



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 2Y4I / pdb_00002y4i
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	:	4-5-2 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

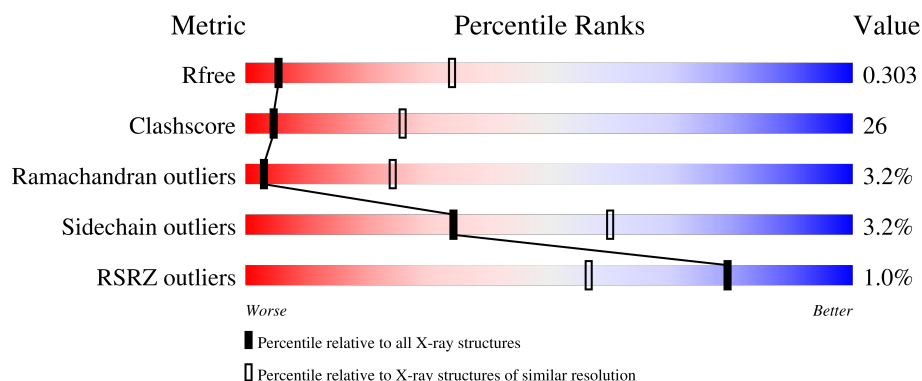
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	B	319	
2	C	395	

2 Entry composition

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
1	B	265	Total	C	N	O	S	0	0	0
			2143	1385	367	379	12			

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
2	C	313	Total	C	N	O	S	0	0	0
			2453	1567	417	452	17			

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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

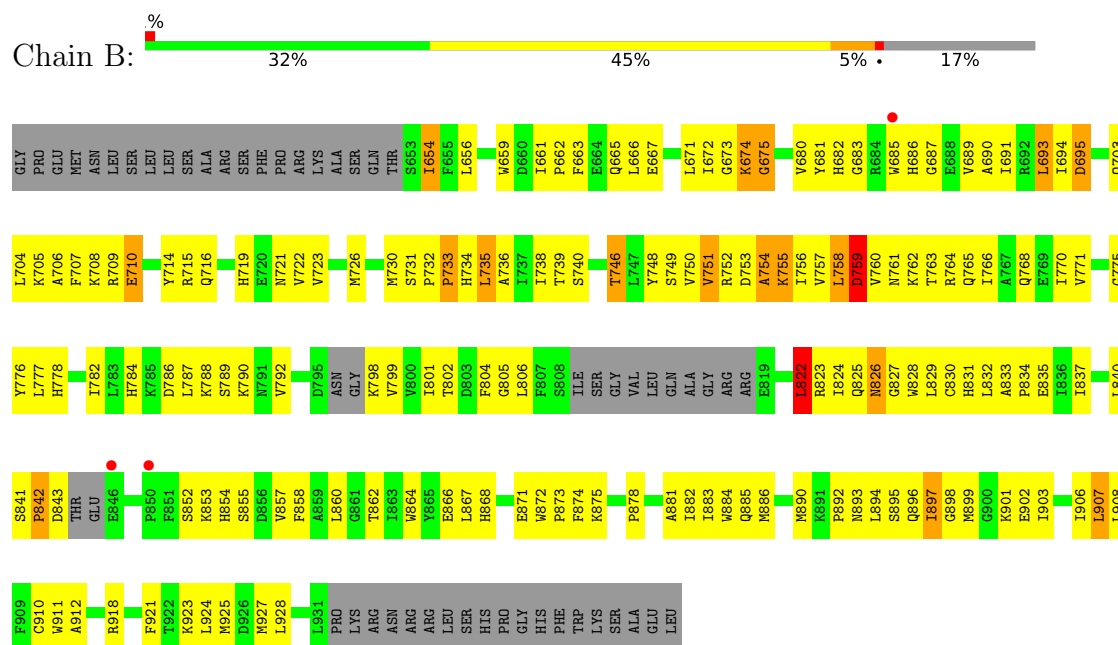
- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

