



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:41 AM UTC

PDB ID : 8HL7 / pdb_00008hl7
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 : 4-5-2 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

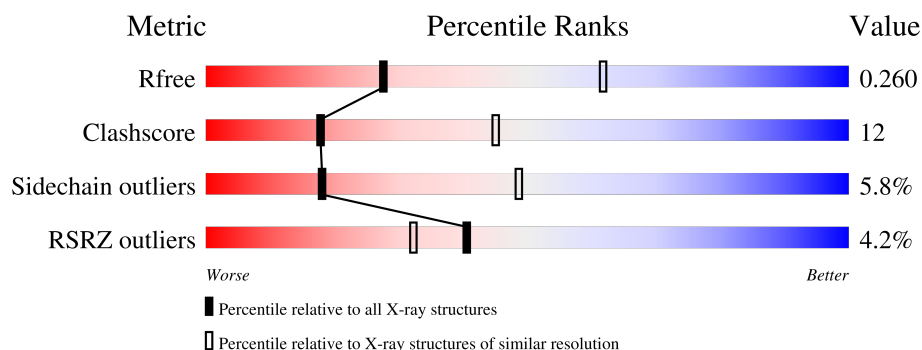
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

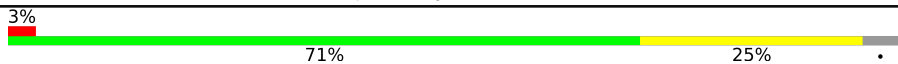
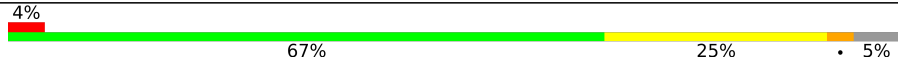
The reported resolution of this entry is 2.80 Å.

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
1	A	200	Total	C	N	O	S	0	0	0
			1528	977	247	293	11			

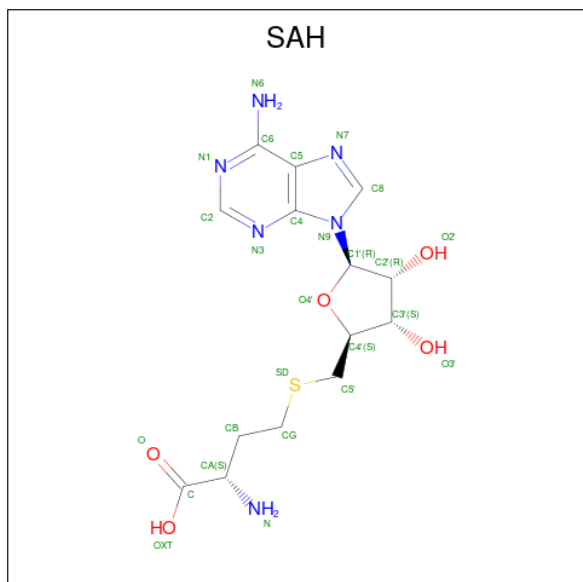
There are 2 discrepancies between the modelled and reference sequences:

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
2	B	416	Total	C	N	O	S	0	0	0
			3046	1932	535	562	17			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



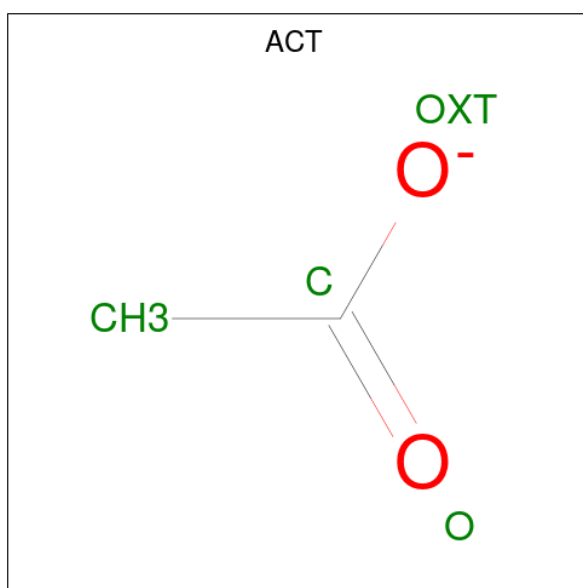
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is FORMIC ACID (CCD ID: 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		

