Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:07 PM EDT

PDB ID	:	2Y4I
Title	:	KSR2-MEK1 heterodimer
Authors	:	Brennan, D.F.; Barford, D.
Deposited on	:	2011-01-06
Resolution	:	3.46 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:

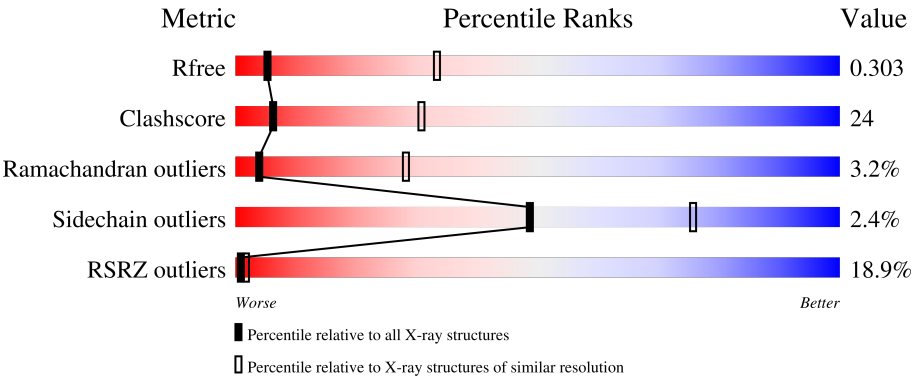
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.46 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	B	319	8% 34% 43% 6% 17%
2	C	395	22% 49% 29% . 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4661 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 KINASE SUPPRESSOR OF RAS 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	265	2143	1385	367	379	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	632	GLY	-	expression tag	UNP Q6VAB6
B	633	PRO	-	expression tag	UNP Q6VAB6

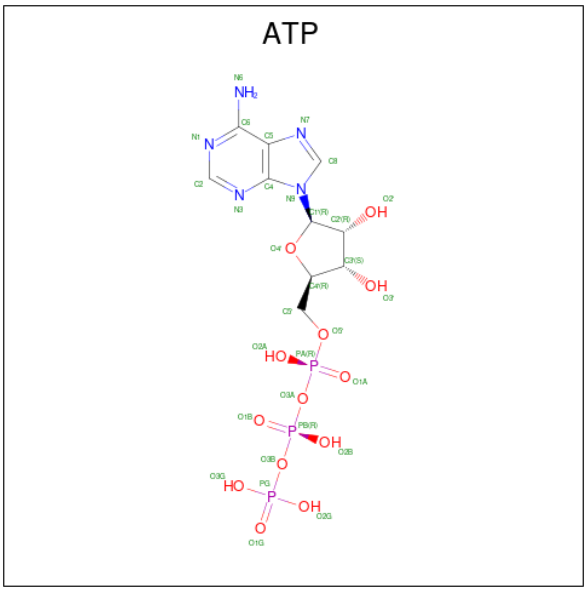
- Molecule 2 is a protein called DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	313	2453	1567	417	452	17	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P29678
C	0	PRO	-	expression tag	UNP P29678
C	38	LEU	GLU	conflict	UNP P29678

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

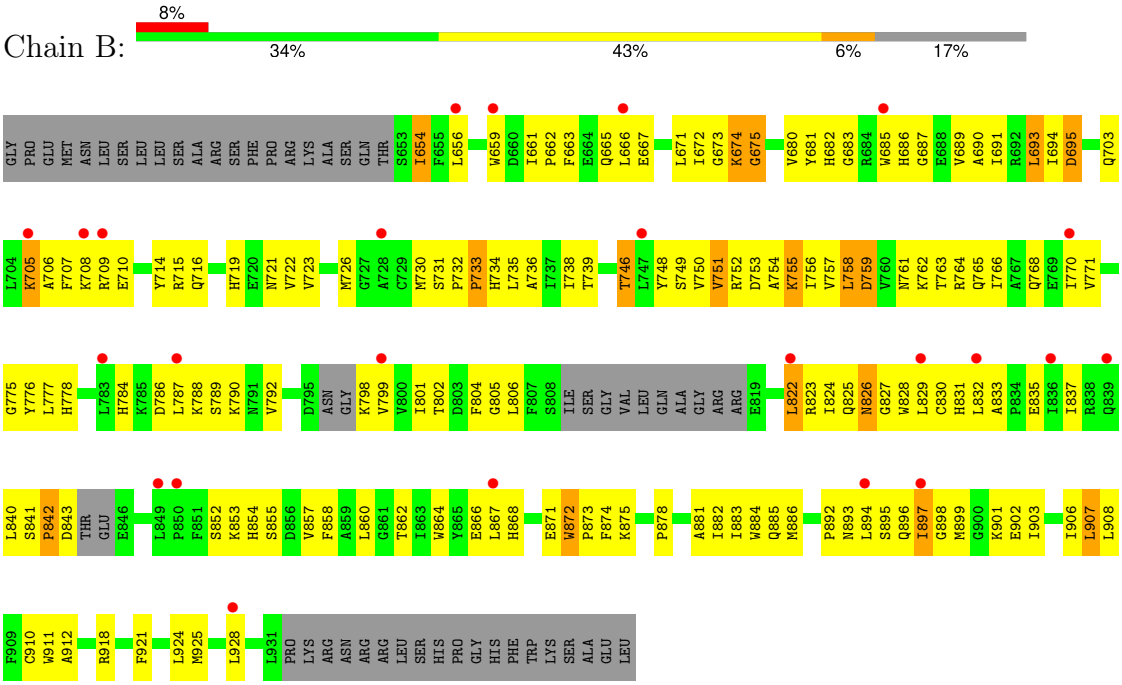
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

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.

