Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 06:27 PM EDT

PDB ID	:	4KBF
Title	:	two different open conformations of the helicase core of the RNA helicase Hera
Authors	:	Rudolph, M.G.; Klostermeier, D.
Deposited on	:	2013-04-23
Resolution	:	1.90 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:

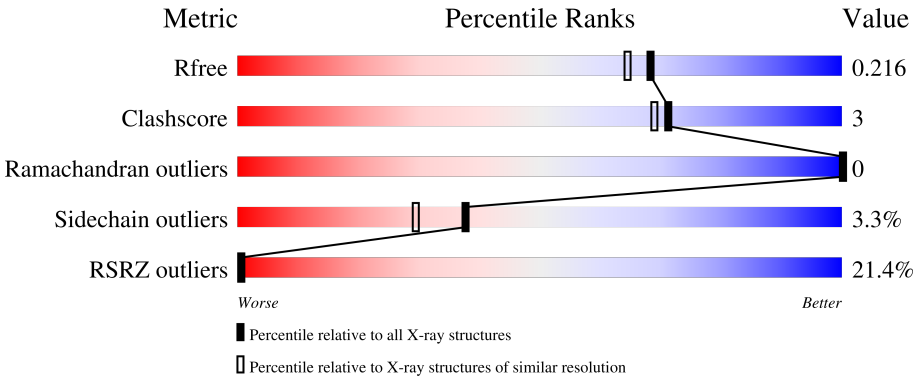
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	365	2% 90% 9%
1	B	365	41% 85% 15%

2 Entry composition

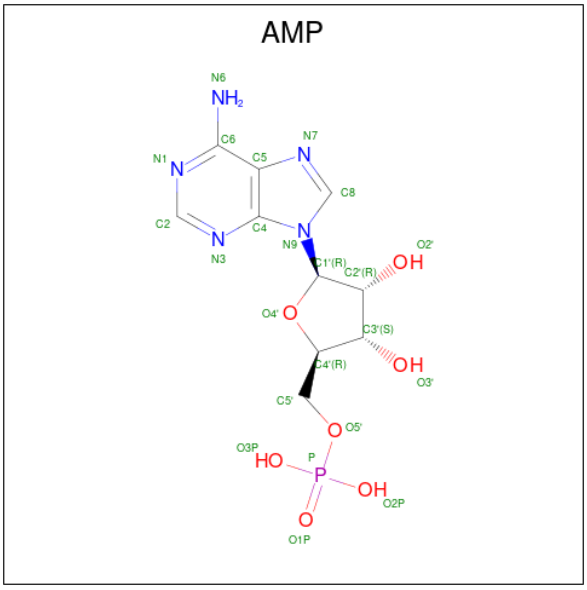
There are 5 unique types of molecules in this entry. The entry contains 5827 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heat resistant RNA dependent ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	1	0
			2823	1775	524	519	5			
1	B	365	Total	C	N	O	S	0	0	0
			2815	1770	521	519	5			

