Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID	:	8BN8 / pdb_00008bn8
Title	:	METTL3-METTL14 heterodimer bound to the SAM competitive small molecule inhibitor STM3006
Authors	:	Pilka, E.S.; Thomas, B.; Blackaby, W.; Hardick, D.; Feeney, K.; Ridgill, M.; Rotty, B.; Rausch, O.
Deposited on	:	2022-11-13
Resolution	:	2.21 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:

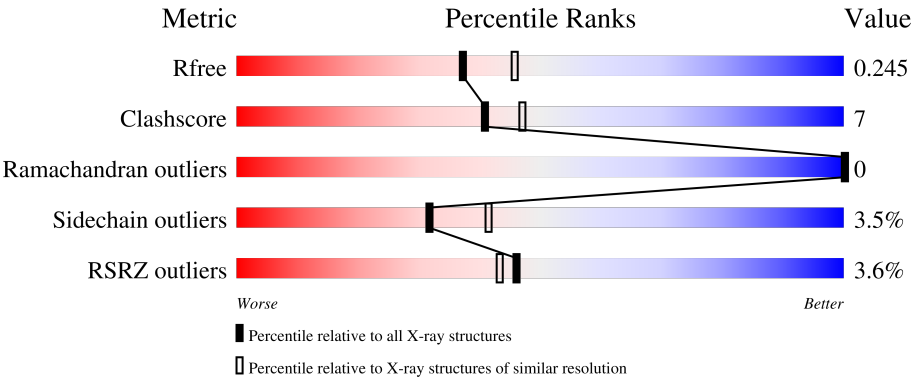
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	AAA	218	2% 75% 16% · 7%
2	BBB	291	4% 66% 15% · 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3735 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 N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	202	Total	C	N	O	S	0	1	0
			1653	1061	292	290	10			

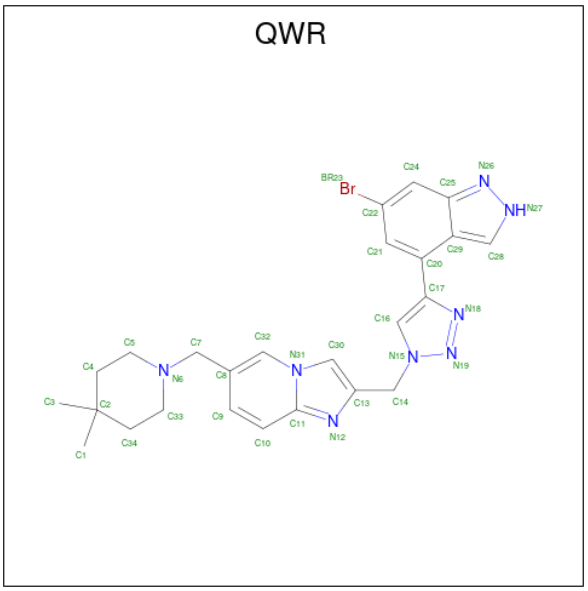
- Molecule 2 is a protein called N6-adenosine-methyltransferase non-catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	239	Total	C	N	O	S	0	1	0
			1965	1256	335	361	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	105	GLY	-	expression tag	UNP Q9HCE5
BBB	106	SER	-	expression tag	UNP Q9HCE5

- Molecule 3 is 2-[[4-(6-bromanyl-2 {H}-indazol-4-yl)-1,2,3-triazol-1-yl]methyl]-6-[(4,4-dimethylpiperidin-1-yl)methyl]imidazo[1,2-a]pyridine (CCD ID: QWR) (formula: $C_{25}H_{27}BrN_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	Br	C	N	0	0
			34	1	25	8		

- Molecule 4 is water.

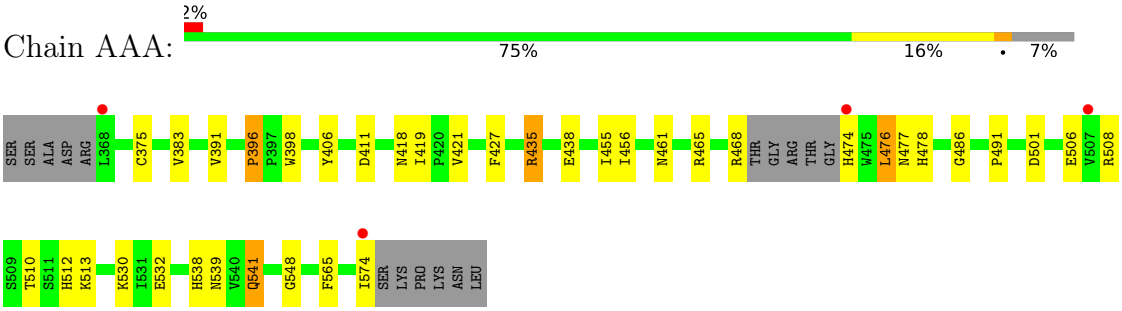
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	37	Total	O	0	0
			37	37		
4	BBB	46	Total	O	0	0
			46	46		

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.

