Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 11:11 am GMT

PDB ID	:	6H2J
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:

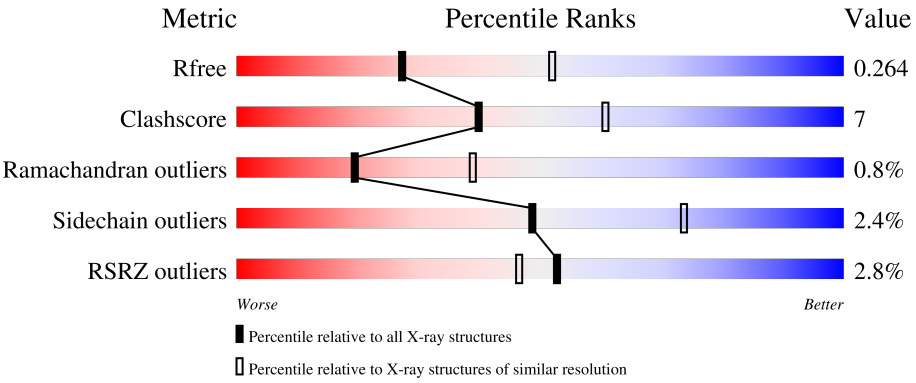
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	% 70% 10% • 19%
1	B	1038	4% 76% 18% • 5%

2 Entry composition

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.

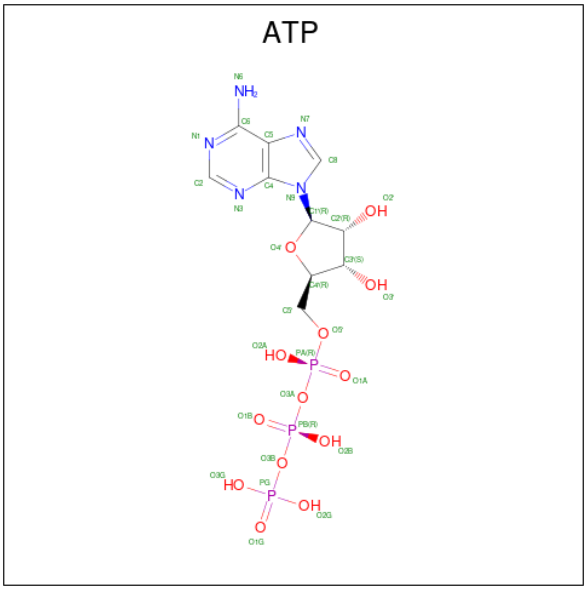
- Molecule 1 is a protein called Type I restriction enzyme R Protein.

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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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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 (three-letter code: 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		

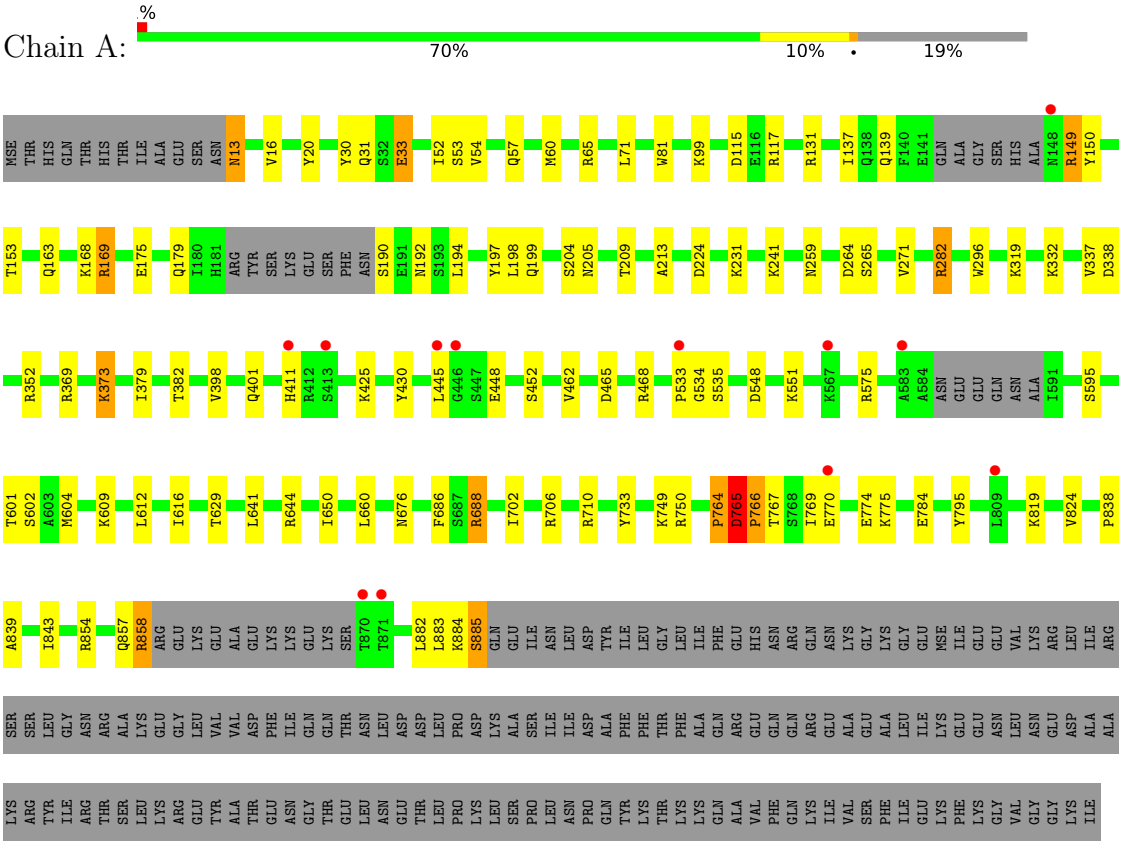
- Molecule 4 is water.

