	O2A-PA-O3A	3.08	115.59	107.27
4	A	1801	ATP	C5-N7-C8	2.84	107.91	103.45
4	B	1801	ATP	N9-C8-N7	-2.77	110.01	113.94
4	A	1801	ATP	N9-C8-N7	-2.71	110.09	113.94
4	B	1801	ATP	C5-N7-C8	2.71	107.71	103.45
4	B	1801	ATP	C4-N9-C8	2.67	108.54	105.74
4	A	1801	ATP	C4-N9-C8	2.65	108.52	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1801	ATP	C3'-C2'-C1'	2.65	106.48	101.46
4	B	1801	ATP	C4-C5-N7	-2.62	107.58	110.58
4	A	1801	ATP	C4-C5-N7	-2.52	107.69	110.58
4	A	1801	ATP	O2B-PB-O1B	2.45	123.82	112.44
4	A	1801	ATP	O2G-PG-O1G	2.39	120.17	110.83
4	B	1801	ATP	C2-N1-C6	2.28	122.48	118.73
4	B	1801	ATP	N6-C6-N1	2.17	123.20	118.38
4	A	1801	ATP	C2-N1-C6	2.05	122.10	118.73
4	A	1801	ATP	O3G-PG-O2G	2.05	115.48	107.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

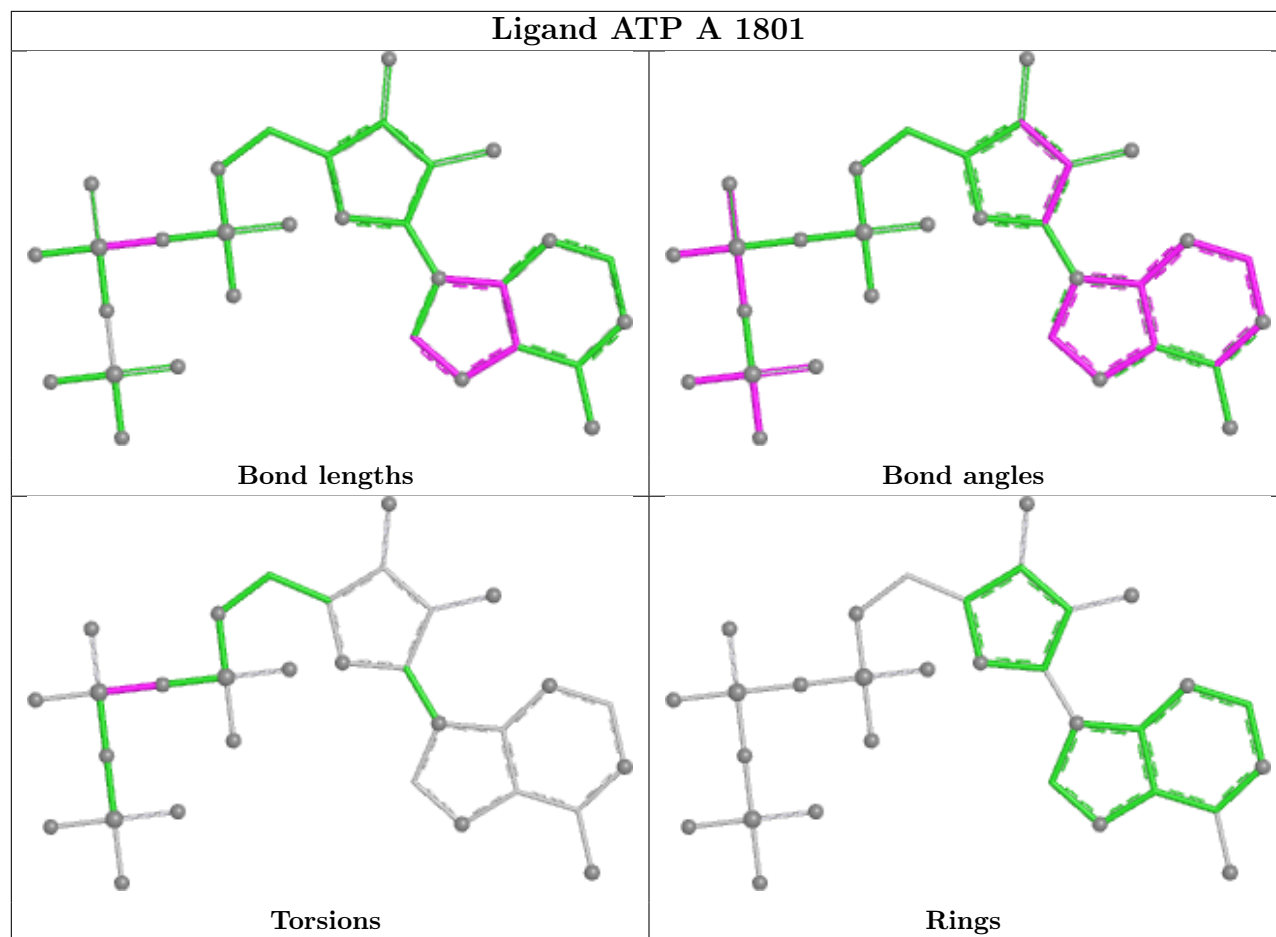
Mol	Chain	Res	Type	Atoms
4	B	1801	ATP	PB-O3B-PG-O2G
4	A	1801	ATP	PA-O3A-PB-O2B
4	B	1801	ATP	PA-O3A-PB-O3B
4	B	1801	ATP	PB-O3B-PG-O3G
4	A	1801	ATP	PA-O3A-PB-O1B
4	B	1801	ATP	PA-O3A-PB-O1B