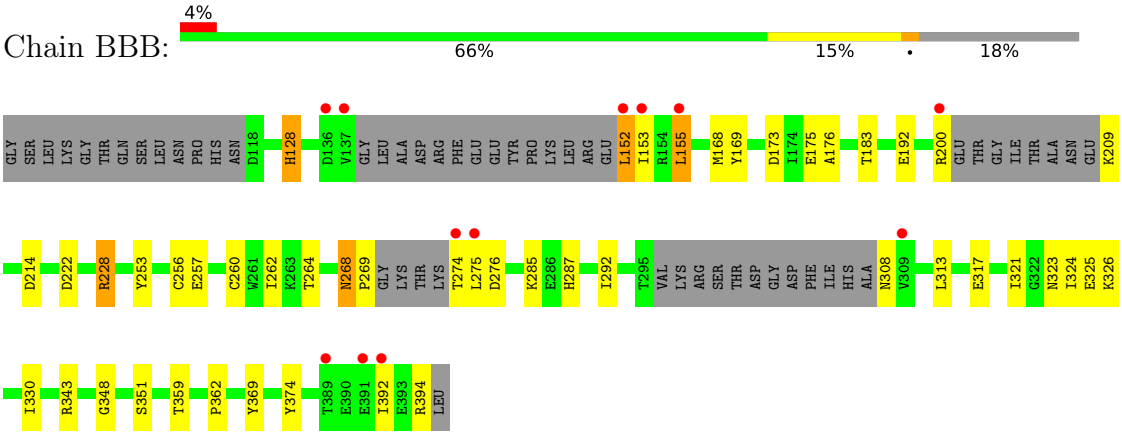
- Molecule 1: N6-adenosine-methyltransferase catalytic subunit

Chain AAA:



- Molecule 2: N6-adenosine-methyltransferase non-catalytic subunit

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	63.97Å 63.97Å 226.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.49 – 2.21 75.49 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (75.49-2.21) 99.9 (75.49-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.184 , 0.244 0.193 , 0.245	Depositor DCC
R_{free} test set	1377 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3735	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: QWR

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	AAA	1.17	2/1701 (0.1%)	1.47	13/2312 (0.6%)
2	BBB	1.18	4/2015 (0.2%)	1.49	7/2728 (0.3%)
All	All	1.17	6/3716 (0.2%)	1.48	20/5040 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	351	SER	C-O	-6.10	1.16	1.24
2	BBB	362	PRO	C-O	-6.05	1.16	1.24
2	BBB	222	ASP	C-O	-5.76	1.16	1.24
1	AAA	491	PRO	C-O	-5.24	1.17	1.23
2	BBB	128	HIS	C-O	5.18	1.30	1.24
1	AAA	438	GLU	C-O	-5.18	1.17	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	418	ASN	CA-C-N	8.14	125.37	120.24
1	AAA	418	ASN	C-N-CA	8.14	125.37	120.24
2	BBB	276	ASP	CA-CB-CG	7.00	119.60	112.60
1	AAA	501	ASP	CA-CB-CG	6.90	119.50	112.60
1	AAA	396	PRO	N-CA-CB	6.74	106.72	103.22
1	AAA	406	TYR	CA-C-N	6.60	126.37	120.10
1	AAA	406	TYR	C-N-CA	6.60	126.37	120.10
1	AAA	418	ASN	CA-CB-CG	-5.93	106.67	112.60
1	AAA	435	ARG	CG-CD-NE	-5.92	98.97	112.00
2	BBB	173	ASP	CB-CA-C	5.68	120.65	111.05
1	AAA	477	ASN	CB-CA-C	5.33	118.75	109.65
2	BBB	253	TYR	CA-C-O	-5.25	115.21	121.56
1	AAA	541	GLN	CB-CA-C	-5.20	100.44	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	214	ASP	CA-CB-CG	5.18	117.78	112.60
2	BBB	183	THR	CB-CA-C	5.17	116.89	108.87
2	BBB	343	ARG	CB-CG-CD	-5.15	99.46	111.30
1	AAA	455	ILE	CA-C-N	-5.15	115.96	123.06
1	AAA	455	ILE	C-N-CA	-5.15	115.96	123.06
1	AAA	419	ILE	CB-CA-C	-5.10	108.94	114.35
2	BBB	256	CYS	CB-CA-C	5.09	117.93	109.38