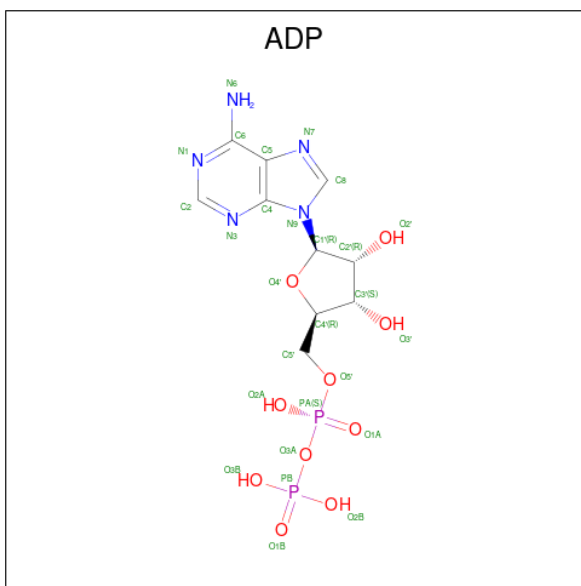
- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



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

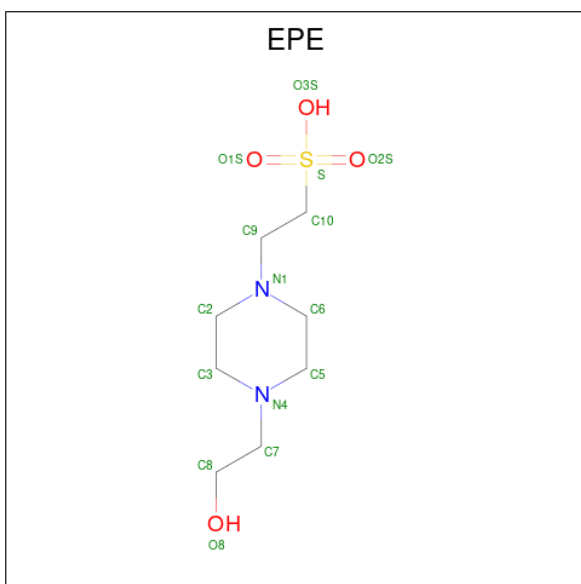
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$)

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



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

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $\text{C}_8\text{H}_{18}\text{N}_2\text{O}_4\text{S}$).



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

- Molecule 9 is water.

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

- Molecule 1: Protein N-lysine methyltransferase METTL21D



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) 99.6 (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)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.217 , 0.261 0.218 , 0.260	Depositor DCC
R_{free} test set	1121 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, M3L, ADP, EPE, ACT, 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	0.40	0/1554	0.59	0/2106
2	B	0.44	0/3083	0.81	18/4200 (0.4%)
All	All	0.43	0/4637	0.75	18/6306 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	170	PRO	CB-CA-C	13.76	129.00	110.98
2	B	170	PRO	N-CA-C	-10.41	94.83	111.38
2	B	171	SER	N-CA-C	10.03	126.38	112.75
2	B	172	PRO	CB-CA-C	8.46	125.51	111.56
2	B	173	TYR	CB-CA-C	8.20	126.73	110.42
2	B	184	CYS	CB-CA-C	-8.03	98.89	110.62
2	B	169	ASP	CB-CA-C	-7.55	95.30	110.17
2	B	184	CYS	N-CA-C	7.06	120.01	107.80
2	B	168	THR	CB-CA-C	6.48	122.24	109.66
2	B	183	HIS	N-CA-C	6.45	118.93	108.41
2	B	169	ASP	CA-C-N	6.33	126.24	119.85
2	B	169	ASP	C-N-CA	6.33	126.24	119.85
2	B	169	ASP	N-CA-C	6.01	123.10	109.81
2	B	183	HIS	CB-CA-C	-6.00	100.20	110.16
2	B	171	SER	CB-CA-C	-5.86	101.86	112.76
2	B	174	CYS	CB-CA-C	5.61	119.69	110.03
2	B	172	PRO	N-CA-C	-5.61	100.92	112.47
2	B	185	GLU	CB-CA-C	5.30	119.39	109.86

