



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:04 PM UTC

PDB ID : 3F9X / pdb_00003f9x
Title : Structural Insights into Lysine Multiple Methylation by SET Domain Methyltransferases, SET8-Y334F / H4-Lys20me2 / AdoHcy
Authors : Couture, J.-F.; Dirk, L.M.A.; Brunzelle, J.S.; Houtz, R.L.; Trievel, R.C.
Deposited on : 2008-11-14
Resolution : 1.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

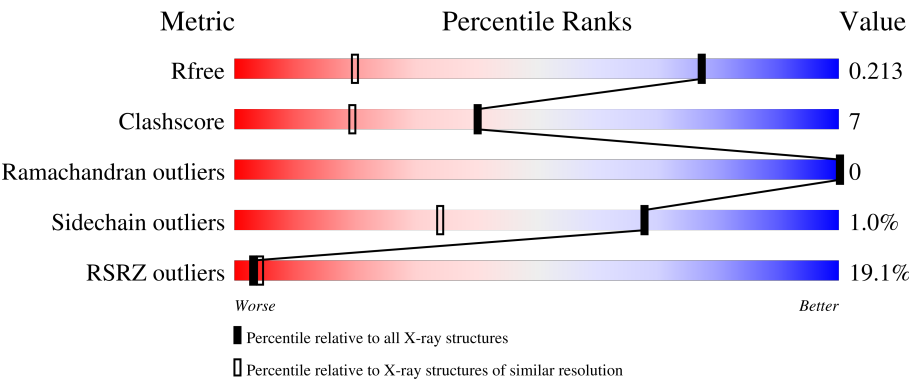
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.25 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.



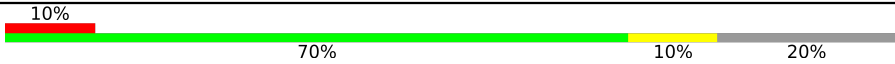
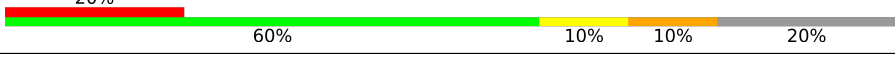
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	166	25% 89% 8% .
1	B	166	14% 87% 9% ..
1	C	166	23% 87% 9% ..
1	D	166	8% 86% 11% ..
2	E	10	30% 40% 50% 10%

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Mol	Chain	Length	Quality of chain
2	F	10	
2	G	10	
2	H	10	

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
2	MLY	H	20	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6407 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 Histone-lysine N-methyltransferase SETD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1278	799	225	248	6			
1	B	160	Total	C	N	O	S	0	0	0
			1278	799	225	248	6			
1	C	160	Total	C	N	O	S	0	0	0
			1278	799	225	248	6			
1	D	161	Total	C	N	O	S	0	0	0
			1283	802	226	249	6			

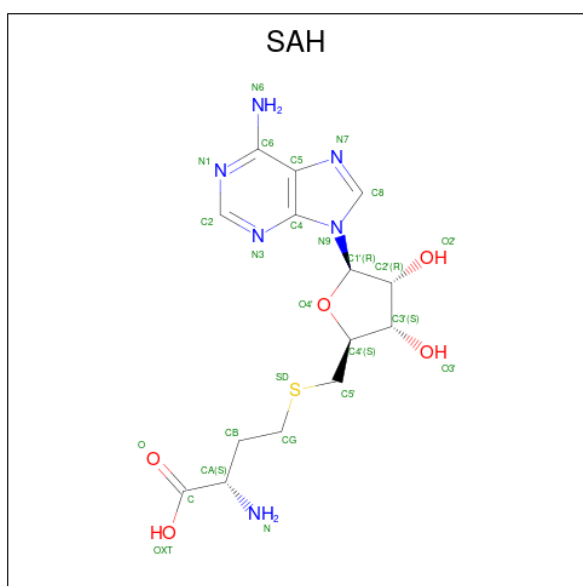
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	expression tag	UNP Q9NQR1
A	188	ALA	-	expression tag	UNP Q9NQR1
A	189	MET	-	expression tag	UNP Q9NQR1
A	190	GLY	-	expression tag	UNP Q9NQR1
A	334	PHE	TYR	engineered mutation	UNP Q9NQR1
B	187	GLY	-	expression tag	UNP Q9NQR1
B	188	ALA	-	expression tag	UNP Q9NQR1
B	189	MET	-	expression tag	UNP Q9NQR1
B	190	GLY	-	expression tag	UNP Q9NQR1
B	334	PHE	TYR	engineered mutation	UNP Q9NQR1
C	187	GLY	-	expression tag	UNP Q9NQR1
C	188	ALA	-	expression tag	UNP Q9NQR1
C	189	MET	-	expression tag	UNP Q9NQR1
C	190	GLY	-	expression tag	UNP Q9NQR1
C	334	PHE	TYR	engineered mutation	UNP Q9NQR1
D	187	GLY	-	expression tag	UNP Q9NQR1
D	188	ALA	-	expression tag	UNP Q9NQR1
D	189	MET	-	expression tag	UNP Q9NQR1
D	190	GLY	-	expression tag	UNP Q9NQR1
D	334	PHE	TYR	engineered mutation	UNP Q9NQR1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	9	Total	C	N	O	0	0	0
			87	53	22	12			
2	F	8	Total	C	N	O	0	0	0
			74	46	20	8			
2	G	9	Total	C	N	O	0	0	0
			83	50	21	12			
2	H	8	Total	C	N	O	0	0	0
			78	49	21	8			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	169	Total	O	0	0
			169	169		

