Full wwPDB X-ray Structure Validation Report (i)

Jul 25, 2022 – 02:33 pm BST

PDB ID	:	7OAT
Title	:	Structural basis for targeted p97 remodelling by ASPL as prerequisite for p97 trimethylation by METTL21D
Authors	:	Petrovic, S.; Heinemann, U.; Roske, Y.
Deposited on	:	2021-04-20
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 3.00 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.
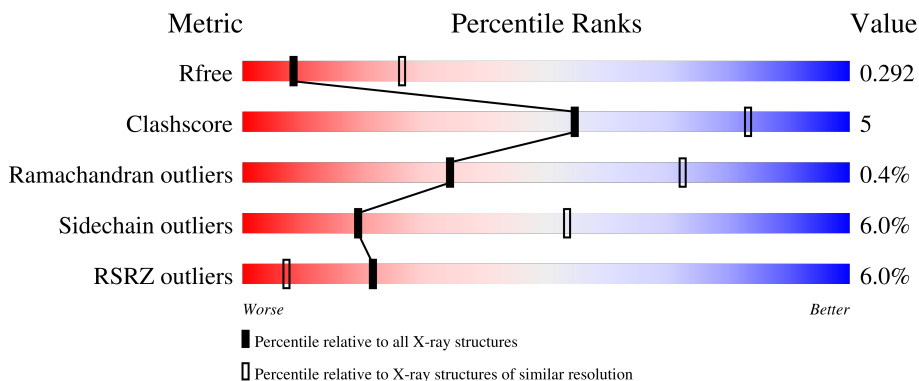
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	A	190	12% / 79% 9% · 10%
2	B	481	4% / 74% 15% · 10%
3	C	224	4% / 79% 14% · 6%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6558 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 Tether containing UBX domain for GLUT4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1382	887	242	251	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	311	GLY	-	expression tag	UNP Q9BZE9
A	312	SER	-	expression tag	UNP Q9BZE9

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	434	Total	C	N	O	S	0	0	0
			3385	2124	599	644	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P55072
B	1	SER	-	expression tag	UNP P55072

- Molecule 3 is a protein called Protein-lysine methyltransferase METTL21D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1659	1061	269	319	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLY	-	expression tag	UNP Q9H867

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	31	10	5	13	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	B	1	1	1	0	0

- Molecule 7 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).
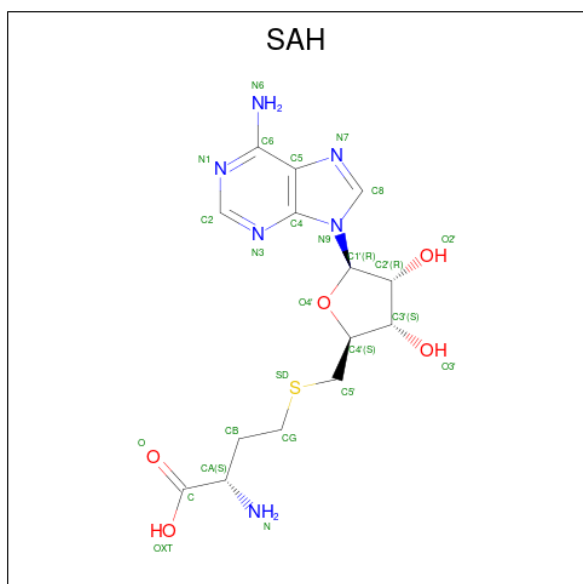
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total 7	O 7	0	0
8	B	40	Total 40	O 40	0	0
8	C	11	Total 11	O 11	0	0

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.
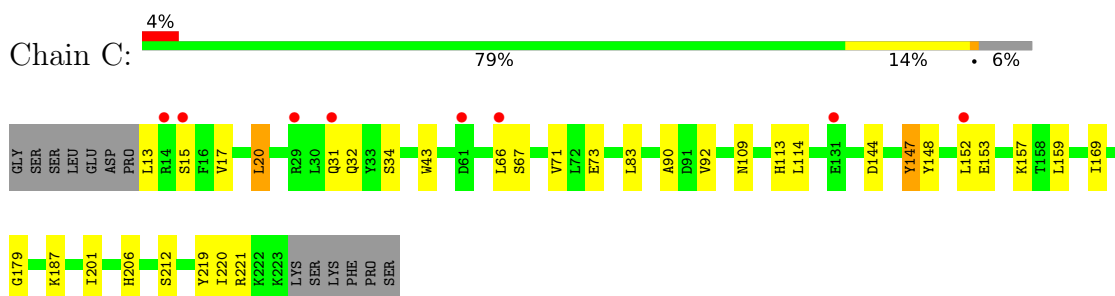
• Molecule 1: Tether containing UBX domain for GLUT4

