



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2023 – 08:08 PM JST

PDB ID : 8HL7
Title : Crystal structure of p97 N/D1 in complex with a valosin-containing protein methyltransferase
Authors : Kang, W.; Yang, J.K.
Deposited on : 2022-11-29
Resolution : 2.80 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 : 2.34
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) : 2.34

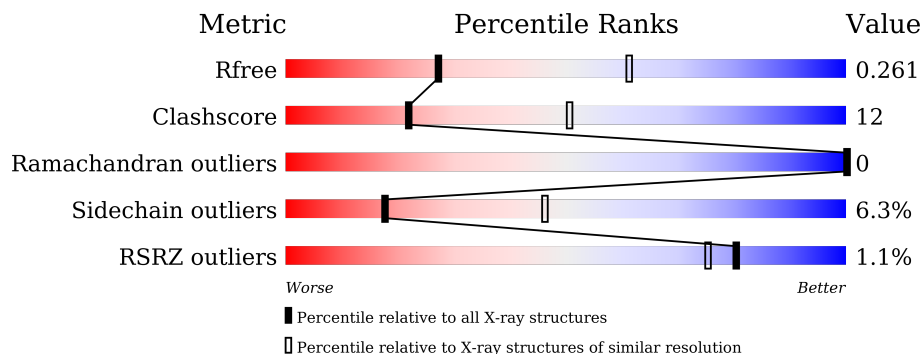
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	208	
2	B	436	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	302	-	X	-	-
4	GOL	B	503	-	X	-	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 4680 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 Protein N-lysine methyltransferase METTL21D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	200	1528	977	247	293	11	0	0	0

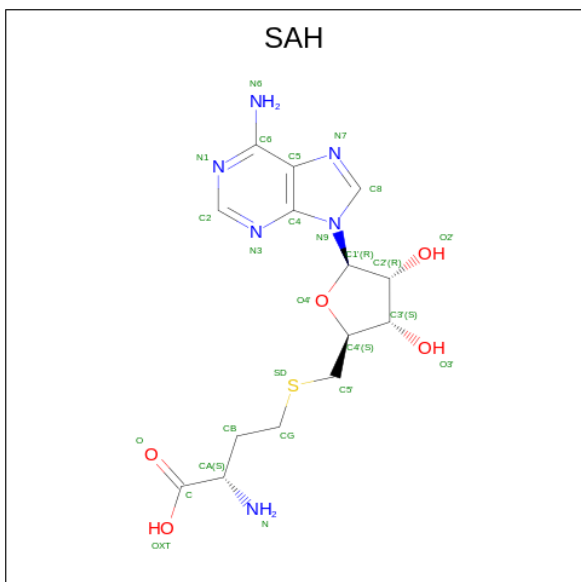
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP Q9H867
A	130	VAL	ILE	engineered mutation	UNP Q9H867

- Molecule 2 is a protein called Transitional endoplasmic reticulum ATPase.

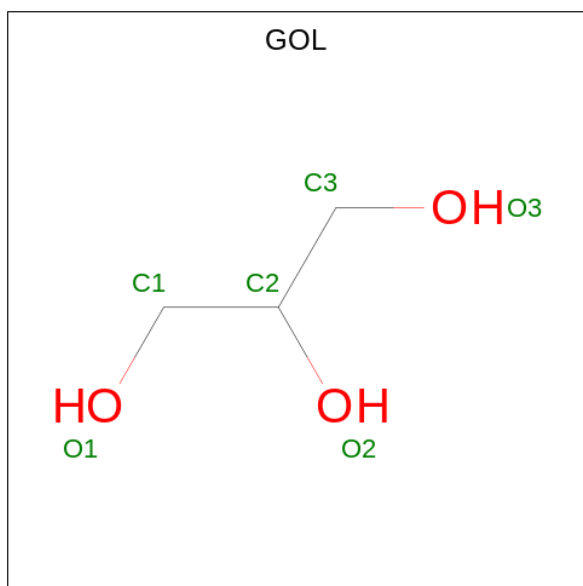
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	416	3046	1932	535	562	17	0	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



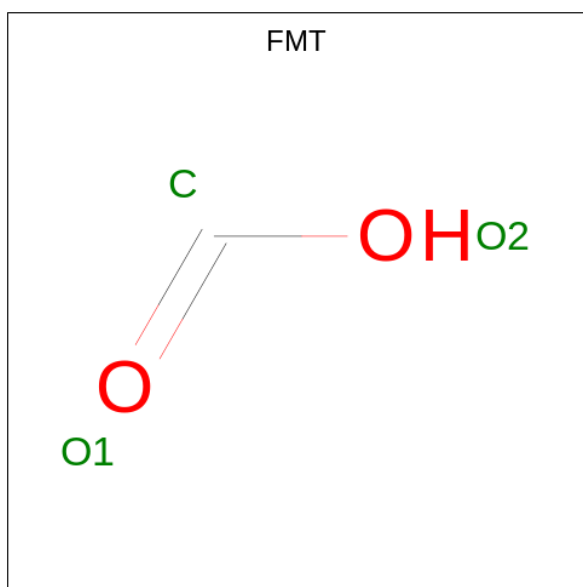
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	26	14	6	5	1	0	0

