



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:46 AM UTC

PDB ID : 8V5I / pdb_00008v5i
Title : Crystal structure of MAP4K4 in complex with an inhibitor
Authors : Greasley, S.E.; Diehl, W.
Deposited on : 2023-11-30
Resolution : 2.18 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

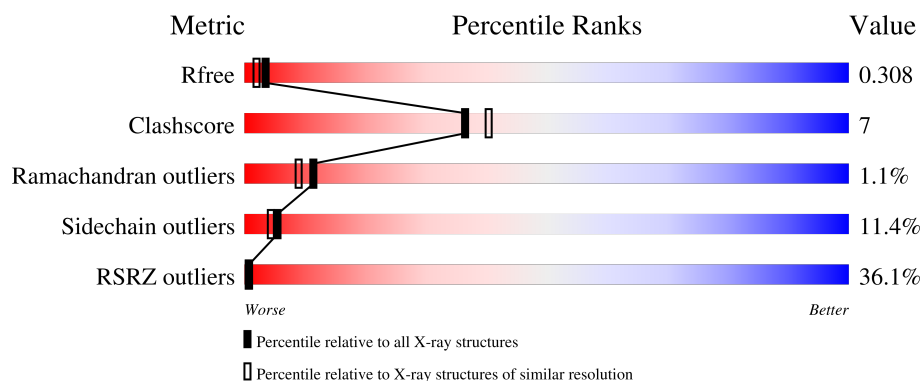
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	320	30% 64% 19% • 12%
1	B	320	34% 68% 19% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4634 atoms, of which 18 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.

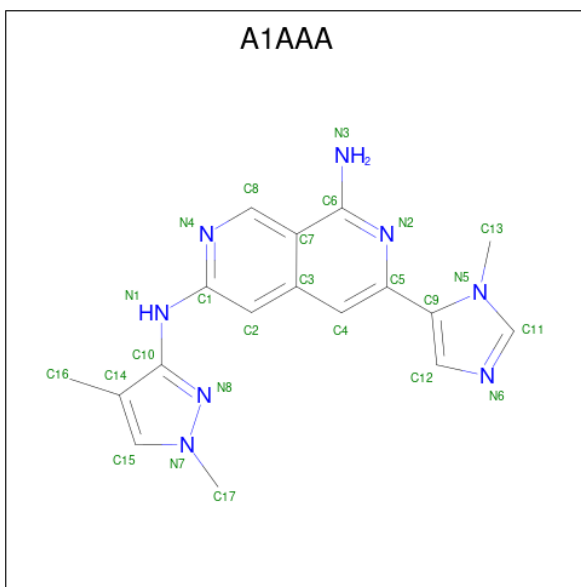
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2260	1441	394	412	13			
1	B	288	Total	C	N	O	S	0	0	0
			2331	1482	416	420	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	LEU	-	expression tag	UNP O95819
A	315	GLU	-	expression tag	UNP O95819
A	316	ASN	-	expression tag	UNP O95819
A	317	LEU	-	expression tag	UNP O95819
A	318	TYR	-	expression tag	UNP O95819
A	319	PHE	-	expression tag	UNP O95819
A	320	GLN	-	expression tag	UNP O95819
B	314	LEU	-	expression tag	UNP O95819
B	315	GLU	-	expression tag	UNP O95819
B	316	ASN	-	expression tag	UNP O95819
B	317	LEU	-	expression tag	UNP O95819
B	318	TYR	-	expression tag	UNP O95819
B	319	PHE	-	expression tag	UNP O95819
B	320	GLN	-	expression tag	UNP O95819

- Molecule 2 is (3M)-N 6 -(1,4-dimethyl-1H-pyrazol-3-yl)-3-(1-methyl-1H-imidazol-5-yl)-2,7-naphthyridine-1,6-diamine (CCD ID: A1AAA) (formula: C₁₇H₁₈N₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
2	A	1	43	17	18	8	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.27Å 93.00Å 99.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.87 – 2.18 67.87 – 2.18	Depositor EDS
% Data completeness (in resolution range)	55.7 (67.87-2.18) 55.7 (67.87-2.18)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.11.7 (29-NOV-2019)	Depositor
R, R_{free}	0.249 , 0.281 0.261 , 0.308	Depositor DCC
R_{free} test set	1038 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4634	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AAA

