



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:14 AM UTC

PDB ID : 4KBF / pdb_00004kbf
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	:	4-5-2 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

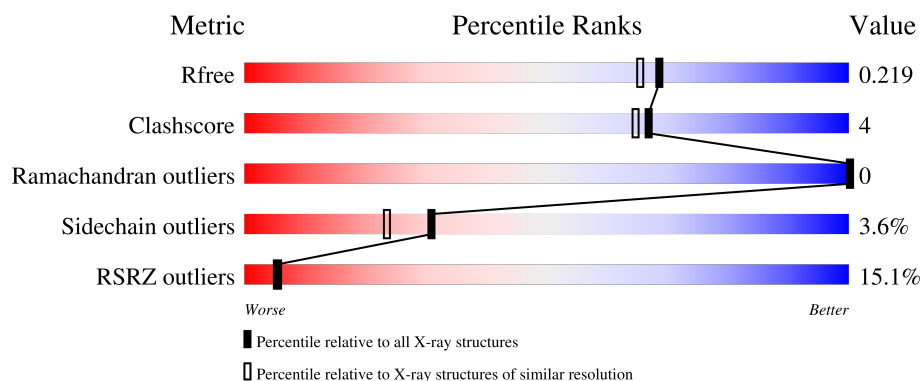
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	2% 90% 9%
1	B	365	28% 84% 15%

2 Entry composition [i](#)

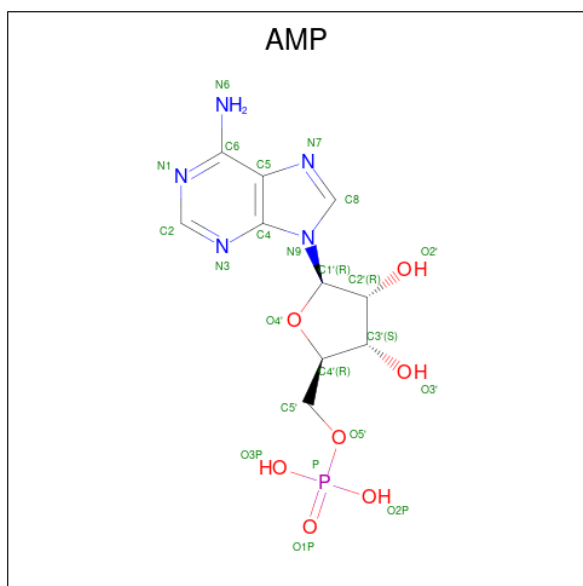
There are 5 unique types of molecules in this entry. The entry contains 5827 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: NA) (formula: Na).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

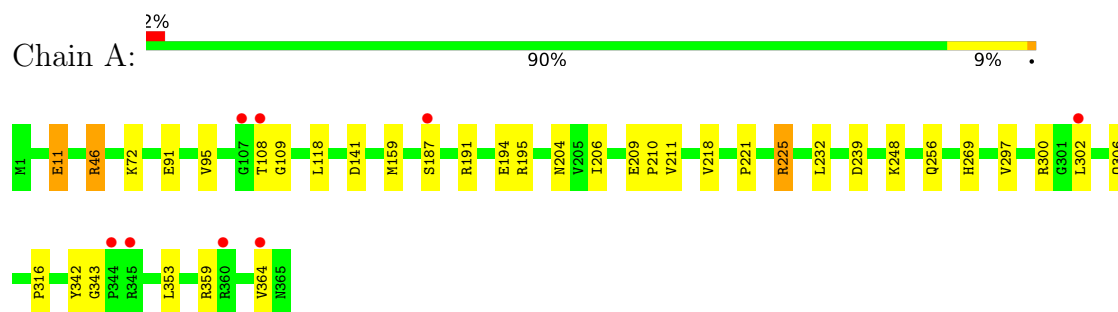
- Molecule 5 is water.