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



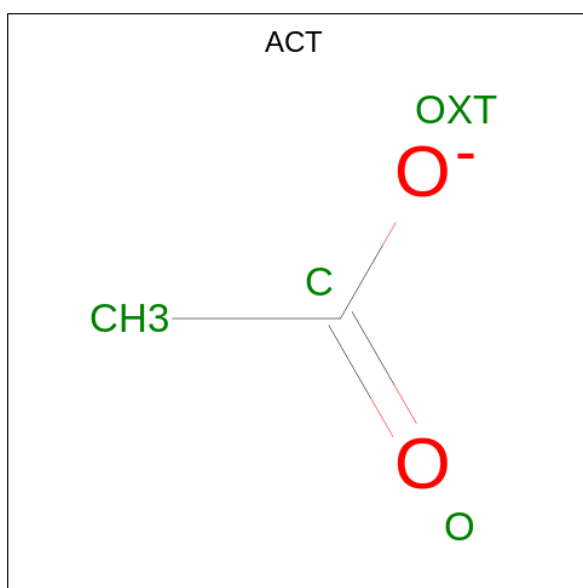
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

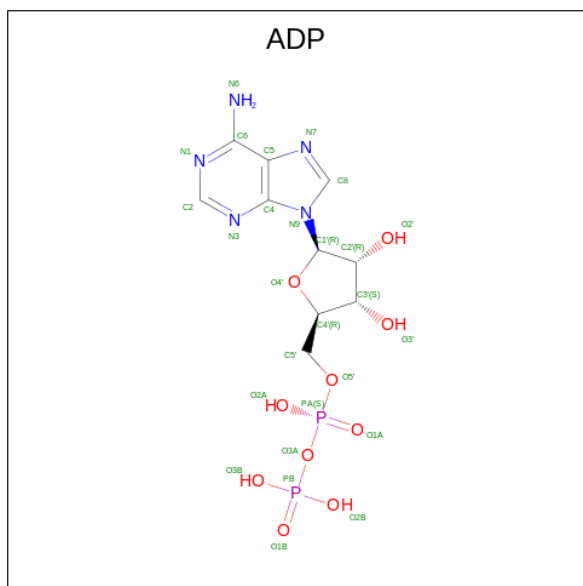
- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

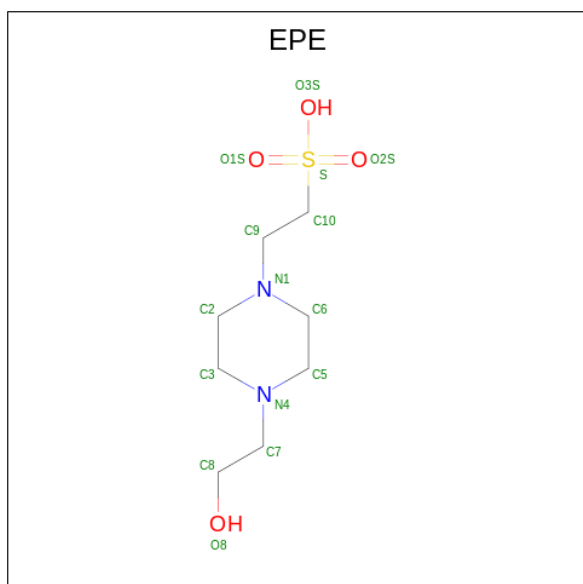
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
7	B	1	27	10	5	10	2	0	0

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	B	1	15	8	2	4	1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	8	Total O 8 8	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.78Å 60.78Å 473.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.57 – 2.80 29.57 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.57-2.80) 99.7 (29.57-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.217 , 0.261 0.217 , 0.261	Depositor DCC
R_{free} test set	1121 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtrriage
Anisotropy	0.308	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4680	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: ACT, EPE, FMT, GOL, ADP, M3L, SAH

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	0.45	0/1554	0.64	0/2106
2	B	0.44	0/3083	0.73	8/4200 (0.2%)
All	All	0.44	0/4637	0.70	8/6306 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	173	TYR	CB-CA-C	8.17	126.73	110.40
2	B	169	ASP	CB-CA-C	-7.55	95.30	110.40
2	B	170	PRO	CB-CA-C	6.80	129.00	112.00
2	B	170	PRO	N-CA-C	-6.64	94.83	112.10
2	B	184	CYS	CB-CA-C	-5.75	98.89	110.40
2	B	171	SER	N-CA-C	5.70	126.38	111.00
2	B	172	PRO	CB-CA-C	5.41	125.51	112.00
2	B	183	HIS	CB-CA-C	-5.10	100.20	110.40

