



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:19 AM UTC

PDB ID : 6H2J / pdb_00006h2j
Title : Crystal structure of the HsdR subunit of the EcoR124I restriction enzyme with the C-terminal domain
Authors : Grinkevich, P.; Mesters, J.R.; Ettrich, R.H.
Deposited on : 2018-07-13
Resolution : 2.60 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

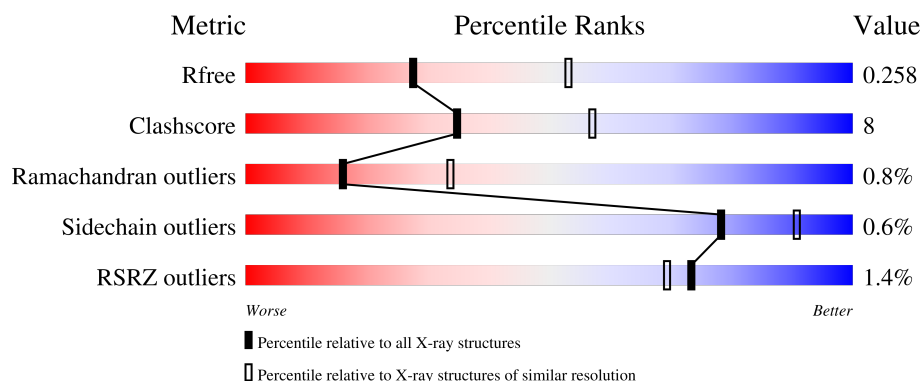
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	1038	
1	B	1038	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15364 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 Type I restriction enzyme R Protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	Se	0	0	0
			6893	4381	1166	1330	3	13			
1	B	990	Total	C	N	O	S	Se	0	0	0
			8024	5099	1360	1549	3	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q304R3
B	1	MSE	-	initiating methionine	UNP Q304R3

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



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

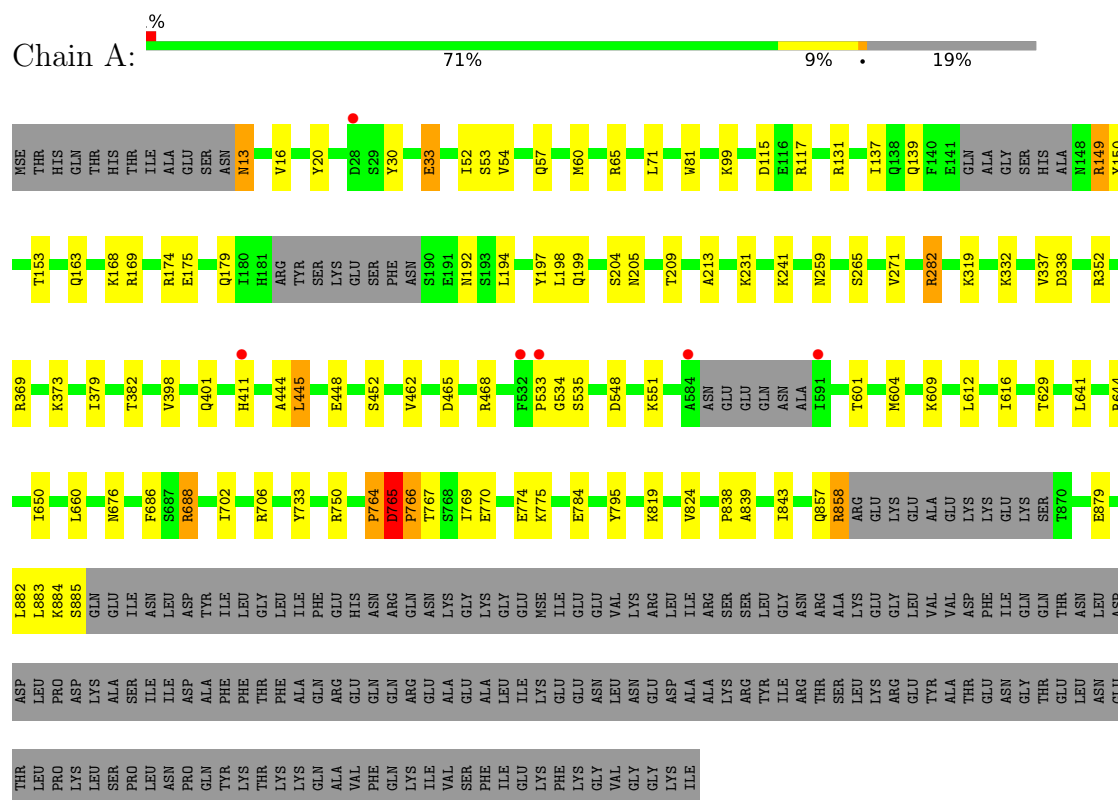
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total	O	0	0
			192	192		
4	B	191	Total	O	0	0
			191	191		