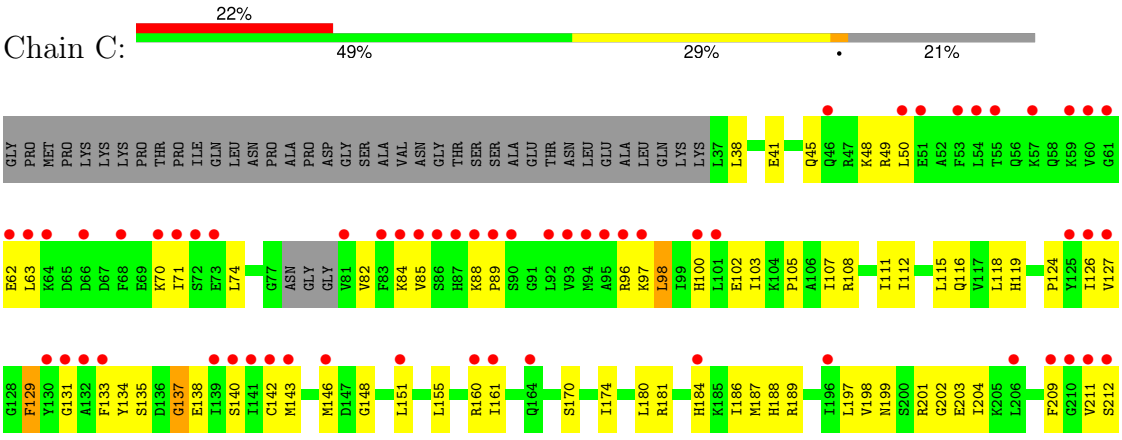
• Molecule 1: KINASE SUPPRESSOR OF RAS 2

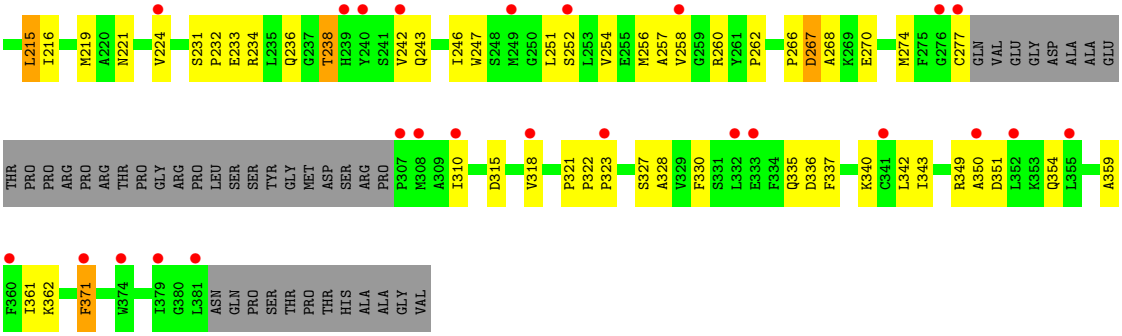
Chain B:



• Molecule 2: DUAL SPECIFICITY MITOGEN-ACTIVATED PROTEIN KINASE KINASE 1

Chain C:




L215 I216 M219 A220 N221 V224 S231 P232 E233 R234 L235 Q236 G237 T238 H239 Y240 S241 V242 Q243 I246 W247 S248 M249 G250 L251 S252 L253 V254 E255 M256 A257 V258 G259 R260 Y261 P262 P266 D267 A268 K269 E270 M274 F275 G276 C277 GLN VAL GLU GLY ASP ALA ALA GLU
THR PRO PRO ARG PRO ARG THR PRO GLY ARG PRO LEU SER SER TYR GLY MET ASP SER ARG PRO P307 M308 A309 I310 D315 V318 P321 P322 P323 S327 A328 V329 F330 S331 L332 E333 F334 Q335 D336 F337 K340 C341 L342 I343 R349 A350 D351 L352 K353 Q354 L355 A359
F360 I361 K362 F371 W374 I379 G380 L381 ASN GLN PRO SER THR PRO THR HIS ALA ALA GLY VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	130.56Å 130.56Å 221.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.86 – 3.46 100.66 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.86-3.46) 99.5 (100.66-3.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.293 0.237 , 0.303	Depositor DCC
R_{free} test set	762 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	133.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 134.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4661	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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, CL

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	B	0.26	0/2192	0.43	0/2955
2	C	0.22	0/2499	0.38	0/3364
All	All	0.24	0/4691	0.41	0/6319

There are no bond length outliers.

There are no bond angle outliers.

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	B	2143	0	2136	148	0
2	C	2453	0	2483	84	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	C	1	0	0	0	0
All	All	4661	0	4643	227	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 24.