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

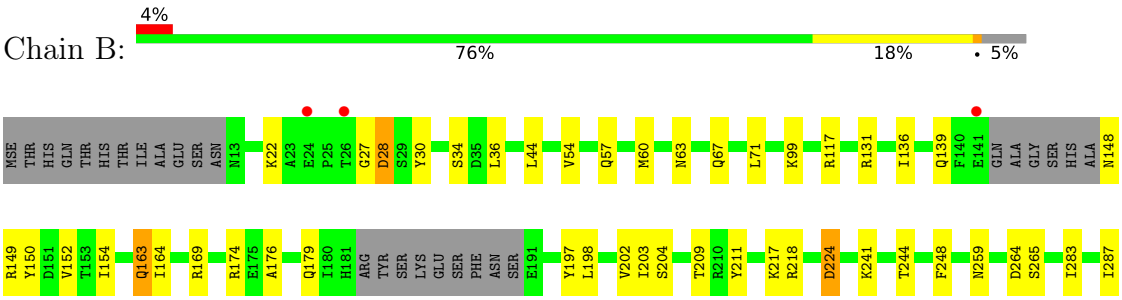
3 Residue-property plots (i)

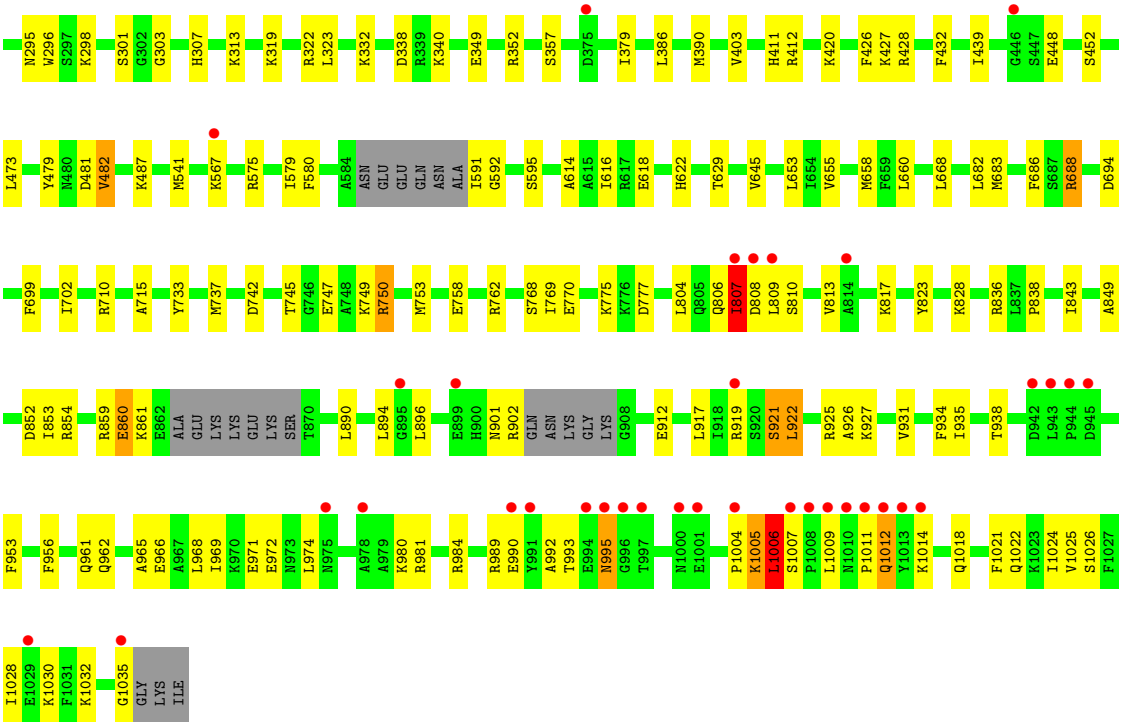
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Type I restriction enzyme R Protein