Chain A:
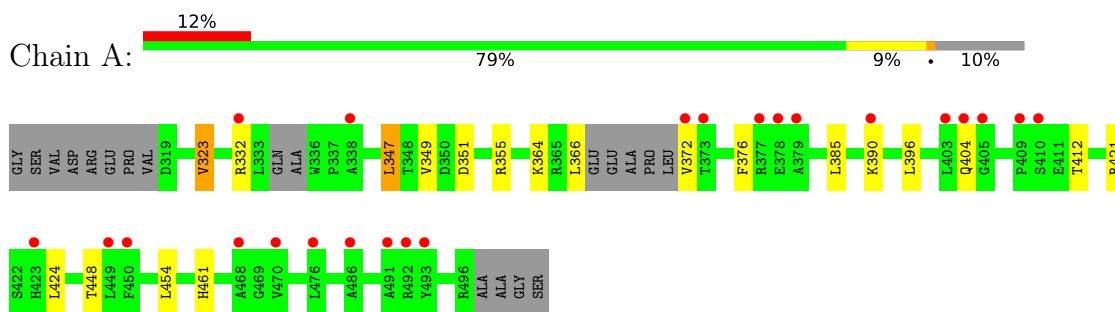
• Molecule 2: Transitional endoplasmic reticulum ATPase

Chain B:
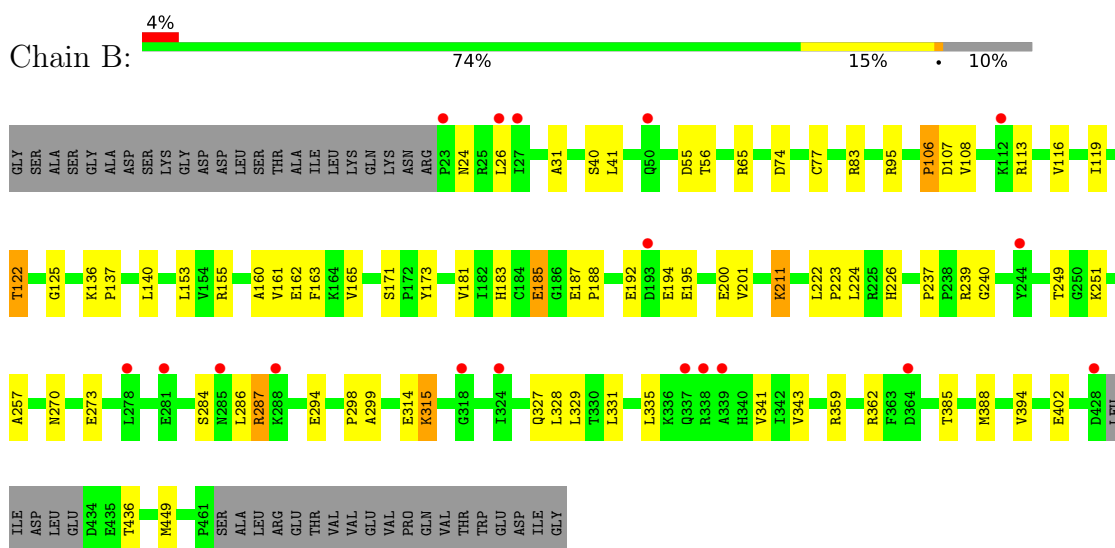
• Molecule 3: Protein-lysine methyltransferase METTL21D

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.26Å 69.62Å 140.18Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	49.32 – 3.00 49.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.32-3.00) 98.1 (49.32-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.3 (6-FEB-2020)	Depositor
R, R_{free}	0.225 , 0.270 0.240 , 0.292	Depositor DCC
R_{free} test set	1042 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	73.6	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6558	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SAH, ATP, EDO, MG, M3L

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	0.30	0/1414	0.23	0/1918
2	B	0.31	0/3426	0.28	1/4633 (0.0%)
3	C	0.28	0/1689	0.25	0/2282
All	All	0.30	0/6529	0.26	1/8833 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	315	M3L	O-C-N	8.31	135.99	122.70

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	1382	0	1374	16	0
2	B	3385	0	3415	44	0
3	C	1659	0	1643	16	0
4	B	8	0	12	0	0
4	C	8	0	12	1	0
5	B	31	0	12	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	26	0	19	0	0
8	A	7	0	0	0	0
8	B	40	0	0	0	0
8	C	11	0	0	0	0
All	All	6558	0	6487	67	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 5.