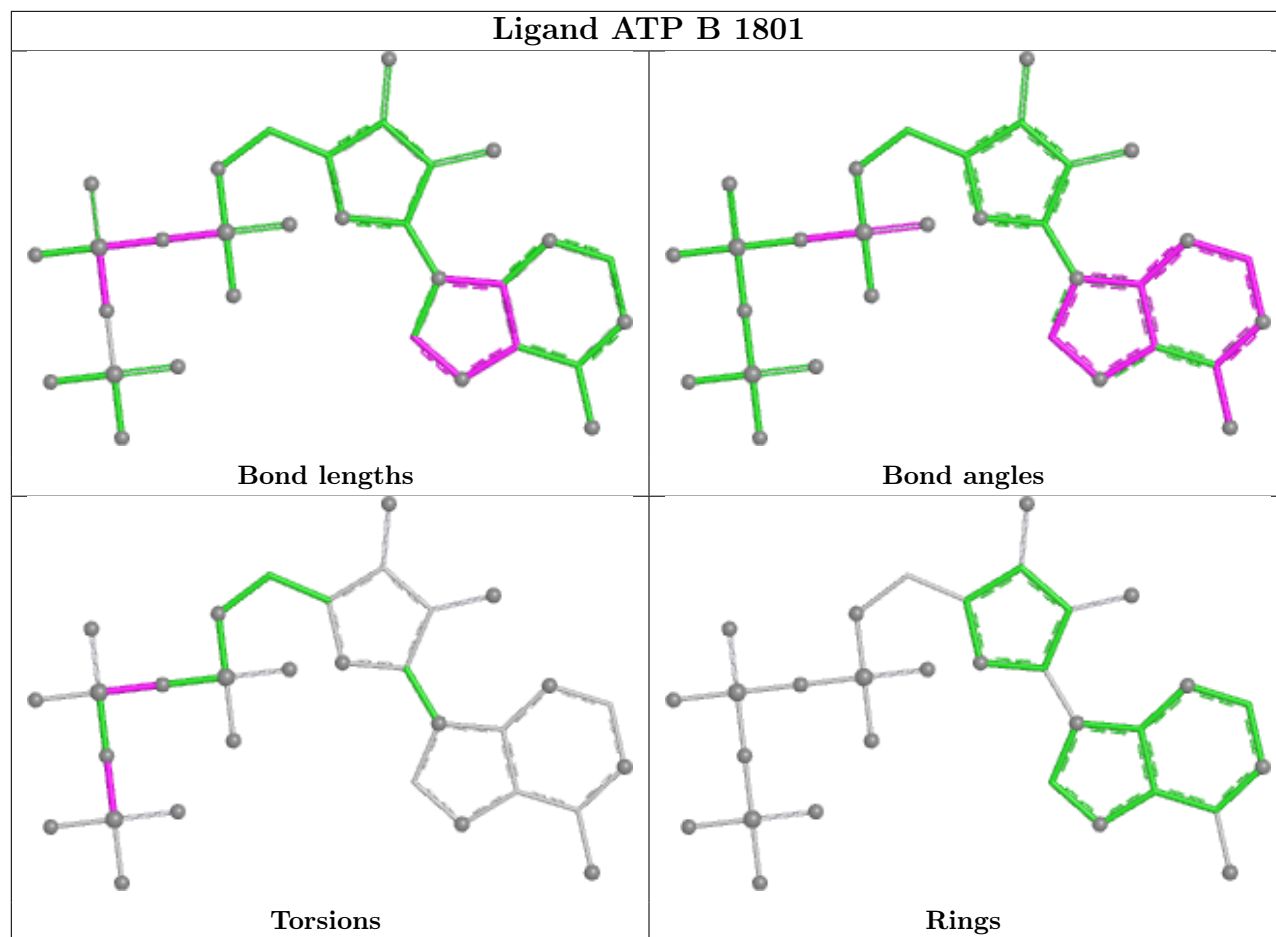
There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	791/800 (98%)	-0.13	11 (1%) 73 75	20, 31, 47, 64	0
1	B	762/800 (95%)	-0.05	15 (1%) 65 66	17, 31, 50, 65	0
2	E	18/30 (60%)	-0.13	1 (5%) 30 31	28, 37, 64, 64	0
3	F	17/30 (56%)	-0.36	0 100 100	25, 36, 63, 64	0
All	All	1588/1660 (95%)	-0.09	27 (1%) 69 70	17, 31, 49, 65	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	ASN	8.2
1	A	444	THR	4.6
1	B	659	ALA	4.4
1	A	659	ALA	3.6
1	A	742	VAL	3.6
1	B	661	ASP	3.4
1	A	439	LEU	3.2
1	B	660	ALA	3.0
1	B	617	MET	3.0
1	A	670	PHE	2.8
1	A	697	ARG	2.7
1	A	658	GLY	2.7
1	B	41	TYR	2.6
1	B	800	SER	2.3
1	B	14	MET	2.3
1	A	669	THR	2.3
2	E	18	DG	2.3
1	A	743	ALA	2.2
1	B	108	ARG	2.2
1	B	759	MET	2.2
1	B	756	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	22	ALA	2.1
1	B	667	ARG	2.1
1	A	64	GLU	2.1
1	B	662	ASP	2.1
1	A	229	ASN	2.0
1	B	24	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