• Molecule 1: Type I restriction enzyme R Protein




N295 W296 S297 K298 S301 G302 G303 H307 K313 K319 R322 L323 K332 D338 R339 K340 E349 R352 S357 D375 I379 L386 M390 V403 H411 R412 K420 F426 K427 R428 F432 I439 G446 S447 E448 S452
L473 Y479 N480 D481 V482 K487 M541 K567 R575 I579 F580 A584 ASN GLU GLU GLN ASN ALA I591 G592 S595 A614 A615 I616 R617 E618 H622 T629 V645 L653 I654 V655 M658 F659 L660 L668 L682 M683 F686 S687 R688 D694
F699 I702 R710 A715 Y733 M737 D742 T745 G746 E747 A748 K749 R750 M753 E758 R762 S768 I769 E770 K775 K776 D777 L804 Q805 Q806 I807 D808 L809 S810 V813 A814 K817 Y823 K828 R836 L837 P838 I843 A849
D852 I853 R854 R859 E860 K861 E862 ALA GLU LYS LYS GLU LYS SER T870 L890 L894 G895 L896 E899 H900 N901 R902 GLN ASN LYS GLY LYS G908 E912 L917 I918 R919 S920 S921 L922 R925 A926 K927 V931 F934 I935 T938 D942 L943 P944 D945
F953 F956 Q961 Q962 A965 E966 A967 L968 I969 K970 E971 E972 N973 L974 N975 A978 A979 K980 R981 R984 R989 E990 Y991 A992 T993 E994 N995 G996 T997 N1000 E1001 P1004 K1005 L1006 S1007 P1008 L1009 N1010 P1011 Q1012 Y1013 K1014 Q1018 F1021 Q1022 K1023 I1024 V1025 S1026 F1027
I1028 E1029 K1030 F1031 K1032 G1035 GLY LYS ILE

4 Data and refinement statistics (i)

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) 100.0 (19.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 2.59Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.203 , 0.264 0.203 , 0.264	Depositor DCC
R_{free} test set	977 reflections (1.22%)	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)	0.28 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.45	0/7013	0.58	1/9437 (0.0%)
1	B	0.45	0/8157	0.61	2/10977 (0.0%)
All	All	0.45	0/15170	0.60	3/20414 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	860	GLU	C-N-CA	6.00	136.70	121.70
1	B	1006	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	264	ASP	CB-CG-OD1	5.09	122.89	118.30

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

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Mol	Chain	Res	Type	Group
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	89	0
1	B	8024	0	7827	128	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	6	0
4	B	191	0	0	5	0
All	All	15364	0	14610	217	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 7.