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

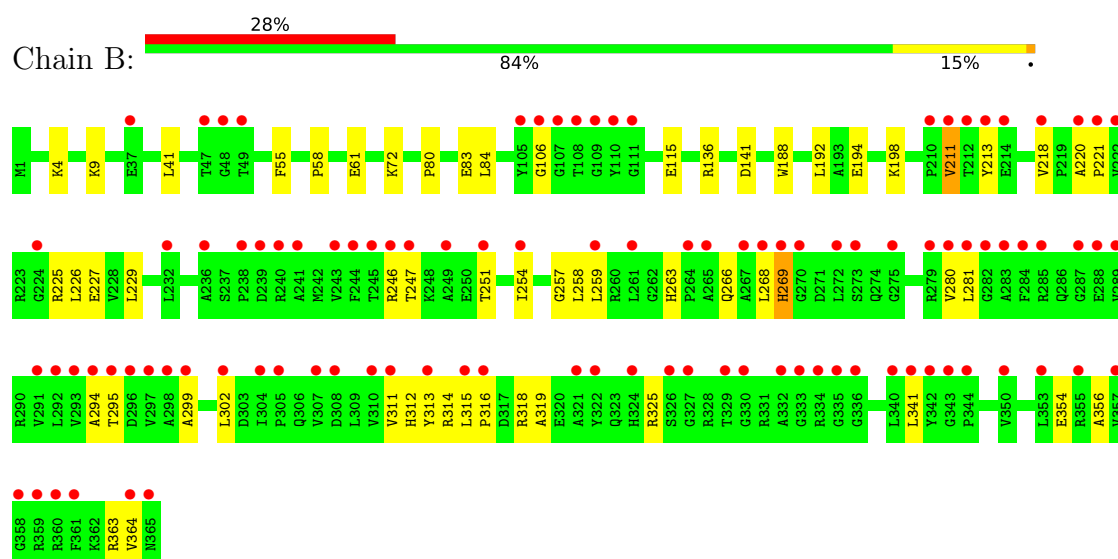
3 Residue-property plots

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: Heat resistant RNA dependent ATPase



- Molecule 1: Heat resistant RNA dependent ATPase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1327)	Depositor
R, R_{free}	0.190 , 0.218 0.192 , 0.219	Depositor DCC
R_{free} test set	3122 reflections (5.07%)	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)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: NA, AMP, 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	0.43	0/2873	0.75	2/3892 (0.1%)
1	B	0.38	0/2862	0.76	1/3878 (0.0%)
All	All	0.41	0/5735	0.76	3/7770 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	GLY	N-CA-C	6.37	120.35	112.64
1	A	343	GLY	CA-C-N	5.82	126.22	119.47
1	A	343	GLY	C-N-CA	5.82	126.22	119.47

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	A	2823	0	2914	18	1
1	B	2815	0	2902	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	58	0	0	1	0
All	All	5827	0	5828	43	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 4.

All (43) 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:A:11:GLU:CD	1:A:11:GLU:H	2.23	0.46
1:B:220:ALA:HA	1:B:221:PRO:HD3	1.79	0.46
1:B:55:PHE:C	1:B:58:PRO:HD2	2.42	0.45
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:B:198:LYS:NZ	5:B:522:HOH:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LEU:HD13	1:B:311:VAL:HG11	2.02	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:A:159:MET:HE2	1:A:159:MET:HA	2.02	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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	283 (97%)	8 (3%)	39	34
1	B	290/290 (100%)	277 (96%)	13 (4%)	24	17
All	All	581/580 (100%)	560 (96%)	21 (4%)	31	23

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	46	ARG
1	A	118	LEU
1	A	225	ARG
1	A	232	LEU
1	A	239	ASP
1	A	256	GLN
1	A	302	LEU
1	B	4	LYS
1	B	41	LEU
1	B	115	GLU
1	B	136	ARG
1	B	194	GLU
1	B	211	VAL
1	B	227	GLU
1	B	247	THR
1	B	259	LEU
1	B	269	HIS
1	B	295	THR
1	B	302	LEU
1	B	318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN