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	0.78	2/2311 (0.1%)	1.21	10/3122 (0.3%)
1	B	0.77	1/2386 (0.0%)	1.14	1/3225 (0.0%)
All	All	0.78	3/4697 (0.1%)	1.17	11/6347 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	MET	SD-CE	-7.96	1.59	1.79
1	B	209	THR	CA-CB	5.59	1.59	1.52
1	A	22	ALA	CA-C	5.15	1.59	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LEU	CA-C-N	6.18	129.40	120.38
1	A	233	LEU	C-N-CA	6.18	129.40	120.38
1	B	191	THR	CB-CA-C	5.98	118.00	109.08
1	A	187	THR	CB-CA-C	5.74	116.91	109.28
1	A	245	ILE	N-CA-CB	5.66	114.31	110.52
1	A	109	GLY	N-CA-C	5.46	119.29	112.73
1	A	271	VAL	CA-C-N	5.38	128.89	120.82
1	A	271	VAL	C-N-CA	5.38	128.89	120.82
1	A	211	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	232	PRO	N-CA-C	5.15	123.08	112.47
1	A	41	LYS	N-CA-C	-5.14	100.70	108.67

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	2260	0	2254	38	0
1	B	2331	0	2326	32	0
2	A	25	18	0	1	0
All	All	4616	18	4580	66	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (66) 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:177:GLN:NE2	1:B:180:ARG:HH11	1.68	0.91
1:A:56:MET:HG3	1:A:66:ILE:HD11	1.60	0.82
1:B:177:GLN:HE21	1:B:180:ARG:HH11	1.28	0.80
1:A:129:TRP:HE1	1:A:301:GLN:HE21	1.31	0.78
1:B:100:GLN:HE21	1:B:102:TRP:HE1	1.33	0.76
1:B:177:GLN:NE2	1:B:180:ARG:NH1	2.33	0.76
1:B:79:HIS:HD2	1:B:81:ASN:H	1.33	0.72
1:A:153:ASP:HB2	1:A:174:VAL:HG11	1.73	0.69
1:B:164:ASN:HA	1:B:303:LYS:HD3	1.73	0.69
1:B:79:HIS:CD2	1:B:81:ASN:H	2.12	0.67
1:A:157:GLN:NE2	1:B:184:ARG:HE	1.98	0.62
1:B:90:ILE:HD11	1:B:99:ASP:HB3	1.82	0.61
1:B:130:ILE:HG23	1:B:226:MET:HE3	1.83	0.60
1:B:151:HIS:HD2	1:B:153:ASP:H	1.49	0.60
1:A:129:TRP:CE2	1:A:302:LEU:HD23	2.36	0.60
1:A:213:ARG:HA	1:A:216:LEU:HD22	1.87	0.56
1:B:198:GLU:HB2	1:B:209:THR:HG23	1.87	0.56
1:A:129:TRP:HE1	1:A:301:GLN:NE2	2.02	0.54
1:A:70:ILE:HD11	1:A:101:LEU:HD21	1.89	0.54
1:A:143:HIS:CE1	1:A:147:HIS:CE1	2.95	0.54
1:A:132:TYR:CD1	1:A:135:ARG:NH2	2.77	0.53
1:B:142:ALA:O	1:B:146:ILE:HG12	2.08	0.53
1:A:130:ILE:HA	1:A:226:MET:CE	2.40	0.52
1:A:117:VAL:HG22	1:A:125:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:PRO:HD3	1:A:272:LYS:HB2	1.93	0.51