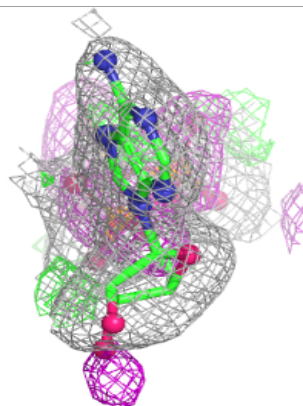
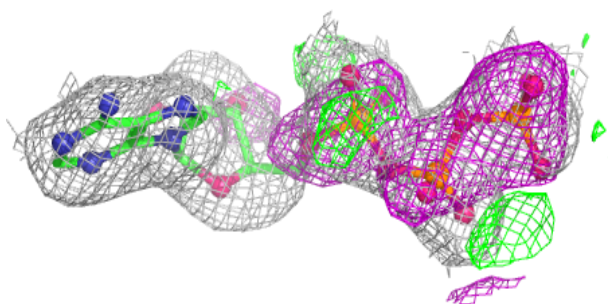
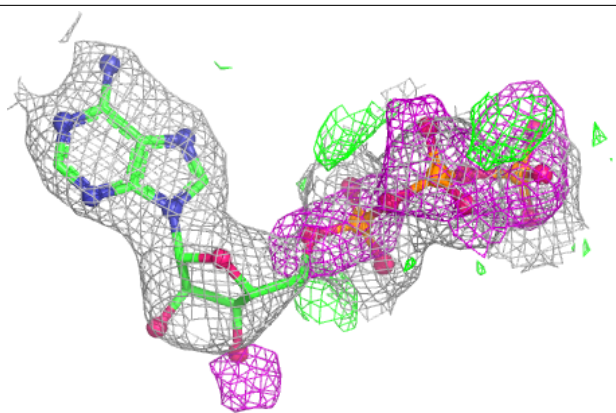
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ATP	B	1801	31/31	0.83	0.15	41,52,58,65	0
4	ATP	A	1801	31/31	0.89	0.12	52,55,63,64	0
5	MG	A	1802	1/1	0.98	0.06	49,49,49,49	0

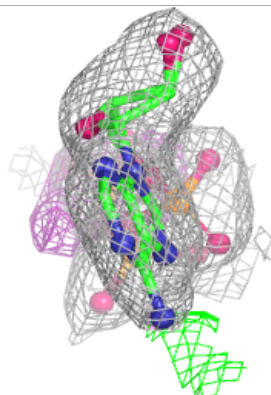
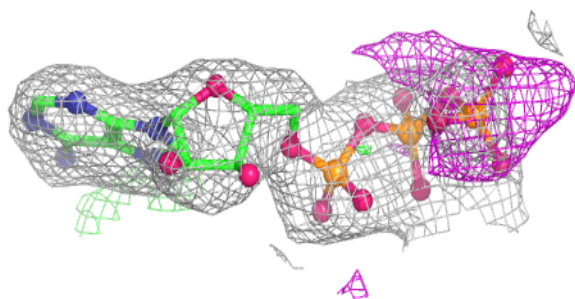
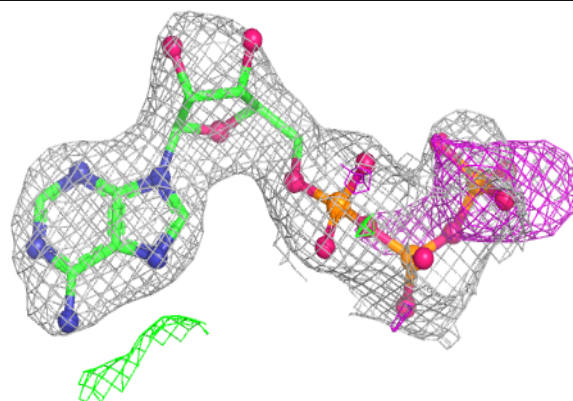
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 1801:

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

**Electron density around ATP A 1801:**

$2mF_o - DF_c$ (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.