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	AAA	1653	0	1631	23	0
2	BBB	1965	0	1921	30	0
3	AAA	34	0	0	0	0
4	AAA	37	0	0	0	0
4	BBB	46	0	0	1	0
All	All	3735	0	3552	47	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 (47) 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:AAA:512:HIS:CE1	1:AAA:538[A]:HIS:CE1	2.56	0.93
1:AAA:391:VAL:HB	1:AAA:530:LYS:HG2	1.68	0.74
2:BBB:168:MET:HE3	2:BBB:369:TYR:HA	1.69	0.74
2:BBB:228:ARG:NH1	2:BBB:292:ILE:HD11	2.07	0.70
2:BBB:260[B]:CYS:SG	2:BBB:287:HIS:CE1	2.86	0.69
1:AAA:456:ILE:HD13	2:BBB:260[A]:CYS:SG	2.43	0.59
2:BBB:168:MET:CE	2:BBB:369:TYR:HD1	2.17	0.58
2:BBB:168:MET:CE	2:BBB:369:TYR:CD1	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:392:ILE:H	2:BBB:392:ILE:HD12	1.72	0.55
1:AAA:396:PRO:HG2	1:AAA:398:TRP:CE2	2.43	0.54
1:AAA:512:HIS:ND1	1:AAA:538[A]:HIS:CE1	2.75	0.53
1:AAA:411:ASP:CG	1:AAA:435:ARG:HH22	2.18	0.52
2:BBB:326:LYS:NZ	4:BBB:403:HOH:O	2.43	0.52
2:BBB:228:ARG:HH12	2:BBB:292:ILE:HD11	1.76	0.51
2:BBB:262:ILE:HD12	2:BBB:313:LEU:HD22	1.93	0.50
1:AAA:456:ILE:HD11	2:BBB:262:ILE:HD11	1.94	0.50
1:AAA:478:HIS:NE2	2:BBB:257:GLU:OE1	2.42	0.49
2:BBB:268:ASN:N	2:BBB:269:PRO:HD3	2.28	0.49
1:AAA:383:VAL:HG23	1:AAA:421:VAL:CG1	2.42	0.48
1:AAA:383:VAL:HG23	1:AAA:421:VAL:HG11	1.95	0.48
2:BBB:168:MET:HE1	2:BBB:374:TYR:HB2	1.94	0.48
1:AAA:411:ASP:OD1	1:AAA:435:ARG:NH2	2.47	0.47
2:BBB:200:ARG:HH12	2:BBB:321:ILE:HD11	1.79	0.47
2:BBB:323:ASN:OD1	2:BBB:325:GLU:HG3	2.15	0.47
2:BBB:169:TYR:HA	2:BBB:359:THR:O	2.15	0.46
2:BBB:192:GLU:O	2:BBB:192:GLU:HG2	2.15	0.45
1:AAA:456:ILE:CD1	2:BBB:260[A]:CYS:SG	3.04	0.45
1:AAA:461:ASN:OD1	1:AAA:461:ASN:C	2.61	0.44
1:AAA:474:HIS:HB3	2:BBB:308:ASN:HD21	1.82	0.44
2:BBB:152:LEU:HD12	2:BBB:155:LEU:HD23	2.00	0.44
1:AAA:456:ILE:HG23	2:BBB:285:LYS:HE2	2.00	0.43
2:BBB:175:GLU:HG2	2:BBB:176:ALA:N	2.33	0.43
2:BBB:264:THR:OG1	2:BBB:317:GLU:HA	2.18	0.43
2:BBB:128:HIS:CE1	2:BBB:269:PRO:HG3	2.54	0.43
2:BBB:200:ARG:HH12	2:BBB:321:ILE:CD1	2.32	0.43
1:AAA:513:LYS:NZ	1:AAA:532:GLU:OE2	2.45	0.43
1:AAA:539:ASN:O	1:AAA:541:GLN:HG2	2.18	0.43
1:AAA:396:PRO:HG2	1:AAA:398:TRP:CZ2	2.54	0.42
1:AAA:508:ARG:HE	1:AAA:508:ARG:HB2	1.61	0.42
2:BBB:348:GLY:HA3	2:BBB:359:THR:HG23	2.00	0.42
1:AAA:375:CYS:HA	1:AAA:548:GLY:O	2.19	0.42
1:AAA:476:LEU:HD12	1:AAA:476:LEU:HA	1.93	0.41
1:AAA:427:PHE:HA	1:AAA:486:GLY:O	2.21	0.41
1:AAA:565:PHE:HE2	1:AAA:574:ILE:HD11	1.84	0.41
2:BBB:153:ILE:HD12	2:BBB:153:ILE:O	2.21	0.41
2:BBB:330:ILE:HD12	2:BBB:330:ILE:HA	1.93	0.40
2:BBB:260[A]:CYS:SG	2:BBB:285:LYS:HD2	2.61	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	AAA	199/218 (91%)	196 (98%)	3 (2%)	0	100	100
2	BBB	230/291 (79%)	220 (96%)	10 (4%)	0	100	100
All	All	429/509 (84%)	416 (97%)	13 (3%)	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	AAA	181/193 (94%)	176 (97%)	5 (3%)	38	50
2	BBB	217/259 (84%)	208 (96%)	9 (4%)	27	35
All	All	398/452 (88%)	384 (96%)	14 (4%)	32	41