1:A:186:ASN:ND2	1:B:237:HIS:CD2	2.79	0.50
1:A:152:ARG:HD2	1:A:175:SER:HA	1.93	0.50
1:A:110:ALA:HB3	1:A:161:LEU:HB2	1.94	0.50
1:B:286:HIS:HD2	1:B:288:PHE:H	1.60	0.50
1:B:130:ILE:HG12	1:B:226:MET:HB3	1.94	0.50
1:B:151:HIS:O	1:B:152:ARG:HB2	2.11	0.49
1:B:177:GLN:HE22	1:B:180:ARG:NH1	2.07	0.49
1:B:73:LEU:HD11	1:B:178:LEU:HD11	1.95	0.48
1:B:128:ASP:HB2	1:B:298:VAL:HG21	1.95	0.47
1:A:186:ASN:ND2	1:B:237:HIS:HD2	2.13	0.47
1:A:216:LEU:HG	1:A:283:LEU:HD12	1.96	0.46
1:B:152:ARG:HG2	1:B:210:TYR:CD1	2.50	0.46
1:A:221:ILE:HG23	1:A:232:PRO:HD2	1.98	0.46
1:B:213:ARG:HA	1:B:216:LEU:HD22	1.98	0.45
1:A:129:TRP:CD1	1:A:298:VAL:HG13	2.52	0.45
1:A:42:GLY:HA3	1:A:53:ILE:HD12	1.98	0.45
1:A:186:ASN:HD22	1:B:237:HIS:CD2	2.36	0.44
1:A:125:LEU:HD23	1:A:226:MET:HE3	2.00	0.44
1:A:130:ILE:HA	1:A:226:MET:HE1	1.99	0.44
1:A:76:TYR:HA	1:A:78:HIS:CE1	2.53	0.44
1:B:42:GLY:HA3	1:B:53:ILE:HD13	1.99	0.44
1:B:216:LEU:HD23	1:B:278:PRO:O	2.18	0.44
1:B:54:LYS:HB2	1:B:172:PHE:CE1	2.53	0.44
1:B:118:LYS:HA	1:B:123:ASN:HD21	1.82	0.43
1:A:132:TYR:HD1	1:A:135:ARG:NH2	2.15	0.43
1:A:196:ALA:HA	1:A:217:TRP:CD1	2.53	0.42
1:A:196:ALA:HB2	1:A:217:TRP:HB3	2.01	0.42
1:A:160:LEU:HD12	1:A:170:VAL:HG11	2.01	0.42
1:A:187:THR:HG22	1:A:188:PHE:CD1	2.55	0.42
1:B:162:THR:OG1	1:B:166:GLU:HB2	2.20	0.42
1:A:130:ILE:HA	1:A:226:MET:HE2	2.02	0.41
1:A:31:VAL:CG2	2:A:401:A1AAA:C14	2.98	0.41
1:B:147:HIS:CD2	1:B:147:HIS:N	2.88	0.41
1:A:161:LEU:HA	1:A:166:GLU:O	2.21	0.41
1:B:41:LYS:HE2	1:B:50:LEU:HD22	2.02	0.41
1:A:136:GLU:HB3	1:A:167:VAL:HB	2.02	0.40
1:A:72:MET:HE2	1:A:149:VAL:HG13	2.03	0.40
1:A:237:HIS:CD2	1:A:238:PRO:HD2	2.55	0.40
1:B:19:ARG:HA	1:B:19:ARG:HD2	1.89	0.40
1:A:250:PRO:HB3	1:A:270:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TRP:CD1	1:A:221:ILE:HG22	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	A	272/320 (85%)	248 (91%)	20 (7%)	4 (2%)	8	5
1	B	284/320 (89%)	265 (93%)	17 (6%)	2 (1%)	18	17
All	All	556/640 (87%)	513 (92%)	37 (7%)	6 (1%)	11	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	LYS
1	A	209	THR
1	A	174	VAL
1	B	121	LYS
1	A	171	ASP
1	A	28	VAL