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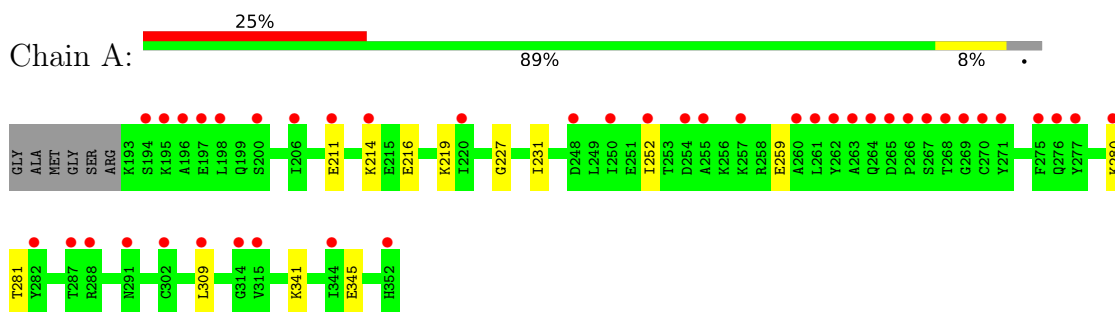
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	213	Total 213	O 213	0	0
4	C	190	Total 190	O 190	0	0
4	D	254	Total 254	O 254	0	0
4	E	15	Total 15	O 15	0	0
4	F	9	Total 9	O 9	0	0
4	G	9	Total 9	O 9	0	0
4	H	5	Total 5	O 5	0	0

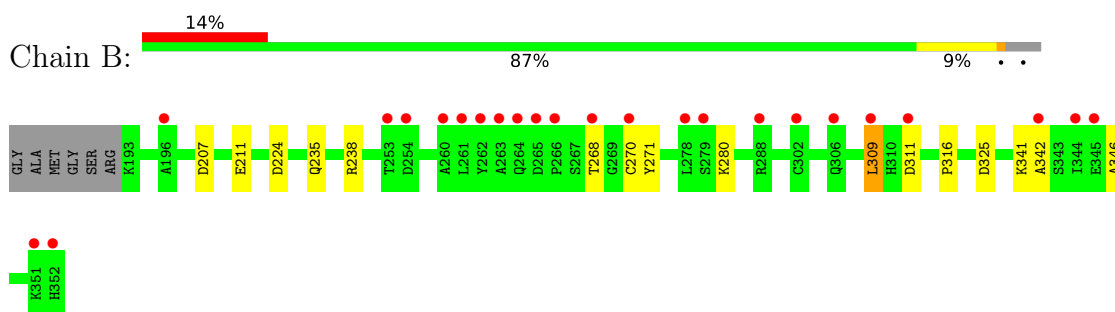
3 Residue-property plots [i](#)

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.

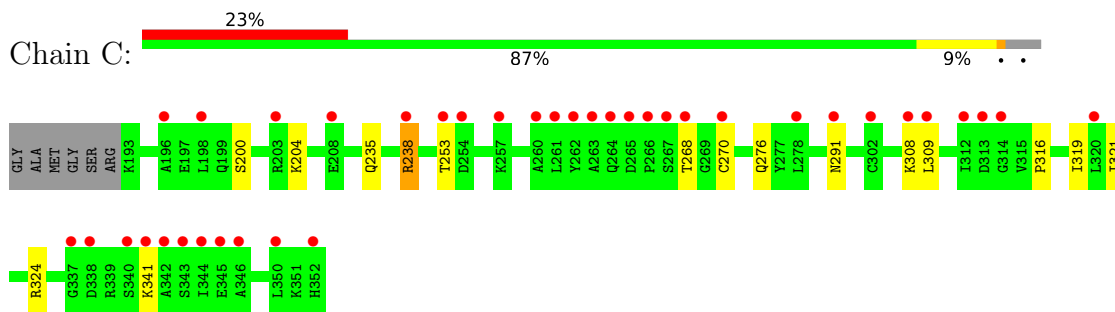
- Molecule 1: Histone-lysine N-methyltransferase SETD8



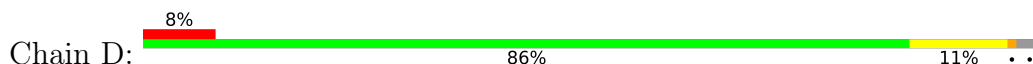
- Molecule 1: Histone-lysine N-methyltransferase SETD8

