



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2021 – 12:08 PM JST

PDB ID : 7DPE
Title : RNA methyltransferase METTL4
Authors : Luo, Q.; Ma, J.B.
Deposited on : 2020-12-18
Resolution : 2.75 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 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 : 2.24
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) : 2.24

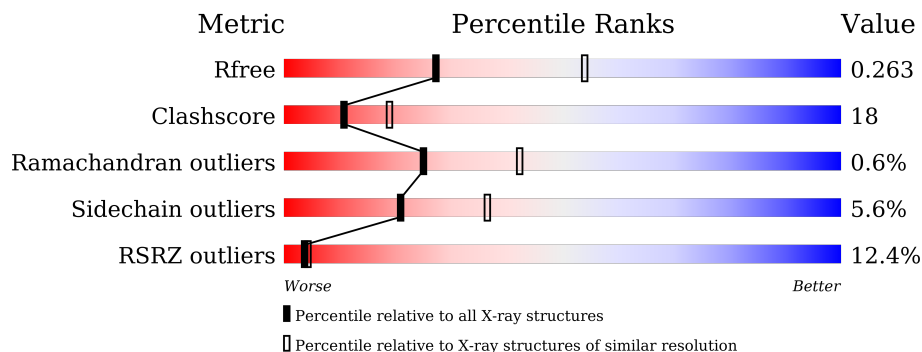
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	18	
2	A	414	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3246 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.

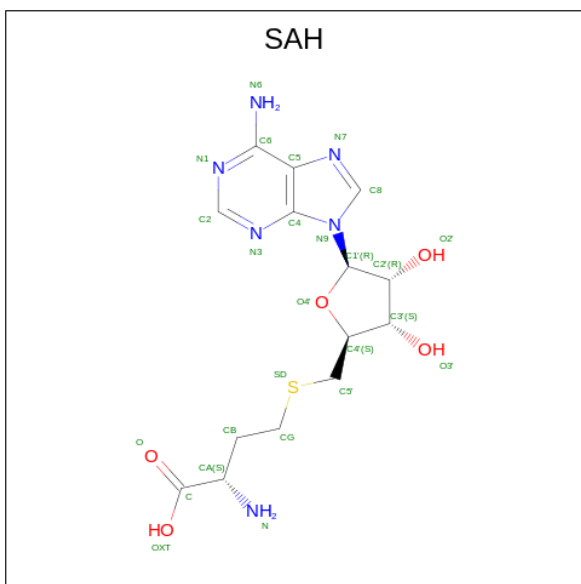
- Molecule 1 is a DNA chain called DNA (5'-D(*GP*CP*CP*GP*CP*GP*TP*GP*AP*TP*CP*AP*CP*GP*CP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	18	Total 365	C 173	N 70	O 105	P 17	0	0	0

- Molecule 2 is a protein called Methyltransferase-like protein 2.

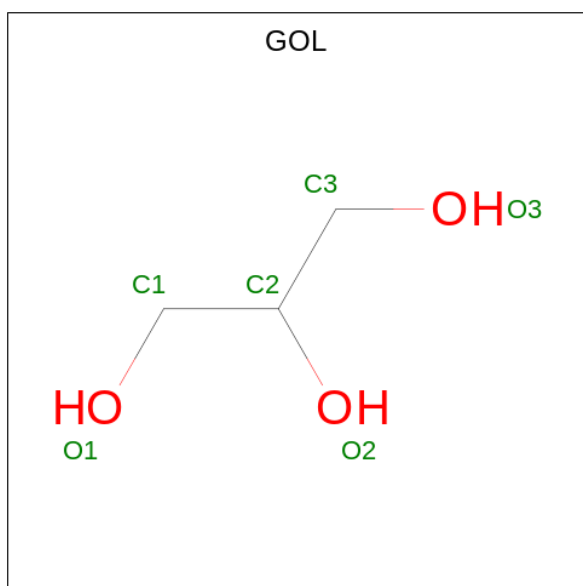
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	336	Total 2789	C 1810	N 467	O 503	S 9	0	1	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

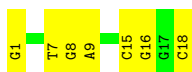
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	10	Total O 10 10	0	0
5	A	32	Total O 32 32	0	0

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.