All (67) 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:A:372:VAL:HG11	1:A:376:PHE:HD2	1.30	0.95
2:B:284:SER:HA	2:B:287:ARG:HD3	1.53	0.90
2:B:394:VAL:HA	2:B:449:MET:HG2	1.54	0.89
1:A:372:VAL:HG13	1:A:376:PHE:HB3	1.64	0.80
1:A:372:VAL:HG11	1:A:376:PHE:CD2	2.18	0.76
1:A:372:VAL:CG1	1:A:376:PHE:CD2	2.71	0.73
1:A:372:VAL:CG1	1:A:376:PHE:HD2	1.99	0.73
1:A:355:ARG:HG2	2:B:222:LEU:HD21	1.74	0.70
2:B:284:SER:HA	2:B:287:ARG:CD	2.21	0.70
2:B:270:ASN:HB3	2:B:273:GLU:HB3	1.77	0.67
2:B:314:GLU:OE2	3:C:179:GLY:HA3	1.95	0.66
3:C:66:LEU:HB3	3:C:90:ALA:HB2	1.76	0.66
2:B:31:ALA:HA	2:B:83:ARG:HB3	1.79	0.64
1:A:372:VAL:CG1	1:A:376:PHE:HB3	2.26	0.63
2:B:116:VAL:HG22	2:B:165:VAL:HG12	1.79	0.62
1:A:347:LEU:HD13	2:B:226:HIS:CE1	2.36	0.61
1:A:372:VAL:HG13	1:A:376:PHE:CB	2.31	0.60
1:A:412:THR:HA	1:A:448:THR:HA	1.84	0.59
2:B:113:ARG:HG3	2:B:181:VAL:HB	1.87	0.56
1:A:372:VAL:HG13	1:A:376:PHE:CD2	2.42	0.56
2:B:211:LYS:HD3	2:B:211:LYS:H	1.73	0.52
2:B:125:GLY:HA2	2:B:436:THR:HG22	1.92	0.52
2:B:40:SER:HB2	2:B:83:ARG:HB2	1.93	0.51
2:B:136:LYS:O	2:B:140:LEU:HB2	2.12	0.50
1:A:421:ARG:HA	1:A:424:LEU:HD12	1.94	0.50
3:C:153:GLU:O	3:C:157:LYS:HG2	2.11	0.49
2:B:181:VAL:HG12	2:B:183:HIS:CD2	2.48	0.48
1:A:396:LEU:HD23	1:A:461:HIS:NE2	2.28	0.48
1:A:323:VAL:HG23	1:A:404:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:THR:HG22	2:B:251:LYS:HD3	1.95	0.47
2:B:119:ILE:O	2:B:122:THR:HG22	2.15	0.46
2:B:74:ASP:HB3	2:B:77:CYS:HB2	1.96	0.46
2:B:185:GLU:H	2:B:185:GLU:HG3	1.44	0.46
2:B:153:LEU:HD11	2:B:160:ALA:HB1	1.97	0.46
2:B:315:M3L:CM2	3:C:43:TRP:CE2	2.99	0.46
3:C:71:VAL:HG13	3:C:92:VAL:HG22	1.97	0.46
1:A:347:LEU:HD13	2:B:226:HIS:NE2	2.31	0.45
2:B:315:M3L:HM13	3:C:147:TYR:CD1	2.53	0.44
2:B:181:VAL:HG12	2:B:183:HIS:HD2	1.83	0.44
2:B:240:GLY:HA2	2:B:343:VAL:O	2.17	0.44
2:B:122:THR:HG23	2:B:161:VAL:HG13	1.99	0.44
2:B:153:LEU:HD23	2:B:162:GLU:HG2	2.00	0.43
2:B:315:M3L:HM13	3:C:147:TYR:CG	2.53	0.43
2:B:187:GLU:HG2	2:B:188:PRO:HD2	2.01	0.43
2:B:136:LYS:HB3	2:B:137:PRO:HD3	2.01	0.43
2:B:56:THR:HG21	2:B:108:VAL:HG21	2.01	0.43
2:B:224:LEU:HD22	2:B:298:PRO:HB2	2.01	0.42
3:C:201:ILE:HD11	3:C:219:TYR:CG	2.54	0.42
2:B:192:GLU:HB2	2:B:195:GLU:HG3	2.02	0.42
2:B:223:PRO:HB3	2:B:237:PRO:HB3	2.00	0.42
2:B:153:LEU:HD21	2:B:160:ALA:HB1	2.00	0.42
2:B:287:ARG:HA	2:B:331:LEU:HD21	2.01	0.42
2:B:26:LEU:HD13	2:B:41:LEU:HD21	2.02	0.41
1:A:347:LEU:HD23	1:A:351:ASP:HB3	2.02	0.41
2:B:106:PRO:HA	2:B:107:ASP:HA	1.87	0.41
2:B:385:THR:HA	2:B:388:MET:HG2	2.03	0.41
3:C:17:VAL:HG12	3:C:31:GLN:HA	2.02	0.41
3:C:152:LEU:HD22	3:C:187:LYS:HB3	2.03	0.41
3:C:169:ILE:HB	3:C:220:ILE:HB	2.03	0.41
2:B:116:VAL:CG1	2:B:163:PHE:HB3	2.51	0.41
3:C:20:LEU:HA	4:C:301:EDO:H22	2.03	0.41
2:B:201:VAL:HG12	2:B:257:ALA:HB2	2.03	0.41
3:C:15:SER:OG	3:C:32:GLN:O	2.28	0.40
2:B:299:ALA:HB3	2:B:341:VAL:HG22	2.02	0.40
3:C:113:HIS:CD2	3:C:114:LEU:HG	2.56	0.40
2:B:315:M3L:HM22	3:C:43:TRP:CE2	2.56	0.40
2:B:359:ARG:HD2	3:C:212:SER:OG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	165/190 (87%)	155 (94%)	10 (6%)	0	100	100
2	B	429/481 (89%)	413 (96%)	14 (3%)	2 (0%)	29	68
3	C	209/224 (93%)	201 (96%)	7 (3%)	1 (0%)	29	68
All	All	803/895 (90%)	769 (96%)	31 (4%)	3 (0%)	34	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	362	ARG
3	C	147	TYR
2	B	106	PRO