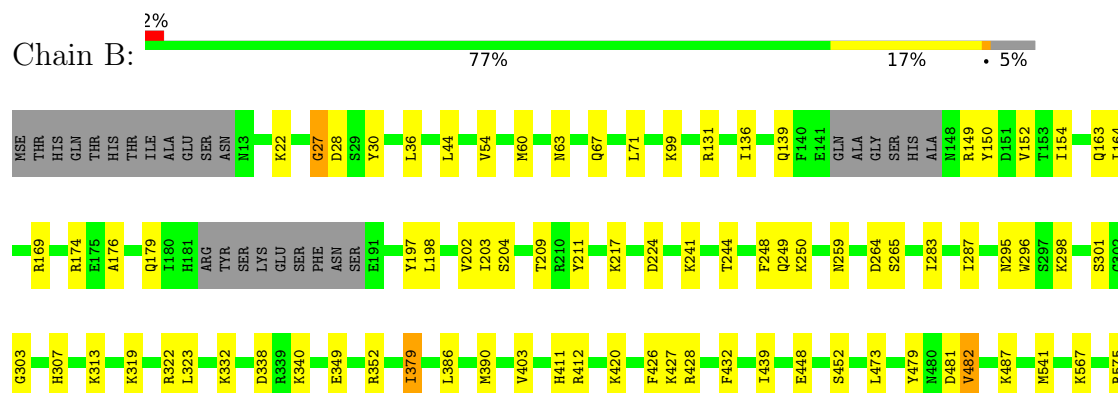
3 Residue-property plots

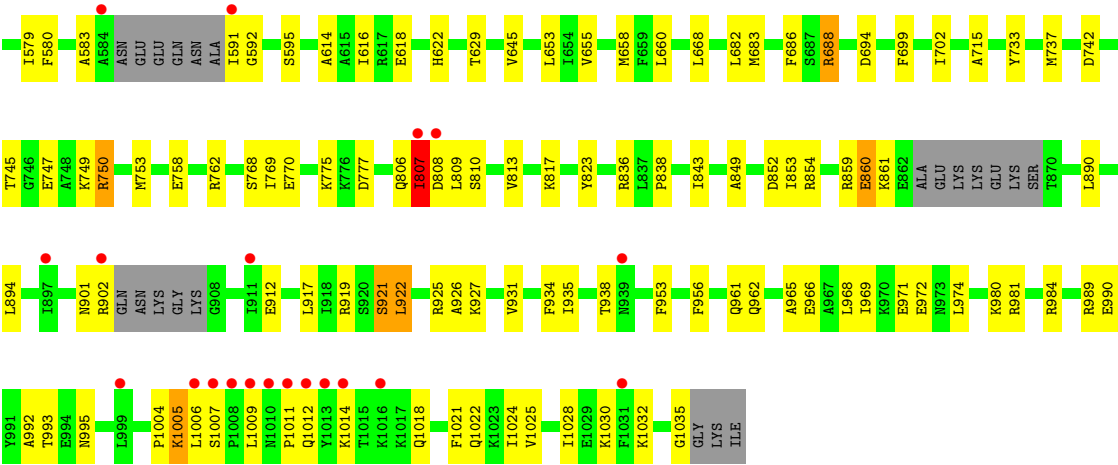
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Type I restriction enzyme R Protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	123.91Å 129.92Å 161.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 19.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.97-2.60) 99.7 (19.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.59Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.203 , 0.264 0.203 , 0.258	Depositor DCC
R_{free} test set	977 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15364	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/7013	0.56	0/9437
1	B	0.39	0/8157	0.62	7/10977 (0.1%)
All	All	0.39	0/15170	0.59	7/20414 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	860	GLU	CA-C-N	8.33	136.70	121.70
1	B	860	GLU	C-N-CA	8.33	136.70	121.70
1	B	583	ALA	CA-C-N	6.01	132.52	121.70
1	B	583	ALA	C-N-CA	6.01	132.52	121.70
1	B	27	GLY	CA-C-N	5.99	132.49	121.70
1	B	27	GLY	C-N-CA	5.99	132.49	121.70
1	B	860	GLU	N-CA-C	5.40	119.64	112.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	764	PRO	Peptide
1	A	765	ASP	Peptide
1	B	750	ARG	Peptide
1	B	768	SER	Peptide
1	B	769	ILE	Peptide
1	B	807	ILE	Peptide
1	B	859	ARG	Peptide