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	1528	0	1475	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3046	0	2957	80	0
3	A	26	0	19	3	0
4	A	12	0	16	4	0
4	B	6	0	8	0	0
5	A	3	0	1	0	0
5	B	3	0	1	0	0
6	A	4	0	3	0	0
7	B	27	0	12	0	0
8	B	15	0	17	0	0
9	A	2	0	0	0	0
9	B	8	0	0	1	0
All	All	4680	0	4509	108	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 12.

All (108) 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:B:153:LEU:HD11	2:B:160:ALA:HB1	1.65	0.78
2:B:117:LEU:CD2	2:B:185:GLU:O	2.32	0.77
2:B:394:VAL:HA	2:B:449:MET:HG2	1.72	0.72
2:B:117:LEU:HD21	2:B:185:GLU:O	1.89	0.71
2:B:452:PHE:O	2:B:456:LEU:HD12	1.94	0.68
2:B:76:THR:O	2:B:83:ARG:NH2	2.29	0.65
2:B:117:LEU:HD22	2:B:185:GLU:O	1.97	0.64
2:B:40:SER:HB2	2:B:83:ARG:HB2	1.81	0.63
1:A:142:MET:HE2	1:A:171:CYS:HB2	1.79	0.62
2:B:118:PRO:O	2:B:188:PRO:HD2	1.99	0.61
1:A:101:GLN:O	1:A:105:LYS:HG3	2.02	0.60
4:A:303:GOL:H32	2:B:329:LEU:HD12	1.83	0.59
2:B:132:GLU:OE2	2:B:136:LYS:NZ	2.23	0.58
2:B:171:SER:CB	2:B:172:PRO:HD3	2.34	0.58
1:A:143:ALA:O	3:A:301:SAH:N	2.37	0.57
2:B:251:LYS:HD2	2:B:346:ALA:HB1	1.88	0.56
2:B:377:ARG:NH1	2:B:403:THR:O	2.39	0.55
1:A:146:ILE:HD11	1:A:173:TYR:CG	2.42	0.55
2:B:169:ASP:CB	2:B:170:PRO:HD3	2.37	0.55
1:A:21:GLU:H	4:A:302:GOL:H2	1.72	0.54
2:B:149:GLY:HA2	2:B:164:LYS:HE2	1.89	0.54
1:A:43:TRP:HA	4:A:303:GOL:H11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:GLN:HG2	2:B:368:ASP:O	2.08	0.53
2:B:225:ARG:HA	2:B:225:ARG:HE	1.73	0.53
2:B:277:LYS:HD2	2:B:281:GLU:HB3	1.89	0.53
2:B:394:VAL:HA	2:B:449:MET:CG	2.39	0.53
1:A:175:GLN:OE1	1:A:216:HIS:NE2	2.42	0.52
2:B:240:GLY:HA2	2:B:343:VAL:O	2.09	0.52
1:A:96:ASP:OD1	1:A:97:LEU:N	2.39	0.51
1:A:170:ILE:HG12	1:A:219:TYR:CE1	2.45	0.51
1:A:44:ASP:CG	4:A:303:GOL:H12	2.32	0.50
1:A:42:VAL:HG22	1:A:78:THR:HG21	1.92	0.50
2:B:329:LEU:HD22	2:B:362:ARG:HD3	1.94	0.50
1:A:204:GLU:HA	1:A:211:ARG:HH12	1.77	0.49
2:B:117:LEU:HB3	2:B:188:PRO:HD3	1.94	0.49
2:B:377:ARG:HD3	2:B:403:THR:O	2.13	0.49
2:B:244:TYR:CE1	2:B:350:PRO:HB3	2.47	0.49
2:B:301:ILE:HB	2:B:343:VAL:HG22	1.94	0.49
2:B:172:PRO:O	2:B:173:TYR:O	2.29	0.49
2:B:298:PRO:HA	2:B:340:HIS:O	2.12	0.48
2:B:208:GLY:HA2	2:B:376:GLY:HA2	1.95	0.48
1:A:147:TYR:OH	3:A:301:SAH:H8	2.14	0.48
1:A:83:LEU:O	1:A:87:THR:HG23	2.13	0.48
1:A:152:LEU:O	1:A:156:LEU:HG	2.13	0.48
2:B:229:LEU:O	2:B:233:ILE:HB	2.14	0.48
2:B:45:LYS:HD2	2:B:49:LEU:HD21	1.96	0.48
2:B:282:SER:OG	2:B:322:ARG:NH2	2.45	0.47
2:B:302:PHE:HA	2:B:344:MET:O	2.13	0.47
2:B:146:ILE:HD12	2:B:165:VAL:HG11	1.97	0.47
2:B:399:VAL:HG13	2:B:456:LEU:HD11	1.95	0.47
2:B:94:VAL:HG22	2:B:98:ASP:CB	2.45	0.47
2:B:111:GLY:HA2	2:B:170:PRO:HD3	1.96	0.47
1:A:137:PRO:O	1:A:167:THR:HG23	2.14	0.47
2:B:111:GLY:HA2	2:B:170:PRO:CD	2.45	0.46
2:B:419:ALA:O	2:B:423:ILE:HG13	2.14	0.46
2:B:338:ARG:HD2	2:B:340:HIS:CE1	2.50	0.46
2:B:147:ARG:HG3	2:B:173:TYR:CD1	2.50	0.46
1:A:144:ASP:O	2:B:315:M3L:HM11	2.16	0.46
1:A:176:ARG:CZ	2:B:315:M3L:HE3	2.45	0.46