All (227) 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:719:HIS:HD2	1:B:721:ASN:H	1.27	0.82
1:B:654:ILE:HG23	1:B:730:MET:H	1.45	0.78
1:B:661:ILE:HD12	1:B:726:MET:HA	1.66	0.78
2:C:252:SER:O	2:C:256:MET:HG2	1.86	0.75
2:C:343:ILE:HD12	2:C:349:ARG:HA	1.67	0.75
1:B:854:HIS:HA	1:B:857:VAL:HG12	1.68	0.74
1:B:735:LEU:HD22	1:B:736:ALA:H	1.52	0.73
1:B:771:VAL:HG23	1:B:921:PHE:HD1	1.53	0.72
1:B:826:ASN:HA	2:C:221:ASN:CG	2.10	0.72
1:B:894:LEU:HD11	1:B:908:LEU:HD21	1.73	0.71
2:C:127:VAL:HG21	2:C:197:LEU:HD12	1.71	0.71
1:B:894:LEU:HD22	1:B:907:LEU:HD13	1.73	0.70
1:B:665:GLN:H	1:B:686:HIS:CE1	2.10	0.69
1:B:685:TRP:HE3	1:B:738:ILE:HG21	1.57	0.68
1:B:735:LEU:HD22	1:B:736:ALA:N	2.08	0.68
2:C:359:ALA:HA	2:C:362:LYS:HE2	1.76	0.67
1:B:878:PRO:O	1:B:882:ILE:HG12	1.95	0.67
1:B:903:ILE:HD12	1:B:903:ILE:H	1.59	0.66
1:B:784:HIS:CD2	1:B:804:PHE:HB3	2.31	0.66
1:B:864:TRP:CH2	1:B:906:ILE:HB	2.30	0.65
3:B:1932:ATP:PB	3:B:1932:ATP:H5'2	2.38	0.64
1:B:719:HIS:CD2	1:B:721:ASN:H	2.14	0.64
1:B:871:GLU:OE1	1:B:875:LYS:HD3	1.98	0.64
2:C:126:ILE:HD11	2:C:180:LEU:CD1	2.27	0.63
1:B:685:TRP:HB3	1:B:689:VAL:HG11	1.81	0.63
1:B:852:SER:O	1:B:855:SER:HB3	1.98	0.63
1:B:730:MET:HG2	1:B:735:LEU:HD23	1.80	0.62
2:C:199:ASN:OD1	2:C:203:GLU:HB2	2.00	0.62
1:B:833:ALA:HB1	1:B:918:ARG:NH2	2.14	0.62
1:B:764:ARG:O	1:B:768:GLN:HG2	2.00	0.62
1:B:829:LEU:HD21	1:B:883:ILE:HG13	1.81	0.62
2:C:70:LYS:HA	2:C:85:VAL:HG12	1.82	0.61
2:C:216:ILE:HA	2:C:219:MET:HB2	1.82	0.61
2:C:262:PRO:HB3	2:C:323:PRO:HB3	1.83	0.61
2:C:181:ARG:HH11	2:C:242:VAL:HG11	1.66	0.61
1:B:673:GLY:HA3	1:B:680:VAL:H	1.67	0.60
1:B:840:LEU:HB2	1:B:843:ASP:HB2	1.84	0.60
1:B:685:TRP:CD1	1:B:685:TRP:O	2.55	0.60
1:B:776:TYR:HD1	1:B:777:LEU:HD23	1.67	0.59
1:B:761:ASN:O	1:B:765:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:LYS:O	1:B:708:LYS:HD3	2.03	0.59
2:C:105:PRO:HA	2:C:108:ARG:NE	2.18	0.58
1:B:862:THR:HA	1:B:911:TRP:HZ2	1.67	0.58
1:B:827:GLY:O	1:B:831:HIS:HD2	1.85	0.58
2:C:112:ILE:O	2:C:116:GLN:HG2	2.04	0.58
1:B:732:PRO:HB2	1:B:733:PRO:HD3	1.85	0.58
1:B:752:ARG:NH2	1:B:866:GLU:OE2	2.36	0.57
1:B:757:VAL:O	1:B:758:LEU:HD23	2.05	0.57
1:B:841:SER:HB3	1:B:842:PRO:HD3	1.86	0.57
2:C:270:GLU:O	2:C:274:MET:HG3	2.03	0.57
1:B:674:LYS:HG3	1:B:675:GLY:H	1.70	0.56
1:B:685:TRP:O	1:B:685:TRP:HD1	1.88	0.56
1:B:824:ILE:HD13	1:B:829:LEU:HD13	1.87	0.56
1:B:719:HIS:HD2	1:B:721:ASN:N	1.99	0.56
1:B:759:ASP:H	1:B:762:LYS:HD2	1.71	0.56
2:C:184:HIS:O	2:C:186:ILE:HG13	2.06	0.56
1:B:778:HIS:HB2	1:B:853:LYS:HE2	1.88	0.55
1:B:864:TRP:CZ3	1:B:906:ILE:HB	2.41	0.55
2:C:146:MET:HG3	2:C:197:LEU:CB	2.36	0.55
2:C:88:LYS:HB3	2:C:89:PRO:HD3	1.88	0.55
2:C:96:ARG:HE	2:C:140:SER:HB3	1.72	0.55
2:C:232:PRO:HD3	2:C:247:TRP:CE2	2.43	0.54
2:C:148:GLY:HA3	2:C:198:VAL:O	2.08	0.54
2:C:126:ILE:HD11	2:C:180:LEU:HD12	1.89	0.54
2:C:155:LEU:HD13	2:C:161:ILE:HG13	1.90	0.54
1:B:726:MET:HB2	1:B:738:ILE:HB	1.89	0.53
1:B:893:ASN:HD22	1:B:896:GLN:HE21	1.56	0.53
1:B:771:VAL:HG13	1:B:925:MET:HG2	1.90	0.53
1:B:901:LYS:O	1:B:902:GLU:HB2	2.08	0.53
2:C:232:PRO:O	2:C:236:GLN:HG3	2.08	0.53
1:B:862:THR:HG22	1:B:911:TRP:HE1	1.72	0.53
1:B:770:ILE:HD11	1:B:792:VAL:HG11	1.90	0.53
1:B:873:PRO:HB3	1:B:892:PRO:HG2	1.91	0.53
1:B:674:LYS:CG	1:B:675:GLY:H	2.20	0.52
1:B:789:SER:HB2	1:B:866:GLU:OE1	2.10	0.52
2:C:71:ILE:HB	2:C:84:LYS:O	2.09	0.52
2:C:146:MET:HG3	2:C:197:LEU:HB3	1.91	0.52
2:C:103:ILE:HB	2:C:107:ILE:HD12	1.91	0.52
1:B:722:VAL:HG21	1:B:777:LEU:HD21	1.92	0.51
2:C:126:ILE:HD11	2:C:180:LEU:HD11	1.90	0.51
1:B:862:THR:HG22	1:B:911:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:672:ILE:HD13	1:B:682:HIS:HB2	1.93	0.51
1:B:903:ILE:HD12	1:B:903:ILE:N	2.26	0.51
2:C:98:LEU:HD22	2:C:138:GLU:OE2	2.11	0.51
1:B:748:TYR:HB2	1:B:790:LYS:HG2	1.93	0.51
2:C:151:LEU:HD13	2:C:256:MET:HE2	1.93	0.50
1:B:654:ILE:HD11	1:B:659:TRP:HE1	1.76	0.50
1:B:694:ILE:O	1:B:695:ASP:C	2.50	0.50
2:C:327:SER:O	2:C:328:ALA:HB3	2.10	0.50
2:C:351:ASP:OD1	2:C:354:GLN:HG3	2.11	0.50
1:B:778:HIS:ND1	1:B:853:LYS:HE2	2.27	0.50
2:C:212:SER:O	2:C:216:ILE:HG13	2.11	0.50
1:B:732:PRO:CB	1:B:733:PRO:HD3	2.42	0.50
1:B:860:LEU:C	1:B:860:LEU:HD23	2.32	0.50
2:C:243:GLN:HA	2:C:246:ILE:HD12	1.92	0.50
1:B:895:SER:HA	1:B:899:MET:CB	2.42	0.49
1:B:893:ASN:ND2	1:B:896:GLN:HE21	2.09	0.49
2:C:74:LEU:HD12	2:C:82:VAL:HG12	1.94	0.49
2:C:187:MET:O	2:C:189:ARG:HG3	2.13	0.49
2:C:233:GLU:HB2	2:C:238:THR:OG1	2.12	0.49
1:B:825:GLN:C	2:C:221:ASN:HB3	2.33	0.49
2:C:180:LEU:HB3	2:C:186:ILE:O	2.12	0.49
2:C:202:GLY:HA2	2:C:371:PHE:CD1	2.48	0.49
1:B:862:THR:HA	1:B:911:TRP:CZ2	2.47	0.48
1:B:775:GLY:O	1:B:778:HIS:HB3	2.13	0.48
1:B:771:VAL:CG1	1:B:925:MET:HG2	2.43	0.48
1:B:756:ILE:HG13	1:B:756:ILE:O	2.12	0.48
1:B:801:ILE:HG22	1:B:802:THR:N	2.29	0.48
1:B:753:ASP:O	1:B:755:LYS:N	2.46	0.48
1:B:835:GLU:OE2	1:B:918:ARG:NH2	2.43	0.48
1:B:756:ILE:HG13	1:B:758:LEU:HD22	1.94	0.48
1:B:862:THR:CG2	1:B:911:TRP:HE1	2.27	0.48
1:B:746:THR:HG23	1:B:749:SER:OG	2.13	0.48
1:B:833:ALA:HB1	1:B:918:ARG:HH22	1.76	0.48
2:C:257:ALA:HB1	2:C:330:PHE:CZ	2.49	0.48
1:B:830:CYS:O	1:B:862:THR:HG21	2.14	0.47