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	6893	0	6759	92	0
1	B	8024	0	7827	130	0
2	A	31	0	12	1	0
2	B	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	192	0	0	5	0
4	B	191	0	0	5	0
All	All	15364	0	14610	222	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 (222) 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:750:ARG:HH21	1:A:784:GLU:CD	1.60	1.09
1:A:57:GLN:OE1	1:A:192:ASN:HB3	1.58	1.03
1:A:533:PRO:HA	1:A:535:SER:H	1.37	0.88
1:A:153:THR:OG1	1:A:163:GLN:OE1	1.94	0.85
1:B:989:ARG:HH22	1:B:993:THR:HB	1.45	0.81
1:A:71:LEU:O	1:A:131:ARG:NH2	2.17	0.77
1:A:115:ASP:OD2	1:A:117:ARG:NE	2.20	0.73
1:B:174:ARG:NH2	4:B:1202:HOH:O	2.20	0.73
1:B:412:ARG:HG2	1:B:439:ILE:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:CG	1:A:117:ARG:HE	1.98	0.71
1:A:369:ARG:HG2	1:A:373:LYS:NZ	2.07	0.70
1:B:927:LYS:NZ	1:B:1032:LYS:O	2.23	0.70
1:B:860:GLU:H	1:B:861:LYS:HB2	1.58	0.69
1:B:54:VAL:HG11	1:B:60:MSE:HG3	1.75	0.69
1:B:390:MSE:HE2	1:B:426:PHE:CE1	2.30	0.67
1:B:688:ARG:NH2	2:B:1101:ATP:O2G	2.20	0.67
1:A:465:ASP:OD1	1:A:468:ARG:NH2	2.28	0.66
1:A:604:MSE:HE3	1:A:609:LYS:HD2	1.77	0.66
1:A:30:TYR:O	1:A:169:ARG:HD3	1.97	0.65
1:B:995:ASN:ND2	4:B:1201:HOH:O	2.20	0.65
1:B:806:GLN:C	1:B:807:ILE:HG13	2.22	0.65
1:A:213:ALA:HB2	1:A:271:VAL:HG23	1.80	0.64
1:A:369:ARG:HG2	1:A:373:LYS:HZ3	1.64	0.62
1:B:332:LYS:HG3	1:B:379:ILE:HD13	1.82	0.62
1:B:541:MSE:HG3	1:B:668:LEU:HD11	1.82	0.61
1:A:838:PRO:HG2	1:A:843:ILE:HD11	1.81	0.61
1:B:295:ASN:O	1:B:301:SER:HB3	2.00	0.61
1:B:813:VAL:O	1:B:817:LYS:N	2.28	0.61
1:B:579:ILE:HG23	1:B:658:MSE:HE3	1.82	0.60
1:B:338:ASP:OD2	1:B:411:HIS:ND1	2.27	0.60
1:B:616:ILE:HD12	1:B:629:THR:HG22	1.82	0.60
1:B:481:ASP:OD1	1:B:487:LYS:HE3	2.01	0.59
1:B:934:PHE:O	1:B:938:THR:OG1	2.19	0.59
1:B:965:ALA:O	1:B:969:ILE:HG12	2.02	0.59
1:A:54:VAL:HG11	1:A:60:MSE:HG3	1.85	0.59
1:A:688:ARG:NH2	2:A:1101:ATP:O2G	2.19	0.59
1:B:972:GLU:HB3	1:B:974:LEU:HD13	1.84	0.59
1:A:750:ARG:NH2	1:A:784:GLU:OE2	2.36	0.58
1:B:747:GLU:OE2	1:B:749:LYS:HE3	2.03	0.58
1:B:71:LEU:O	1:B:131:ARG:NH2	2.32	0.58
1:A:770:GLU:HG2	1:A:774:GLU:OE1	2.04	0.58
1:A:750:ARG:NH2	1:A:784:GLU:CD	2.45	0.57
1:A:839:ALA:O	1:A:843:ILE:HG12	2.04	0.57
1:B:1005:LYS:CG	1:B:1006:LEU:H	2.16	0.57
1:B:1014:LYS:HB2	1:B:1018:GLN:HG3	1.86	0.57
1:A:115:ASP:CG	1:A:117:ARG:HH21	2.13	0.56
1:A:764:PRO:O	1:A:765:ASP:HB2	2.04	0.56
1:A:139:GLN:HB2	1:A:149:ARG:HH12	1.70	0.56
1:A:175:GLU:O	1:A:179:GLN:HG3	2.05	0.56
1:B:981:ARG:HG3	1:B:984:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:838:PRO:HG2	1:B:843:ILE:HD11	1.87	0.56
1:A:139:GLN:CB	1:A:149:ARG:HH12	2.20	0.55
1:B:968:LEU:HA	1:B:971:GLU:HG2	1.86	0.55
1:B:30:TYR:O	1:B:169:ARG:HD2	2.06	0.55
1:B:163:GLN:HG3	1:B:198:LEU:HD11	1.88	0.55
1:B:217:LYS:HE2	4:B:1345:HOH:O	2.05	0.55
1:A:338:ASP:OD2	1:A:411:HIS:HD2	1.88	0.55
1:B:163:GLN:HG3	1:B:198:LEU:CD1	2.37	0.55
1:A:33:GLU:OE2	1:A:168:LYS:HE2	2.08	0.54
1:A:601:THR:O	1:A:604:MSE:HG3	2.08	0.54
1:A:60:MSE:HE2	1:A:194:LEU:HD13	1.90	0.54
1:B:139:GLN:NE2	1:B:149:ARG:O	2.40	0.54
1:B:807:ILE:HD12	1:B:808:ASP:HA	1.90	0.54
1:A:548:ASP:HA	1:A:551:LYS:HD3	1.90	0.53
1:B:390:MSE:HE2	1:B:426:PHE:HE1	1.73	0.53
1:B:139:GLN:NE2	1:B:150:TYR:HA	2.22	0.53
1:B:733:TYR:OH	1:B:737:MSE:HE2	2.09	0.53
1:A:338:ASP:OD2	1:A:411:HIS:CD2	2.62	0.53
1:A:115:ASP:CG	1:A:117:ARG:NE	2.66	0.52
1:B:27:GLY:CA	1:B:28:ASP:HB2	2.40	0.52