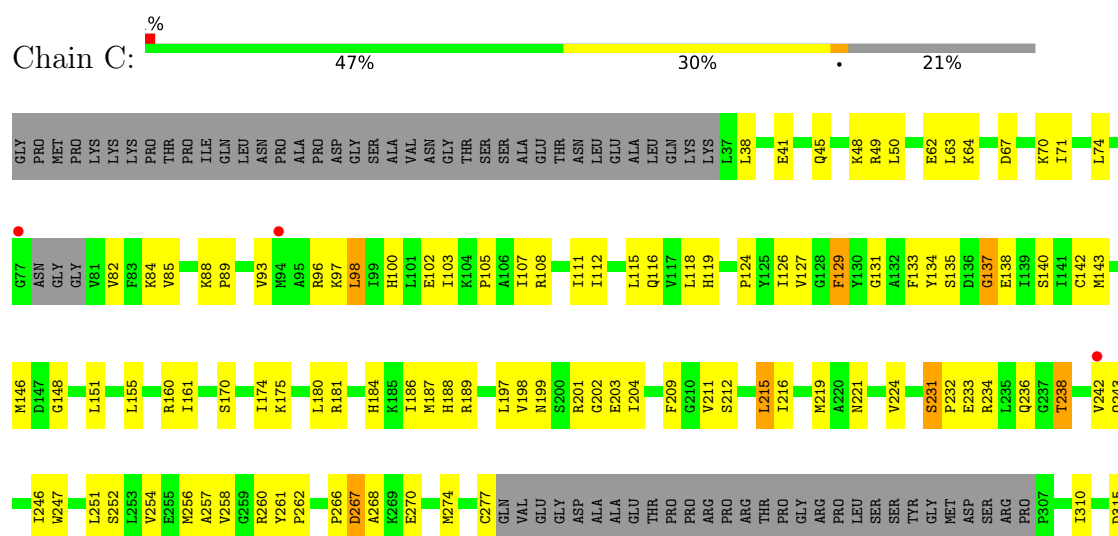
3 Residue-property plots

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: KINASE SUPPRESSOR OF RAS 2



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



V318	P321	P322	P323	S327	A328	V329	F330	Q335	D336	F337	K340	G341	L342	I343	R349	A350	D351	L352	K353	Q354	L355	M356	A359	F360	I361	K362	F371	L381	ASN	GLN	PRO	SER	THR	PRO	THR	HIS	ALA	ALA	GLY	VAL
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

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 39.86 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.86-3.46) 99.5 (39.86-3.46)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.36 , 169.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/2192	0.73	1/2955 (0.0%)
2	C	0.27	0/2499	0.74	4/3364 (0.1%)
All	All	0.29	0/4691	0.74	5/6319 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	760	VAL	N-CA-C	-5.81	107.15	112.96
2	C	231	SER	CA-C-N	5.59	125.96	119.47
2	C	231	SER	C-N-CA	5.59	125.96	119.47
2	C	261	TYR	CA-C-N	5.32	126.49	119.84
2	C	261	TYR	C-N-CA	5.32	126.49	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2143	0	2136	157	0
2	C	2453	0	2483	90	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	242	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 26.