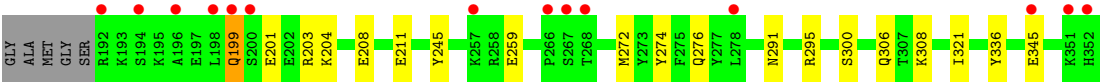


- Molecule 1: Histone-lysine N-methyltransferase SETD8

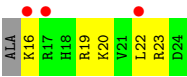


- Molecule 1: Histone-lysine N-methyltransferase SETD8

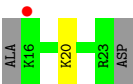




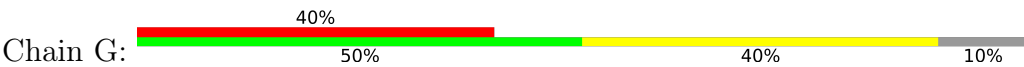
● Molecule 2: Histone H4



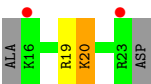
● Molecule 2: Histone H4



● Molecule 2: Histone H4



● Molecule 2: Histone H4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.11Å 45.74Å 94.76Å 89.45° 87.59° 89.90°	Depositor
Resolution (Å)	47.35 – 1.25 47.35 – 1.25	Depositor EDS
% Data completeness (in resolution range)	94.3 (47.35-1.25) 94.3 (47.35-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.207 0.187 , 0.213	Depositor DCC
R_{free} test set	9694 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,-h,l 0.000 for -k,h,l 0.011 for h,-k,-l 0.013 for -h,k,-l 0.003 for -h,-k,l 0.003 for k,h,-l 0.001 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4848e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MLY, 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	0.69	0/1300	0.79	0/1743
1	B	0.75	0/1300	0.85	1/1743 (0.1%)
1	C	0.71	0/1300	0.81	2/1743 (0.1%)
1	D	0.81	1/1305 (0.1%)	0.82	0/1750
2	E	1.23	1/76 (1.3%)	0.81	0/97
2	F	0.67	0/63	0.82	0/82
2	G	0.67	0/72	0.79	0/93
2	H	0.75	0/67	0.82	0/86
All	All	0.75	2/5483 (0.0%)	0.82	3/7337 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	22	LEU	CA-C	8.56	1.62	1.52
1	D	321	ILE	CA-CB	5.44	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	268	THR	N-CA-C	7.14	118.85	111.14
1	B	268	THR	N-CA-C	5.57	117.03	111.07
1	C	238	ARG	NE-CZ-NH1	5.18	126.68	121.50