1:B:54:VAL:HG11	1:B:60:MSE:CG	2.39	0.52
1:B:1022:GLN:HA	1:B:1025:VAL:HG22	1.92	0.52
1:B:27:GLY:HA2	1:B:28:ASP:HB2	1.90	0.52
1:A:369:ARG:CG	1:A:373:LYS:NZ	2.72	0.52
1:A:204:SER:HB2	1:A:209:THR:HG23	1.92	0.51
1:A:601:THR:HB	1:A:604:MSE:HE2	1.93	0.51
1:B:849:ALA:O	1:B:852:ASP:HB2	2.11	0.51
1:A:465:ASP:HA	1:A:468:ARG:NH2	2.26	0.51
1:B:961:GLN:NE2	1:B:1035:GLY:O	2.38	0.50
1:A:616:ILE:HD12	1:A:629:THR:HG22	1.92	0.50
1:A:882:LEU:O	1:A:885:SER:HB3	2.11	0.50
1:A:16:VAL:O	1:A:282:ARG:NH2	2.44	0.50
1:A:604:MSE:HE1	1:A:612:LEU:HD23	1.94	0.50
1:B:1009:LEU:HB3	1:B:1012:GLN:HG3	1.93	0.50
1:B:152:VAL:O	1:B:164:ILE:HD12	2.12	0.49
1:B:403:VAL:HG21	1:B:426:PHE:HE2	1.77	0.49
1:A:688:ARG:HD2	1:A:688:ARG:N	2.27	0.49
1:A:398:VAL:HA	1:A:401:GLN:HG3	1.95	0.49
1:A:448:GLU:HG3	1:A:452:SER:OG	2.12	0.49
1:A:99:LYS:HD2	1:A:197:TYR:CZ	2.48	0.49
1:B:244:THR:HA	1:B:248:PHE:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LYS:O	1:B:301:SER:OG	2.31	0.49
1:B:860:GLU:N	1:B:861:LYS:HB2	2.28	0.49
1:B:303:GLY:O	1:B:432:PHE:HA	2.13	0.49
1:A:53:SER:HA	4:A:1208:HOH:O	2.13	0.49
1:A:398:VAL:HB	4:A:1257:HOH:O	2.12	0.48
1:B:660:LEU:C	1:B:688:ARG:HD3	2.37	0.48
1:A:858:ARG:NE	4:A:1207:HOH:O	2.30	0.48
1:B:295:ASN:HD21	1:B:298:LYS:HE2	1.79	0.48
1:A:57:GLN:CD	1:A:192:ASN:HB3	2.34	0.48
1:B:448:GLU:HG2	1:B:452:SER:OG	2.13	0.48
1:B:890:LEU:O	1:B:894:LEU:HG	2.13	0.48
1:A:332:LYS:HG3	1:A:379:ILE:HD12	1.96	0.48
1:A:533:PRO:HA	1:A:535:SER:N	2.17	0.48
1:B:921:SER:O	1:B:922:LEU:HB2	2.14	0.48
1:A:139:GLN:O	1:A:139:GLN:HG2	2.13	0.47
1:B:386:LEU:HD11	1:B:390:MSE:HE3	1.96	0.47
1:A:33:GLU:H	1:A:33:GLU:HG2	1.27	0.47
1:A:660:LEU:O	1:A:688:ARG:HD3	2.15	0.47
1:A:765:ASP:O	1:A:767:THR:N	2.48	0.47
1:B:482:VAL:HG21	1:B:823:TYR:CG	2.49	0.47
1:B:962:GLN:O	1:B:966:GLU:HG2	2.14	0.47
1:B:980:LYS:HB3	1:B:984:ARG:NH2	2.30	0.47
1:B:1018:GLN:O	1:B:1022:GLN:HG2	2.15	0.47
1:A:369:ARG:HG2	1:A:373:LYS:HZ2	1.80	0.47
1:B:750:ARG:NH1	1:B:758:GLU:OE2	2.48	0.47
1:A:265:SER:HB3	1:A:352:ARG:HD2	1.96	0.46
1:B:836:ARG:HG3	1:B:836:ARG:HH11	1.80	0.46
1:B:775:LYS:HD3	1:B:853:ILE:HG12	1.96	0.46
1:B:264:ASP:HB2	1:B:349:GLU:OE2	2.16	0.46
1:B:265:SER:HB3	1:B:352:ARG:HD2	1.98	0.46
1:A:163:GLN:HG2	1:A:198:LEU:HD21	1.98	0.46
1:B:307:HIS:O	1:B:313:LYS:HD3	2.15	0.46
1:A:533:PRO:HB2	1:A:534:GLY:HA2	1.97	0.46
1:B:204:SER:HB2	1:B:209:THR:HG23	1.98	0.46
1:A:676:ASN:OD1	1:A:706:ARG:NH1	2.47	0.46
1:A:769:ILE:O	1:A:775:LYS:NZ	2.48	0.46
1:B:259:ASN:O	1:B:319:LYS:HE3	2.15	0.46
1:B:567:LYS:HE3	1:B:567:LYS:HB3	1.77	0.46
1:A:115:ASP:OD1	1:A:117:ARG:NE	2.49	0.45
1:A:686:PHE:CZ	1:A:702:ILE:HG21	2.52	0.45
1:B:660:LEU:O	1:B:688:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:O	1:B:67:GLN:HG2	2.16	0.45
1:B:479:TYR:CD2	1:B:481:ASP:HB2	2.52	0.45
1:B:473:LEU:HB3	1:B:699:PHE:HA	1.98	0.45
1:B:224:ASP:OD1	1:B:694:ASP:HA	2.17	0.45
1:B:580:PHE:HA	1:B:658:MSE:HE2	1.98	0.45
1:A:733:TYR:HB2	1:A:795:TYR:CD2	2.52	0.44
1:A:765:ASP:HB3	1:A:766:PRO:CD	2.47	0.44
1:B:202:VAL:HG22	1:B:211:TYR:HB3	2.00	0.44
1:B:1021:PHE:O	1:B:1025:VAL:HG13	2.17	0.44
1:A:660:LEU:C	1:A:688:ARG:HD3	2.43	0.44
1:B:332:LYS:HG3	1:B:379:ILE:CD1	2.47	0.44
1:A:462:VAL:O	1:A:465:ASP:HB2	2.18	0.44
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.82	0.44
1:B:762:ARG:HH22	1:B:777:ASP:HB3	1.83	0.44
1:A:199:GLN:NE2	4:A:1227:HOH:O	2.51	0.44
1:A:369:ARG:CG	1:A:373:LYS:HZ3	2.29	0.44
1:B:686:PHE:CZ	1:B:702:ILE:HG21	2.53	0.44