2:B:381:LEU:HD21	2:B:411:LEU:HD12	1.97	0.46
1:A:165:PHE:CE2	1:A:222:LYS:HE2	2.51	0.46
2:B:120:ASP:N	2:B:120:ASP:OD1	2.49	0.46
2:B:177:ALA:N	2:B:180:THR:HG1	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:SER:CB	2:B:172:PRO:CD	2.94	0.45
2:B:117:LEU:CD2	2:B:185:GLU:H	2.30	0.45
1:A:29:ARG:HE	1:A:29:ARG:HB2	1.40	0.45
2:B:229:LEU:HB3	2:B:233:ILE:HD12	1.99	0.45
2:B:118:PRO:HA	2:B:163:PHE:HA	1.99	0.45
2:B:130:LEU:HD23	2:B:130:LEU:HA	1.82	0.45
2:B:71:VAL:O	2:B:72:LEU:HD23	2.17	0.44
2:B:274:ILE:HD11	2:B:285:ASN:HB3	2.00	0.44
1:A:29:ARG:NH2	1:A:110:MET:O	2.50	0.44
2:B:430:ILE:HD12	2:B:430:ILE:O	2.17	0.44
2:B:404:HIS:C	2:B:406:HIS:H	2.22	0.44
2:B:245:GLY:O	2:B:348:ASN:HA	2.18	0.44
1:A:214:ASP:OD2	2:B:359:ARG:NH2	2.46	0.43
2:B:129:ASN:ND2	2:B:132:GLU:HB2	2.33	0.43
2:B:329:LEU:HD23	2:B:329:LEU:HA	1.78	0.43
2:B:95:ARG:HG2	2:B:273:GLU:HG3	2.01	0.43
2:B:46:MET:HG2	2:B:51:LEU:HB2	2.00	0.43
2:B:312:LYS:HE3	2:B:351:ASN:O	2.18	0.43
2:B:388:MET:SD	2:B:419:ALA:HB2	2.59	0.43
1:A:187:LYS:O	1:A:191:LEU:HD12	2.19	0.43
2:B:45:LYS:HA	2:B:45:LYS:HD3	1.78	0.43
2:B:147:ARG:HG3	2:B:173:TYR:CE1	2.54	0.43
2:B:220:VAL:HG13	2:B:224:LEU:HG	2.01	0.42
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.87	0.42
2:B:29:ASP:OD1	2:B:30:GLU:N	2.52	0.42
2:B:170:PRO:HD2	2:B:174:CYS:HB2	2.01	0.42
2:B:406:HIS:HB3	2:B:411:LEU:CD2	2.50	0.42
2:B:177:ALA:N	2:B:180:THR:OG1	2.53	0.42
1:A:46:ALA:HB2	3:A:301:SAH:O	2.20	0.42
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.89	0.41
1:A:51:LYS:HA	1:A:51:LYS:HD2	1.88	0.41
2:B:23:PRO:O	2:B:45:LYS:NZ	2.49	0.41
2:B:246:PRO:HD2	2:B:249:THR:HG21	2.02	0.41
1:A:95:THR:HA	1:A:122:LYS:O	2.20	0.41
1:A:156:LEU:HD21	1:A:188:TYR:CE1	2.55	0.41
2:B:205:ASP:N	2:B:205:ASP:OD1	2.52	0.41
1:A:23:ARG:HH21	1:A:55:THR:HG22	1.86	0.41
2:B:249:THR:HB	2:B:369:ILE:HG22	2.02	0.41
2:B:25:ARG:HA	2:B:25:ARG:HD3	1.88	0.41
2:B:157:GLY:C	2:B:159:ARG:H	2.25	0.41
2:B:285:ASN:ND2	9:B:602:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:LYS:HA	2:B:237:PRO:HD3	1.95	0.41
1:A:126:TRP:HB3	1:A:155:LEU:HA	2.02	0.40
2:B:385:THR:HG22	2:B:388:MET:CE	2.51	0.40
2:B:444:SER:HB3	2:B:445:LEU:H	1.76	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	194/208 (93%)	184 (95%)	10 (5%)	0	100	100
2	B	409/436 (94%)	373 (91%)	36 (9%)	0	100	100
All	All	603/644 (94%)	557 (92%)	46 (8%)	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	162/182 (89%)	150 (93%)	12 (7%)	13	37
2	B	301/372 (81%)	284 (94%)	17 (6%)	21	51
All	All	463/554 (84%)	434 (94%)	29 (6%)	18	46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	18	ARG
1	A	35	SER
1	A	67	SER
1	A	102	ASP
1	A	142	MET
1	A	144	ASP
1	A	149	GLU
1	A	192	LEU
1	A	198	PHE
1	A	212	SER
1	A	222	LYS
2	B	52	PHE
2	B	73	SER
2	B	94	VAL
2	B	99	VAL
2	B	101	SER
2	B	116	VAL
2	B	164	LYS
2	B	168	THR
2	B	174	CYS
2	B	180	THR
2	B	184	CYS
2	B	276	SER
2	B	324	ILE
2	B	340	HIS
2	B	342	ILE
2	B	351	ASN
2	B	358	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](#)