5.3.2 Protein sidechains ⓘ

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	149/164 (91%)	140 (94%)	9 (6%)	19	53
2	B	367/409 (90%)	346 (94%)	21 (6%)	20	56
3	C	180/197 (91%)	168 (93%)	12 (7%)	16	49
All	All	696/770 (90%)	654 (94%)	42 (6%)	19	53

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	VAL
1	A	332	ARG
1	A	347	LEU
1	A	349	VAL
1	A	364	LYS
1	A	366	LEU
1	A	385	LEU
1	A	390	LYS
1	A	454	LEU
2	B	24	ASN
2	B	55	ASP
2	B	65	ARG
2	B	95	ARG
2	B	122	THR
2	B	155	ARG
2	B	171	SER
2	B	173	TYR
2	B	185	GLU
2	B	194	GLU
2	B	200	GLU
2	B	211	LYS
2	B	239	ARG
2	B	286	LEU
2	B	287	ARG
2	B	294	GLU
2	B	327	GLN
2	B	328	LEU
2	B	329	LEU
2	B	335	LEU
2	B	402	GLU
3	C	13	LEU
3	C	20	LEU
3	C	34	SER
3	C	67	SER
3	C	73	GLU
3	C	83	LEU
3	C	109	ASN
3	C	144	ASP
3	C	148	TYR
3	C	159	LEU
3	C	206	HIS
3	C	221	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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	0.99	1 (10%)	9,14,16	0.25	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	-	1/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	M3L	O-C	3.02	1.32	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	315	M3L	4	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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	EDO	B	501	-	3,3,3	0.64	0	2,2,2	0.29	0
7	SAH	C	302	-	24,28,28	0.68	0	25,40,40	1.12	3 (12%)
4	EDO	C	303	-	3,3,3	0.55	0	2,2,2	0.35	0
4	EDO	B	502	-	3,3,3	0.56	0	2,2,2	0.35	0
4	EDO	C	301	-	3,3,3	0.57	0	2,2,2	0.34	0
5	ATP	B	503	6	26,33,33	0.62	0	31,52,52	0.62	1 (3%)

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	EDO	B	501	-	-	0/1/1/1	-
7	SAH	C	302	-	-	5/11/31/31	0/3/3/3
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	B	502	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
5	ATP	B	503	6	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	302	SAH	CB-CG-SD	-3.23	106.07	113.31
7	C	302	SAH	CB-CA-N	2.78	117.46	110.17
7	C	302	SAH	C5-C6-N6	2.30	123.84	120.35
5	B	503	ATP	C5-C6-N6	2.23	123.75	120.35

There are no chirality outliers.