1:B:762:ARG:NH2	1:B:777:ASP:HB3	2.33	0.44
1:B:750:ARG:O	4:B:1203:HOH:O	2.21	0.43
1:A:139:GLN:NE2	1:A:150:TYR:HA	2.33	0.43
1:B:745:THR:HG23	1:B:747:GLU:H	1.83	0.43
1:B:854:ARG:HG3	1:B:854:ARG:HH11	1.83	0.43
1:A:259:ASN:O	1:A:319:LYS:HE3	2.19	0.43
1:B:579:ILE:HG23	1:B:658:MSE:CE	2.47	0.43
1:B:591:ILE:HB	1:B:592:GLY:H	1.72	0.43
1:A:115:ASP:CG	1:A:117:ARG:NH2	2.76	0.43
1:A:169:ARG:HG2	1:A:205:ASN:O	2.19	0.43
1:B:934:PHE:CE1	1:B:953:PHE:HA	2.53	0.43
1:A:241:LYS:HB3	1:A:241:LYS:HE3	1.85	0.43
1:A:883:LEU:HD23	1:A:883:LEU:HA	1.89	0.43
1:B:575:ARG:HD2	1:B:622:HIS:CD2	2.54	0.43
1:A:99:LYS:HD2	1:A:197:TYR:CE2	2.52	0.43
1:A:174:ARG:HH22	1:A:879:GLU:CD	2.27	0.43
1:A:13:ASN:HD22	1:A:13:ASN:N	2.17	0.43
1:A:644:ARG:CB	1:A:650:ILE:HD12	2.49	0.43
1:B:683:MSE:HE3	1:B:715:ALA:HB3	2.00	0.43
1:B:579:ILE:HG12	1:B:658:MSE:HE1	2.01	0.42
1:B:682:LEU:CD2	1:B:683:MSE:HE2	2.49	0.42
1:B:479:TYR:CE2	1:B:481:ASP:HB2	2.55	0.42
1:B:176:ALA:HB1	1:B:203:ILE:HD11	2.01	0.42
1:A:20:TYR:HB3	1:A:231:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:917:LEU:HD23	1:B:917:LEU:HA	1.92	0.42
1:B:809:LEU:HA	1:B:810:SER:HA	1.66	0.42
1:A:13:ASN:N	1:A:13:ASN:ND2	2.66	0.42
1:A:52:ILE:HG13	1:A:137:ILE:HG22	2.01	0.42
1:A:337:VAL:O	1:A:382:THR:HA	2.20	0.42
1:A:858:ARG:NH2	4:A:1207:HOH:O	2.51	0.42
1:B:901:ASN:HA	1:B:902:ARG:HA	1.72	0.42
1:B:579:ILE:C	1:B:658:MSE:HE1	2.45	0.42
1:B:179:GLN:HE21	1:B:179:GLN:HB2	1.66	0.41
1:B:614:ALA:O	1:B:618:GLU:HG3	2.20	0.41
1:B:989:ARG:O	1:B:990:GLU:HB2	2.20	0.41
1:A:65:ARG:HB2	1:A:81:TRP:CZ2	2.55	0.41
1:B:645:VAL:HG21	1:B:653:LEU:HD22	2.02	0.41
1:B:742:ASP:HB3	1:B:745:THR:HG22	2.02	0.41
1:A:163:GLN:HG3	1:A:198:LEU:HD11	2.01	0.41
1:B:992:ALA:HB3	1:B:1025:VAL:HG12	2.01	0.41
1:A:604:MSE:HE3	1:A:609:LYS:CD	2.48	0.41
1:B:248:PHE:HD1	1:B:248:PHE:HA	1.75	0.41
1:B:340:LYS:NZ	1:B:595:SER:O	2.53	0.41
1:B:953:PHE:O	1:B:956:PHE:HB3	2.21	0.41
1:B:420:LYS:HE3	1:B:420:LYS:HB3	1.86	0.41
1:B:745:THR:HG23	1:B:747:GLU:HB3	2.02	0.41
1:B:44:LEU:HD13	1:B:136:ILE:HG21	2.02	0.41
1:B:296:TRP:CE2	1:B:428:ARG:HG2	2.55	0.41
1:B:99:LYS:HD2	1:B:197:TYR:CZ	2.56	0.41
1:B:249:GLN:O	1:B:250:LYS:C	2.64	0.41
1:A:644:ARG:HB3	1:A:650:ILE:HD12	2.03	0.41
1:B:919:ARG:O	1:B:925:ARG:NE	2.44	0.41
1:B:926:ALA:O	1:B:1030:LYS:HD2	2.21	0.41
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.93	0.40
1:B:403:VAL:HG21	1:B:426:PHE:CE2	2.56	0.40
1:B:1006:LEU:HG	1:B:1007:SER:H	1.85	0.40
1:A:444:ALA:O	1:A:445:LEU:C	2.64	0.40
1:A:660:LEU:HD23	1:A:660:LEU:HA	1.90	0.40
1:A:858:ARG:H	1:A:858:ARG:HG3	1.40	0.40
1:B:22:LYS:HB3	1:B:22:LYS:HE3	1.87	0.40
1:B:931:VAL:O	1:B:935:ILE:HG23	2.22	0.40
1:B:1024:ILE:O	1:B:1028:ILE:HG12	2.21	0.40
1:A:641:LEU:HD12	1:A:650:ILE:HD13	2.02	0.40
1:B:30:TYR:OH	1:B:241:LYS:HG2	2.22	0.40
1:B:427:LYS:HA	1:B:427:LYS:HD3	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:O	1:B:287:ILE:HG13	2.21	0.40
1:B:682:LEU:HD22	1:B:683:MSE:HE2	2.03	0.40
1:B:861:LYS:HE3	1:B:861:LYS:HA	2.02	0.40
1:A:819:LYS:HA	1:A:824:VAL:HG22	2.03	0.40
1:B:27:GLY:HA2	1:B:28:ASP:CB	2.51	0.40
1:B:136:ILE:HG22	1:B:154:ILE:HG12	2.03	0.40
1:B:753:MSE:HE3	4:B:1281:HOH:O	2.20	0.40
1:B:806:GLN:O	1:B:807:ILE:HG13	2.21	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	832/1038 (80%)	784 (94%)	42 (5%)	6 (1%)	18	38
1	B	978/1038 (94%)	915 (94%)	54 (6%)	9 (1%)	14	30
All	All	1810/2076 (87%)	1699 (94%)	96 (5%)	15 (1%)	16	34