1 non-standard protein/DNA/RNA residue 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	M3L	B	315	2	10,11,12	0.59	0	9,14,16	0.78	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	M3L	B	315	2	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	315	M3L	CG-CD-CE-NZ
2	B	315	M3L	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	315	M3L	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry i

9 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
5	FMT	B	502	-	2,2,2	0.65	0	1,1,1	0.19	0
4	GOL	A	302	-	5,5,5	1.50	2 (40%)	5,5,5	1.00	0
3	SAH	A	301	-	24,28,28	1.18	2 (8%)	25,40,40	1.71	4 (16%)
5	FMT	A	304	-	2,2,2	0.62	0	1,1,1	0.02	0
6	ACT	A	305	-	3,3,3	1.82	1 (33%)	3,3,3	1.44	0
7	ADP	B	501	-	24,29,29	1.12	2 (8%)	29,45,45	1.35	4 (13%)
8	EPE	B	504	-	15,15,15	0.86	1 (6%)	18,20,20	2.32	8 (44%)
4	GOL	B	503	-	5,5,5	2.16	2 (40%)	5,5,5	1.12	0
4	GOL	A	303	-	5,5,5	1.35	1 (20%)	5,5,5	1.01	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	302	-	-	4/4/4/4	-
3	SAH	A	301	-	-	3/11/31/31	0/3/3/3
7	ADP	B	501	-	-	2/12/32/32	0/3/3/3
8	EPE	B	504	-	-	5/9/19/19	0/1/1/1
4	GOL	B	503	-	-	4/4/4/4	-
4	GOL	A	303	-	-	4/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	GOL	C1-C2	3.69	1.66	1.51
3	A	301	SAH	C2-N3	3.38	1.37	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	ADP	C5-C4	3.11	1.49	1.40
4	B	503	GOL	C3-C2	3.08	1.64	1.51
8	B	504	EPE	C10-S	2.99	1.81	1.77
6	A	305	ACT	CH3-C	2.81	1.60	1.49
7	B	501	ADP	O4'-C1'	2.74	1.44	1.41
4	A	302	GOL	C3-C2	2.45	1.61	1.51
3	A	301	SAH	C2-N1	2.32	1.38	1.33
4	A	302	GOL	C1-C2	2.24	1.60	1.51
4	A	303	GOL	C1-C2	2.14	1.60	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	SAH	N3-C2-N1	-5.88	119.48	128.68
8	B	504	EPE	O3S-S-C10	5.71	115.00	105.77
8	B	504	EPE	C5-N4-C3	4.48	118.92	108.83
3	A	301	SAH	C5'-SD-CG	-2.84	93.74	102.27
8	B	504	EPE	C7-N4-C5	2.83	118.46	111.23
8	B	504	EPE	O2S-S-C10	-2.77	103.58	106.92
8	B	504	EPE	C7-N4-C3	2.75	118.26	111.23
3	A	301	SAH	OXT-C-CA	2.64	122.38	113.38
7	B	501	ADP	C3'-C2'-C1'	2.61	104.91	100.98
3	A	301	SAH	C2'-C3'-C4'	2.55	107.59	102.64
8	B	504	EPE	O3S-S-O1S	-2.51	105.14	111.27
8	B	504	EPE	O1S-S-C10	2.33	109.72	106.92
8	B	504	EPE	C6-C5-N4	2.31	115.38	110.64
7	B	501	ADP	N3-C2-N1	-2.23	125.20	128.68
7	B	501	ADP	C4-C5-N7	-2.10	107.21	109.40
7	B	501	ADP	N6-C6-N1	2.07	122.88	118.57