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	248/282 (88%)	223 (90%)	25 (10%)	7	6
1	B	253/282 (90%)	221 (87%)	32 (13%)	4	3
All	All	501/564 (89%)	444 (89%)	57 (11%)	5	4

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	29	GLU
1	A	56	MET
1	A	72	MET
1	A	73	LEU
1	A	98	ASP
1	A	101	LEU
1	A	103	LEU
1	A	105	MET
1	A	124	THR
1	A	125	LEU
1	A	155	LYS
1	A	157	GLN
1	A	161	LEU
1	A	186	ASN
1	A	187	THR
1	A	199	VAL
1	A	204	GLU
1	A	216	LEU
1	A	236	MET
1	A	256	LYS
1	A	280	THR
1	A	281	GLU
1	A	301	GLN
1	A	302	LEU
1	B	16	SER
1	B	19	ARG
1	B	20	ASP
1	B	24	ILE
1	B	29	GLU
1	B	45	VAL
1	B	49	GLN
1	B	57	ASP
1	B	60	GLU
1	B	68	LEU

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Mol	Chain	Res	Type
1	B	91	LYS
1	B	100	GLN
1	B	121	LYS
1	B	123	ASN
1	B	126	LYS
1	B	128	ASP
1	B	146	ILE
1	B	157	GLN
1	B	180	ARG
1	B	184	ARG
1	B	185	ARG
1	B	186	ASN
1	B	199	VAL
1	B	203	ASP
1	B	207	ASP
1	B	209	THR
1	B	233	LEU
1	B	239	MET
1	B	252	ARG
1	B	281	GLU
1	B	289	ILE
1	B	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	A	147	HIS
1	A	157	GLN
1	A	186	ASN
1	A	301	GLN
1	B	79	HIS
1	B	97	HIS
1	B	100	GLN
1	B	123	ASN
1	B	143	HIS
1	B	151	HIS
1	B	177	GLN
1	B	205	ASN
1	B	286	HIS
1	B	301	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	A1AAA	A	401	-	27,28,28	1.37	1 (3%)	30,41,41	1.62	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1AAA	A	401	-	-	2/8/8/8	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A1AAA	C6-C7	-4.63	1.40	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	A1AAA	C5-C4-C3	-4.63	118.24	119.73
2	A	401	A1AAA	C9-C5-N2	-3.94	111.20	117.12
2	A	401	A1AAA	C12-C9-N5	-2.79	103.96	105.21
2	A	401	A1AAA	C11-N5-C9	2.78	107.72	106.38
2	A	401	A1AAA	C17-N7-C15	-2.34	125.59	127.94

There are no chirality outliers.

All (2) torsion outliers are listed below:

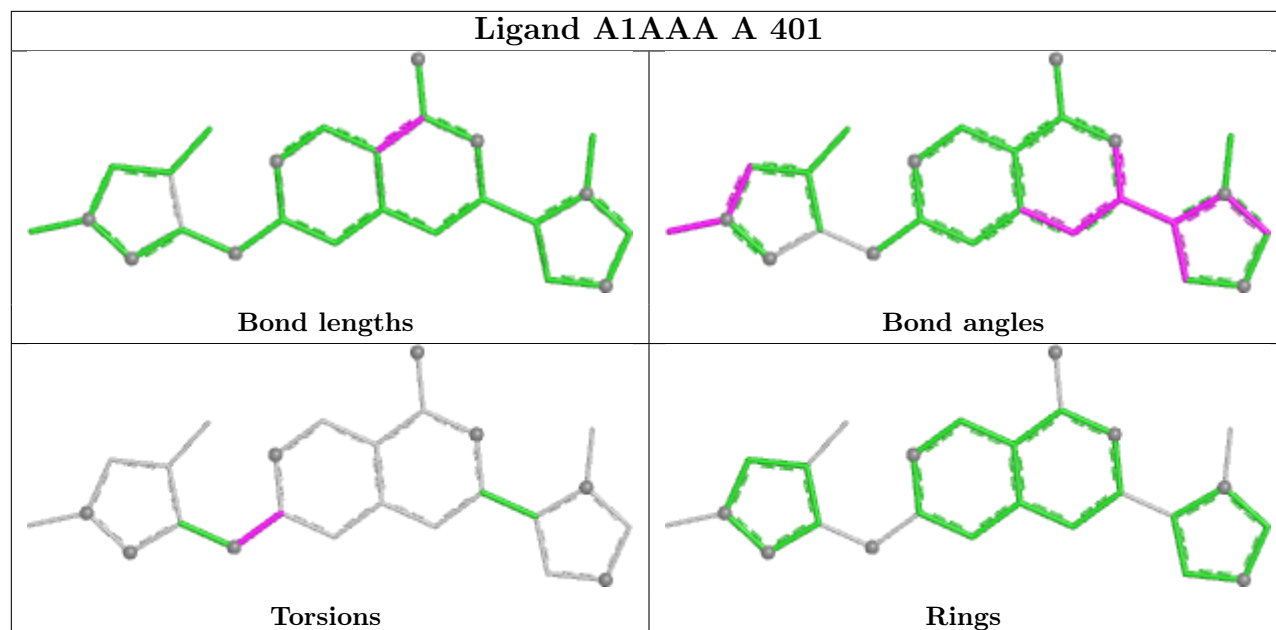
Mol	Chain	Res	Type	Atoms
2	A	401	A1AAA	C2-C1-N1-C10
2	A	401	A1AAA	N4-C1-N1-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	A1AAA	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