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

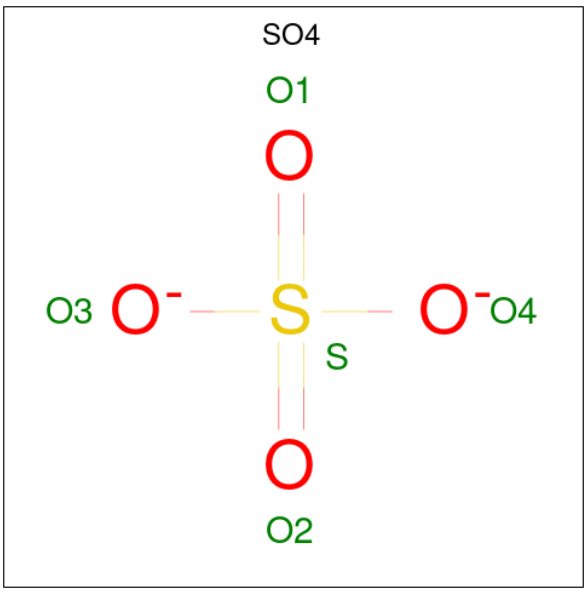


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

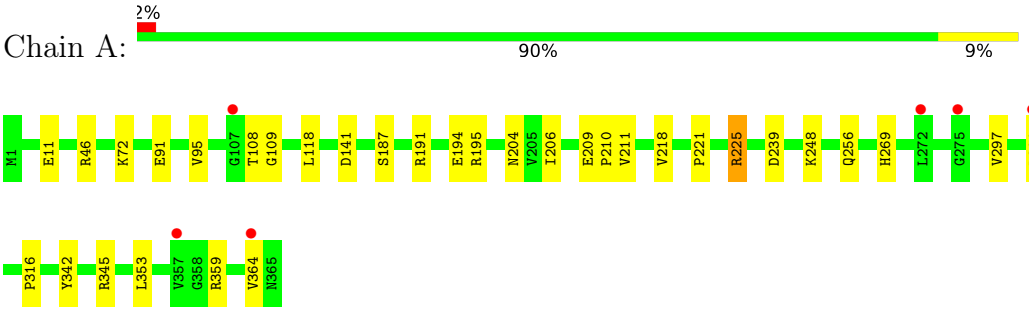
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	101	Total O 101 101	0	0
5	B	58	Total O 58 58	0	0

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.

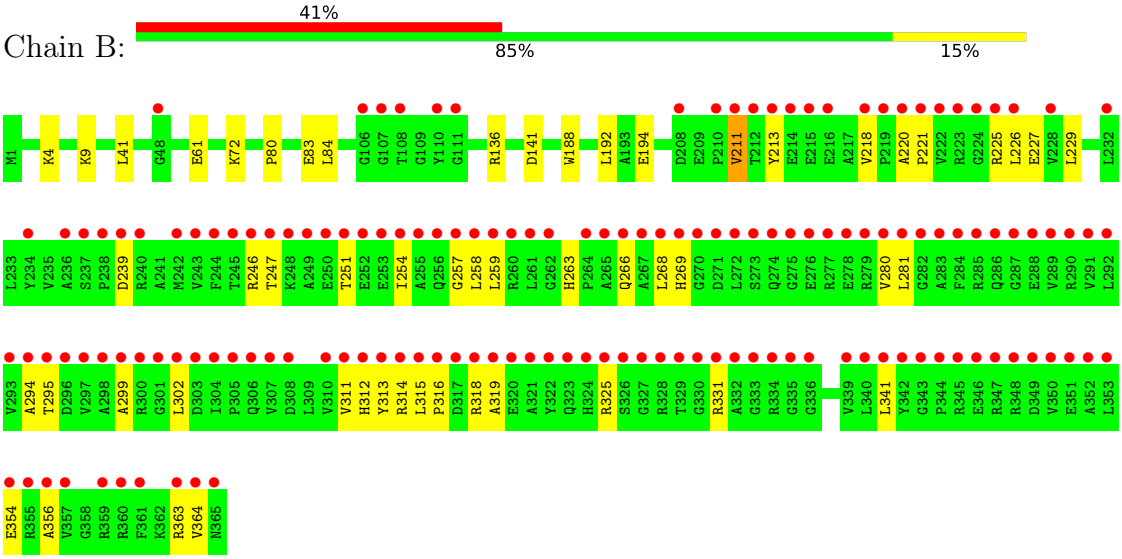
• Molecule 1: Heat resistant RNA dependent ATPase

Chain A:



• Molecule 1: Heat resistant RNA dependent ATPase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.64Å 119.64Å 107.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 1.90 48.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.88-1.90) 91.6 (48.88-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1327)	Depositor
R, R_{free}	0.190 , 0.218 0.190 , 0.216	Depositor DCC
R_{free} test set	3122 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5827	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: AMP, NA, SO4

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	0.32	0/2873	0.51	0/3892
1	B	0.28	0/2862	0.47	0/3878
All	All	0.30	0/5735	0.49	0/7770

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	A	2823	0	2914	17	1
1	B	2815	0	2902	23	1
2	A	23	0	12	0	0
3	A	2	0	0	0	0
4	B	5	0	0	0	0
5	A	101	0	0	0	0
5	B	58	0	0	0	0
All	All	5827	0	5828	40	1

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 3.