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Mol	Chain	Res	Type
1	B	256	GLN
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 oligosaccharides 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	-	25,25,25	1.42	4 (16%)	37,38,38	1.98	8 (21%)
4	SO4	B	401	-	4,4,4	0.19	0	6,6,6	0.27	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	-	-	0/10/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AMP	C5-C4	4.80	1.47	1.39
2	A	401	AMP	C5-C6	2.66	1.48	1.41
2	A	401	AMP	C5-N7	-2.32	1.34	1.39
2	A	401	AMP	C8-N7	2.26	1.36	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AMP	C5-C4-N3	-6.14	118.26	126.72
2	A	401	AMP	N3-C4-N9	5.25	136.10	127.17
2	A	401	AMP	C2-N3-C4	3.86	121.25	111.83
2	A	401	AMP	N3-C2-N1	-3.27	123.63	128.58
2	A	401	AMP	C4-C5-N7	-3.00	107.15	110.58
2	A	401	AMP	C4-N9-C8	2.85	108.73	105.74
2	A	401	AMP	C5-N7-C8	2.46	107.32	103.45
2	A	401	AMP	O3P-P-O2P	2.11	115.72	107.80

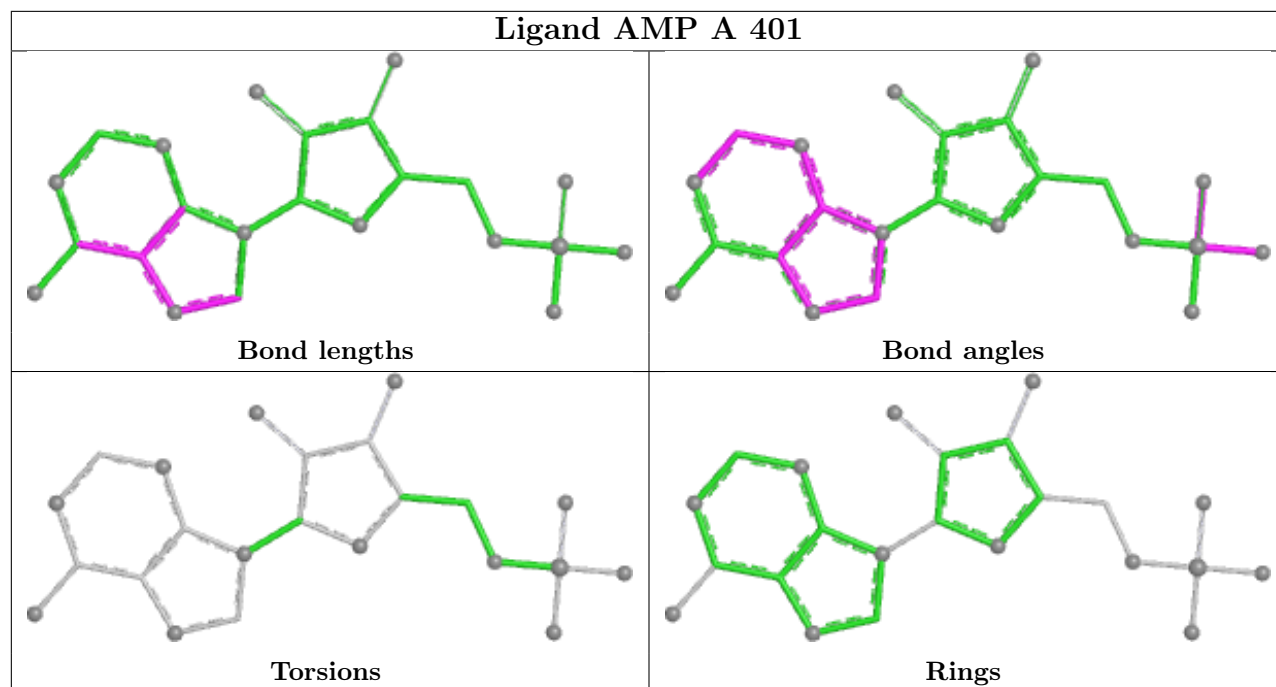
There are no chirality outliers.