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	1278	0	1259	9	0
1	B	1278	0	1259	16	0
1	C	1278	0	1259	17	0
1	D	1283	0	1261	19	0
2	E	87	0	97	10	0
2	F	74	0	82	2	0
2	G	83	0	86	2	0
2	H	78	0	93	10	0
3	A	26	0	19	2	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
4	A	169	0	0	3	1
4	B	213	0	0	9	0
4	C	190	0	0	6	1
4	D	254	0	0	16	1
4	E	15	0	0	5	0
4	F	9	0	0	0	0
4	G	9	0	0	0	0
4	H	5	0	0	0	0
All	All	6407	0	5472	73	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (73) 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:E:19:ARG:C	4:E:824:HOH:O	2.00	1.03
1:D:291:ASN:HB3	4:D:828:HOH:O	1.58	1.02
4:D:833:HOH:O	2:H:19:ARG:HB2	1.60	0.99
1:C:235:GLN:HG3	4:C:825:HOH:O	1.70	0.91
1:D:345:GLU:HG2	4:D:764:HOH:O	1.72	0.88
4:C:627:HOH:O	2:H:19:ARG:HD2	1.75	0.85
1:B:311:ASP:CG	4:B:843:HOH:O	2.24	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:GLU:HG3	4:D:473:HOH:O	1.83	0.77
1:C:235:GLN:CG	4:C:825:HOH:O	2.30	0.74
1:D:245:TYR:OH	2:H:20:MLY:HH12	1.87	0.74
1:B:325:ASP:HB3	4:B:829:HOH:O	1.90	0.71
1:C:291:ASN:HB2	4:C:457:HOH:O	1.90	0.71
1:B:346:ALA:HB2	2:E:16:LYS:HE3	1.73	0.70
1:D:203:ARG:HD3	4:D:706:HOH:O	1.90	0.70
1:B:270:CYS:O	2:E:20:MLY:HH21	1.93	0.69
1:B:235:GLN:CG	4:B:829:HOH:O	2.42	0.68
1:A:341:LYS:O	1:A:345:GLU:HG3	1.94	0.67
4:A:845:HOH:O	1:C:253:THR:HG21	1.95	0.66
1:A:219:LYS:HE2	1:A:231:ILE:HD11	1.78	0.66
1:D:201:GLU:OE2	4:D:384:HOH:O	2.15	0.62
4:A:450:HOH:O	1:C:341:LYS:HB2	1.99	0.62
2:E:19:ARG:O	4:E:824:HOH:O	2.11	0.60
1:B:311:ASP:CB	4:B:843:HOH:O	2.50	0.59
3:A:801:SAH:SD	2:F:20:MLY:CH2	2.90	0.59
1:A:259:GLU:CD	4:A:820:HOH:O	2.47	0.58
3:A:801:SAH:SD	2:F:20:MLY:HH23	2.44	0.58
1:A:252:ILE:H	1:A:280:LYS:HZ1	1.52	0.57
1:B:207:ASP:O	1:B:211:GLU:HG3	2.05	0.55
1:C:270:CYS:O	2:G:20:MLY:HH21	2.06	0.55
1:D:276:GLN:NE2	4:D:777:HOH:O	2.39	0.55
1:C:308:LYS:HG3	1:C:319:ILE:CG1	2.36	0.55
1:D:259:GLU:HG2	1:D:272:MET:SD	2.46	0.55
4:D:835:HOH:O	2:H:20:MLY:CD	2.55	0.55
2:E:23:ARG:HB3	4:E:334:HOH:O	2.06	0.54
1:B:235:GLN:CD	4:B:829:HOH:O	2.51	0.53
4:D:835:HOH:O	2:H:20:MLY:HD3	2.10	0.51
1:D:306:GLN:HG2	1:D:308:LYS:HE3	1.91	0.51
1:D:211:GLU:CD	4:D:434:HOH:O	2.54	0.50
1:D:204:LYS:NZ	4:D:851:HOH:O	2.44	0.49
4:D:835:HOH:O	2:H:20:MLY:HE2	2.12	0.49
1:C:238:ARG:CZ	1:C:324:ARG:HA	2.42	0.49
1:B:341:LYS:HD2	4:B:377:HOH:O	2.12	0.49
1:B:271:TYR:HA	2:E:20:MLY:HH12	1.95	0.48
1:D:274:TYR:CE2	2:H:19:ARG:HD3	2.49	0.48
2:E:19:ARG:CB	4:E:824:HOH:O	2.61	0.48
1:C:308:LYS:HG3	1:C:319:ILE:HG12	1.95	0.48
1:B:342:ALA:HB1	2:E:16:LYS:HD2	1.96	0.47
2:E:19:ARG:HB2	4:E:824:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:GLU:CG	4:D:473:HOH:O	2.55	0.46
1:B:235:GLN:HG3	4:B:829:HOH:O	2.10	0.46
1:A:214:LYS:HG2	1:A:216:GLU:HG3	1.98	0.46
1:A:280:LYS:HG3	1:A:281:THR:N	2.29	0.46
1:D:300:SER:OG	4:D:390:HOH:O	2.21	0.46
1:A:309:LEU:HD13	1:A:309:LEU:C	2.41	0.45
1:C:308:LYS:HE3	1:C:321:ILE:HD13	1.98	0.45
1:D:295:ARG:O	2:H:20:MLY:HH11	2.17	0.45
1:A:280:LYS:HD2	1:B:224:ASP:OD2	2.16	0.45
1:D:336:TYR:CE1	2:H:20:MLY:HH22	2.52	0.45
2:E:23:ARG:HD2	2:E:23:ARG:C	2.41	0.45
1:C:200:SER:OG	1:C:204:LYS:NZ	2.49	0.45
1:B:238:ARG:NH1	4:B:387:HOH:O	2.50	0.45
1:A:227:GLY:HA2	1:C:276:GLN:NE2	2.33	0.44
1:B:311:ASP:HB2	4:B:843:HOH:O	2.17	0.44
1:C:308:LYS:HD2	1:C:321:ILE:HG21	2.01	0.42
1:D:199:GLN:NE2	4:D:503:HOH:O	2.50	0.42
4:C:667:HOH:O	2:G:22:LEU:HD23	2.20	0.42
1:D:291:ASN:CB	4:D:828:HOH:O	2.39	0.41
1:C:309:LEU:HD11	1:C:316:PRO:HB2	2.02	0.41
1:C:235:GLN:CD	4:C:825:HOH:O	2.60	0.41
1:C:308:LYS:CG	1:C:319:ILE:HG13	2.51	0.41
1:B:309:LEU:HD21	1:B:316:PRO:HB2	2.03	0.41
1:C:308:LYS:HG3	1:C:319:ILE:HG13	2.02	0.40
1:D:336:TYR:CZ	2:H:20:MLY:HH22	2.56	0.40

All (2) 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)
4:A:841:HOH:O	4:C:383:HOH:O[1_545]	1.94	0.26
4:D:404:HOH:O	4:D:851:HOH:O[1_455]	2.14	0.06

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	158/166 (95%)	155 (98%)	3 (2%)	0	100	100
1	B	158/166 (95%)	155 (98%)	3 (2%)	0	100	100
1	C	158/166 (95%)	157 (99%)	1 (1%)	0	100	100
1	D	159/166 (96%)	158 (99%)	1 (1%)	0	100	100
2	E	6/10 (60%)	6 (100%)	0	0	100	100
2	F	5/10 (50%)	5 (100%)	0	0	100	100
2	G	6/10 (60%)	6 (100%)	0	0	100	100
2	H	5/10 (50%)	5 (100%)	0	0	100	100
All	All	655/704 (93%)	647 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	136/139 (98%)	135 (99%)	1 (1%)	76	47
1	B	136/139 (98%)	134 (98%)	2 (2%)	57	20
1	C	136/139 (98%)	136 (100%)	0	100	100
1	D	136/139 (98%)	135 (99%)	1 (1%)	76	47
2	E	8/8 (100%)	8 (100%)	0	100	100
2	F	6/8 (75%)	6 (100%)	0	100	100
2	G	7/8 (88%)	5 (71%)	2 (29%)	0	0
2	H	7/8 (88%)	7 (100%)	0	100	100
All	All	572/588 (97%)	566 (99%)	6 (1%)	68	34