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	ASP
1	B	921	SER
1	B	1005	LYS
1	B	807	ILE
1	B	912	GLU
1	B	922	LEU
1	B	1011	PRO
1	A	766	PRO
1	B	482	VAL
1	A	445	LEU

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Mol	Chain	Res	Type
1	A	884	LYS
1	B	1004	PRO
1	A	149	ARG
1	A	857	GLN
1	B	770	GLU

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	756/912 (83%)	751 (99%)	5 (1%)	76	89
1	B	860/912 (94%)	856 (100%)	4 (0%)	81	92
All	All	1616/1824 (89%)	1607 (99%)	9 (1%)	78	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	33	GLU
1	A	282	ARG
1	A	688	ARG
1	A	858	ARG
1	B	36	LEU
1	B	379	ILE
1	B	655	VAL
1	B	688	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	63	ASN
1	A	67	GLN
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	387	ASN
1	A	411	HIS
1	A	414	GLN
1	A	632	ASN
1	A	723	ASN
1	A	726	ASN
1	A	805	GLN
1	A	806	GLN
1	A	844	GLN
1	A	857	GLN
1	B	42	GLN
1	B	179	GLN
1	B	192	ASN
1	B	295	ASN
1	B	414	GLN
1	B	485	GLN
1	B	518	GLN
1	B	622	HIS
1	B	632	ASN
1	B	723	ASN
1	B	726	ASN
1	B	806	GLN
1	B	851	ASN
1	B	958	GLN
1	B	1022	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	B	1101	3	32,33,33	1.39	5 (15%)	48,52,52	1.68	8 (16%)
2	ATP	A	1101	3	32,33,33	1.40	5 (15%)	48,52,52	1.87	14 (29%)

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	B	1101	3	-	0/22/38/38	0/3/3/3
2	ATP	A	1101	3	-	0/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ATP	C5-C4	4.23	1.46	1.39
2	A	1101	ATP	C5-C4	4.07	1.46	1.39
2	A	1101	ATP	PA-O3A	3.22	1.63	1.59
2	B	1101	ATP	PB-O3B	2.84	1.62	1.59
2	B	1101	ATP	C5-N7	-2.52	1.34	1.39
2	B	1101	ATP	C5-C6	2.51	1.48	1.41
2	A	1101	ATP	C5-N7	-2.49	1.34	1.39
2	A	1101	ATP	C5-C6	2.43	1.47	1.41
2	B	1101	ATP	C4-N9	-2.20	1.33	1.37
2	A	1101	ATP	C8-N7	2.11	1.35	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	ATP	C5-C4-N3	-5.61	119.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	ATP	C5-C4-N3	-5.25	119.49	126.72
2	A	1101	ATP	N3-C4-N9	4.72	135.20	127.17
2	B	1101	ATP	N3-C4-N9	4.48	134.79	127.17
2	A	1101	ATP	C4-N9-C8	3.77	109.69	105.74
2	A	1101	ATP	N3-C2-N1	-3.54	123.22	128.58
2	A	1101	ATP	C2-N3-C4	3.50	120.39	111.83
2	B	1101	ATP	C4-C5-N7	-3.35	106.75	110.58
2	B	1101	ATP	C2-N3-C4	3.18	119.60	111.83
2	A	1101	ATP	C4-C5-N7	-3.05	107.09	110.58
2	A	1101	ATP	C5-N7-C8	2.96	108.10	103.45
2	A	1101	ATP	N9-C8-N7	-2.92	109.80	113.94
2	B	1101	ATP	C4-N9-C8	2.88	108.76	105.74
2	B	1101	ATP	C5-N7-C8	2.69	107.67	103.45
2	A	1101	ATP	C2'-C1'-N9	-2.62	106.80	113.30
2	A	1101	ATP	O2B-PB-O3A	-2.44	100.68	107.27
2	B	1101	ATP	N3-C2-N1	-2.38	124.97	128.58
2	A	1101	ATP	C2-N1-C6	2.35	122.59	118.73
2	B	1101	ATP	N9-C8-N7	-2.35	110.61	113.94
2	A	1101	ATP	O2B-PB-O1B	2.25	122.89	112.44
2	A	1101	ATP	C6-C5-N7	2.04	136.02	132.09
2	A	1101	ATP	O3G-PG-O1G	2.00	118.64	110.83

There are no chirality outliers.

There are no torsion outliers.