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	1528	0	1475	32	0
2	B	3046	0	2957	84	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	113	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 (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: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
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:241:ILE:HD12	2:B:344:MET:HE3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:MET:HE1	2:B:73:SER:HA	1.86	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
1:A:44:ASP:CG	4:A:303:GOL:H12	2.32	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
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: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:404:HIS:C	2:B:406:HIS:H	2.22	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:332:MET:HB3	2:B:332:MET:HE2	1.83	0.46
2:B:171:SER:CB	2:B:172:PRO:CD	2.94	0.45
2:B:157:GLY:C	2:B:159:ARG:H	2.25	0.45
2:B:348:ASN:C	2:B:349:ARG:HG3	2.42	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
1:A:142:MET:HE1	1:A:188:TYR:OH	2.15	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: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:HE1	2:B:73:SER:CA	2.47	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:120:ASP:OD1	2:B:120:ASP:N	2.49	0.42
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
1:A:59:SER:C	1:A:65:ALA:HB3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:285:ASN:ND2	9:B:602:HOH:O	2.53	0.41
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](#)

There are no protein backbone outliers to report in this entry.

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%)	155 (96%)	7 (4%)	26	60
2	B	301/372 (81%)	281 (93%)	20 (7%)	15	43
All	All	463/554 (84%)	436 (94%)	27 (6%)	18	49

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	92	VAL
1	A	100	LEU
1	A	144	ASP
1	A	149	GLU
1	A	192	LEU
1	A	212	SER
2	B	73	SER
2	B	94	VAL
2	B	99	VAL
2	B	101	SER
2	B	108	VAL
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	201	VAL
2	B	276	SER
2	B	324	ILE
2	B	342	ILE
2	B	353	ILE
2	B	357	LEU
2	B	358	ARG
2	B	367	VAL
2	B	399	VAL

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

Mol	Chain	Res	Type
2	B	129	ASN
2	B	226	HIS
2	B	406	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.61	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
4	GOL	A	302	-	5,5,5	1.61	2 (40%)	5,5,5	1.07	0
4	GOL	A	303	-	5,5,5	1.44	1 (20%)	5,5,5	1.08	0
5	FMT	B	502	-	2,2,2	0.67	0	1,1,1	0.18	0
6	ACT	A	305	-	3,3,3	1.94	1 (33%)	3,3,3	1.43	0
4	GOL	B	503	-	5,5,5	2.32	2 (40%)	5,5,5	1.19	0
7	ADP	B	501	-	28,29,29	1.70	5 (17%)	43,45,45	1.78	7 (16%)
8	EPE	B	504	-	15,15,15	0.86	1 (6%)	19,20,20	2.09	7 (36%)
5	FMT	A	304	-	2,2,2	0.63	0	1,1,1	0.01	0
3	SAH	A	301	-	27,28,28	1.09	3 (11%)	36,40,40	1.94	10 (27%)

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	302	-	-	4/4/4/4	-
4	GOL	A	303	-	-	4/4/4/4	-
4	GOL	B	503	-	-	4/4/4/4	-
7	ADP	B	501	-	-	2/16/32/32	0/3/3/3
8	EPE	B	504	-	-	5/9/19/19	0/1/1/1
3	SAH	A	301	-	-	3/15/31/31	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	ADP	C5-C4	5.65	1.49	1.39
7	B	501	ADP	PA-O3A	4.23	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	GOL	C1-C2	3.97	1.66	1.51
4	B	503	GOL	C3-C2	3.31	1.64	1.51
6	A	305	ACT	CH3-C	3.00	1.60	1.49
8	B	504	EPE	C10-S	2.98	1.81	1.77
7	B	501	ADP	C5-C6	2.69	1.48	1.41
7	B	501	ADP	C8-N7	2.65	1.36	1.31
4	A	302	GOL	C3-C2	2.62	1.61	1.51
3	A	301	SAH	C2-N1	2.41	1.38	1.33
4	A	302	GOL	C1-C2	2.40	1.60	1.51
4	A	303	GOL	C1-C2	2.29	1.60	1.51
3	A	301	SAH	C8-N7	2.25	1.36	1.31
7	B	501	ADP	C5-N7	-2.24	1.35	1.39
3	A	301	SAH	C2-N3	2.03	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	501	ADP	C5-C4-N3	-6.33	118.00	126.72
3	A	301	SAH	N3-C2-N1	-6.01	119.48	128.58
7	B	501	ADP	N3-C4-N9	5.01	135.68	127.17
8	B	504	EPE	C5-N4-C3	4.68	118.92	108.84
8	B	504	EPE	O3S-S-C10	4.60	115.00	106.00
3	A	301	SAH	C5-C4-N3	-3.61	121.75	126.72
3	A	301	SAH	N9-C8-N7	-3.47	109.01	113.94
3	A	301	SAH	C2-N3-C4	3.29	119.87	111.83
7	B	501	ADP	C2-N3-C4	3.29	119.86	111.83
7	B	501	ADP	C4-C5-N7	-2.95	107.21	110.58
3	A	301	SAH	C5'-SD-CG	-2.87	93.74	102.26
3	A	301	SAH	C5-N7-C8	2.76	107.79	103.45
8	B	504	EPE	C7-N4-C5	2.71	118.46	111.24
8	B	504	EPE	C7-N4-C3	2.63	118.26	111.24
3	A	301	SAH	C2'-C3'-C4'	2.58	107.59	102.61
8	B	504	EPE	O3S-S-O1S	-2.50	105.14	111.40
8	B	504	EPE	C6-C5-N4	2.34	115.38	110.65
3	A	301	SAH	O4'-C1'-N9	-2.26	103.74	108.09
3	A	301	SAH	C2'-C1'-N9	2.26	118.92	113.30
7	B	501	ADP	N3-C2-N1	-2.24	125.20	128.58
3	A	301	SAH	N3-C4-N9	2.23	130.97	127.17
8	B	504	EPE	O2S-S-C10	-2.08	103.58	106.73
7	B	501	ADP	C5-N7-C8	2.05	106.67	103.45
7	B	501	ADP	N6-C6-N1	2.02	122.88	118.38