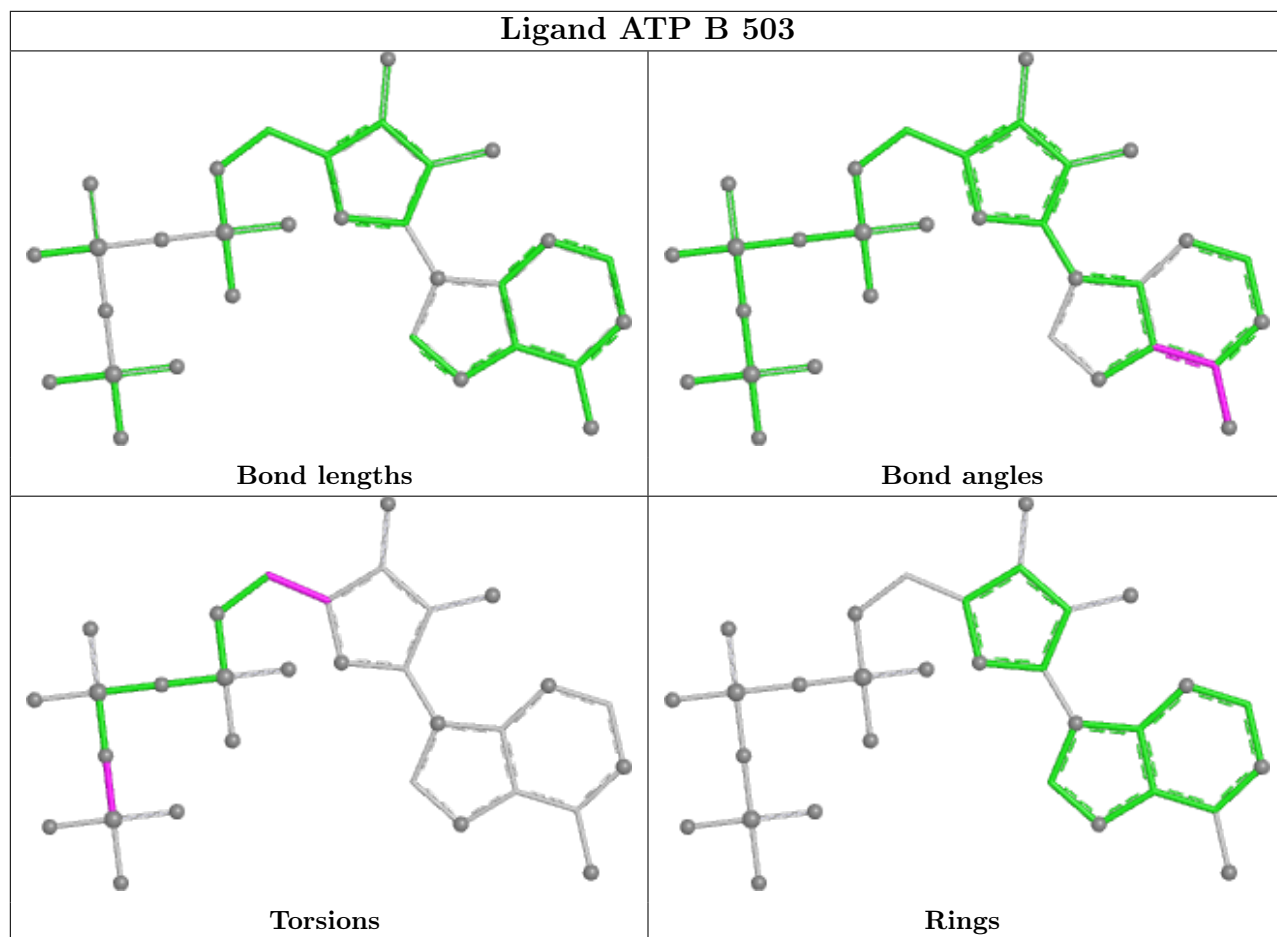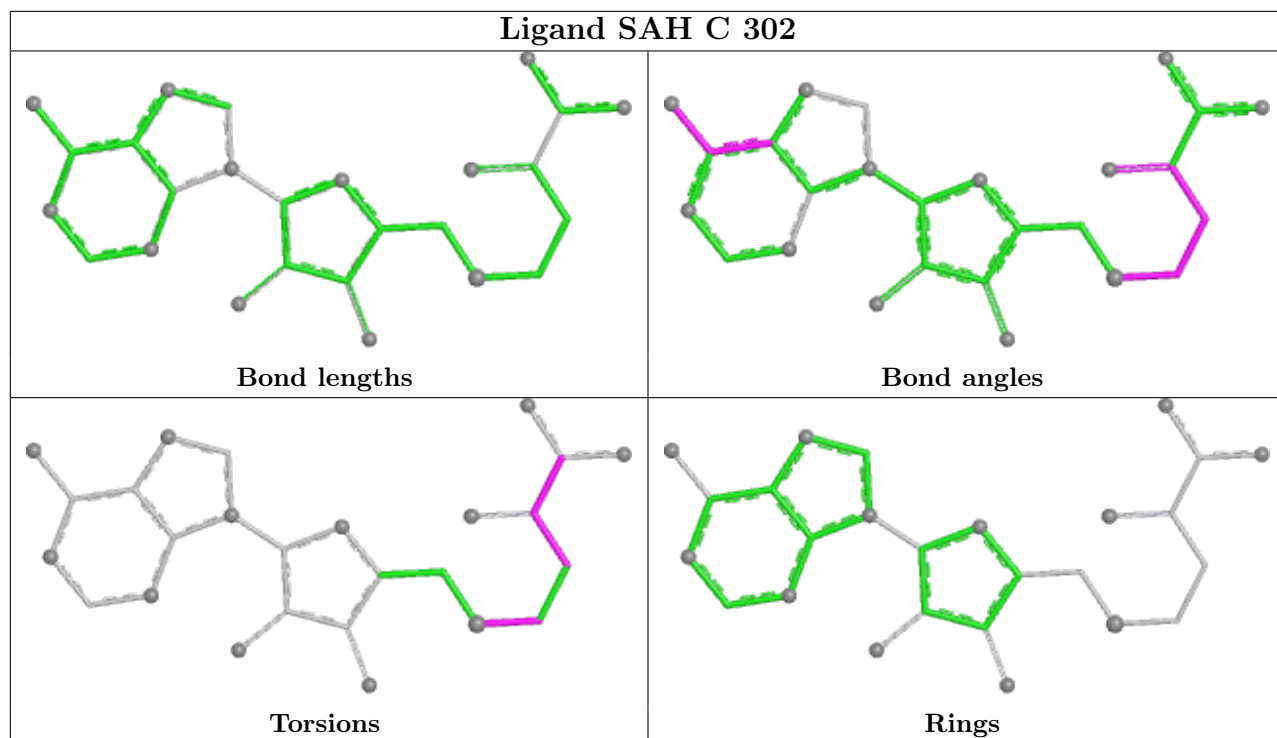All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	503	ATP	PB-O3B-PG-O2G
5	B	503	ATP	O4'-C4'-C5'-O5'
5	B	503	ATP	C3'-C4'-C5'-O5'
7	C	302	SAH	N-CA-CB-CG
7	C	302	SAH	C-CA-CB-CG
7	C	302	SAH	O-C-CA-N
7	C	302	SAH	OXT-C-CA-N
7	C	302	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SAH C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 503