All (242) 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
1:B:826:ASN:HA	2:C:221:ASN:CG	2.10	0.77
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: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
1:B:689:VAL:HG12	1:B:726:MET:HE3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:175:LYS:HG2	2:C:356:MET:HE1	1.84	0.59
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
2:C:151:LEU:HB3	2:C:256:MET:HE1	1.86	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
1:B:694:ILE:O	1:B:695:ASP:C	2.50	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
1:B:860:LEU:C	1:B:860:LEU:HD23	2.32	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:GLN:C	2:C:221:ASN:HB3	2.33	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
2:C:135:SER:C	2:C:137:GLY:H	2.18	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
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
1:B:654:ILE:HD11	1:B:659:TRP:HE1	1.76	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
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
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:923:LYS:HG2	1:B:927:MET:HE3	1.95	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:735:LEU:HD13	1:B:735:LEU:C	2.39	0.48
1:B:756:ILE:O	1:B:756:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:842:PRO:O	1:B:843:ASP:C	2.56	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:CD1	1:B:685:TRP:C	2.93	0.47
1:B:685:TRP:O	1:B:686:HIS:HB2	2.13	0.47
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
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:45:GLN:CD	2:C:49:ARG:HH21	2.24	0.46
2:C:50:LEU:HD11	2:C:124:PRO:HG3	1.97	0.46
2:C:233:GLU:HG2	2:C:234:ARG:N	2.29	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
1:B:707:PHE:C	1:B:709:ARG:N	2.72	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: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
2:C:161:ILE:HD12	2:C:256:MET:HE3	1.98	0.46
1:B:666:LEU:HD12	1:B:667:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:267:ASP:CG	2:C:268:ALA:H	2.24	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
1:B:911:TRP:O	1:B:912:ALA:C	2.58	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:184:HIS:C	2:C:186:ILE:H	2.27	0.42
1:B:884:TRP:HE1	2:C:315:ASP:HA	1.85	0.42
1:B:890:MET:HE3	1:B:890:MET:HB2	1.85	0.42
1:B:834:PRO:O	1:B:835:GLU:C	2.63	0.42
2:C:129:PHE:CD1	2:C:129:PHE:C	2.97	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
2:C:353:LYS:O	2:C:354:GLN:C	2.63	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
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:753:ASP:O	1:B:754:ALA:C	2.64	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:750:VAL:C	1:B:752:ARG:H	2.28	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: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:707:PHE:C	1:B:709:ARG:H	2.28	0.40
2:C:64:LYS:HB2	2:C:67:ASP:CG	2.46	0.40
1:B:726:MET:HE2	1:B:740:SER:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:704:LEU:C	1:B:706:ALA:N	2.80	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	17
2	C	307/395 (78%)	261 (85%)	40 (13%)	6 (2%)	6	32
All	All	564/714 (79%)	464 (82%)	82 (14%)	18 (3%)	3	24

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	217 (95%)	11 (5%)	23	50
2	C	270/339 (80%)	265 (98%)	5 (2%)	50	68
All	All	498/617 (81%)	482 (97%)	16 (3%)	34	60

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	654	ILE
1	B	693	LEU
1	B	710	GLU
1	B	735	LEU
1	B	746	THR
1	B	751	VAL
1	B	759	ASP
1	B	782	ILE
1	B	822	LEU
1	B	907	LEU
1	B	928	LEU
2	C	93	VAL
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	700	ASN
1	B	734	HIS
1	B	765	GLN
1	B	854	HIS
1	B	896	GLN
1	B	915	GLN
2	C	116	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	32,33,33	1.40	5 (15%)	48,52,52	1.83	9 (18%)
3	ATP	C	1382	4	32,33,33	1.41	4 (12%)	48,52,52	1.79	9 (18%)

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	-	5/22/38/38	0/3/3/3
3	ATP	C	1382	4	-	2/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1382	ATP	C5-C4	4.77	1.47	1.39
3	B	1932	ATP	C5-C4	4.59	1.47	1.39
3	B	1932	ATP	C5-C6	2.73	1.48	1.41
3	C	1382	ATP	C5-C6	2.70	1.48	1.41
3	B	1932	ATP	C8-N7	2.29	1.36	1.31
3	C	1382	ATP	C8-N7	2.26	1.36	1.31
3	C	1382	ATP	C5-N7	-2.26	1.35	1.39
3	B	1932	ATP	C5-N7	-2.23	1.35	1.39
3	B	1932	ATP	PB-O3A	2.20	1.61	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1932	ATP	C5-C4-N3	-5.96	118.51	126.72
3	C	1382	ATP	C5-C4-N3	-5.88	118.62	126.72
3	B	1932	ATP	N3-C4-N9	4.90	135.50	127.17
3	C	1382	ATP	N3-C4-N9	4.85	135.42	127.17
3	B	1932	ATP	C2-N3-C4	3.74	120.96	111.83
3	C	1382	ATP	C2-N3-C4	3.68	120.83	111.83
3	B	1932	ATP	C4-C5-N7	-3.53	106.55	110.58
3	C	1382	ATP	C4-C5-N7	-3.33	106.77	110.58
3	C	1382	ATP	N3-C2-N1	-3.21	123.72	128.58
3	B	1932	ATP	N3-C2-N1	-3.18	123.77	128.58
3	B	1932	ATP	C4-N9-C8	3.14	109.03	105.74
3	C	1382	ATP	C4-N9-C8	2.87	108.76	105.74
3	B	1932	ATP	C5-N7-C8	2.75	107.78	103.45
3	C	1382	ATP	C5-N7-C8	2.53	107.42	103.45
3	C	1382	ATP	C3'-C2'-C1'	2.36	105.94	101.46
3	B	1932	ATP	N9-C8-N7	-2.31	110.66	113.94
3	B	1932	ATP	C3'-C2'-C1'	2.29	105.79	101.46
3	C	1382	ATP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (7) torsion outliers are listed below:

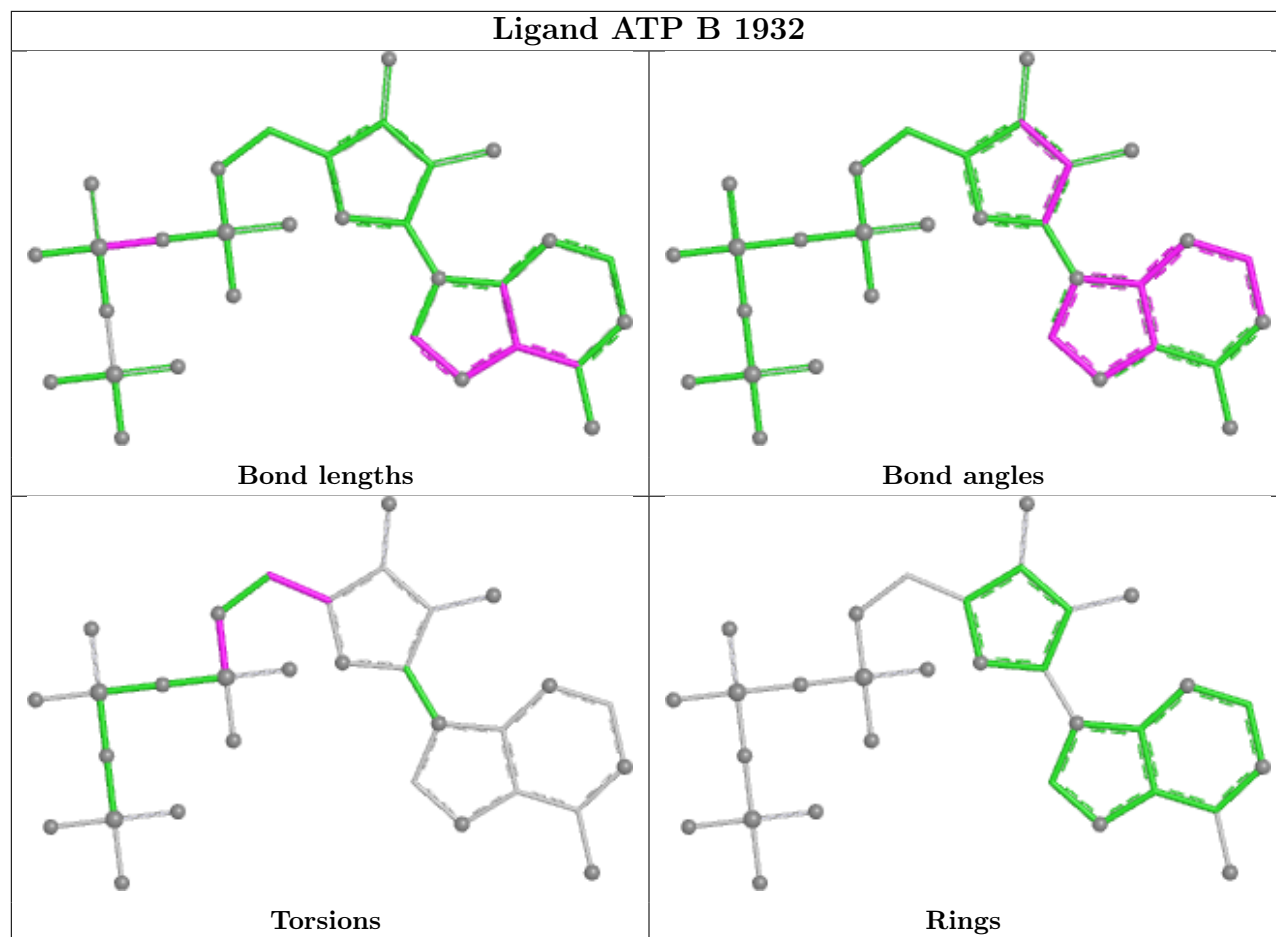
Mol	Chain	Res	Type	Atoms
3	B	1932	ATP	C5'-O5'-PA-O2A
3	B	1932	ATP	O4'-C4'-C5'-O5'
3	B	1932	ATP	C3'-C4'-C5'-O5'
3	C	1382	ATP	C3'-C4'-C5'-O5'
3	C	1382	ATP	O4'-C4'-C5'-O5'
3	B	1932	ATP	C5'-O5'-PA-O1A
3	B	1932	ATP	C5'-O5'-PA-O3A