All (217) 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	1.04
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
1:A:369:ARG:HG2	1:A:373:LYS:NZ	2.07	0.70
1:B:860:GLU:H	1:B:861:LYS:HB2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:927:LYS:NZ	1:B:1032:LYS:O	2.23	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:115:ASP:CG	1:A:117:ARG:HE	1.98	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:A:213:ALA:HB2	1:A:271:VAL:HG23	1.80	0.64
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:A:369:ARG:HG2	1:A:373:LYS:HZ2	1.65	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:806:GLN:C	1:B:807:ILE:HG13	2.22	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: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: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
1:B:838:PRO:HG2	1:B:843:ILE:HD11	1.87	0.56
1:A:425:LYS:NZ	4:A:1211:HOH:O	2.39	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:934:PHE:O	1:B:938:THR:OG1	2.19	0.53
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: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:115:ASP:CG	1:A:117:ARG:HH21	2.13	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:750:ARG:NH2	1:A:784:GLU:CD	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:115:ASP:CG	1:A:117:ARG:NE	2.66	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: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:A:369:ARG:CG	1:A:373:LYS:HZ2	2.28	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: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:369:ARG:HG2	1:A:373:LYS:HZ3	1.79	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:13:ASN:N	1:A:13:ASN:ND2	2.66	0.44
1:B:660:LEU:C	1:B:688:ARG:HD3	2.37	0.44
1:A:199:GLN:NE2	4:A:1227:HOH:O	2.51	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:57:GLN:CD	1:A:192:ASN:HB3	2.34	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: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:13:ASN:N	1:A:13:ASN:HD22	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:769:ILE:O	1:A:775:LYS:NZ	2.48	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	22	43
1	B	978/1038 (94%)	915 (94%)	54 (6%)	9 (1%)	17	35
All	All	1810/2076 (87%)	1699 (94%)	96 (5%)	15 (1%)	19	39

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
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 (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	756/912 (83%)	737 (98%)	19 (2%)	47 73
1	B	860/912 (94%)	840 (98%)	20 (2%)	50 75
All	All	1616/1824 (89%)	1577 (98%)	39 (2%)	49 74

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	31	GLN
1	A	33	GLU
1	A	169	ARG
1	A	190	SER
1	A	224	ASP
1	A	282	ARG
1	A	296	TRP
1	A	373	LYS
1	A	430	TYR
1	A	575	ARG
1	A	595	SER
1	A	602	SER
1	A	688	ARG
1	A	710	ARG
1	A	749	LYS
1	A	854	ARG
1	A	858	ARG
1	A	885	SER
1	B	28	ASP
1	B	34	SER
1	B	36	LEU
1	B	57	GLN
1	B	117	ARG
1	B	148	ASN
1	B	163	GLN
1	B	218	ARG

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Mol	Chain	Res	Type
1	B	224	ASP
1	B	357	SER
1	B	655	VAL
1	B	688	ARG
1	B	710	ARG
1	B	804	LEU
1	B	828	LYS
1	B	896	LEU
1	B	995	ASN
1	B	1006	LEU
1	B	1012	GLN
1	B	1026	SER

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

Mol	Chain	Res	Type
1	A	13	ASN
1	A	148	ASN
1	A	387	ASN
1	A	411	HIS
1	A	414	GLN
1	A	806	GLN
1	A	844	GLN
1	B	179	GLN
1	B	192	ASN
1	B	295	ASN
1	B	485	GLN
1	B	622	HIS
1	B	958	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	1101	3	26,33,33	0.88	1 (3%)	31,52,52	1.32	5 (16%)
2	ATP	B	1101	3	26,33,33	0.91	2 (7%)	31,52,52	1.29	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	1101	3	-	0/18/38/38	0/3/3/3
2	ATP	B	1101	3	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ATP	C5-C4	2.16	1.46	1.40
2	A	1101	ATP	C5-C4	2.05	1.46	1.40
2	B	1101	ATP	O4'-C1'	2.05	1.43	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ATP	N3-C2-N1	-3.49	123.22	128.68
2	B	1101	ATP	C4-C5-N7	-2.54	106.75	109.40
2	B	1101	ATP	O4'-C1'-C2'	-2.52	103.24	106.93
2	B	1101	ATP	N3-C2-N1	-2.37	124.97	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ATP	C2-N1-C6	2.24	122.59	118.75
2	A	1101	ATP	C4-C5-N7	-2.21	107.09	109.40
2	A	1101	ATP	O2B-PB-O1B	2.15	122.89	112.24
2	B	1101	ATP	PB-O3B-PG	-2.10	125.63	132.83
2	B	1101	ATP	PA-O3A-PB	-2.09	125.64	132.83
2	A	1101	ATP	O3G-PG-O1G	2.03	118.64	110.68

There are no chirality outliers.