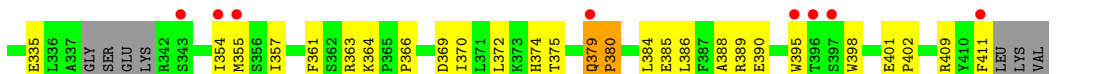
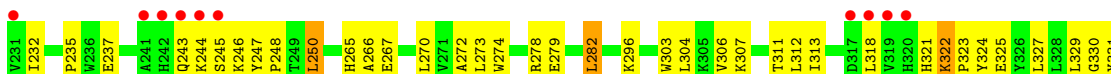
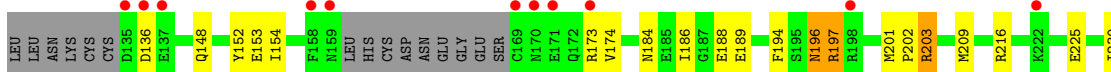
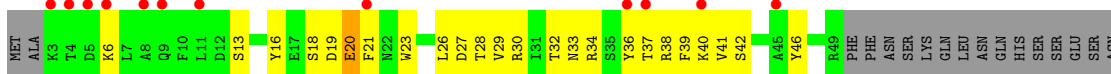
- Molecule 1: DNA (5'-D(*GP*CP*CP*GP*CP*GP*TP*GP*AP*TP*CP*AP*CP*GP*CP*GP*GP*C)-3')

Chain B:  61% 39%



- Molecule 2: Methyltransferase-like protein 2

Chain A:  11% 52% 27% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.66Å 93.49Å 70.89Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	29.32 – 2.75 29.32 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.32-2.75) 99.3 (29.32-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.76Å)	Xtrriage
Refinement program	REFMAC v1.0	Depositor
R, R_{free}	0.210 , 0.262 0.215 , 0.263	Depositor DCC
R_{free} test set	759 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: SAH, GOL

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	0.60	0/409	0.91	0/630
2	A	0.35	0/2868	0.55	2/3884 (0.1%)
All	All	0.39	0/3277	0.61	2/4514 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	374	HIS	C-N-CA	-5.49	107.99	121.70
2	A	380	PRO	N-CA-C	-5.41	98.04	112.10

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	365	0	199	4	1
2	A	2789	0	2715	109	0
3	A	26	0	19	5	0
4	A	24	0	32	6	0
5	A	32	0	0	0	0
5	B	10	0	0	0	0
All	All	3246	0	2965	113	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 18.