Bond lengths

Bond angles

Torsions

Rings

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	171/190 (90%)	0.97	23 (13%)	3	1	66, 84, 118, 129	0
2	B	433/481 (90%)	0.52	18 (4%)	36	14	52, 75, 94, 99	0
3	C	211/224 (94%)	0.53	8 (3%)	40	16	61, 75, 88, 102	0
All	All	815/895 (91%)	0.61	49 (6%)	21	7	52, 77, 101, 129	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	THR	5.6
2	B	338	ARG	5.6
1	A	372	VAL	4.6
3	C	14	ARG	4.3
2	B	337	GLN	3.8
3	C	61	ASP	3.6
1	A	338	ALA	3.5
2	B	278	LEU	3.5
2	B	193	ASP	3.2
3	C	15	SER	3.1
1	A	332	ARG	3.0
1	A	379	ALA	2.9
2	B	27	ILE	2.9
1	A	450	PHE	2.9
2	B	281	GLU	2.8
2	B	50	GLN	2.7
1	A	377	ARG	2.7
1	A	390	LYS	2.7
2	B	244	TYR	2.6
1	A	404	GLN	2.5
2	B	288	LYS	2.5
1	A	470	VAL	2.5
3	C	31	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	29	ARG	2.5
1	A	486	ALA	2.5
1	A	423	HIS	2.5
1	A	403	LEU	2.4
1	A	410	SER	2.3
3	C	152	LEU	2.3
1	A	491	ALA	2.3
1	A	449	LEU	2.3
2	B	318	GLY	2.3
2	B	364	ASP	2.2
3	C	131	GLU	2.2
2	B	324	ILE	2.2
1	A	378	GLU	2.2
1	A	492	ARG	2.2
1	A	409	PRO	2.1
1	A	493	TYR	2.1
1	A	468	ALA	2.1
2	B	339	ALA	2.1
2	B	23	PRO	2.1
2	B	112	LYS	2.1
1	A	405	GLY	2.1
2	B	26	LEU	2.0
3	C	66	LEU	2.0
2	B	285	ASN	2.0
1	A	476	LEU	2.0
2	B	428	ASP	2.0