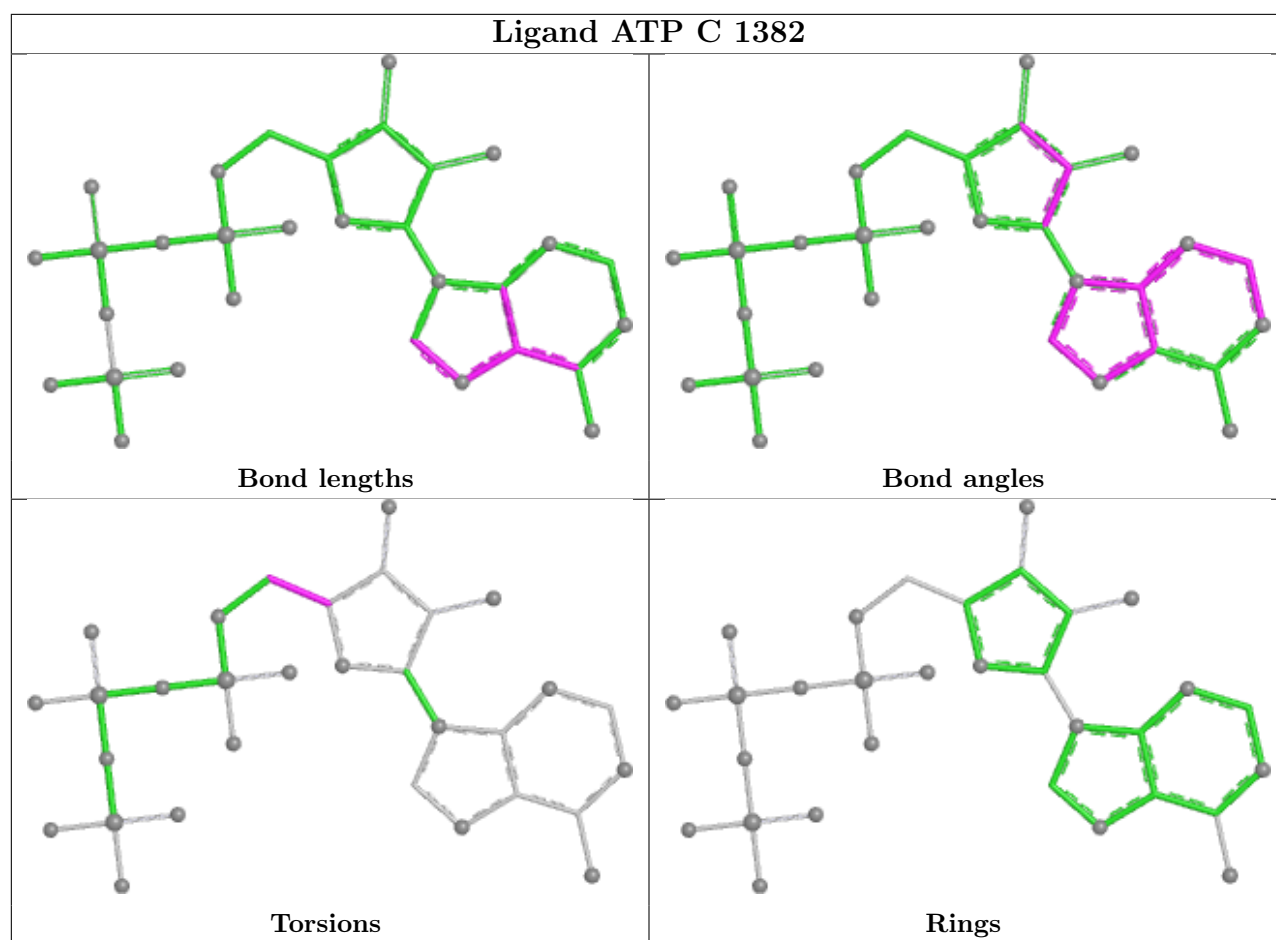
There are no ring outliers.