All (113) 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)
2:A:379:GLN:CB	2:A:380:PRO:HD2	1.38	1.44
2:A:379:GLN:HB3	2:A:380:PRO:CD	1.22	1.43
2:A:322:LYS:NZ	2:A:324:TYR:O	1.66	1.28
2:A:379:GLN:HB3	2:A:380:PRO:HD3	1.33	1.07
2:A:196:ASN:HD22	2:A:196:ASN:H	1.07	1.00
2:A:379:GLN:HB2	2:A:380:PRO:HD2	1.52	0.89
2:A:379:GLN:CB	2:A:380:PRO:CD	2.05	0.88
2:A:197:ARG:HH22	2:A:409:ARG:HD3	1.42	0.84
2:A:32:THR:HG22	2:A:36:TYR:HE2	1.43	0.82
2:A:322:LYS:HZ3	2:A:324:TYR:C	1.85	0.79
2:A:196:ASN:H	2:A:196:ASN:ND2	1.83	0.76
2:A:33:ASN:HA	2:A:36:TYR:HD2	1.51	0.76
2:A:209:MET:HE2	2:A:401:GLU:HA	1.71	0.71
2:A:6:LYS:NZ	2:A:19:ASP:OD2	2.24	0.71
2:A:379:GLN:HB3	2:A:380:PRO:HD2	0.72	0.70
2:A:29:VAL:O	2:A:33:ASN:ND2	2.25	0.69
1:B:8:DG:H2'	1:B:9:DA:C8	2.28	0.69
2:A:27:ASP:OD2	2:A:30:ARG:NE	2.25	0.69
2:A:26:LEU:HD21	2:A:370:ILE:HD11	1.77	0.67
2:A:237:GLU:O	2:A:278:ARG:NH2	2.28	0.67
2:A:209:MET:HG3	2:A:402:PRO:HD2	1.77	0.66
2:A:389:ARG:HG3	3:A:501:SAH:HB1	1.77	0.65
2:A:265:HIS:CD2	2:A:267:GLU:H	2.14	0.65
2:A:246:LYS:HG3	4:A:505:GOL:H2	1.78	0.65
2:A:186:ILE:HD12	2:A:188:GLU:H	1.62	0.64
2:A:244:LYS:N	2:A:244:LYS:HD2	2.13	0.64
2:A:265:HIS:HD2	2:A:267:GLU:H	1.44	0.64
2:A:364:LYS:HB2	4:A:503:GOL:H12	1.80	0.63
2:A:270:LEU:HD23	2:A:375:THR:HG22	1.84	0.59
2:A:13:SER:O	2:A:34:ARG:NH2	2.36	0.59
2:A:34:ARG:O	2:A:203[A]:ARG:NH1	2.28	0.58
2:A:307:LYS:HE3	2:A:313:ILE:HA	1.84	0.58
2:A:33:ASN:HA	2:A:36:TYR:CD2	2.37	0.56
2:A:154:ILE:CD1	2:A:194:PHE:HB2	2.35	0.56
2:A:385:GLU:HG2	2:A:388:ALA:HB2	1.88	0.55
2:A:108:GLU:HA	2:A:111:LEU:HD13	1.88	0.55
2:A:93:GLU:OE1	2:A:94:ALA:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:197:ARG:HH22	2:A:409:ARG:CD	2.17	0.54
2:A:184:ASN:ND2	2:A:202:PRO:O	2.40	0.54
2:A:153:GLU:HB3	2:A:174:VAL:HG22	1.89	0.54
2:A:232:ILE:HB	2:A:273:LEU:HD12	1.90	0.54
2:A:335:GLU:N	2:A:335:GLU:OE1	2.41	0.54
2:A:366:PRO:HB3	4:A:502:GOL:H32	1.90	0.53
2:A:90:ARG:HG2	2:A:93:GLU:OE1	2.09	0.53
2:A:318:LEU:HD11	2:A:321:HIS:O	2.09	0.53
2:A:6:LYS:HD3	2:A:16:TYR:HE1	1.73	0.52
2:A:244:LYS:N	2:A:244:LYS:CD	2.72	0.52
2:A:322:LYS:CE	2:A:324:TYR:O	2.56	0.52
2:A:244:LYS:HG2	2:A:361:PHE:CD2	2.45	0.51
2:A:307:LYS:HD2	2:A:311:THR:HG23	1.93	0.50
2:A:363:ARG:HH21	2:A:390:GLU:CD	2.15	0.50
2:A:96:LEU:O	2:A:100:LYS:HE2	2.11	0.50
2:A:196:ASN:HD22	2:A:196:ASN:N	1.90	0.49
2:A:322:LYS:CD	2:A:324:TYR:O	2.60	0.49
2:A:386:LEU:HD23	2:A:398:TRP:HB3	1.93	0.49
2:A:106:LEU:HD23	2:A:109:ILE:HG21	1.95	0.49
2:A:20:GLU:OE1	2:A:21:PHE:CD1	2.65	0.49