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	GLU
1	B	280	LYS
1	B	309	LEU
1	D	199	GLN
2	G	23	ARG
2	G	24	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	199	GLN
1	D	276	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	MLY	G	20	2	9,10,11	0.67	0	6,11,13	0.57	0
2	MLY	H	20	2	9,10,11	1.17	0	6,11,13	1.88	1 (16%)
2	MLY	E	20	2	9,10,11	0.70	0	6,11,13	0.69	0
2	MLY	F	20	2	9,10,11	0.58	0	6,11,13	0.77	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	MLY	G	20	2	-	0/8/9/11	-
2	MLY	H	20	2	-	1/8/9/11	-
2	MLY	E	20	2	-	1/8/9/11	-
2	MLY	F	20	2	-	0/8/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	20	MLY	CH1-NZ-CE	3.99	126.59	110.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	20	MLY	O-C-CA-CB
2	H	20	MLY	CD-CE-NZ-CH2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	20	MLY	1	0
2	H	20	MLY	7	0
2	E	20	MLY	2	0
2	F	20	MLY	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	SAH	C	801	-	27,28,28	0.87	0	36,40,40	1.41	6 (16%)
3	SAH	D	801	-	27,28,28	0.93	1 (3%)	36,40,40	1.09	4 (11%)
3	SAH	B	801	-	27,28,28	0.88	1 (3%)	36,40,40	1.28	6 (16%)
3	SAH	A	801	-	27,28,28	1.00	2 (7%)	36,40,40	1.77	8 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	C	801	-	-	1/15/31/31	0/3/3/3
3	SAH	D	801	-	-	1/15/31/31	0/3/3/3
3	SAH	B	801	-	-	1/15/31/31	0/3/3/3
3	SAH	A	801	-	-	1/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	SAH	C2-N1	2.55	1.38	1.33
3	A	801	SAH	C2-N3	2.16	1.37	1.33
3	B	801	SAH	OXT-C	-2.16	1.23	1.30
3	D	801	SAH	OXT-C	-2.13	1.23	1.30

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	SAH	N3-C2-N1	-5.33	120.52	128.58
3	A	801	SAH	N9-C8-N7	-4.09	108.14	113.94
3	C	801	SAH	N3-C2-N1	-4.07	122.43	128.58
3	A	801	SAH	C5-N7-C8	3.56	109.05	103.45
3	A	801	SAH	C5-C4-N3	-3.05	122.52	126.72
3	C	801	SAH	N9-C8-N7	-3.04	109.62	113.94
3	B	801	SAH	N9-C8-N7	-3.02	109.64	113.94
3	C	801	SAH	CB-CG-SD	-2.93	106.91	113.45
3	B	801	SAH	N3-C2-N1	-2.79	124.36	128.58
3	A	801	SAH	C4-C5-N7	-2.68	107.52	110.58
3	D	801	SAH	N9-C8-N7	-2.64	110.19	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	SAH	C5-C4-N3	-2.60	123.13	126.72
3	B	801	SAH	C4-C5-N7	-2.59	107.62	110.58
3	A	801	SAH	C2-N3-C4	2.54	118.04	111.83
3	A	801	SAH	C4-N9-C8	2.46	108.32	105.74
3	B	801	SAH	C5-N7-C8	2.43	107.27	103.45
3	D	801	SAH	C4-C5-N7	-2.43	107.81	110.58
3	C	801	SAH	C2-N1-C6	2.33	122.56	118.73
3	D	801	SAH	C5-N7-C8	2.31	107.08	103.45
3	C	801	SAH	C4-N9-C8	2.30	108.16	105.74
3	B	801	SAH	C4-N9-C8	2.25	108.10	105.74
3	C	801	SAH	C5-N7-C8	2.21	106.92	103.45
3	A	801	SAH	C2-N1-C6	2.11	122.19	118.73
3	D	801	SAH	C5-C4-N9	2.10	108.11	105.81

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	801	SAH	CB-CG-SD-C5'
3	D	801	SAH	CB-CG-SD-C5'
3	B	801	SAH	CB-CG-SD-C5'
3	A	801	SAH	CB-CG-SD-C5'