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 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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/365 (100%)	0.12	8 (2%) 62 66	24, 40, 77, 106	1 (0%)
1	B	365/365 (100%)	1.06	102 (27%) 1 1	27, 62, 200, 233	0
All	All	730/730 (100%)	0.59	110 (15%) 5 5	24, 46, 181, 233	1 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	VAL	6.0
1	B	108	THR	5.9
1	B	211	VAL	5.5
1	B	109	GLY	5.3
1	A	302	LEU	5.0
1	B	284	PHE	4.9
1	B	222	VAL	4.9
1	B	267	ALA	4.9
1	B	281	LEU	4.8
1	B	297	VAL	4.7
1	B	110	TYR	4.6
1	B	265	ALA	4.3
1	B	236	ALA	4.2
1	B	106	GLY	4.2
1	B	249	ALA	4.1
1	B	268	LEU	4.1
1	B	212	THR	4.1
1	B	305	PRO	4.0
1	B	357	VAL	4.0
1	B	107	GLY	3.9
1	B	272	LEU	3.8
1	B	254	ILE	3.8
1	B	364	VAL	3.8
1	B	213	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	3.7
1	B	302	LEU	3.7
1	B	287	GLY	3.6
1	B	282	GLY	3.5
1	B	47	THR	3.5
1	B	270	GLY	3.5
1	B	49	THR	3.4
1	B	111	GLY	3.4
1	B	105	TYR	3.4
1	B	307	VAL	3.3
1	B	238	PRO	3.3
1	B	332	ALA	3.3
1	B	245	THR	3.3
1	B	247	THR	3.3
1	B	289	VAL	3.2
1	B	299	ALA	3.2
1	A	344	PRO	3.2
1	B	243	VAL	3.2
1	B	341	LEU	3.1
1	B	304	ILE	3.0
1	B	344	PRO	3.0
1	B	313	TYR	3.0
1	B	48	GLY	3.0
1	B	316	PRO	2.9
1	B	322	TYR	2.9
1	B	269	HIS	2.9
1	B	221	PRO	2.9
1	B	353	LEU	2.9
1	B	264	PRO	2.8
1	B	298	ALA	2.8
1	B	326	SER	2.7
1	B	340	LEU	2.7
1	A	364	VAL	2.7
1	B	333	GLY	2.7
1	B	324	HIS	2.7
1	B	294	ALA	2.6
1	B	291	VAL	2.6
1	B	336	GLY	2.6
1	B	330	GLY	2.5
1	B	283	ALA	2.5
1	B	244	PHE	2.5
1	B	259	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	310	VAL	2.5
1	B	275	GLY	2.4
1	B	365	ASN	2.4
1	B	360	ARG	2.4
1	B	358	GLY	2.4
1	B	329	THR	2.4
1	B	321	ALA	2.4
1	B	261	LEU	2.4
1	B	308	ASP	2.3
1	B	232	LEU	2.3
1	B	343	GLY	2.3
1	B	246	ARG	2.3
1	B	296	ASP	2.3
1	A	108	THR	2.3
1	B	342	TYR	2.3
1	B	220	ALA	2.3
1	B	292	LEU	2.3
1	B	251	THR	2.3
1	B	293	VAL	2.3
1	B	218	VAL	2.2
1	B	327	GLY	2.2
1	B	335	GLY	2.2
1	B	241	ALA	2.2
1	B	361	PHE	2.2
1	B	311	VAL	2.2
1	B	295	THR	2.2
1	B	240	ARG	2.2
1	B	37	GLU	2.1
1	B	273	SER	2.1
1	B	334	ARG	2.1
1	B	288	GLU	2.1
1	A	345	ARG	2.1
1	A	360	ARG	2.1
1	B	279	ARG	2.1
1	B	239	ASP	2.1
1	B	359	ARG	2.1
1	B	210	PRO	2.1
1	B	285	ARG	2.1
1	B	355	ARG	2.1
1	B	350	VAL	2.0
1	B	214	GLU	2.0
1	A	187	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	107	GLY	2.0
1	B	224	GLY	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](#)