2:A:246:LYS:O	2:A:246:LYS:HD2	2.12	0.49
2:A:106:LEU:HA	2:A:109:ILE:HG12	1.95	0.48
2:A:329:LEU:HD22	2:A:329:LEU:N	2.29	0.48
2:A:41:VAL:HA	2:A:411:PHE:HB3	1.96	0.48
2:A:152:TYR:HB3	2:A:194:PHE:HE1	1.78	0.47
2:A:265:HIS:CD2	2:A:266:ALA:N	2.82	0.47
2:A:154:ILE:O	2:A:174:VAL:HA	2.15	0.47
2:A:306:VAL:HG12	2:A:312:LEU:HD12	1.96	0.47
2:A:322:LYS:HD2	2:A:322:LYS:C	2.35	0.47
2:A:322:LYS:HD2	2:A:324:TYR:H	1.81	0.46
2:A:304:LEU:O	2:A:355:MET:HA	2.15	0.46
2:A:154:ILE:HD12	2:A:194:PHE:HB2	1.97	0.46
2:A:272:ALA:HB1	2:A:327:LEU:HD11	1.97	0.46
2:A:38:ARG:HG2	2:A:39:PHE:CD1	2.51	0.46
2:A:28:THR:HG21	2:A:46:TYR:OH	2.15	0.46
2:A:250:LEU:HD21	3:A:501:SAH:N6	2.31	0.46
2:A:108:GLU:HB3	2:A:111:LEU:HB2	1.97	0.45
2:A:20:GLU:OE1	2:A:21:PHE:CG	2.69	0.45
2:A:27:ASP:OD2	2:A:30:ARG:HB2	2.17	0.45
2:A:273:LEU:C	2:A:327:LEU:HD12	2.37	0.45
2:A:401:GLU:OE2	4:A:505:GOL:H32	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:154:ILE:HD13	2:A:194:PHE:HB2	1.98	0.44
2:A:385:GLU:OE2	4:A:503:GOL:H2	2.17	0.44
2:A:38:ARG:HG2	2:A:39:PHE:CE1	2.53	0.44
2:A:270:LEU:HD12	2:A:330:GLY:O	2.18	0.44
2:A:153:GLU:HB3	2:A:174:VAL:CG2	2.47	0.43
2:A:107:LYS:NZ	2:A:108:GLU:OE1	2.48	0.43
2:A:230:ILE:HA	2:A:384:LEU:O	2.19	0.43
2:A:235:PRO:HG3	3:A:501:SAH:C8	2.48	0.43
2:A:209:MET:CE	2:A:401:GLU:HA	2.44	0.43
2:A:279:GLU:HA	2:A:282:LEU:HB2	2.01	0.43
2:A:395:TRP:CE2	4:A:502:GOL:H2	2.53	0.43
2:A:322:LYS:NZ	2:A:325:GLU:HG2	2.34	0.43
2:A:18:SER:HB3	2:A:23:TRP:O	2.19	0.42
2:A:369:ASP:HA	2:A:372:LEU:HD12	2.01	0.42
1:B:7:DT:H2'	1:B:8:DG:C8	2.54	0.42
2:A:94:ALA:O	2:A:97:PHE:N	2.51	0.42
2:A:94:ALA:O	2:A:98:LEU:HD12	2.18	0.42
2:A:248:PRO:O	3:A:501:SAH:H8	2.19	0.42
2:A:265:HIS:HD2	2:A:266:ALA:N	2.17	0.42
2:A:184:ASN:HB2	2:A:201:MET:HE2	2.01	0.42
1:B:15:DC:H2''	1:B:16:DG:C8	2.54	0.42
2:A:243:GLN:N	2:A:243:GLN:CD	2.72	0.42
2:A:303:TRP:HA	2:A:354:ILE:HG12	2.01	0.42
2:A:386:LEU:CD2	2:A:398:TRP:HB3	2.49	0.42
2:A:306:VAL:HG23	2:A:357:ILE:HD13	2.03	0.41
2:A:197:ARG:NH2	2:A:409:ARG:HD3	2.23	0.41
2:A:274:TRP:CZ2	2:A:364:LYS:HB3	2.56	0.41
2:A:247:TYR:HB2	3:A:501:SAH:H2'	2.03	0.41
2:A:136:ASP:OD1	2:A:136:ASP:N	2.43	0.41
2:A:37:THR:N	2:A:189:GLU:OE1	2.54	0.40
2:A:96:LEU:O	2:A:100:LYS:HG3	2.22	0.40
2:A:225:GLU:HB2	2:A:265:HIS:CE1	2.56	0.40
2:A:311:THR:OG1	2:A:312:LEU:N	2.54	0.40
1:B:7:DT:H2'	1:B:8:DG:O4'	2.21	0.40
2:A:98:LEU:HD23	2:A:304:LEU:HD13	2.03	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:B:1:DG:N2	1:B:18:DC:O2[2_558]	2.08	0.12