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	280/320 (87%)	1.82	97 (34%)  	41, 70, 107, 117	0
1	B	288/320 (90%)	1.77	108 (37%)  	42, 71, 104, 111	0
All	All	568/640 (88%)	1.79	205 (36%)  	41, 71, 105, 117	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	VAL	9.0
1	A	188	PHE	8.5
1	B	302	LEU	7.9
1	A	94	PRO	7.5
1	B	311	LYS	7.3
1	B	137	ILE	6.6
1	A	309	THR	6.5
1	A	210	TYR	6.3
1	A	50	LEU	6.1
1	A	173	GLY	6.0
1	B	165	ALA	5.8
1	B	95	PRO	5.6
1	A	161	LEU	5.2
1	A	66	ILE	5.1
1	A	171	ASP	5.0
1	A	302	LEU	5.0
1	B	177	GLN	4.9
1	B	174	VAL	4.8
1	A	109	GLY	4.7
1	B	167	VAL	4.6
1	B	66	ILE	4.6
1	B	154	ILE	4.6
1	A	93	SER	4.6
1	B	216	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	167	VAL	4.4
1	B	93	SER	4.4
1	B	133	ILE	4.4
1	B	94	PRO	4.3
1	A	157	GLN	4.3
1	A	37	GLY	4.2
1	A	186	ASN	4.2
1	A	306	ILE	4.1
1	A	174	VAL	4.1
1	A	120	THR	4.1
1	B	212	TYR	4.1
1	B	129	TRP	4.1
1	A	165	ALA	4.1
1	B	169	LEU	4.0
1	B	29	GLU	3.9
1	A	137	ILE	3.9
1	A	169	LEU	3.9
1	A	22	ALA	3.9
1	B	16	SER	3.8
1	B	182	VAL	3.8
1	B	39	VAL	3.8
1	B	45	VAL	3.8
1	A	103	LEU	3.7
1	A	163	GLU	3.7
1	B	50	LEU	3.7
1	B	180	ARG	3.7
1	A	113	ILE	3.6
1	A	129	TRP	3.6
1	B	109	GLY	3.6
1	B	209	THR	3.5
1	A	172	PHE	3.4
1	B	27	LEU	3.4
1	B	210	TYR	3.4
1	B	28	VAL	3.4
1	A	133	ILE	3.4
1	B	24	ILE	3.4
1	A	68	LEU	3.4
1	B	150	ILE	3.4
1	A	18	LEU	3.4
1	B	141	LEU	3.4
1	A	281	GLU	3.3
1	A	59	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	3.3
1	B	113	ILE	3.3
1	B	116	LEU	3.3
1	A	72	MET	3.3
1	A	110	ALA	3.2
1	A	208	ALA	3.2
1	A	107	PHE	3.1
1	B	117	VAL	3.1
1	B	298	VAL	3.1
1	A	141	LEU	3.1
1	B	91	LYS	3.0
1	A	283	LEU	3.0
1	A	146	ILE	3.0
1	A	265	PHE	3.0
1	A	121	LYS	3.0
1	B	46	LYS	3.0
1	A	73	LEU	3.0
1	B	185	ARG	3.0
1	A	124	THR	3.0
1	B	132	TYR	3.0
1	B	172	PHE	3.0
1	A	70	ILE	3.0
1	A	263	PHE	2.9
1	A	27	LEU	2.9
1	A	30	VAL	2.9
1	A	300	ILE	2.9
1	B	90	ILE	2.9
1	B	96	GLY	2.9
1	A	122	GLY	2.9
1	B	103	LEU	2.8
1	A	132	TYR	2.8
1	A	58	VAL	2.8
1	B	104	VAL	2.8
1	A	164	ASN	2.8
1	B	56	MET	2.8
1	A	116	LEU	2.8
1	B	101	LEU	2.8
1	A	104	VAL	2.8
1	A	154	ILE	2.8
1	A	289	ILE	2.8
1	B	297	GLN	2.8
1	A	98	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	308	ARG	2.7
1	B	204	GLU	2.7
1	B	23	GLY	2.7
1	B	186	ASN	2.7
1	B	110	ALA	2.7
1	B	160	LEU	2.7
1	B	143	HIS	2.7
1	B	188	PHE	2.6
1	B	125	LEU	2.6
1	B	296	ARG	2.6
1	A	117	VAL	2.6
1	A	219	CYS	2.6
1	A	232	PRO	2.6
1	B	283	LEU	2.6
1	A	48	GLY	2.6
1	B	184	ARG	2.6
1	A	175	SER	2.6
1	A	45	VAL	2.5
1	B	146	ILE	2.5
1	A	32	GLY	2.5
1	B	176	ALA	2.5
1	B	18	LEU	2.5
1	B	25	PHE	2.5
1	B	102	TRP	2.5
1	B	42	GLY	2.5
1	A	92	LYS	2.5
1	B	238	PRO	2.5
1	B	149	VAL	2.5
1	B	289	ILE	2.5
1	A	304	ASP	2.5
1	A	15	LEU	2.5
1	B	75	LYS	2.5
1	A	62	GLU	2.4
1	A	64	GLU	2.4
1	A	46	LYS	2.4
1	B	148	HIS	2.4
1	A	288	PHE	2.4
1	B	40	TYR	2.4
1	A	125	LEU	2.4
1	B	161	LEU	2.4
1	B	107	PHE	2.4
1	A	299	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	76	TYR	2.4
1	A	305	HIS	2.4
1	B	52	ALA	2.4
1	B	138	LEU	2.4
1	A	295	GLU	2.4
1	A	159	VAL	2.4
1	B	44	HIS	2.4
1	A	242	LEU	2.3
1	B	178	LEU	2.3
1	B	252	ARG	2.3
1	A	130	ILE	2.3
1	B	53	ILE	2.3
1	A	33	ASN	2.3
1	A	101	LEU	2.3
1	A	152	ARG	2.3
1	B	22	ALA	2.3
1	A	307	ASP	2.3
1	B	19	ARG	2.3
1	B	173	GLY	2.3
1	B	239	MET	2.3
1	B	157	GLN	2.3
1	A	31	VAL	2.2
1	B	43	ARG	2.2
1	B	85	TYR	2.2
1	A	151	HIS	2.2
1	A	292	GLN	2.2
1	B	299	ARG	2.2
1	B	26	GLU	2.2
1	A	293	PRO	2.2
1	B	124	THR	2.2
1	B	263	PHE	2.2
1	B	48	GLY	2.2
1	B	68	LEU	2.2
1	B	121	LYS	2.2
1	A	111	GLY	2.1
1	B	51	ALA	2.1
1	A	56	MET	2.1
1	A	63	GLU	2.1
1	A	209	THR	2.1
1	B	47	THR	2.1
1	B	120	THR	2.1
1	B	83	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	234	CYS	2.1
1	A	128	ASP	2.1
1	A	291	ASP	2.1
1	B	86	TYR	2.1
1	B	181	THR	2.1
1	B	300	ILE	2.1
1	B	269	CYS	2.0
1	B	308	ARG	2.0
1	A	67	LYS	2.0
1	B	268	GLY	2.0
1	A	301	GLN	2.0
1	B	144	LEU	2.0
1	B	97	HIS	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](#)