All (40) 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:258:LEU:HB3	1:B:263:HIS:HB2	1.75	0.67
1:B:319:ALA:HB2	1:B:356:ALA:HB1	1.80	0.62
1:B:266:GLN:HB3	1:B:280:VAL:HG13	1.81	0.61
1:A:46:ARG:HD3	1:A:206:ILE:HD12	1.84	0.59
1:B:313:TYR:HA	1:B:341:LEU:HD12	1.87	0.56
1:A:316:PRO:HD2	1:A:353:LEU:HD11	1.87	0.56
1:B:80:PRO:HD2	1:B:84:LEU:HD23	1.90	0.54
1:A:218:VAL:HG22	1:A:364:VAL:HG21	1.90	0.54
1:B:226:LEU:HD21	1:B:257:GLY:HA3	1.89	0.54
1:B:72:LYS:HD2	1:B:141:ASP:HB3	1.92	0.52
1:B:218:VAL:HG22	1:B:364:VAL:HG21	1.91	0.51
1:A:187:SER:OG	1:A:191:ARG:NH1	2.44	0.51
1:A:72:LYS:HD2	1:A:141:ASP:HB3	1.94	0.49
1:A:91:GLU:O	1:A:95:VAL:HG23	2.13	0.49
1:B:354:GLU:OE2	1:B:363:ARG:NH1	2.45	0.49
1:B:188:TRP:CH2	1:B:192:LEU:HD11	2.48	0.49
1:B:221:PRO:O	1:B:225:ARG:HD2	2.13	0.48
1:B:211:VAL:HB	1:B:213:TYR:CD1	2.48	0.48
1:A:221:PRO:O	1:A:225:ARG:HD3	2.14	0.48
1:B:220:ALA:HA	1:B:221:PRO:HD3	1.79	0.46
1:B:246:ARG:NH1	1:B:314:ARG:HG2	2.32	0.45
1:B:294:ALA:HB1	1:B:299:ALA:HB2	1.99	0.44
1:A:204:ASN:OD1	1:A:206:ILE:HG12	2.17	0.44
1:B:312:HIS:CE1	1:B:325:ARG:HD2	2.53	0.44
1:B:251:THR:HG21	1:B:269:HIS:HB3	1.99	0.44
1:A:46:ARG:HG2	1:A:306:GLN:NE2	2.34	0.43
1:A:211:VAL:HG21	1:A:359:ARG:CZ	2.49	0.42
1:A:248:LYS:HG3	1:A:269:HIS:CG	2.55	0.42
1:B:268:LEU:HD22	1:B:281:LEU:HD21	2.00	0.42
1:B:229:LEU:HD13	1:B:311:VAL:HG11	2.02	0.42
1:A:11:GLU:CD	1:A:11:GLU:H	2.23	0.42
1:A:194:GLU:HG2	1:A:195:ARG:HG3	2.01	0.42
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.83	0.42
1:A:108:THR:OG1	1:A:109:GLY:N	2.53	0.41
1:B:9:LYS:HG3	1:B:61:GLU:OE1	2.20	0.41
1:A:297:VAL:HA	1:A:300:ARG:NH1	2.36	0.41
1:B:254:ILE:HD11	1:B:313:TYR:CE2	2.56	0.41
1:B:315:LEU:HA	1:B:316:PRO:HD3	1.92	0.41
1:A:209:GLU:HA	1:A:210:PRO:HD3	1.96	0.40
1:B:211:VAL:HB	1:B:213:TYR:HD1	1.85	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:OH	1:B:83:GLU:OE1[6_545]	2.17	0.03

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	364/365 (100%)	357 (98%)	7 (2%)	0	100	100
1	B	363/365 (100%)	341 (94%)	22 (6%)	0	100	100
All	All	727/730 (100%)	698 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	291/290 (100%)	285 (98%)	6 (2%)	53	48
1	B	290/290 (100%)	277 (96%)	13 (4%)	27	18
All	All	581/580 (100%)	562 (97%)	19 (3%)	38	29

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	225	ARG
1	A	239	ASP
1	A	256	GLN
1	A	302	LEU
1	A	345	ARG
1	B	4	LYS
1	B	41	LEU
1	B	136	ARG
1	B	194	GLU
1	B	211	VAL
1	B	227	GLU
1	B	239	ASP
1	B	247	THR
1	B	259	LEU
1	B	295	THR
1	B	302	LEU
1	B	318	ARG
1	B	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	312	HIS

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	AMP	A	401	-	22,25,25	0.92	1 (4%)	25,38,38	1.23	3 (12%)
4	SO4	B	401	-	4,4,4	0.08	0	6,6,6	0.25	0

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	AMP	A	401	-	-	0/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AMP	C5-C4	2.54	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	AMP	N3-C2-N1	-3.23	123.63	128.68
2	A	401	AMP	C4-C5-N7	-2.16	107.15	109.40
2	A	401	AMP	O3P-P-O2P	2.12	115.72	107.64

There are no chirality outliers.