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	GOL	O1-C1-C2-C3
4	A	302	GOL	C1-C2-C3-O3
4	A	302	GOL	O2-C2-C3-O3
4	A	303	GOL	O1-C1-C2-O2
4	A	303	GOL	O1-C1-C2-C3
4	A	303	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

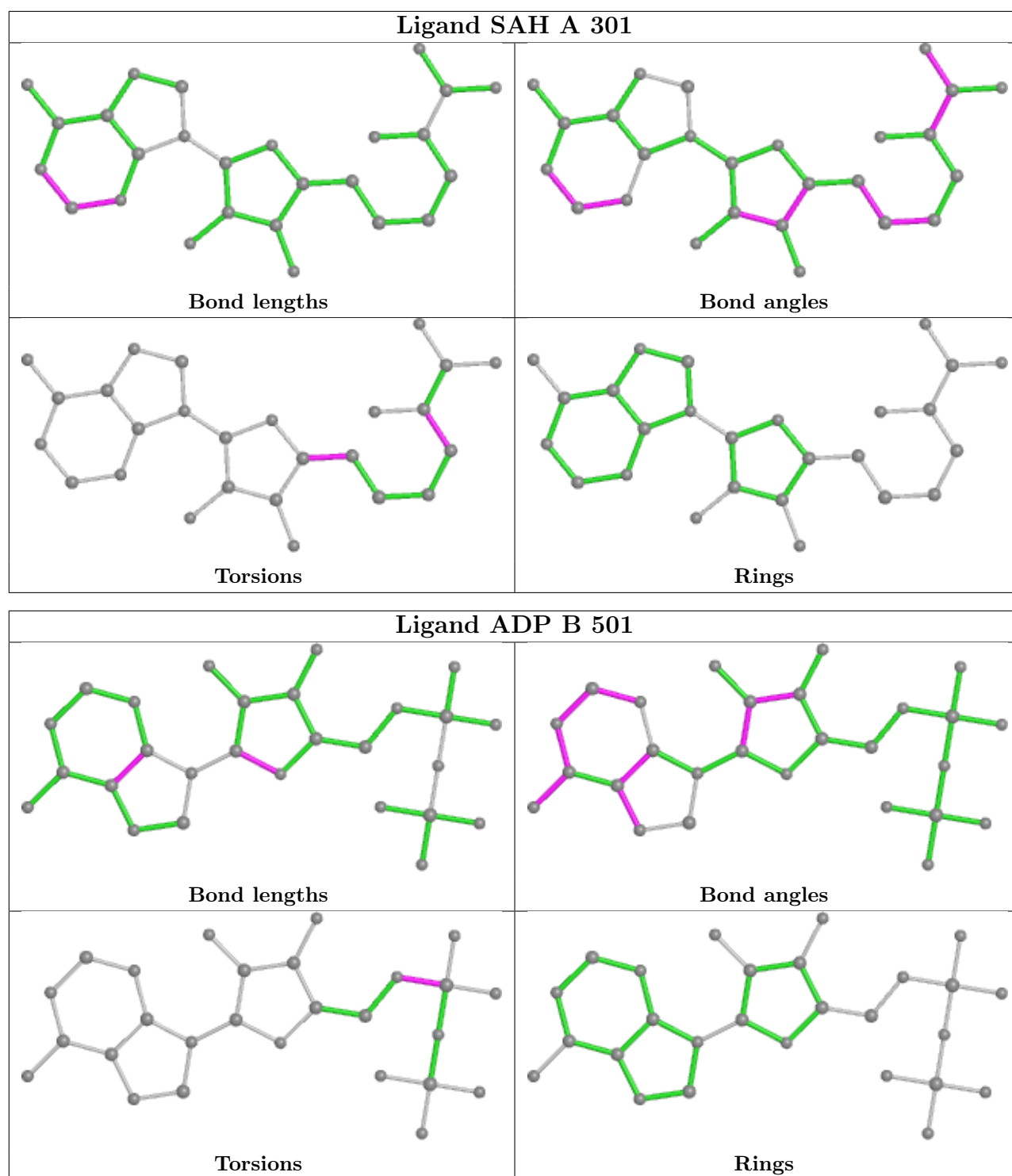
Mol	Chain	Res	Type	Atoms
7	B	501	ADP	C5'-O5'-PA-O3A
8	B	504	EPE	C8-C7-N4-C3
8	B	504	EPE	C9-C10-S-O1S
8	B	504	EPE	C9-C10-S-O3S
4	A	302	GOL	O1-C1-C2-O2
4	A	303	GOL	O2-C2-C3-O3
4	B	503	GOL	O1-C1-C2-O2
3	A	301	SAH	C-CA-CB-CG
4	B	503	GOL	O2-C2-C3-O3
3	A	301	SAH	N-CA-CB-CG
7	B	501	ADP	C5'-O5'-PA-O1A
8	B	504	EPE	C9-C10-S-O2S
3	A	301	SAH	O4'-C4'-C5'-SD
8	B	504	EPE	N4-C7-C8-O8