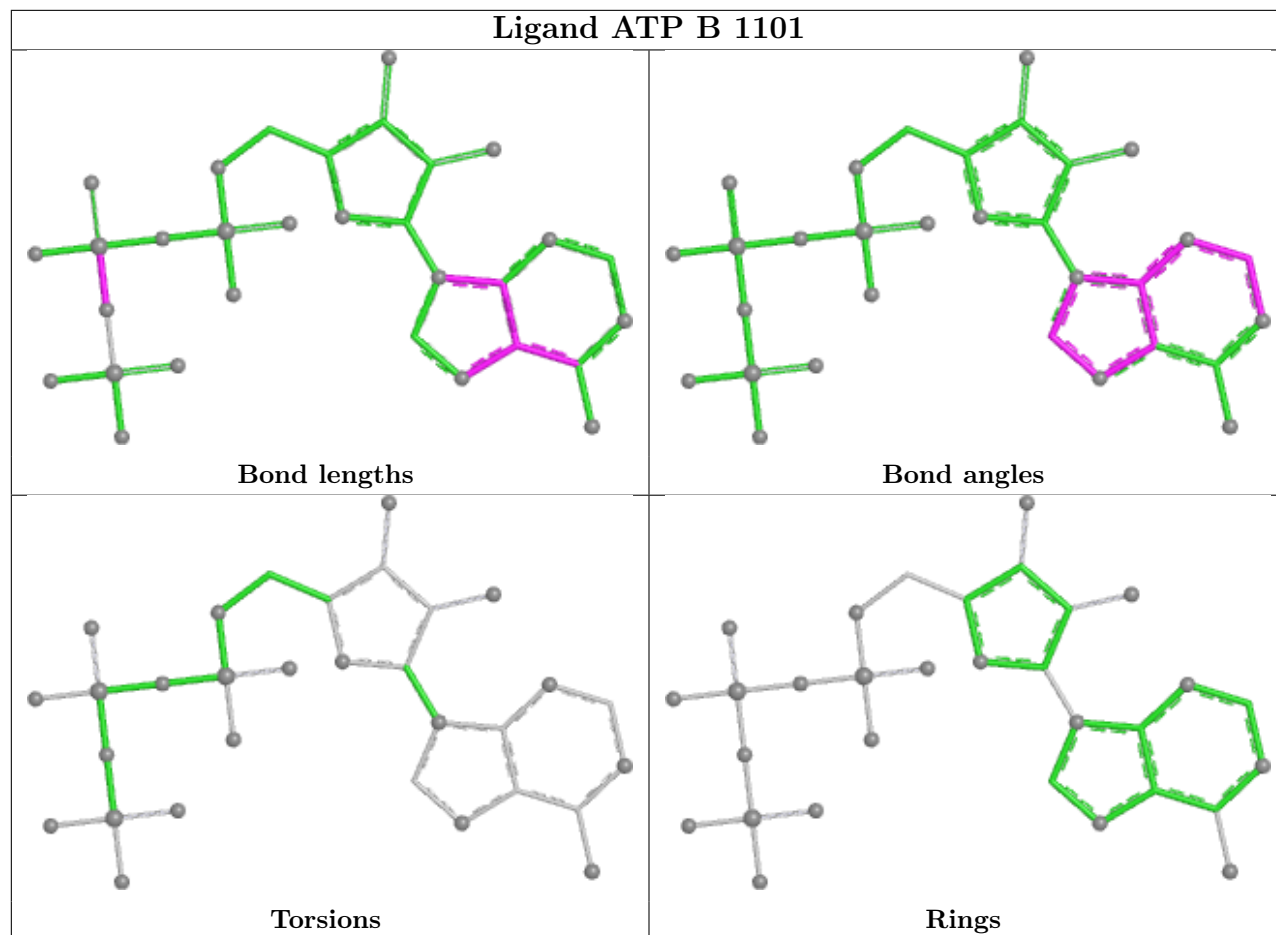
There are no ring outliers.

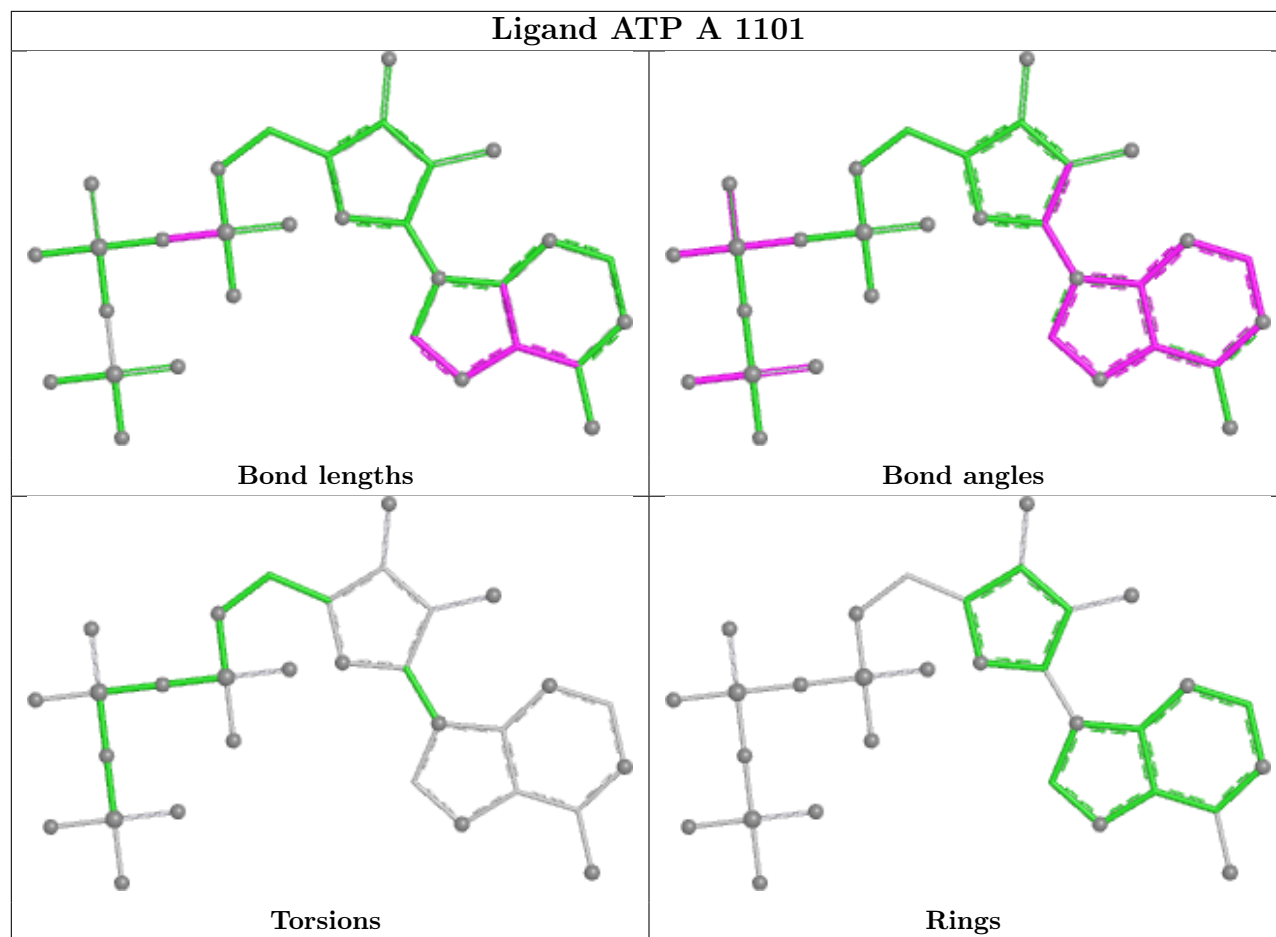
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	ATP	1	0
2	A	1101	ATP	1	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 [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	829/1038 (79%)	-0.50	6 (0%) 84 82	26, 46, 81, 110	0
1	B	976/1038 (94%)	-0.27	20 (2%) 65 60	27, 50, 106, 149	0
All	All	1805/2076 (86%)	-0.38	26 (1%) 73 69	26, 48, 99, 149	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1011	PRO	4.7
1	B	1007	SER	4.7
1	B	1013	TYR	4.2
1	B	1009	LEU	4.2
1	B	1010	ASN	4.0
1	A	591	ILE	3.8
1	B	1008	PRO	3.5
1	B	807	ILE	3.4
1	A	411	HIS	3.0
1	B	591	ILE	2.9
1	B	1006	LEU	2.9
1	B	584	ALA	2.9
1	B	1014	LYS	2.8
1	B	897	ILE	2.7
1	B	902	ARG	2.6
1	A	532	PHE	2.6
1	B	999	LEU	2.6
1	B	1012	GLN	2.5
1	B	939	ASN	2.4
1	B	1016	LYS	2.4
1	A	584	ALA	2.3
1	B	911	ILE	2.3
1	B	1031	PHE	2.2
1	A	533	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	808	ASP	2.2
1	A	28	ASP	2.1