There are no torsion outliers.

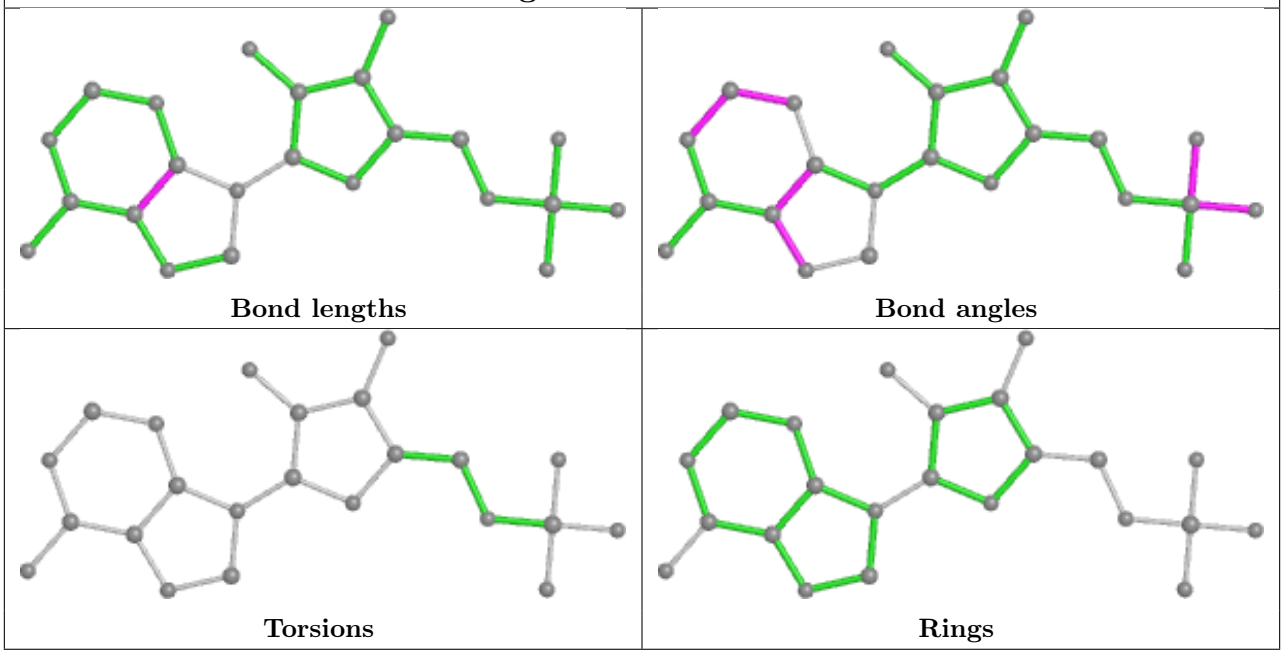
There are no ring outliers.

No monomer is involved in short contacts.

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 AMP A 401



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	365/365 (100%)	0.31	7 (1%) 66 69	25, 40, 77, 106	0
1	B	365/365 (100%)	3.16	149 (40%) 0 0	27, 62, 200, 233	0
All	All	730/730 (100%)	1.74	156 (21%) 0 0	25, 46, 181, 233	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	VAL	49.4
1	B	281	LEU	33.5
1	B	332	ALA	25.4
1	B	279	ARG	18.1
1	B	344	PRO	17.1
1	B	297	VAL	17.0
1	B	284	PHE	15.7
1	B	271	ASP	15.5
1	B	275	GLY	14.9
1	B	272	LEU	14.0
1	B	268	LEU	14.0
1	B	302	LEU	13.5
1	B	304	ILE	13.5
1	B	249	ALA	13.3
1	B	336	GLY	12.6
1	B	333	GLY	12.6
1	B	345	ARG	12.3
1	B	288	GLU	12.2
1	B	334	ARG	12.0
1	B	315	LEU	11.9
1	B	273	SER	11.9
1	B	247	THR	11.8
1	B	254	ILE	11.8
1	B	347	ARG	10.9