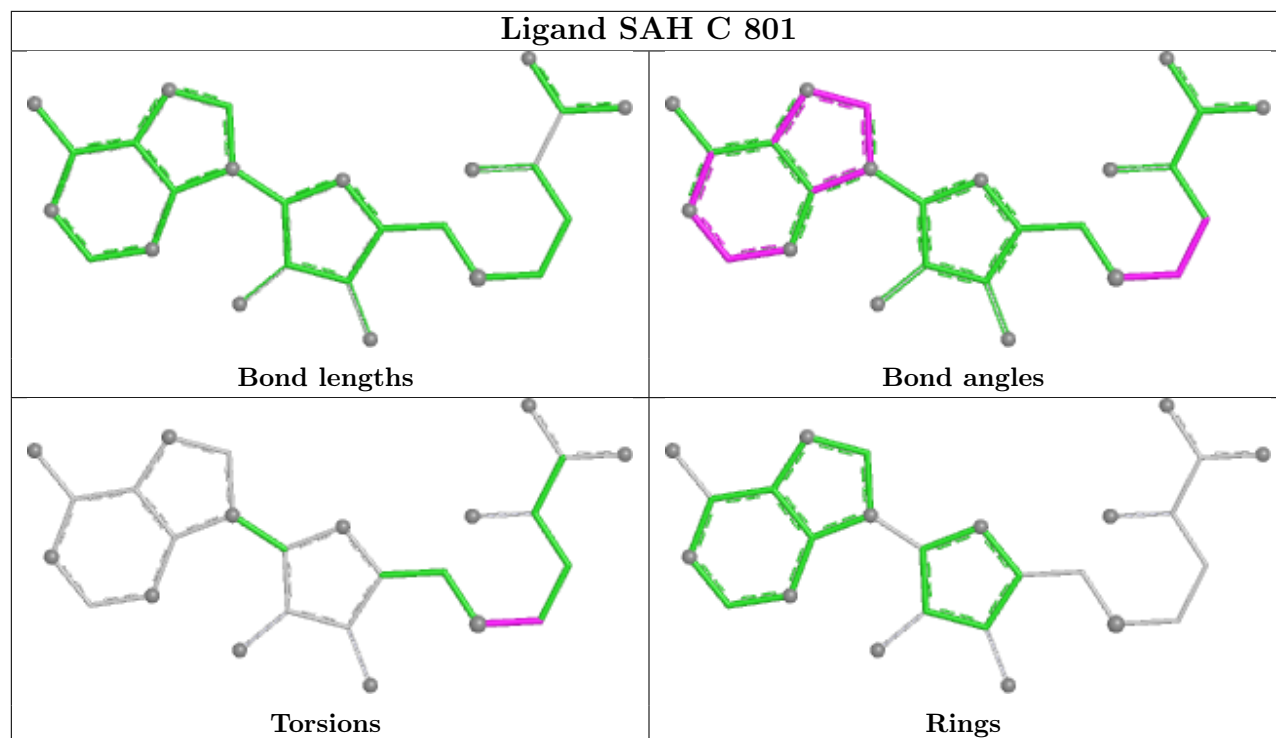
There are no ring outliers.

1 monomer is involved in 2 short contacts:

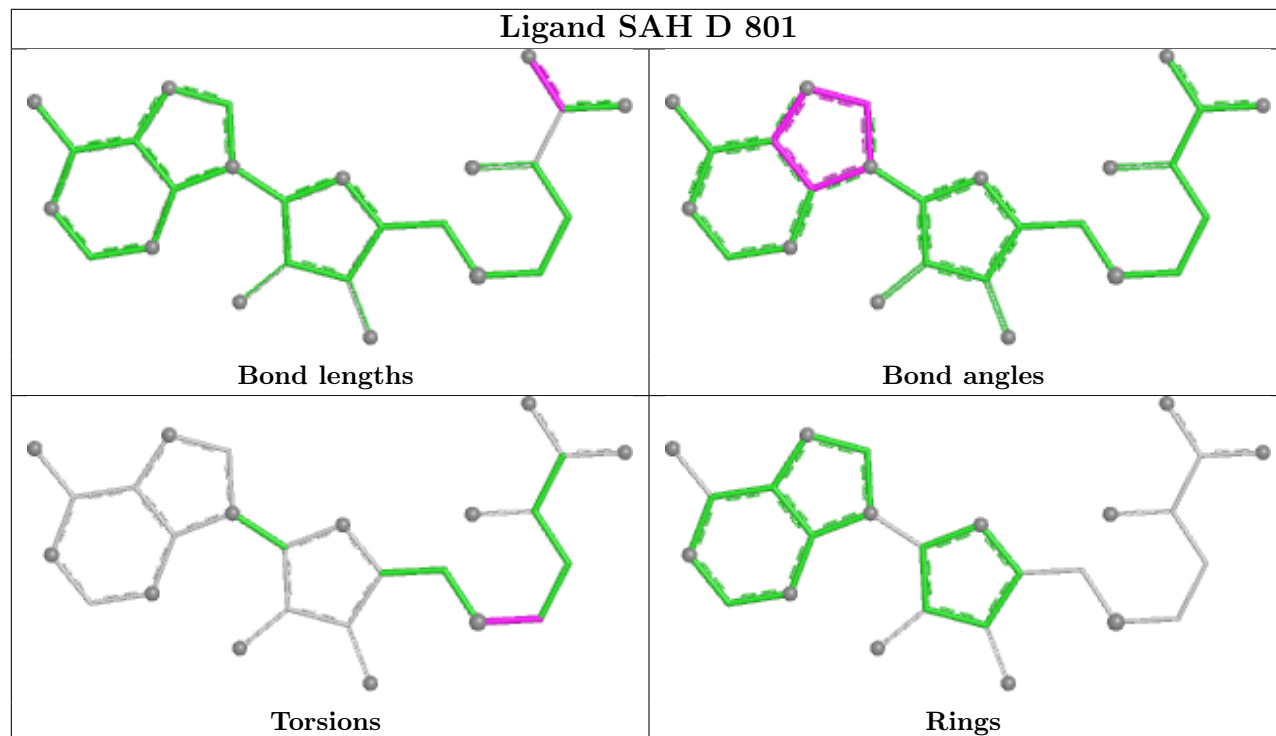
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	SAH	2	0