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

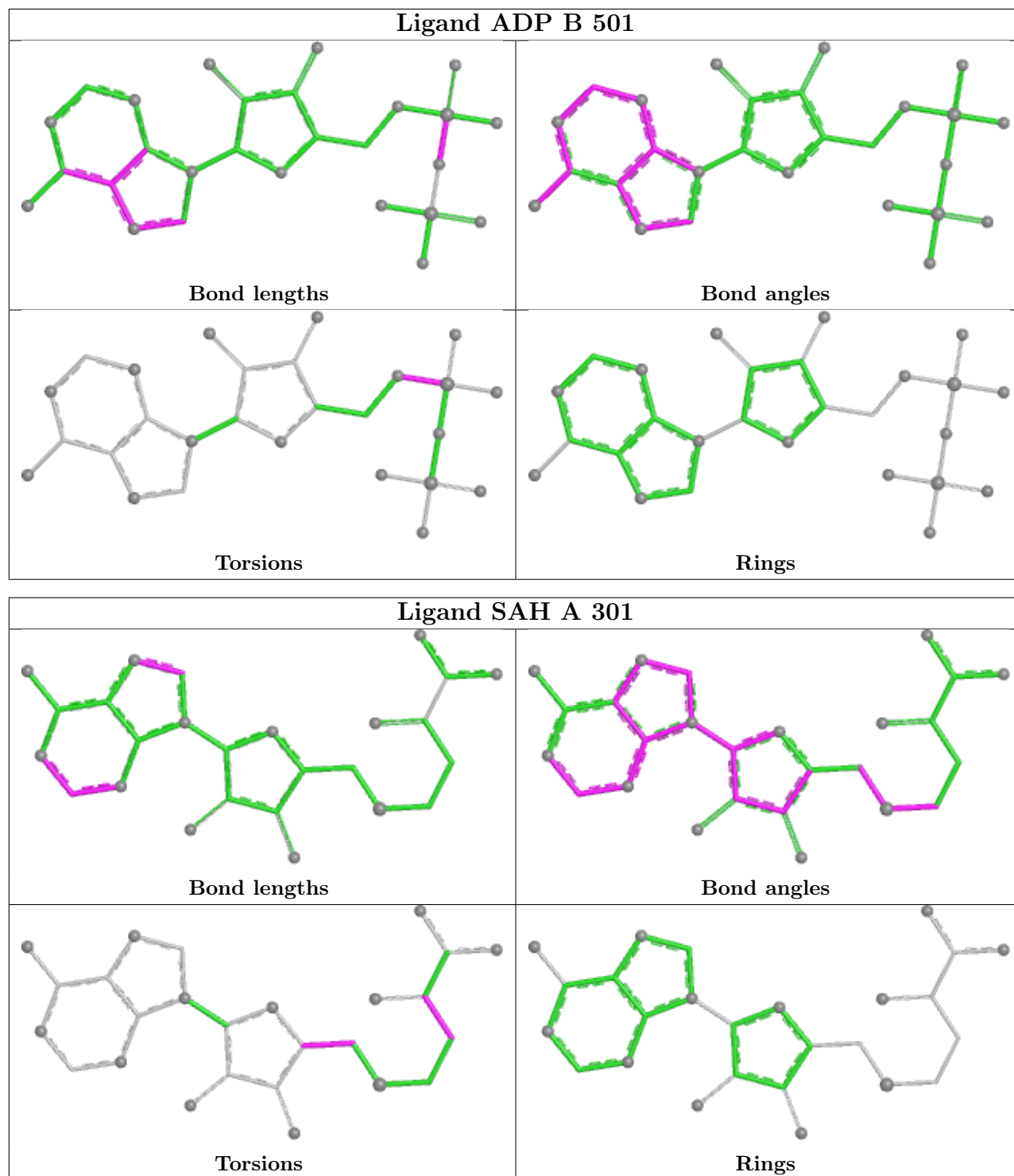
There are no ring outliers.