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	
2	A	327/414 (79%)	310 (95%)	15 (5%)	2 (1%)	25	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	379	GLN
2	A	323	PRO

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	
2	A	303/374 (81%)	285 (94%)	18 (6%)	19	34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	20	GLU
2	A	40	LYS
2	A	42	SER
2	A	93	GLU
2	A	97	PHE
2	A	148	GLN
2	A	173	ARG
2	A	196	ASN
2	A	197	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	203[A]	ARG
2	A	203[B]	ARG
2	A	216	ARG
2	A	245	SER
2	A	250	LEU
2	A	282	LEU
2	A	296	LYS
2	A	322	LYS
2	A	331	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	196	ASN
2	A	243	GLN
2	A	265	HIS
2	A	404	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](#)

5 ligands are 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	$\# Z > 2$
4	GOL	A	505	-	5,5,5	0.85	0	5,5,5	1.37	1 (20%)
4	GOL	A	502	-	5,5,5	0.89	0	5,5,5	1.02	0
4	GOL	A	504	-	5,5,5	0.88	0	5,5,5	0.98	0
3	SAH	A	501	-	21,28,28	1.22	2 (9%)	20,40,40	1.71	2 (10%)
4	GOL	A	503	-	5,5,5	0.88	0	5,5,5	0.92	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
4	GOL	A	505	-	-	4/4/4/4	-
4	GOL	A	502	-	-	2/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
3	SAH	A	501	-	-	3/7/31/31	0/3/3/3
4	GOL	A	503	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	SAH	C2-N3	4.01	1.38	1.32
3	A	501	SAH	C2-N1	2.56	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	SAH	N3-C2-N1	-5.57	119.97	128.68
3	A	501	SAH	C5'-SD-CG	-2.91	93.54	102.27
4	A	505	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	SAH	N-CA-CB-CG
3	A	501	SAH	C-CA-CB-CG

Continued on next page...

Continued from previous page...