1:B:715:ARG:HG2	1:B:716:GLN:HG3	1.96	0.47
1:B:833:ALA:HB2	1:B:858:PHE:CG	2.48	0.47
1:B:864:TRP:HZ3	1:B:907:LEU:N	2.12	0.47
1:B:874:PHE:CE2	1:B:886:MET:HG2	2.49	0.47
1:B:663:PHE:HB2	1:B:685:TRP:CZ2	2.50	0.47
1:B:685:TRP:O	1:B:686:HIS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:TRP:O	1:B:687:GLY:N	2.47	0.47
1:B:853:LYS:HE3	1:B:921:PHE:CD2	2.49	0.47
2:C:254:VAL:O	2:C:258:VAL:HG22	2.15	0.47
2:C:233:GLU:HG2	2:C:234:ARG:N	2.29	0.47
1:B:766:ILE:O	1:B:770:ILE:HG12	2.15	0.47
2:C:174:ILE:HD11	2:C:337:PHE:HZ	1.79	0.47
1:B:826:ASN:N	2:C:221:ASN:HB3	2.30	0.46
1:B:706:ALA:O	1:B:710:GLU:HB2	2.16	0.46
1:B:787:LEU:O	1:B:787:LEU:HG	2.14	0.46
1:B:666:LEU:HD11	1:B:691:ILE:HD11	1.98	0.46
2:C:50:LEU:HD11	2:C:124:PRO:HG3	1.97	0.46
2:C:260:ARG:HH12	2:C:266:PRO:HA	1.79	0.46
1:B:656:LEU:HD12	1:B:663:PHE:CZ	2.50	0.46
2:C:188:HIS:CD2	2:C:209:PHE:HB3	2.51	0.46
2:C:118:LEU:HD21	2:C:211:VAL:HG11	1.98	0.46
2:C:160:ARG:HH21	2:C:277:CYS:H	1.62	0.46
2:C:135:SER:C	2:C:137:GLY:H	2.18	0.46
2:C:327:SER:HA	2:C:335:GLN:NE2	2.30	0.46
1:B:874:PHE:HB3	1:B:882:ILE:CD1	2.46	0.46
2:C:111:ILE:O	2:C:115:LEU:HB2	2.14	0.46
2:C:49:ARG:HB3	2:C:201:ARG:NH1	2.31	0.46
1:B:666:LEU:HD12	1:B:667:GLU:N	2.31	0.45
1:B:837:ILE:HD12	1:B:886:MET:HB2	1.97	0.45
2:C:118:LEU:HB2	2:C:129:PHE:CZ	2.51	0.45
1:B:770:ILE:O	1:B:801:ILE:HD11	2.17	0.45
1:B:798:LYS:HB3	1:B:799:VAL:H	1.61	0.45
1:B:723:VAL:HG22	1:B:802:THR:HA	1.98	0.45
1:B:714:TYR:N	1:B:714:TYR:CD1	2.84	0.45
1:B:864:TRP:CH2	1:B:903:ILE:HA	2.52	0.45
1:B:674:LYS:HG3	1:B:675:GLY:N	2.32	0.45
1:B:910:CYS:SG	1:B:924:LEU:HD11	2.57	0.45
1:B:690:ALA:O	1:B:739:THR:HG22	2.17	0.45
2:C:170:SER:O	2:C:174:ILE:HG13	2.16	0.45
1:B:703:GLN:HB3	1:B:706:ALA:HB3	1.99	0.44
1:B:763:THR:HG23	1:B:867:LEU:HB3	2.00	0.44
2:C:63:LEU:HD11	2:C:131:GLY:HA3	1.99	0.44
2:C:119:HIS:HA	2:C:129:PHE:HE1	1.82	0.44
2:C:133:PHE:HD1	2:C:134:TYR:O	2.00	0.44
1:B:805:GLY:O	1:B:806:LEU:HD23	2.17	0.44
2:C:224:VAL:HG11	2:C:310:ILE:HD13	2.00	0.44
1:B:830:CYS:HA	1:B:886:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:ILE:H	1:B:903:ILE:CD1	2.28	0.44
1:B:881:ALA:O	1:B:885:GLN:HG3	2.17	0.44
2:C:215:LEU:O	2:C:219:MET:HG2	2.17	0.44
2:C:254:VAL:HG12	2:C:262:PRO:HG3	2.00	0.44
1:B:763:THR:HG21	1:B:868:HIS:CE1	2.53	0.44
1:B:924:LEU:O	1:B:924:LEU:HD23	2.18	0.44
2:C:198:VAL:HG22	2:C:204:ILE:HG12	2.00	0.44
1:B:666:LEU:HD13	1:B:685:TRP:HA	1.99	0.44
2:C:129:PHE:HA	2:C:143:MET:HA	1.99	0.44
1:B:735:LEU:HD13	1:B:735:LEU:C	2.39	0.43
1:B:771:VAL:HG23	1:B:921:PHE:CD1	2.42	0.43
2:C:45:GLN:O	2:C:48:LYS:HB3	2.18	0.43
1:B:842:PRO:HB2	1:B:843:ASP:H	1.53	0.43
1:B:750:VAL:HG22	1:B:756:ILE:HD13	1.99	0.43
2:C:82:VAL:HG22	2:C:97:LYS:HB2	2.00	0.43
1:B:751:VAL:HG12	1:B:752:ARG:HG3	2.00	0.43
1:B:661:ILE:HA	1:B:662:PRO:HD3	1.91	0.43
1:B:842:PRO:O	1:B:843:ASP:C	2.56	0.43
1:B:751:VAL:CG1	1:B:752:ARG:HG3	2.48	0.43
2:C:327:SER:HA	2:C:335:GLN:HE22	1.83	0.43
2:C:349:ARG:HG2	2:C:350:ALA:N	2.34	0.43
1:B:758:LEU:HA	1:B:762:LYS:HD2	2.01	0.43
1:B:654:ILE:CG2	1:B:730:MET:H	2.23	0.43
1:B:683:GLY:HA3	1:B:691:ILE:CD1	2.48	0.43
2:C:251:LEU:N	2:C:342:LEU:HD21	2.34	0.43
1:B:681:TYR:CE1	1:B:693:LEU:HD22	2.54	0.42
1:B:714:TYR:N	1:B:714:TYR:HD1	2.17	0.42
2:C:231:SER:OG	2:C:234:ARG:HG3	2.19	0.42
1:B:750:VAL:CG2	1:B:756:ILE:HD13	2.48	0.42
1:B:671:LEU:HB2	1:B:681:TYR:CE2	2.54	0.42
1:B:874:PHE:CB	1:B:882:ILE:HD12	2.50	0.42
1:B:685:TRP:CD1	1:B:685:TRP:C	2.93	0.42
1:B:884:TRP:HE1	2:C:315:ASP:HA	1.85	0.42
2:C:63:LEU:HD13	2:C:133:PHE:HD2	1.85	0.42
2:C:321:PRO:HA	2:C:322:PRO:HD3	1.78	0.42
1:B:707:PHE:C	1:B:709:ARG:N	2.72	0.41
2:C:45:GLN:CD	2:C:49:ARG:HH21	2.24	0.41
2:C:105:PRO:O	2:C:108:ARG:HG2	2.20	0.41
2:C:361:ILE:HD13	2:C:361:ILE:HA	1.96	0.41
1:B:822:LEU:HD12	1:B:823:ARG:N	2.36	0.41
1:B:884:TRP:NE1	2:C:315:ASP:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:186:ILE:HD13	2:C:211:VAL:HG23	2.02	0.41
1:B:748:TYR:CB	1:B:790:LYS:HG2	2.49	0.41
1:B:853:LYS:HE3	1:B:921:PHE:CE2	2.55	0.41
1:B:705:LYS:HG3	1:B:709:ARG:HD2	2.02	0.41
1:B:723:VAL:HG13	1:B:801:ILE:O	2.20	0.41
1:B:731:SER:OG	1:B:734:HIS:CE1	2.74	0.41
1:B:786:ASP:OD1	1:B:788:LYS:HG3	2.20	0.41
1:B:897:ILE:HA	1:B:898:GLY:HA2	1.63	0.41
2:C:45:GLN:O	2:C:49:ARG:HG3	2.20	0.41
1:B:723:VAL:CG1	1:B:802:THR:HB	2.51	0.41
1:B:864:TRP:HH2	1:B:903:ILE:HA	1.85	0.41
1:B:872:TRP:HB2	1:B:873:PRO:HD2	2.03	0.41
1:B:893:ASN:O	1:B:894:LEU:HD23	2.21	0.41
2:C:267:ASP:CG	2:C:268:ALA:H	2.24	0.41
2:C:336:ASP:O	2:C:340:LYS:HG2	2.21	0.41
2:C:215:LEU:HG	2:C:219:MET:HG2	2.03	0.41
1:B:911:TRP:O	1:B:912:ALA:C	2.58	0.40
1:B:884:TRP:CZ2	2:C:318:VAL:HG11	2.57	0.40
2:C:133:PHE:HE2	2:C:142:CYS:SG	2.44	0.40
1:B:663:PHE:HB2	1:B:685:TRP:CE2	2.57	0.40
1:B:828:TRP:CZ2	1:B:832:LEU:HD11	2.56	0.40
1:B:837:ILE:HD12	1:B:886:MET:CB	2.51	0.40
2:C:100:HIS:CE1	2:C:102:GLU:HG2	2.56	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	B	257/319 (81%)	203 (79%)	42 (16%)	12 (5%)	2 19
2	C	307/395 (78%)	261 (85%)	40 (13%)	6 (2%)	7 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	564/714 (79%)	464 (82%)	82 (14%)	18 (3%)	4 28