3 monomers are involved in 7 short contacts:

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

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

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	200/208 (96%)	0.04	7 (3%) 47 38	40, 62, 104, 127	0
2	B	415/436 (95%)	0.13	19 (4%) 37 29	36, 65, 100, 131	0
All	All	615/644 (95%)	0.10	26 (4%) 40 32	36, 64, 103, 131	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	185	GLU	4.5
2	B	172	PRO	4.0
2	B	348	ASN	3.5
1	A	190	GLU	3.2
2	B	430	ILE	3.1
2	B	432	LEU	2.9
2	B	364	ASP	2.9
2	B	173	TYR	2.8
2	B	171	SER	2.8
2	B	395	ASP	2.4
1	A	134	PRO	2.4
1	A	135	SER	2.4
2	B	320	VAL	2.3
2	B	340	HIS	2.3
2	B	394	VAL	2.3
2	B	157	GLY	2.3
1	A	59	SER	2.2
2	B	187	GLU	2.2
2	B	428	ASP	2.1
2	B	170	PRO	2.1
1	A	219	TYR	2.1
2	B	398	GLN	2.1
2	B	23	PRO	2.1
1	A	220	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	189	ILE	2.1
1	A	130	VAL	2.0

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	0.93	0.12	62,69,77,77	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

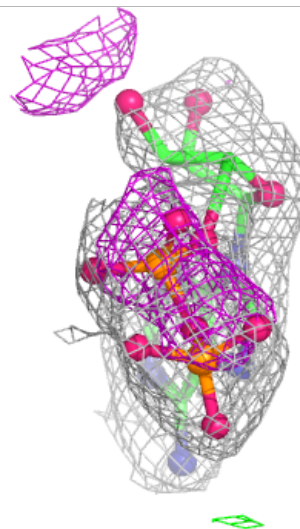
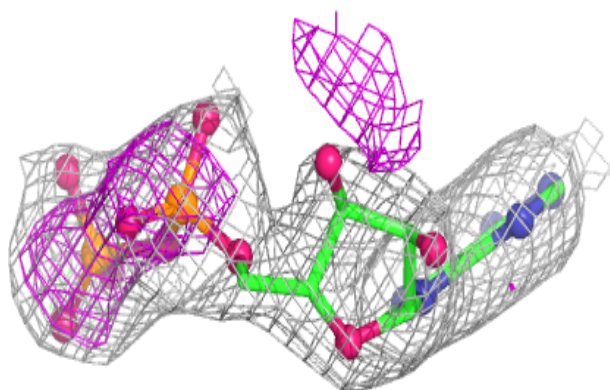
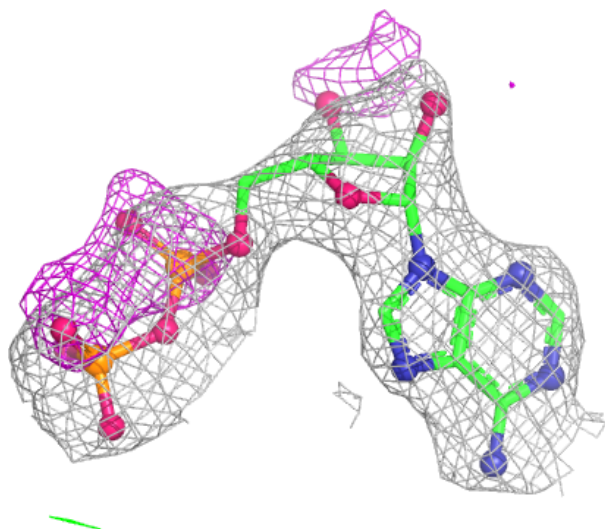
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