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	465	ARG
1	AAA	468	ARG
1	AAA	476	LEU
1	AAA	506	GLU
1	AAA	510	THR
2	BBB	152	LEU
2	BBB	155	LEU
2	BBB	209	LYS

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Mol	Chain	Res	Type
2	BBB	228	ARG
2	BBB	268	ASN
2	BBB	274	THR
2	BBB	275	LEU
2	BBB	324	ILE
2	BBB	394	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
3	QWR	AAA	601	-	38,39,39	1.50	6 (15%)	42,58,58	2.89	18 (42%)

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	QWR	AAA	601	-	-	3/12/24/24	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AAA	601	QWR	C14-C13	-4.30	1.44	1.50
3	AAA	601	QWR	C5-N6	3.00	1.55	1.46
3	AAA	601	QWR	C20-C29	-2.71	1.40	1.44
3	AAA	601	QWR	BR23-C22	2.63	1.95	1.90
3	AAA	601	QWR	C24-C25	-2.28	1.38	1.40
3	AAA	601	QWR	C25-N26	2.05	1.35	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	601	QWR	C22-C24-C25	-6.72	112.04	118.67
3	AAA	601	QWR	C29-C28-N27	6.66	113.80	107.05
3	AAA	601	QWR	C28-N27-N26	-6.32	102.92	112.59
3	AAA	601	QWR	C1-C2-C4	-5.93	101.49	110.04
3	AAA	601	QWR	C34-C2-C4	4.56	114.60	108.67
3	AAA	601	QWR	N31-C11-N12	4.47	113.08	110.64
3	AAA	601	QWR	C25-N26-N27	4.02	113.80	105.24
3	AAA	601	QWR	C21-C20-C17	4.01	124.78	117.64
3	AAA	601	QWR	C3-C2-C34	-3.98	104.31	110.04
3	AAA	601	QWR	C21-C20-C29	-3.51	114.28	119.55
3	AAA	601	QWR	C17-C16-N15	-2.76	103.06	105.28
3	AAA	601	QWR	C30-N31-C11	-2.69	105.38	106.90
3	AAA	601	QWR	C34-C33-N6	2.59	113.80	111.16
3	AAA	601	QWR	C7-C8-C32	2.46	124.95	121.10
3	AAA	601	QWR	C30-C13-N12	2.32	112.63	110.65
3	AAA	601	QWR	C3-C2-C4	2.31	113.37	110.04
3	AAA	601	QWR	C20-C21-C22	2.19	122.26	118.83
3	AAA	601	QWR	C4-C5-N6	2.16	113.36	111.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	601	QWR	N6-C7-C8-C32