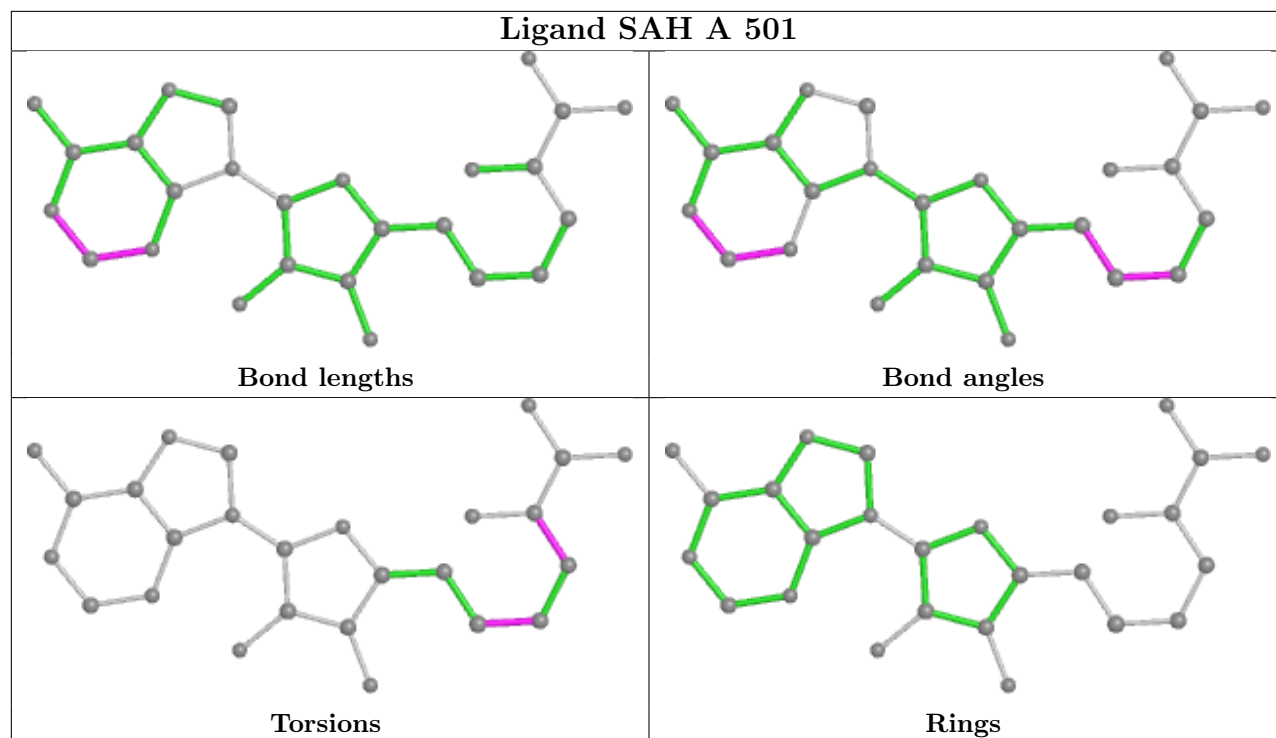
Mol	Chain	Res	Type	Atoms
4	A	502	GOL	C1-C2-C3-O3
4	A	505	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	A	502	GOL	O2-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	A	505	GOL	O1-C1-C2-O2
3	A	501	SAH	CB-CG-SD-C5'

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	GOL	2	0
4	A	502	GOL	2	0
3	A	501	SAH	5	0
4	A	503	GOL	2	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	B	18/18 (100%)	-0.32	0 100 100	66, 105, 163, 176	0
2	A	336/414 (81%)	0.62	44 (13%) 3 4	36, 90, 159, 204	0
All	All	354/432 (81%)	0.58	44 (12%) 4 4	36, 90, 160, 204	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	110	GLU	10.5
2	A	320	HIS	7.7
2	A	318	LEU	6.6
2	A	136	ASP	4.9
2	A	6	LYS	4.5
2	A	242	HIS	4.4
2	A	169	CYS	4.2
2	A	3	LYS	4.0
2	A	4	THR	3.9
2	A	8	ALA	3.6
2	A	5	ASP	3.5
2	A	40	LYS	3.3
2	A	319	VAL	3.2
2	A	92	GLN	3.2
2	A	135	ASP	3.1
2	A	244	LYS	3.1
2	A	11	LEU	3.0
2	A	37	THR	3.0
2	A	243	GLN	2.9
2	A	137	GLU	2.9
2	A	159	ASN	2.9
2	A	170	ASN	2.9
2	A	45	ALA	2.9
2	A	198	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	36	TYR	2.8
2	A	411	PHE	2.8
2	A	397	SER	2.6
2	A	379	GLN	2.6
2	A	171	GLU	2.6
2	A	109	ILE	2.5
2	A	343	SER	2.4
2	A	9	GLN	2.4
2	A	222	LYS	2.4
2	A	355	MET	2.3
2	A	241	ALA	2.3
2	A	396	THR	2.3
2	A	354	ILE	2.2
2	A	245	SER	2.1
2	A	21	PHE	2.1
2	A	158	PHE	2.1
2	A	317	ASP	2.1
2	A	231	VAL	2.1
2	A	173	ARG	2.0
2	A	395	TRP	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 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, 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.