There are no torsion outliers.

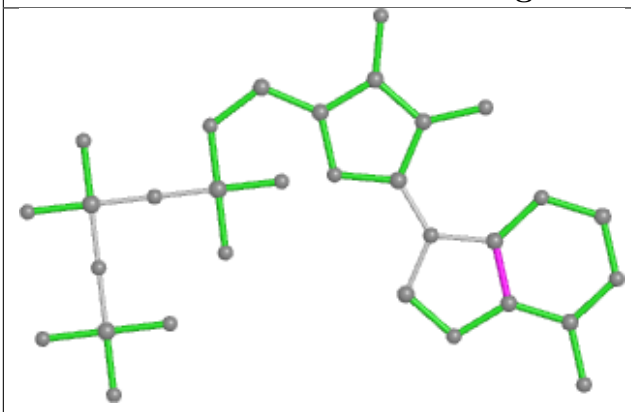
There are no ring outliers.

2 monomers are involved in 2 short contacts:

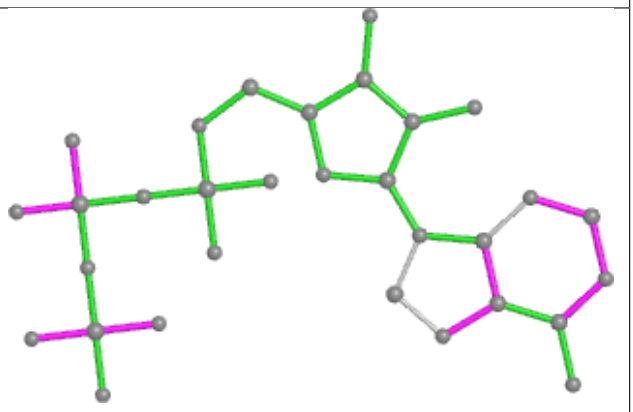
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	ATP	1	0
2	B	1101	ATP	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