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 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	B	265/319 (83%)	-0.05	3 (1%)	78 54	97, 135, 226, 274	0
2	C	313/395 (79%)	-0.22	3 (0%)	79 56	95, 168, 234, 302	0
All	All	578/714 (80%)	-0.14	6 (1%)	79 56	95, 151, 232, 302	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	685	TRP	3.4
2	C	94	MET	2.7
1	B	850	PRO	2.4
2	C	77	GLY	2.4
1	B	846	GLU	2.2
2	C	242	VAL	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

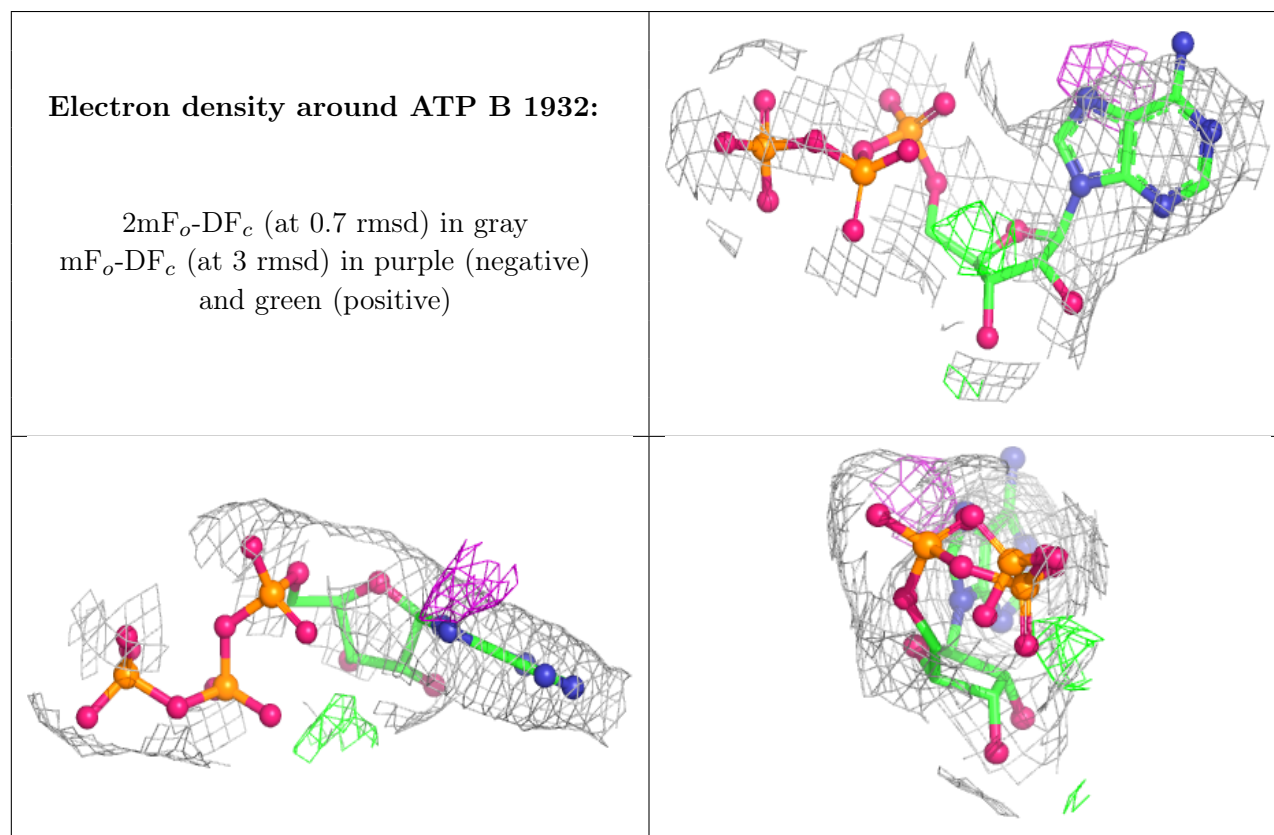
There are no oligosaccharides in this entry.