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

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.

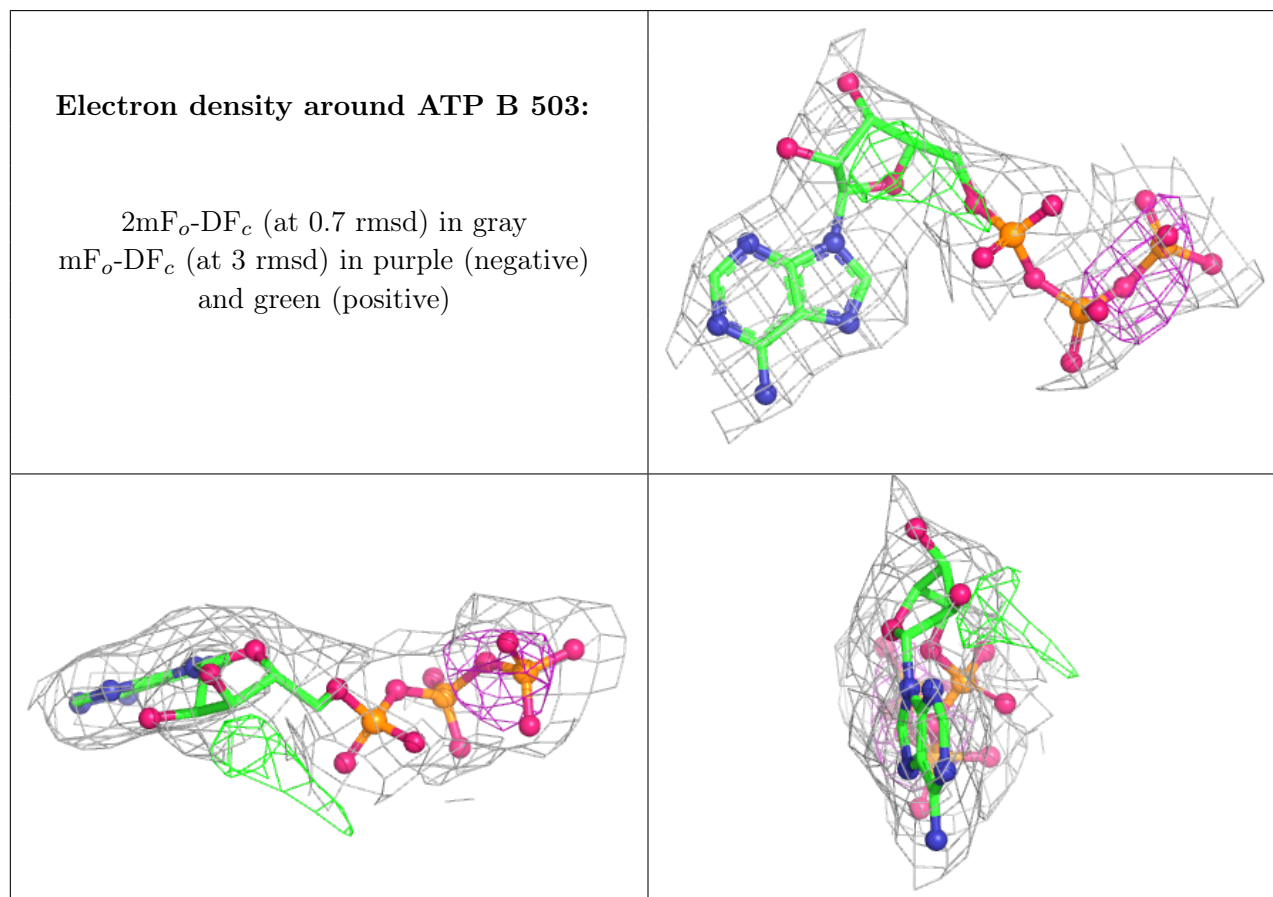| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	M3L	B	315	12/13	0.94	0.36	79,79,81,129	0