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Mol	Chain	Res	Type	RSRZ
1	B	270	GLY	10.7
1	B	307	VAL	10.6
1	B	299	ALA	10.4
1	B	245	THR	10.4
1	B	267	ALA	10.4
1	B	277	ARG	10.4
1	B	285	ARG	10.2
1	B	221	PRO	9.8
1	B	298	ALA	9.6
1	B	295	THR	9.5
1	B	269	HIS	9.1
1	B	365	ASN	9.0
1	B	322	TYR	8.9
1	B	327	GLY	8.8
1	B	240	ARG	8.7
1	B	348	ARG	8.6
1	B	318	ARG	8.6
1	B	289	VAL	8.5
1	B	212	THR	8.4
1	B	222	VAL	8.3
1	B	305	PRO	8.3
1	B	342	TYR	8.3
1	B	303	ASP	8.2
1	B	357	VAL	8.2
1	A	302	LEU	8.1
1	B	211	VAL	8.1
1	B	276	GLU	8.0
1	B	107	GLY	7.9
1	B	321	ALA	7.8
1	B	296	ASP	7.8
1	B	341	LEU	7.7
1	B	335	GLY	7.6
1	B	219	PRO	7.5
1	B	223	ARG	7.4
1	B	213	TYR	7.3
1	B	250	GLU	7.3
1	B	224	GLY	7.3
1	B	265	ALA	7.3
1	B	244	PHE	7.2
1	B	331	ARG	7.1
1	B	110	TYR	7.0
1	B	253	GLU	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	356	ALA	6.7
1	B	246	ARG	6.6
1	B	106	GLY	6.5
1	B	300	ARG	6.5
1	B	220	ALA	6.4
1	B	274	GLN	6.3
1	B	313	TYR	6.3
1	B	355	ARG	6.2
1	B	314	ARG	6.2
1	B	301	GLY	6.1
1	B	317	ASP	6.0
1	B	259	LEU	5.9
1	B	316	PRO	5.9
1	B	330	GLY	5.9
1	B	243	VAL	5.7
1	B	320	GLU	5.6
1	B	236	ALA	5.6
1	B	352	ALA	5.6
1	B	293	VAL	5.5
1	B	248	LYS	5.5
1	B	283	ALA	5.4
1	B	306	GLN	5.3
1	B	282	GLY	5.3
1	B	210	PRO	5.2
1	B	228	VAL	5.2
1	B	353	LEU	5.1
1	B	294	ALA	5.1
1	B	239	ASP	4.9
1	B	328	ARG	4.8
1	B	364	VAL	4.6
1	B	286	GLN	4.5
1	B	329	THR	4.4
1	B	287	GLY	4.4
1	B	226	LEU	4.3
1	B	325	ARG	4.3
1	B	323	GLN	4.2
1	B	361	PHE	4.2
1	B	238	PRO	4.1
1	B	218	VAL	4.1
1	B	214	GLU	4.1
1	B	343	GLY	4.1
1	B	340	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	258	LEU	4.0
1	B	324	HIS	4.0
1	B	308	ASP	3.9
1	B	108	THR	3.8
1	B	255	ALA	3.7
1	B	319	ALA	3.7
1	B	225	ARG	3.7
1	B	351	GLU	3.6
1	B	363	ARG	3.6
1	B	346	GLU	3.5
1	B	262	GLY	3.5
1	B	291	VAL	3.4
1	B	48	GLY	3.4
1	B	266	GLN	3.4
1	B	278	GLU	3.4
1	B	264	PRO	3.3
1	B	292	LEU	3.2
1	B	359	ARG	3.2
1	B	326	SER	3.2
1	B	260	ARG	3.1
1	B	252	GLU	3.1
1	B	216	GLU	2.8
1	A	107	GLY	2.8
1	B	354	GLU	2.8
1	B	261	LEU	2.8
1	B	360	ARG	2.8
1	B	311	VAL	2.8
1	B	215	GLU	2.8
1	B	242	MET	2.7
1	B	312	HIS	2.6
1	A	272	LEU	2.6
1	B	232	LEU	2.5
1	B	111	GLY	2.5
1	B	256	GLN	2.5
1	B	237	SER	2.4
1	B	310	VAL	2.4
1	B	251	THR	2.4
1	A	300	ARG	2.4
1	B	234	TYR	2.4
1	B	290	ARG	2.3
1	B	350	VAL	2.3
1	B	339	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	208	ASP	2.3
1	A	275	GLY	2.3
1	A	357	VAL	2.2
1	A	364	VAL	2.2
1	B	349	ASP	2.2
1	B	257	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