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](#)

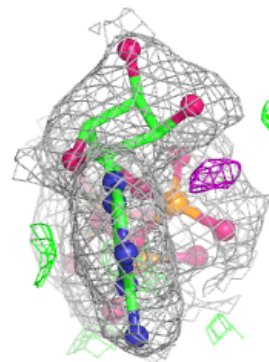
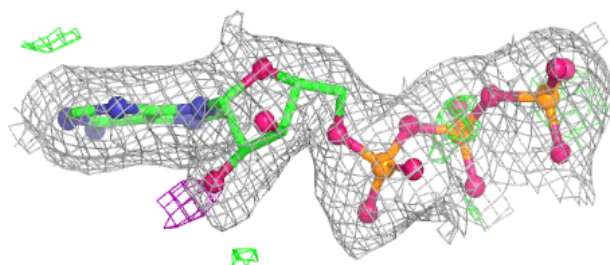
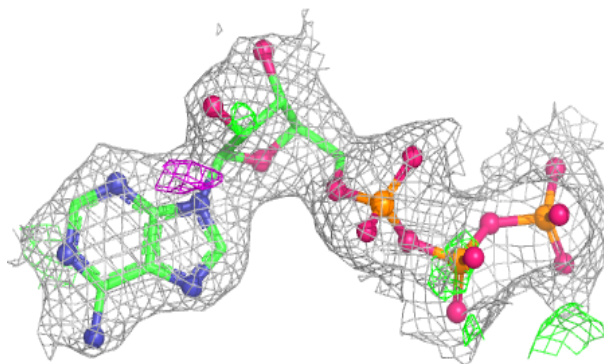
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
3	MG	A	1102	1/1	0.97	0.18	33,33,33,33	0
2	ATP	B	1101	31/31	0.98	0.05	23,31,36,39	0
2	ATP	A	1101	31/31	0.98	0.05	19,28,35,42	0
3	MG	B	1102	1/1	1.00	0.02	13,13,13,13	0

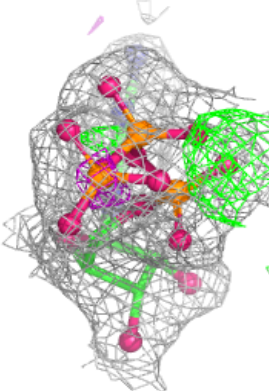
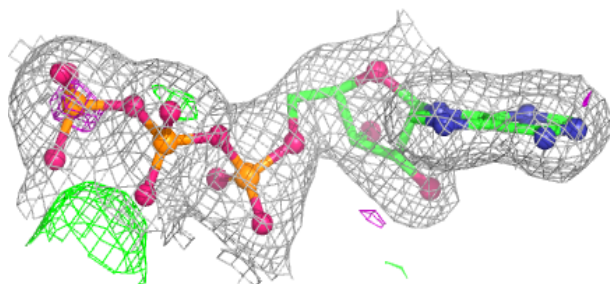
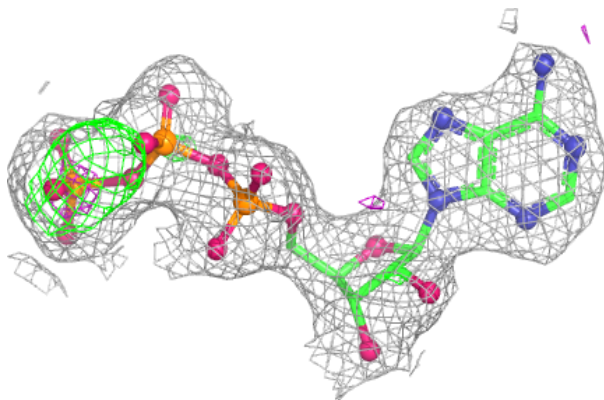
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP B 1101:

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

**Electron density around ATP A 1101:**

$2mF_o - DF_c$ (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.