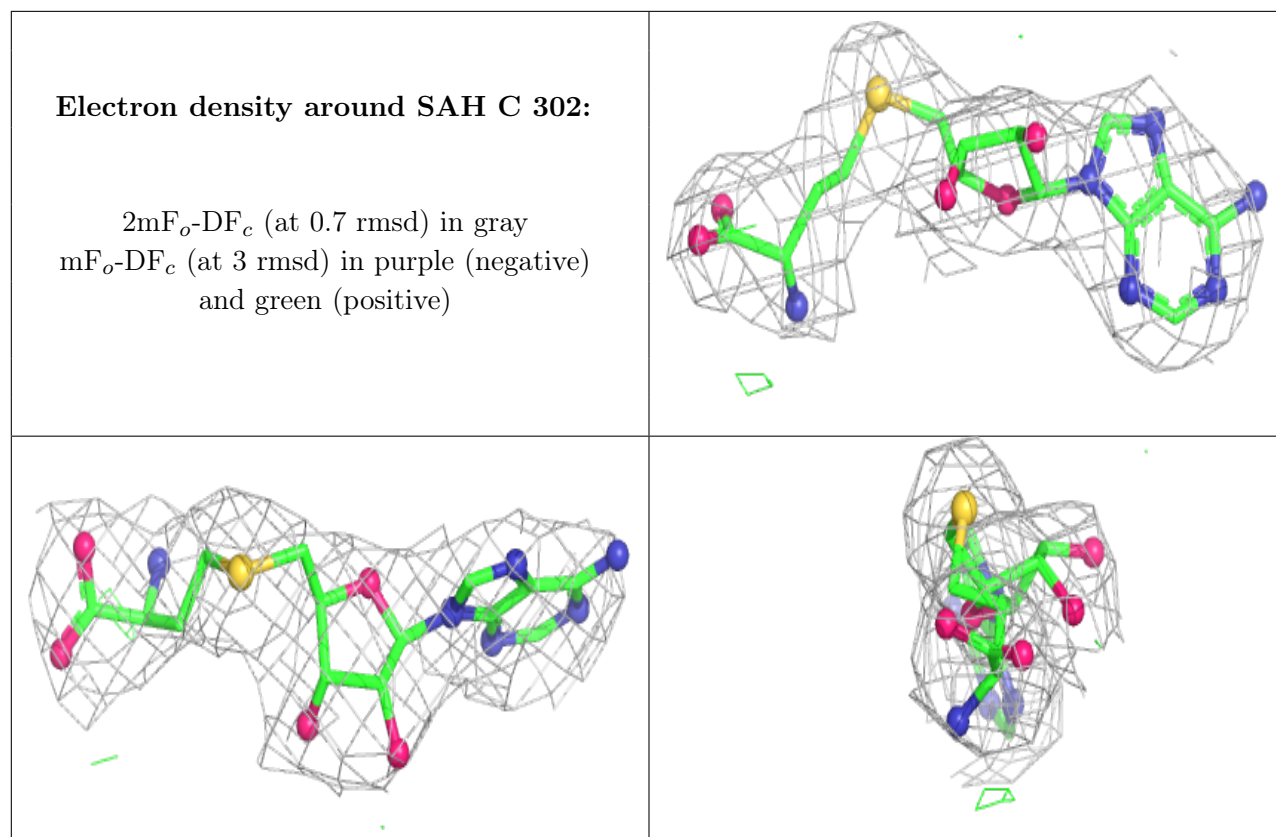## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	EDO	C	303	4/4	0.82	0.27	87,87,87,87	0
4	EDO	B	502	4/4	0.87	0.18	72,72,72,72	0
4	EDO	C	301	4/4	0.89	0.20	73,73,73,73	0
5	ATP	B	503	31/31	0.91	0.21	75,77,81,81	0
4	EDO	B	501	4/4	0.92	0.23	60,60,60,60	0
6	MG	B	504	1/1	0.93	0.10	72,72,72,72	0
7	SAH	C	302	26/26	0.94	0.23	75,77,77,77	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 ATP B 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around SAH C 302:

$2mF_o$-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 ⓘ

There are no such residues in this entry.