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	754	ALA
1	B	758	LEU
1	B	822	LEU
1	B	826	ASN
2	C	267	ASP
1	B	675	GLY
1	B	755	LYS
1	B	759	ASP
1	B	842	PRO
2	C	41	GLU
2	C	371	PHE
1	B	674	LYS
1	B	695	ASP
1	B	733	PRO
1	B	897	ILE
2	C	38	LEU
2	C	62	GLU
2	C	137	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	228/278 (82%)	220 (96%)	8 (4%)	36 67
2	C	270/339 (80%)	266 (98%)	4 (2%)	65 84
All	All	498/617 (81%)	486 (98%)	12 (2%)	49 76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	654	ILE
1	B	693	LEU
1	B	705	LYS
1	B	746	THR
1	B	751	VAL
1	B	872	TRP
1	B	907	LEU
1	B	928	LEU
2	C	98	LEU
2	C	129	PHE
2	C	215	LEU
2	C	238	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	734	HIS
1	B	765	GLN
1	B	831	HIS
1	B	896	GLN
1	B	915	GLN
2	C	116	GLN
2	C	335	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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	B	1932	4	28,33,33	1.00	1 (3%)	34,52,52	1.16	2 (5%)
3	ATP	C	1382	4	28,33,33	0.99	0	34,52,52	1.16	2 (5%)