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	GOL	1	0
3	A	301	SAH	3	0
4	A	303	GOL	3	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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	200/208 (96%)	-0.01	4 (2%) 65 56	40, 62, 104, 127	0
2	B	415/436 (95%)	-0.18	3 (0%) 87 84	36, 65, 100, 131	0
All	All	615/644 (95%)	-0.12	7 (1%) 80 75	36, 64, 103, 131	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	320	VAL	2.9
1	A	56	PRO	2.6
2	B	278	LEU	2.3
1	A	141	LEU	2.3
2	B	37	SER	2.2
1	A	190	GLU	2.1
1	A	172	CYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	M3L	B	315	12/13	0.95	0.15	62,69,77,77	0

6.3 Carbohydrates [i](#)

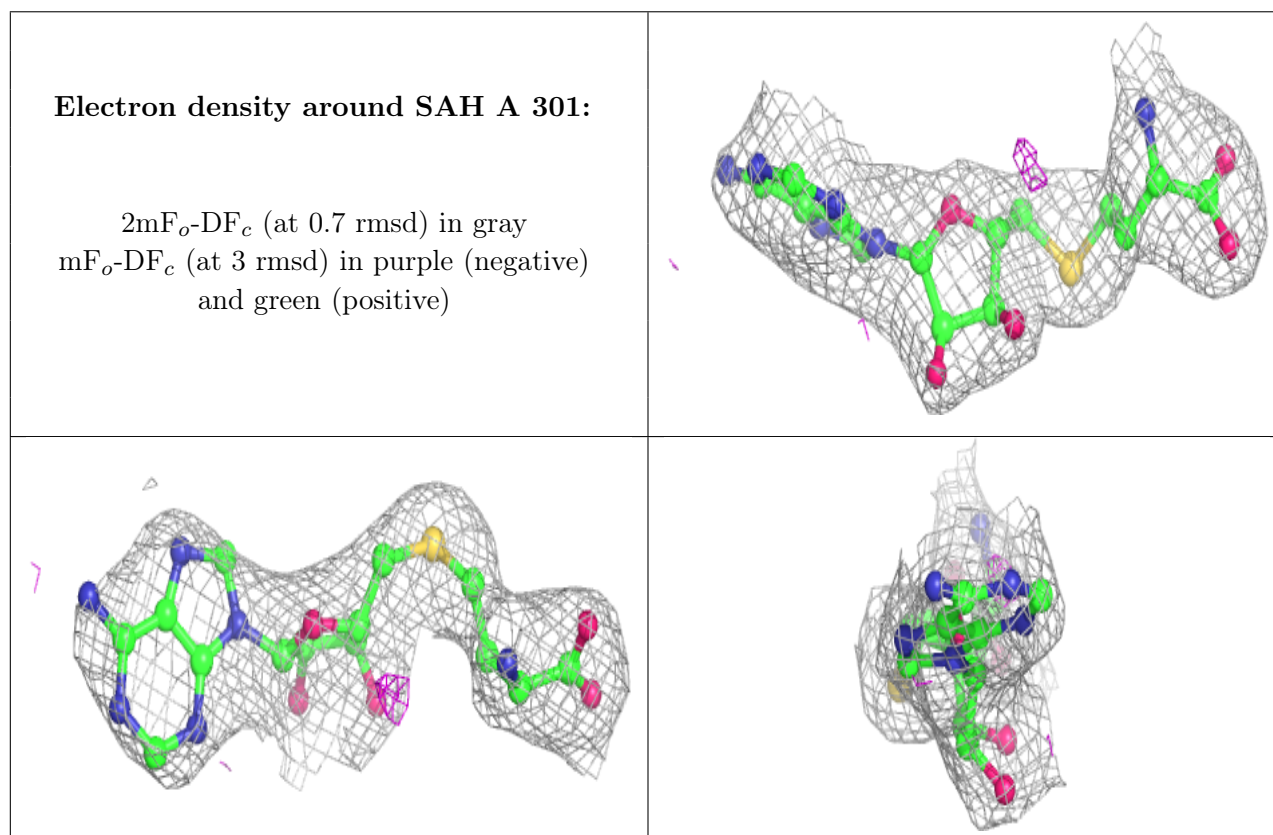
There are no monosaccharides in this entry.