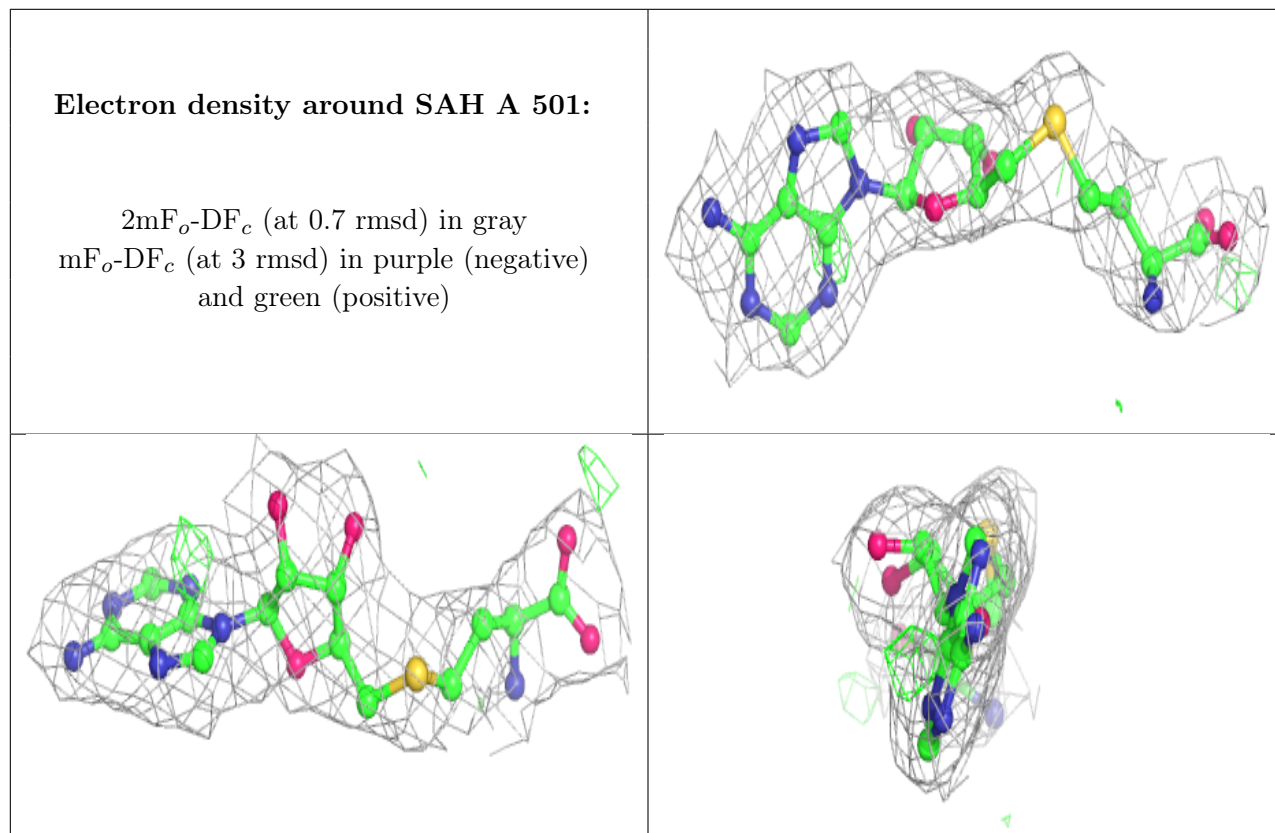
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	505	6/6	0.83	0.42	86,96,119,139	0
4	GOL	A	502	6/6	0.84	0.59	80,87,97,101	0
4	GOL	A	503	6/6	0.90	0.27	60,79,101,108	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	504	6/6	0.92	0.15	70,73,76,76	0
3	SAH	A	501	26/26	0.97	0.18	35,51,61,67	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.