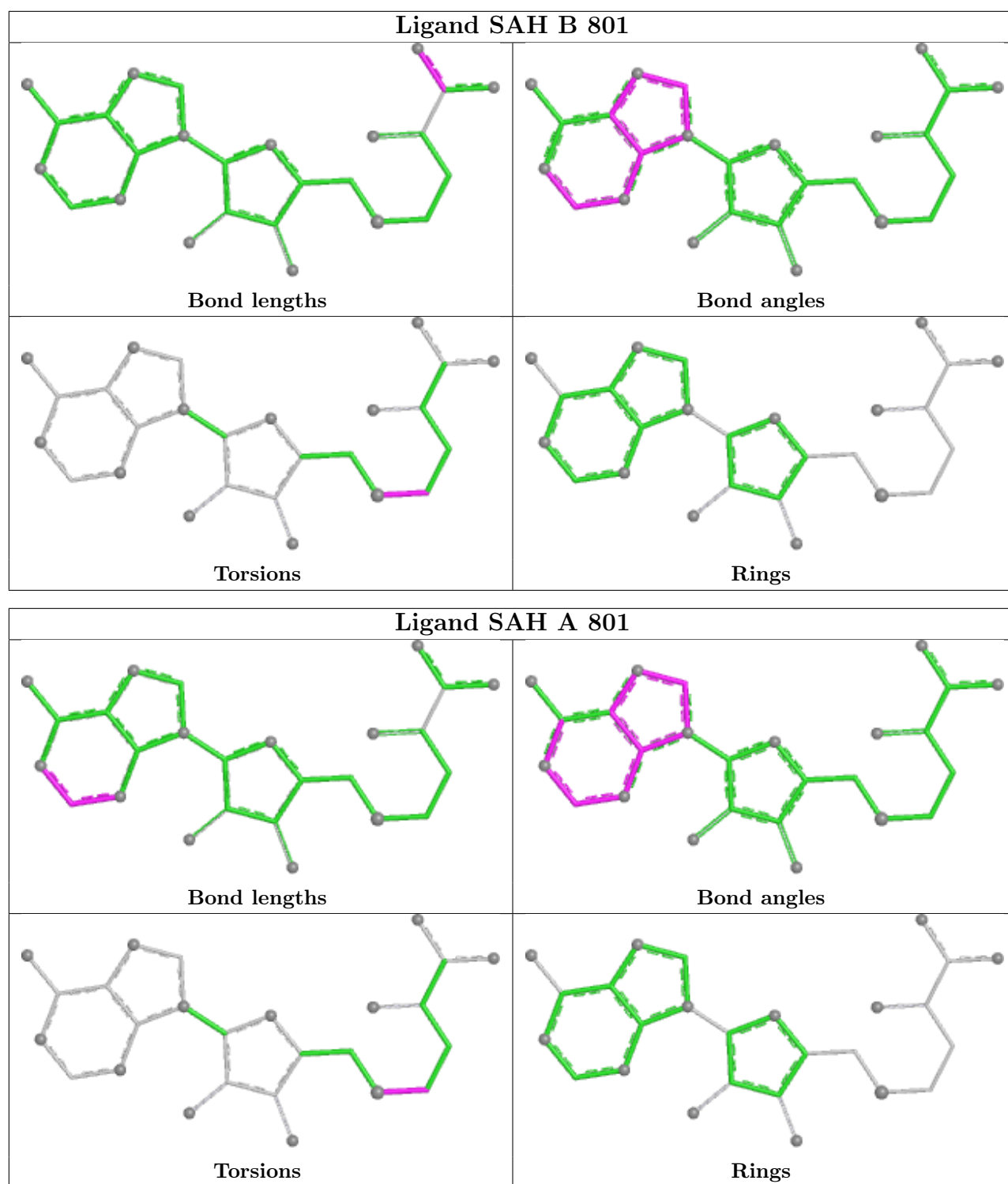
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand SAH C 801