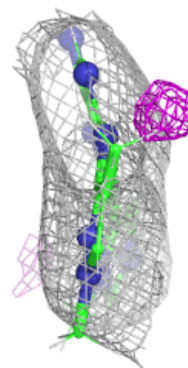
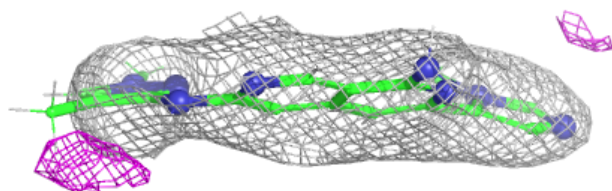
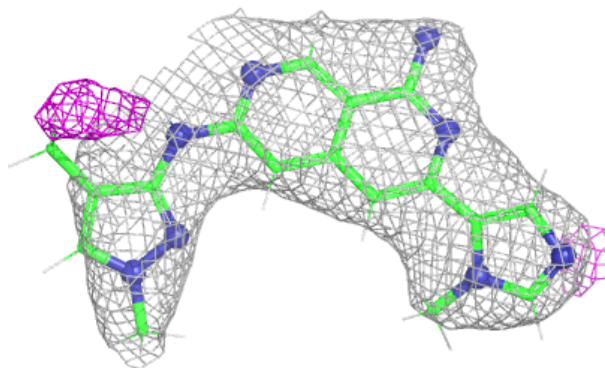
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1AAA	A	401	25/25	0.87	0.12	70,77,93,93	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 A1AAA 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.