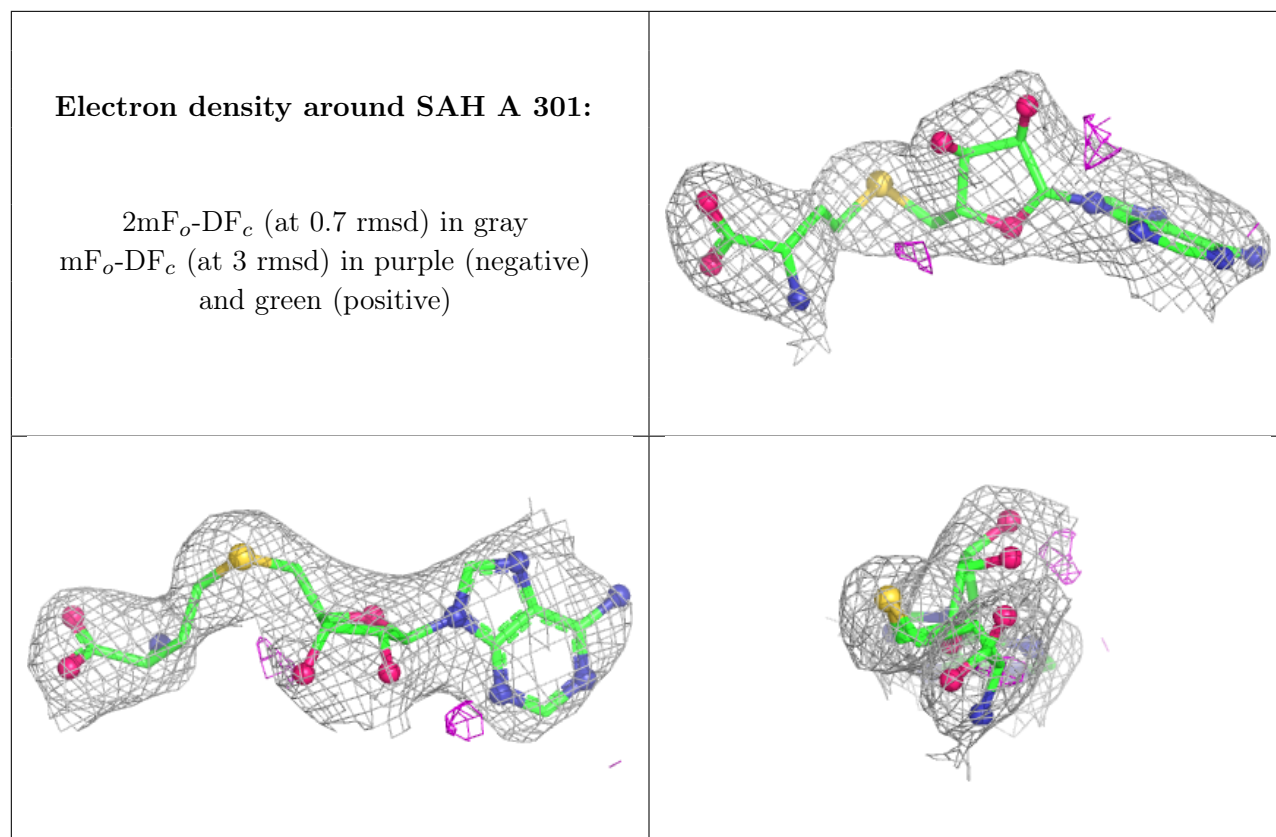
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	A	305	4/4	0.75	0.13	63,66,67,67	0
4	GOL	B	503	6/6	0.79	0.17	44,49,53,57	0
5	FMT	B	502	3/3	0.90	0.10	54,54,55,56	0
4	GOL	A	302	6/6	0.90	0.10	47,52,56,57	0
4	GOL	A	303	6/6	0.91	0.16	46,49,50,51	0
7	ADP	B	501	27/27	0.91	0.10	56,64,68,69	0
5	FMT	A	304	3/3	0.92	0.09	55,55,60,61	0
8	EPE	B	504	15/15	0.94	0.12	50,72,79,79	0
3	SAH	A	301	26/26	0.95	0.08	38,58,69,74	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 ADP B 501:

$2mF_o-DF_c$ (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.