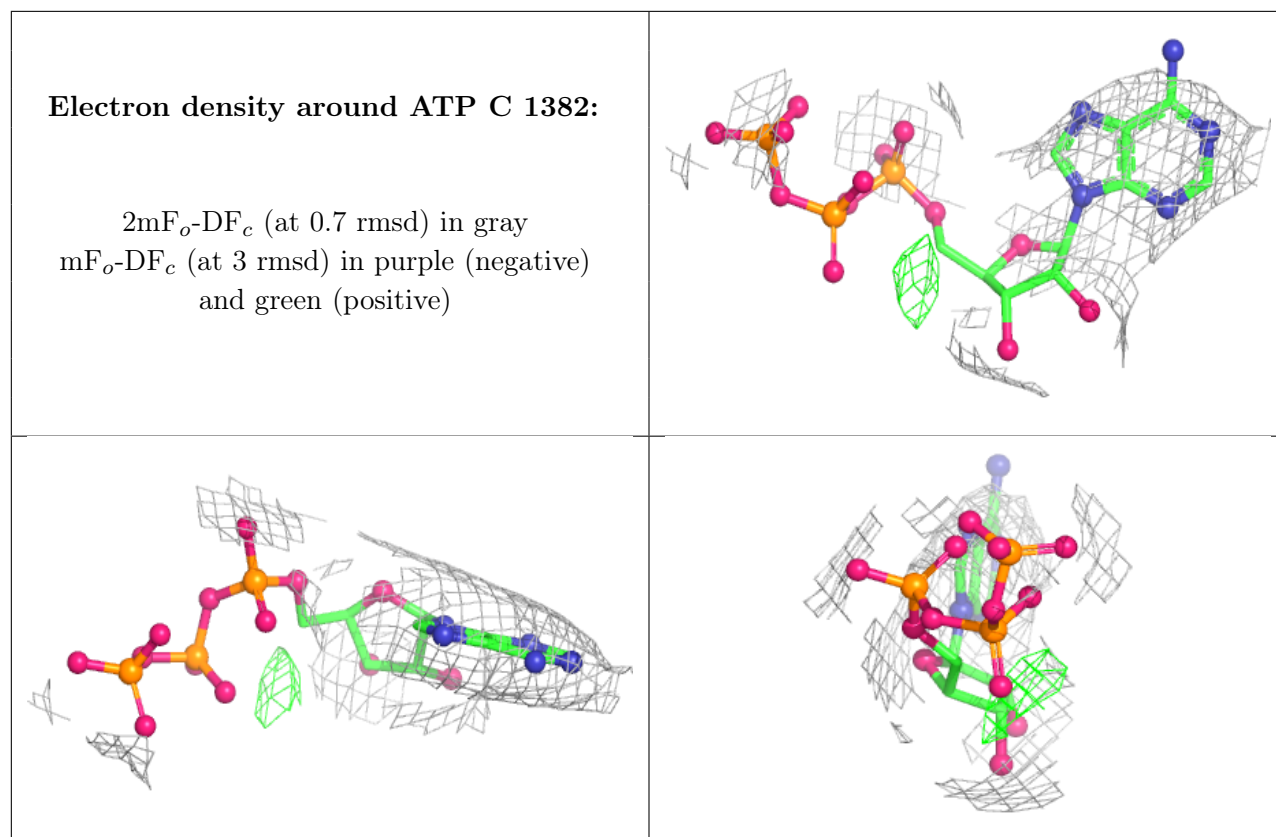
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	1383	1/1	0.92	0.12	185,185,185,185	0
5	CL	C	1384	1/1	0.93	0.08	143,143,143,143	0
4	MG	B	1933	1/1	0.95	0.06	94,94,94,94	0
3	ATP	B	1932	31/31	0.95	0.07	86,105,134,268	0
3	ATP	C	1382	31/31	0.95	0.07	110,136,174,305	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.