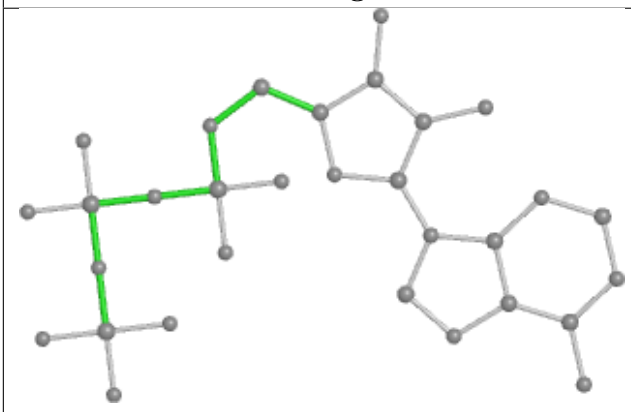
Ligand ATP A 1101



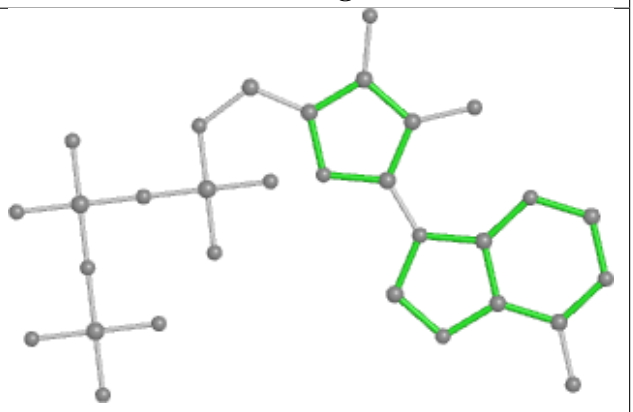
Bond lengths



Bond angles

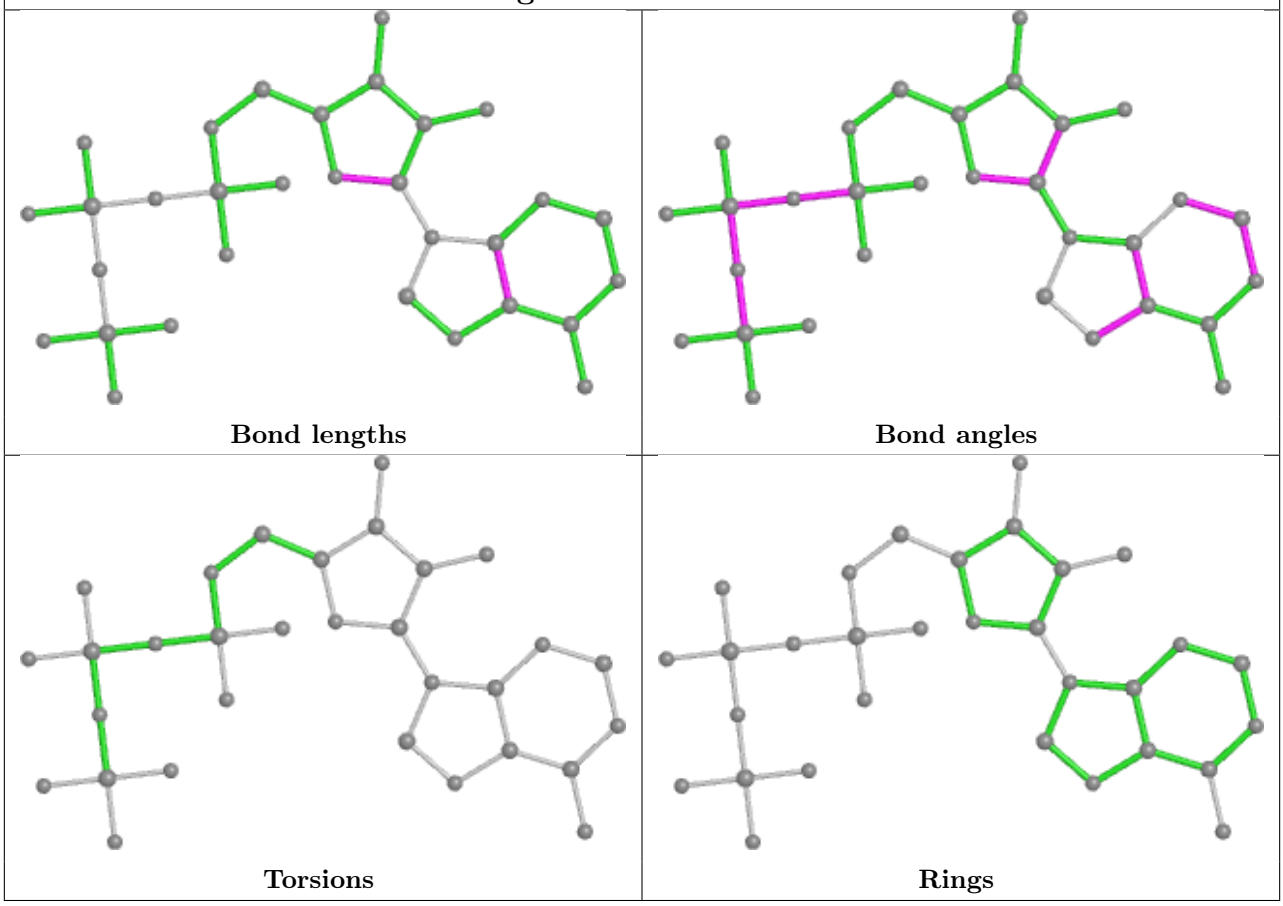


Torsions



Rings

Ligand ATP B 1101



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, 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	829/1038 (79%)	-0.53	12 (1%)	75	71	26, 46, 81, 110	0
1	B	976/1038 (94%)	-0.28	38 (3%)	39	32	27, 50, 106, 149	0
All	All	1805/2076 (86%)	-0.40	50 (2%)	53	46	26, 48, 99, 149	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1013	TYR	14.9
1	B	1011	PRO	11.8
1	B	1012	GLN	8.2
1	B	1010	ASN	6.8
1	B	1008	PRO	6.4
1	B	1014	LYS	6.4
1	B	1007	SER	5.1
1	B	26	THR	5.0
1	A	446	GLY	4.1
1	B	1009	LEU	4.0
1	B	975	ASN	3.8
1	B	944	PRO	3.7
1	B	1000	ASN	3.5
1	B	375	ASP	3.3
1	B	567	LYS	3.2
1	A	445	LEU	3.2
1	B	808	ASP	3.1
1	A	871	THR	3.1
1	B	996	GLY	3.0
1	B	1004	PRO	3.0