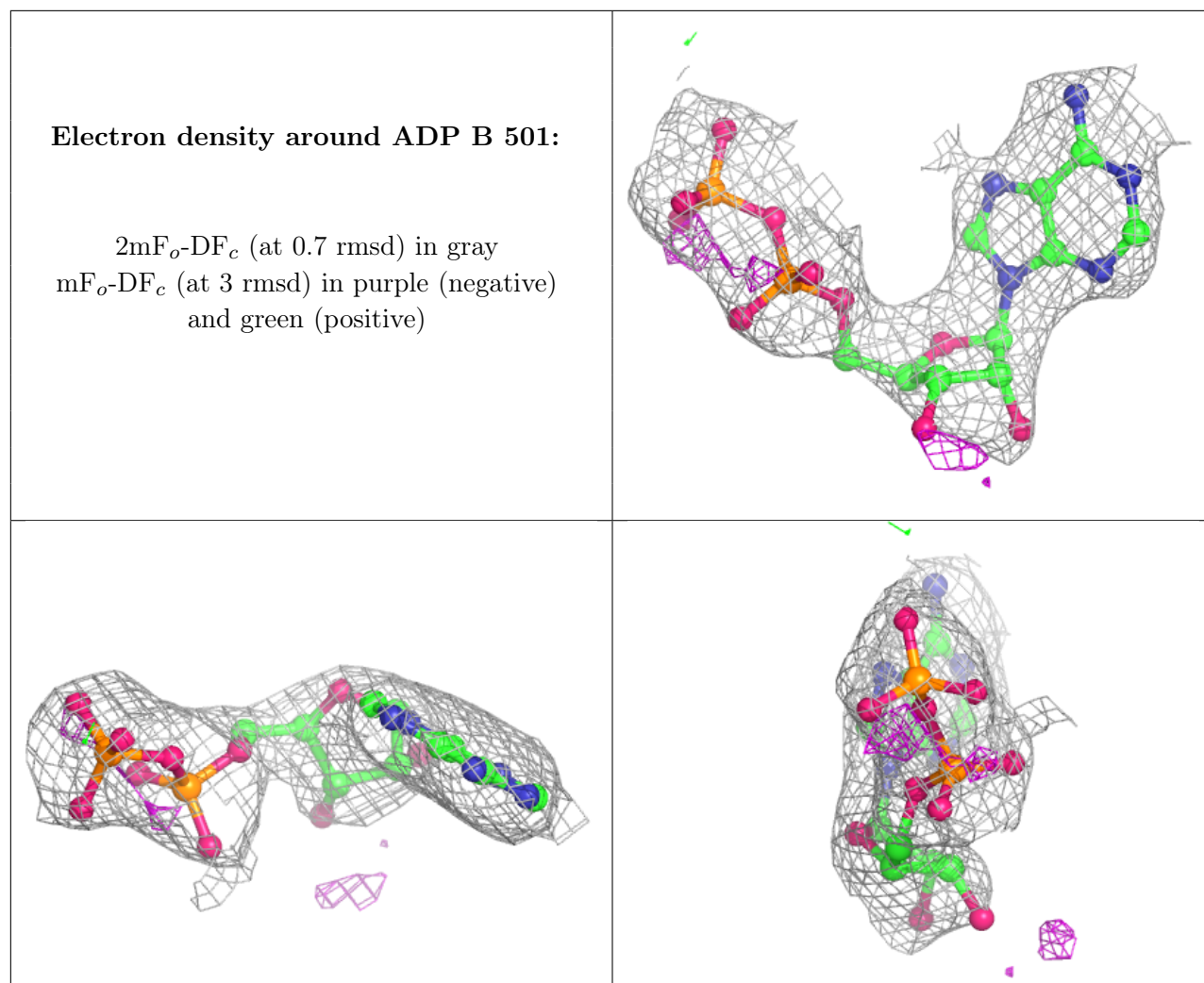
6.4 Ligands [i](#)

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	B	503	6/6	0.79	0.29	44,49,53,57	0
4	GOL	A	302	6/6	0.86	0.20	47,52,56,57	0
6	ACT	A	305	4/4	0.89	0.44	63,66,67,67	0
3	SAH	A	301	26/26	0.90	0.18	38,58,69,74	0
8	EPE	B	504	15/15	0.92	0.39	50,72,79,79	0
5	FMT	A	304	3/3	0.93	0.25	55,55,60,61	0
5	FMT	B	502	3/3	0.94	0.15	54,54,55,56	0
4	GOL	A	303	6/6	0.95	0.21	46,49,50,51	0
7	ADP	B	501	27/27	0.96	0.16	56,64,68,69	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.