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
3	ATP	B	1932	4	-	5/18/38/38	0/3/3/3
3	ATP	C	1382	4	-	2/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1932	ATP	PB-O3A	2.20	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1382	ATP	N3-C2-N1	-3.65	123.72	128.67
3	B	1932	ATP	N3-C2-N1	-3.61	123.77	128.67
3	B	1932	ATP	C4-C5-N7	-2.64	106.55	109.34
3	C	1382	ATP	C4-C5-N7	-2.43	106.77	109.34

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1932	ATP	C5'-O5'-PA-O2A
3	B	1932	ATP	O4'-C4'-C5'-O5'
3	B	1932	ATP	C3'-C4'-C5'-O5'
3	C	1382	ATP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	C	1382	ATP	O4'-C4'-C5'-O5'
3	B	1932	ATP	C5'-O5'-PA-O1A
3	B	1932	ATP	C5'-O5'-PA-O3A

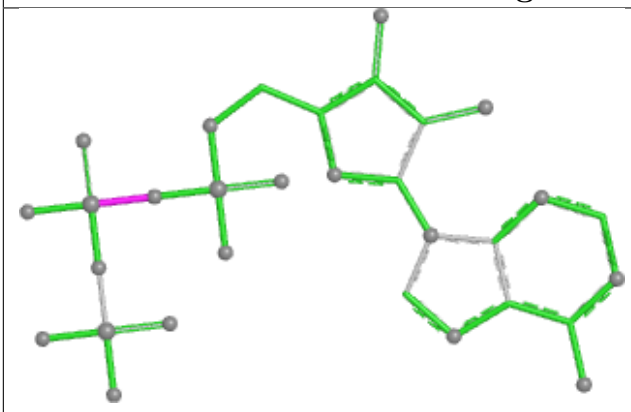
There are no ring outliers.

1 monomer is involved in 1 short contact:

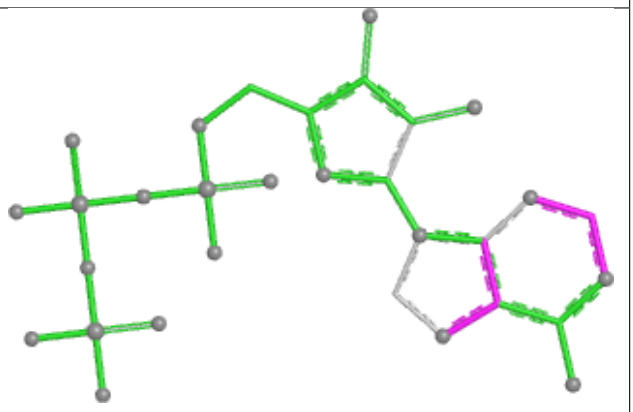
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1932	ATP	1	0

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.