1	B	943	LEU	3.0
1	B	141	GLU	2.9
1	B	809	LEU	2.9
1	A	870	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	446	GLY	2.8
1	B	1035	GLY	2.8
1	A	411	HIS	2.8
1	A	148	ASN	2.7
1	B	1029	GLU	2.7
1	A	809	LEU	2.7
1	B	995	ASN	2.7
1	B	978	ALA	2.6
1	B	24	GLU	2.6
1	B	807	ILE	2.5
1	B	990	GLU	2.5
1	B	1001	GLU	2.3
1	A	770	GLU	2.3
1	B	895	GLY	2.2
1	A	533	PRO	2.2
1	B	994	GLU	2.2
1	B	814	ALA	2.2
1	A	583	ALA	2.2
1	B	942	ASP	2.1
1	A	567	LYS	2.1
1	B	997	THR	2.1
1	B	991	TYR	2.1
1	B	899	GLU	2.1
1	A	413	SER	2.0
1	B	945	ASP	2.0
1	B	919	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

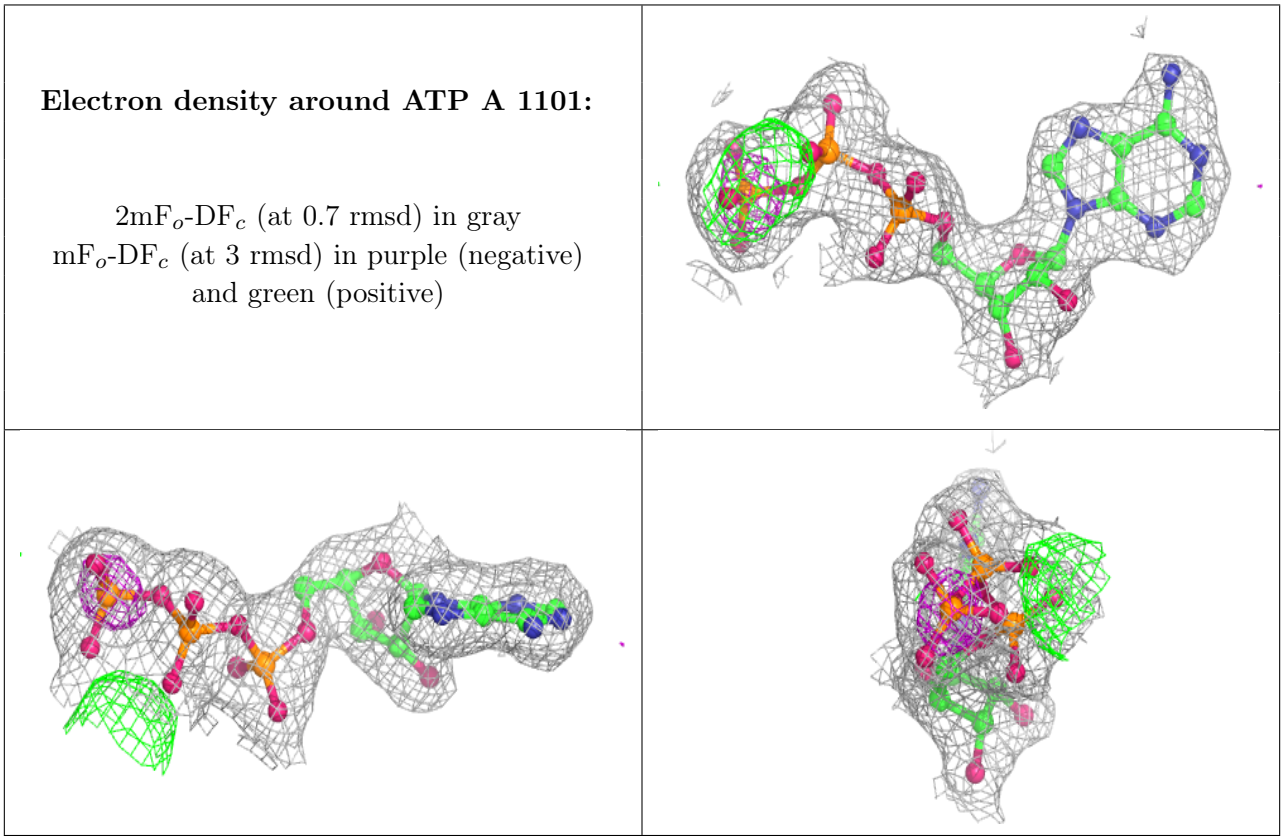
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1102	1/1	0.93	0.26	33,33,33,33	0
2	ATP	A	1101	31/31	0.97	0.10	19,28,35,42	0
3	MG	B	1102	1/1	0.97	0.11	13,13,13,13	0
2	ATP	B	1101	31/31	0.98	0.09	23,31,36,39	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.