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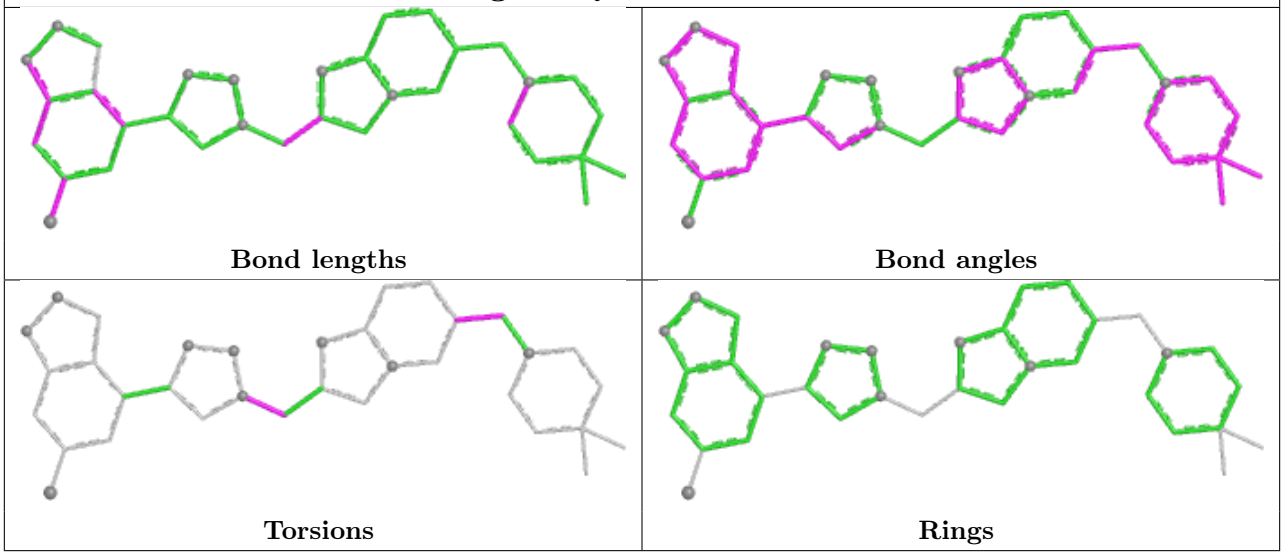
Mol	Chain	Res	Type	Atoms
3	AAA	601	QWR	C13-C14-N15-C16
3	AAA	601	QWR	C13-C14-N15-N19

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 QWR AAA 601



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	AAA	202/218 (92%)	-0.11	4 (1%)	65	63	29, 45, 81, 101	1 (0%)
2	BBB	239/291 (82%)	0.05	12 (5%)	34	31	23, 44, 94, 114	1 (0%)
All	All	441/509 (86%)	-0.02	16 (3%)	46	43	23, 44, 87, 114	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	152	LEU	4.6
1	AAA	368	LEU	3.6
2	BBB	155	LEU	3.3
2	BBB	275	LEU	3.2
2	BBB	153	ILE	3.2
2	BBB	392	ILE	2.7
2	BBB	274	THR	2.5
1	AAA	574	ILE	2.5
2	BBB	391	GLU	2.4
2	BBB	137	VAL	2.4
1	AAA	474	HIS	2.3
1	AAA	507	VAL	2.3
2	BBB	309	VAL	2.2
2	BBB	200	ARG	2.2
2	BBB	136	ASP	2.1
2	BBB	389	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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)

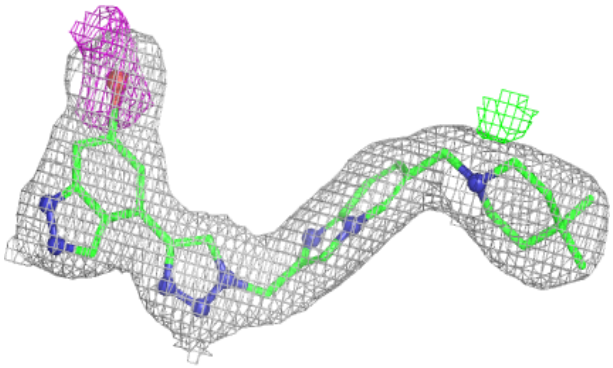
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

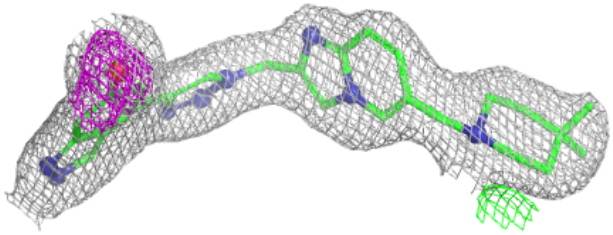
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QWR	AAA	601	34/34	0.95	0.09	36,43,53,63	0

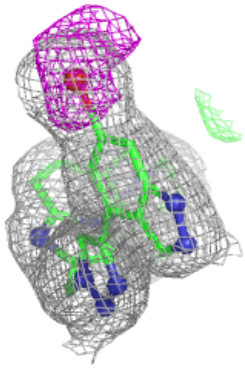
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QWR AAA 601:

$2mF_o$-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.