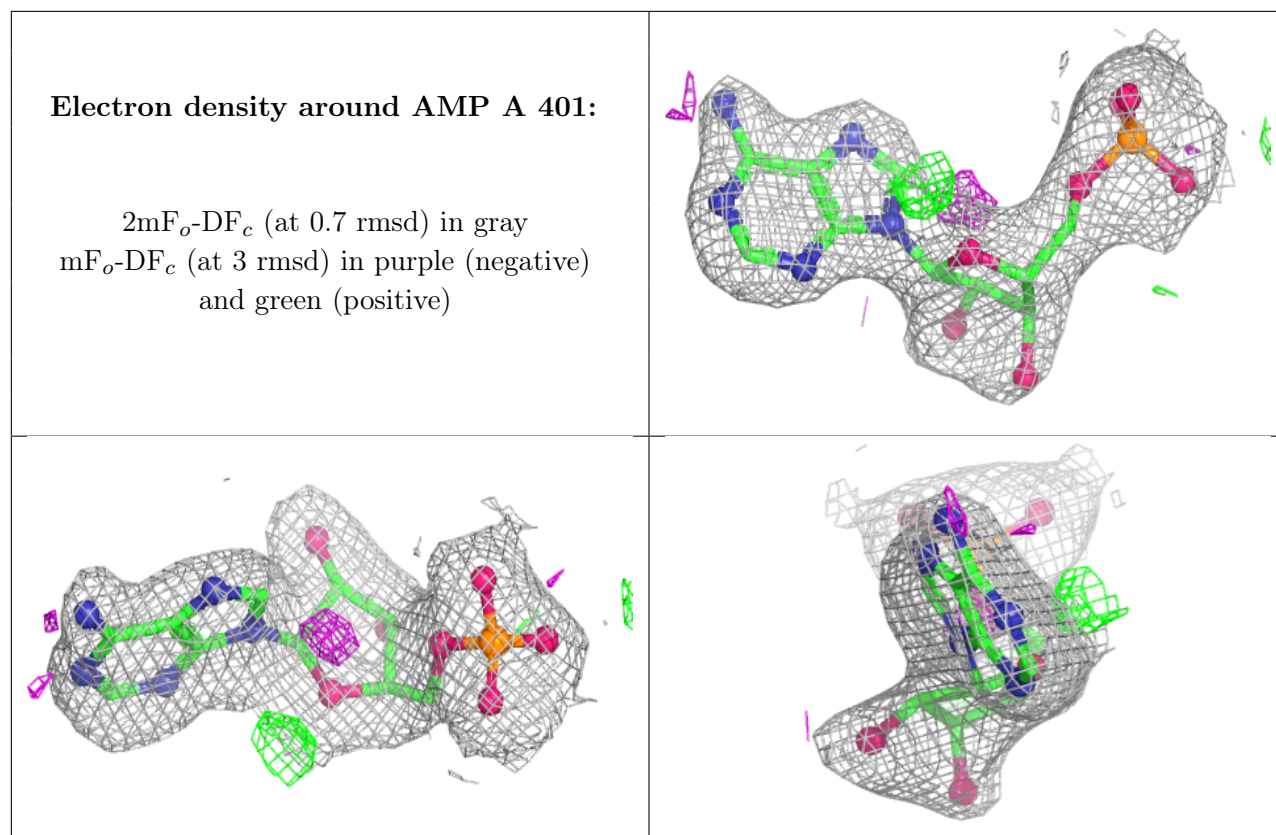
There are no oligosaccharides in this entry.

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	SO4	B	401	5/5	0.78	0.12	43,73,73,79	0
2	AMP	A	401	23/23	0.90	0.10	40,61,72,72	0
3	NA	A	403	1/1	0.93	0.10	51,51,51,51	0
3	NA	A	402	1/1	0.98	0.04	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.