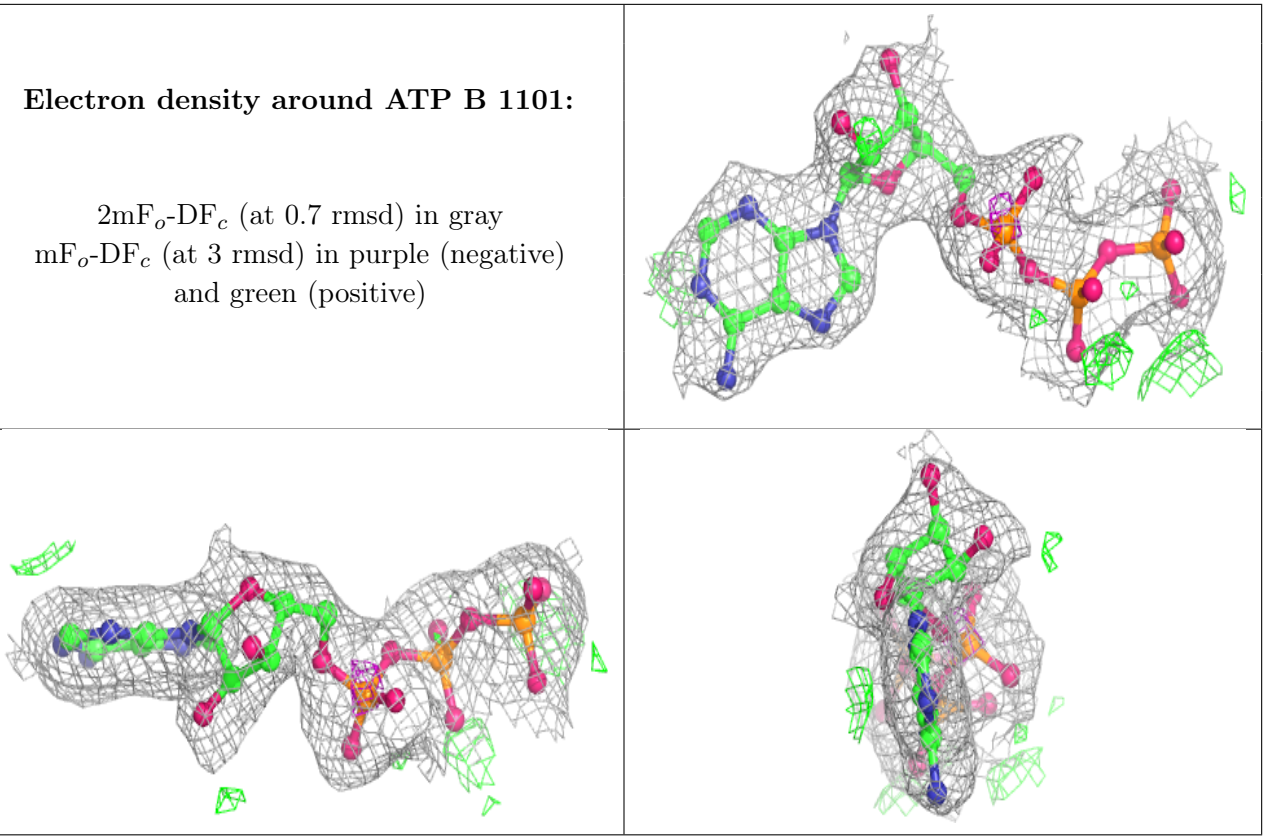
Electron density around ATP A 1101:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.