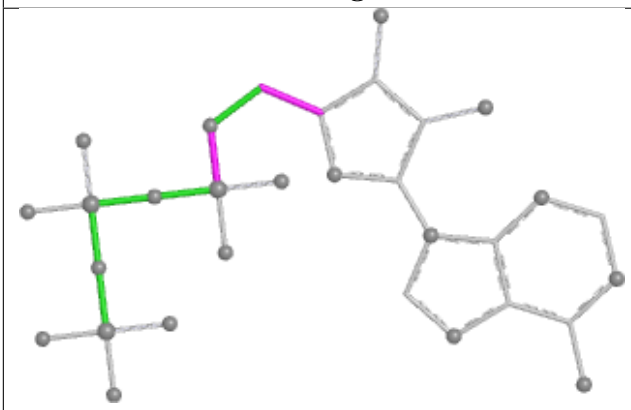
Ligand ATP B 1932



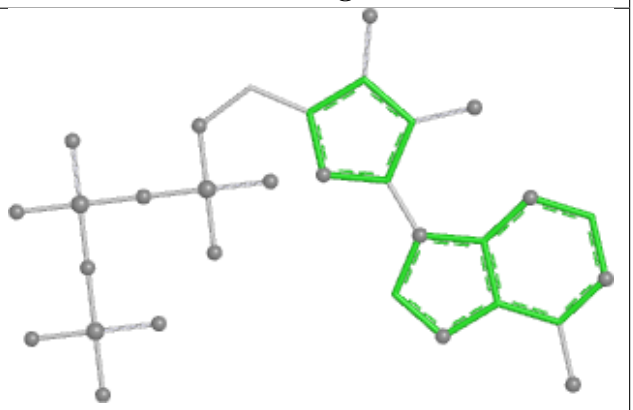
Bond lengths



Bond angles

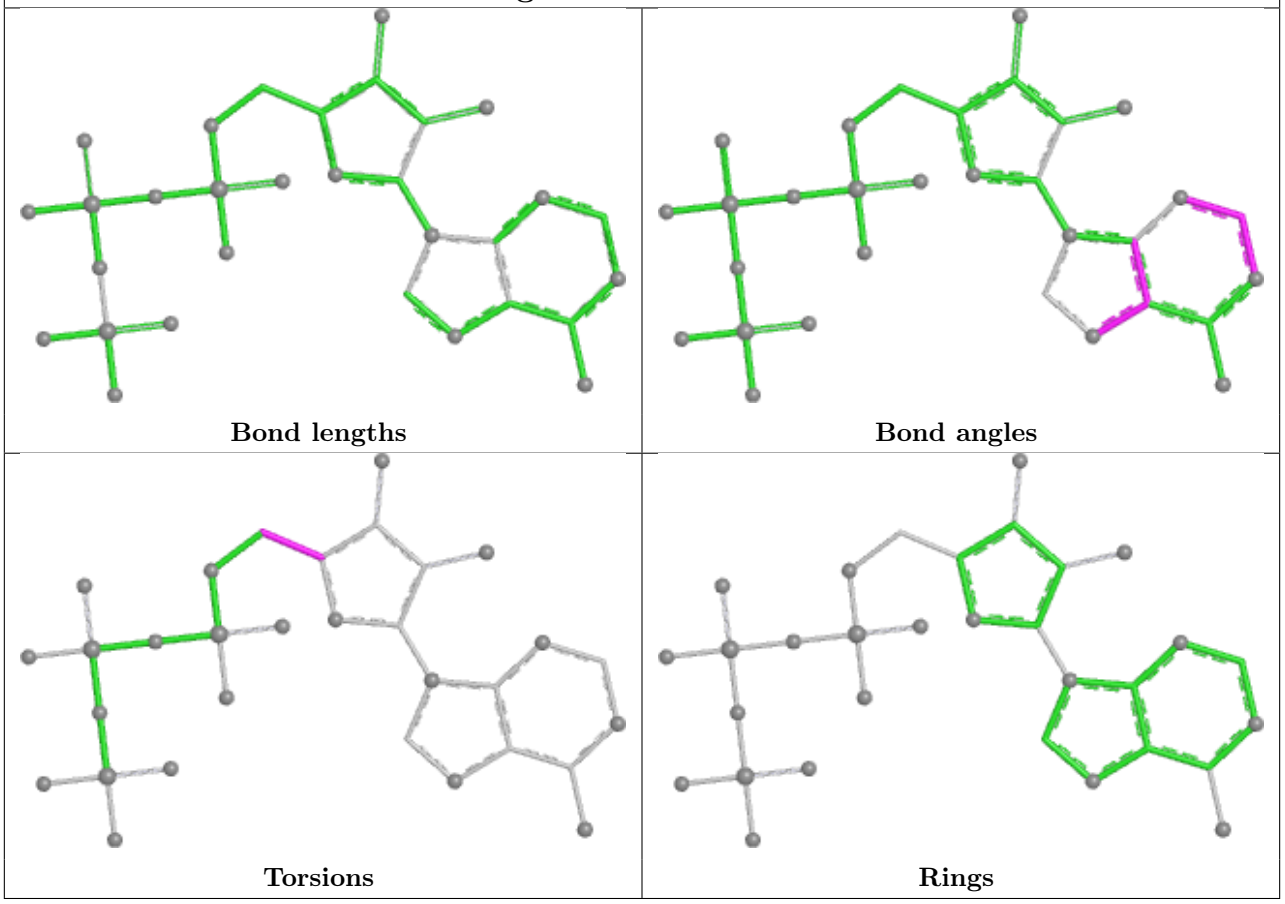


Torsions



Rings

Ligand ATP C 1382



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	B	265/319 (83%)	0.87	24 (9%) 9 11	97, 135, 226, 274	0
2	C	313/395 (79%)	1.25	85 (27%) 0 0	95, 168, 234, 302	0
All	All	578/714 (80%)	1.08	109 (18%) 1 2	95, 151, 232, 302	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	94	MET	7.5
2	C	63	LEU	5.7
1	B	685	TRP	5.4
2	C	139	ILE	5.1
2	C	93	VAL	5.1
2	C	141	ILE	5.0
2	C	85	VAL	5.0
2	C	60	VAL	5.0
2	C	132	ALA	4.6
2	C	68	PHE	4.2
2	C	90	SER	4.2
2	C	352	LEU	4.0
2	C	310	ILE	4.0
2	C	53	PHE	3.8
1	B	822	LEU	3.8
2	C	240	TYR	3.7
2	C	211	VAL	3.6
2	C	210	GLY	3.6
1	B	728	ALA	3.5
2	C	46	GLN	3.5
2	C	50	LEU	3.4
2	C	142	CYS	3.4
2	C	95	ALA	3.4
2	C	84	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	89	PRO	3.3
2	C	87	HIS	3.3
2	C	374	TRP	3.2
2	C	277	CYS	3.2
2	C	88	LYS	3.1
1	B	850	PRO	3.1
2	C	125	TYR	3.1
2	C	64	LYS	3.0
1	B	656	LEU	3.0
2	C	308	MET	3.0
2	C	151	LEU	2.9
2	C	55	THR	2.9
2	C	70	LYS	2.9
1	B	897	ILE	2.8
1	B	705	LYS	2.8
2	C	307	PRO	2.8
2	C	161	ILE	2.8
1	B	708	LYS	2.8
1	B	894	LEU	2.8
1	B	829	LEU	2.7
2	C	127	VAL	2.7
2	C	97	LYS	2.7
1	B	787	LEU	2.7
1	B	747	LEU	2.7
2	C	62	GLU	2.6
2	C	73	GLU	2.6
2	C	184	HIS	2.6
2	C	212	SER	2.6
2	C	57	LYS	2.6
2	C	131	GLY	2.6
2	C	92	LEU	2.6
2	C	96	ARG	2.6
2	C	242	VAL	2.5
2	C	276	GLY	2.5
2	C	224	VAL	2.5
1	B	783	LEU	2.5
2	C	59	LYS	2.5
1	B	709	ARG	2.5
2	C	379	ILE	2.5
2	C	341	CYS	2.4
2	C	239	HIS	2.4
2	C	83	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	66	ASP	2.4
2	C	209	PHE	2.4
2	C	164	GLN	2.4
1	B	928	LEU	2.3
2	C	332	LEU	2.3
1	B	659	TRP	2.3
2	C	206	LEU	2.3
2	C	130	TYR	2.3
1	B	770	ILE	2.3
2	C	196	ILE	2.3
2	C	51	GLU	2.3
2	C	249	MET	2.3
1	B	839	GLN	2.3
2	C	86	SER	2.3
2	C	160	ARG	2.2
2	C	61	GLY	2.2
2	C	252	SER	2.2
2	C	318	VAL	2.2
1	B	867	LEU	2.2
2	C	81	VAL	2.2
2	C	140	SER	2.2
2	C	355	LEU	2.2
2	C	360	PHE	2.2
2	C	72	SER	2.2
2	C	101	LEU	2.1
1	B	799	VAL	2.1
1	B	849	LEU	2.1
2	C	126	ILE	2.1
2	C	143	MET	2.1
1	B	666	LEU	2.1
1	B	836	ILE	2.1
2	C	146	MET	2.1
2	C	333	GLU	2.1
2	C	323	PRO	2.1
2	C	350	ALA	2.1
2	C	100	HIS	2.1
2	C	381	LEU	2.0
2	C	71	ILE	2.0
2	C	371	PHE	2.0
1	B	832	LEU	2.0
2	C	133	PHE	2.0
2	C	258	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	54	LEU	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)