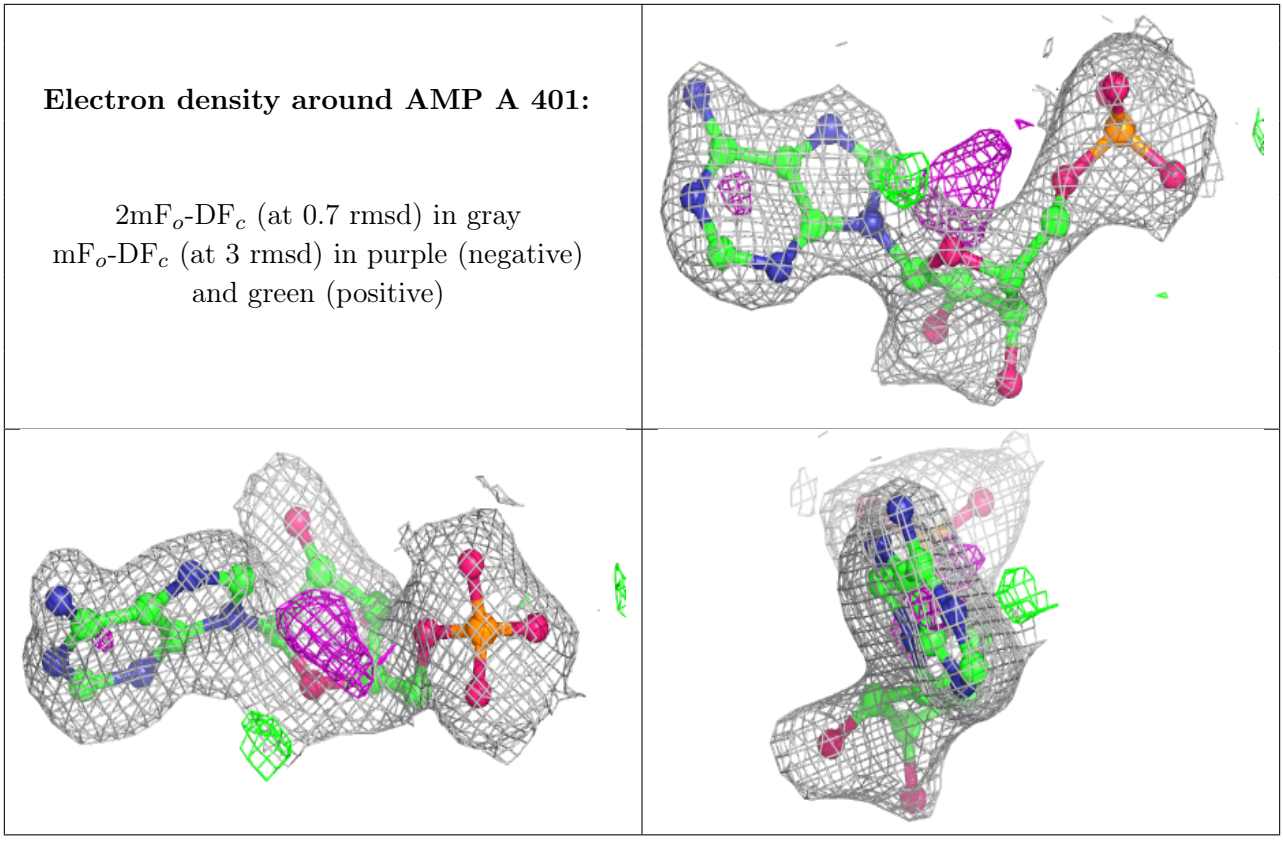
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NA	A	403	1/1	0.81	0.12	51,51,51,51	0
2	AMP	A	401	23/23	0.92	0.17	40,61,72,72	0
4	SO4	B	401	5/5	0.94	0.11	43,73,73,79	0
3	NA	A	402	1/1	0.98	0.12	31,31,31,31	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 AMP A 401:

$2mF_o$-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.