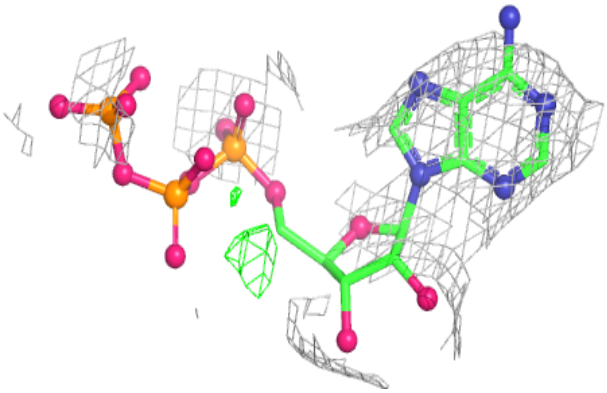
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

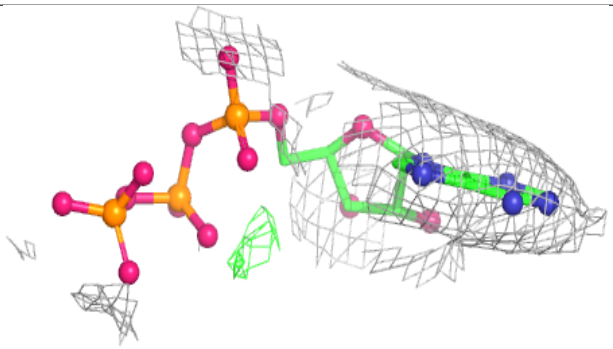
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	C	1384	1/1	0.59	0.31	143,143,143,143	0
3	ATP	C	1382	31/31	0.84	0.27	110,136,174,305	0
3	ATP	B	1932	31/31	0.95	0.27	86,105,134,268	0
4	MG	C	1383	1/1	0.97	0.20	185,185,185,185	0
4	MG	B	1933	1/1	0.99	0.23	94,94,94,94	0

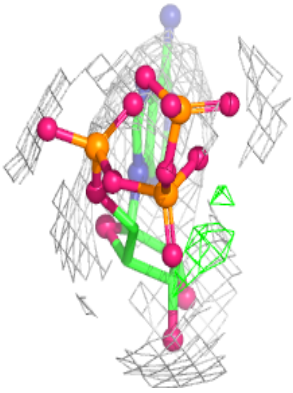
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP C 1382:

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

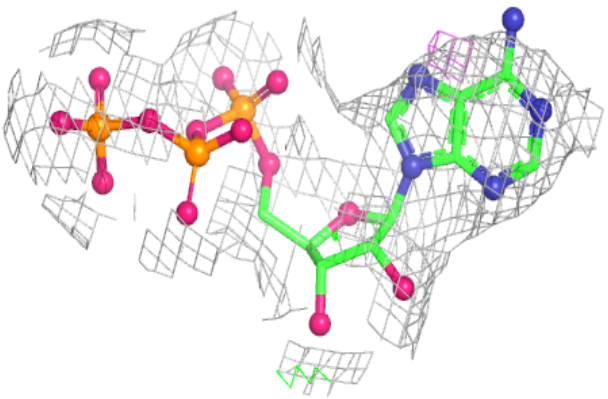


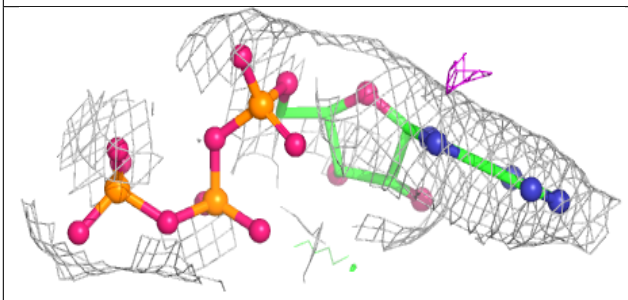


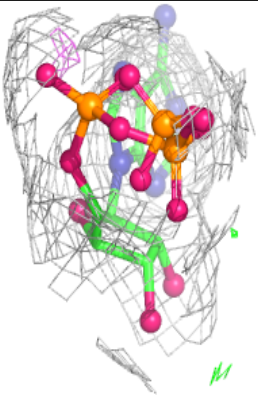


Electron density around ATP B 1932:

$2mF_o$-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.