Ligand SAH D 801





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 ⓘ

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	160/166 (96%)	1.43	42 (26%) 1 2	14, 22, 44, 49	0
1	B	160/166 (96%)	1.05	24 (15%) 5 7	11, 19, 31, 39	0
1	C	160/166 (96%)	1.30	38 (23%) 2 2	13, 21, 35, 41	0
1	D	161/166 (96%)	0.60	14 (8%) 16 17	9, 16, 25, 30	0
2	E	8/10 (80%)	1.72	3 (37%) 1 1	15, 24, 29, 37	0
2	F	7/10 (70%)	1.49	1 (14%) 6 7	19, 21, 30, 36	0
2	G	8/10 (80%)	2.34	4 (50%) 0 1	22, 34, 42, 44	0
2	H	7/10 (70%)	1.29	2 (28%) 1 2	14, 18, 29, 33	0
All	All	671/704 (95%)	1.12	128 (19%) 3 4	9, 20, 35, 49	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	ALA	7.7
1	A	266	PRO	6.5
1	C	261	LEU	5.9
1	A	260	ALA	5.1
1	C	266	PRO	4.7
1	A	277	TYR	4.5
1	A	263	ALA	4.5
1	A	268	THR	4.4
1	A	261	LEU	4.4
1	C	264	GLN	4.2
1	C	265	ASP	4.0
1	B	196	ALA	3.9
1	B	261	LEU	3.9
1	C	268	THR	3.8
2	G	24	ASP	3.7
1	A	262	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	16	LYS	3.7
1	C	302	CYS	3.7
1	A	282	TYR	3.6
1	A	267	SER	3.6
1	C	342	ALA	3.5
1	A	315	VAL	3.5
1	D	266	PRO	3.5
1	A	291	ASN	3.5
1	D	352	HIS	3.5
1	D	196	ALA	3.4
1	A	250	ILE	3.4
1	B	270	CYS	3.4
1	B	352	HIS	3.4
1	B	263	ALA	3.4
1	C	344	ILE	3.3
1	C	263	ALA	3.3
1	B	260	ALA	3.2
1	B	288	ARG	3.2
1	B	302	CYS	3.2
1	B	268	THR	3.2
1	C	262	TYR	3.1
1	C	350	LEU	3.1
1	C	313	ASP	3.1
1	D	268	THR	3.1
1	B	264	GLN	3.0
2	H	23	ARG	3.0
1	C	340	SER	3.0
2	G	17	ARG	3.0
1	A	248	ASP	3.0
1	D	192	ARG	2.9
1	A	194	SER	2.9
1	B	262	TYR	2.9
1	D	199	GLN	2.9
1	A	214	LYS	2.9
1	C	309	LEU	2.9
1	B	266	PRO	2.9
1	C	308	LYS	2.9
2	G	23	ARG	2.9
1	C	270	CYS	2.9
1	D	267	SER	2.9
1	B	279	SER	2.8
1	B	345	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	253	THR	2.8
1	C	343	SER	2.8
1	A	255	ALA	2.8
1	C	346	ALA	2.8
1	A	352	HIS	2.7
1	C	337	GLY	2.7
1	A	280	LYS	2.7
1	C	257	LYS	2.7
1	A	257	LYS	2.7
1	C	267	SER	2.7
2	G	21	VAL	2.7
1	C	203	ARG	2.6
1	A	200	SER	2.6
1	C	341	LYS	2.6
1	D	257	LYS	2.6
1	C	352	HIS	2.6
1	B	278	LEU	2.6
1	A	254	ASP	2.5
1	C	254	ASP	2.5
1	A	271	TYR	2.5
2	E	22	LEU	2.5
1	A	265	ASP	2.5
1	B	265	ASP	2.5
1	A	309	LEU	2.5
1	D	278	LEU	2.5
1	C	208	GLU	2.5
1	B	254	ASP	2.4
1	A	252	ILE	2.4
1	A	264	GLN	2.4
1	A	269	GLY	2.4
1	A	302	CYS	2.4
1	D	198	LEU	2.4
1	B	351	LYS	2.3
1	C	312	ILE	2.3
1	A	211	GLU	2.3
1	C	291	ASN	2.3
1	C	196	ALA	2.3
1	B	253	THR	2.3
2	E	16	LYS	2.3
1	C	320	LEU	2.3
1	C	338	ASP	2.3
1	A	276	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	16	LYS	2.2
1	D	194	SER	2.2
1	A	196	ALA	2.2
1	B	311	ASP	2.2
1	C	238	ARG	2.2
1	A	198	LEU	2.2
1	A	275	PHE	2.2
1	A	270	CYS	2.2
1	A	195	LYS	2.2
1	B	309	LEU	2.1
1	C	198	LEU	2.1
1	C	278	LEU	2.1
1	C	345	GLU	2.1
1	D	351	LYS	2.1
1	D	345	GLU	2.1
1	A	287	THR	2.1
1	A	220	ILE	2.1
1	D	200	SER	2.1
1	A	288	ARG	2.1
2	E	17	ARG	2.1
1	A	197	GLU	2.1
1	B	342	ALA	2.1
1	A	206	ILE	2.1
1	A	314	GLY	2.0
1	C	314	GLY	2.0
1	A	344	ILE	2.0
1	B	306	GLN	2.0
1	B	344	ILE	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	MLY	H	20	11/12	0.88	0.12	14,15,20,22	0
2	MLY	G	20	11/12	0.90	0.13	21,25,27,27	0
2	MLY	F	20	11/12	0.90	0.10	18,19,26,28	0
2	MLY	E	20	11/12	0.96	0.09	14,15,19,20	0

6.3 Carbohydrates [i](#)

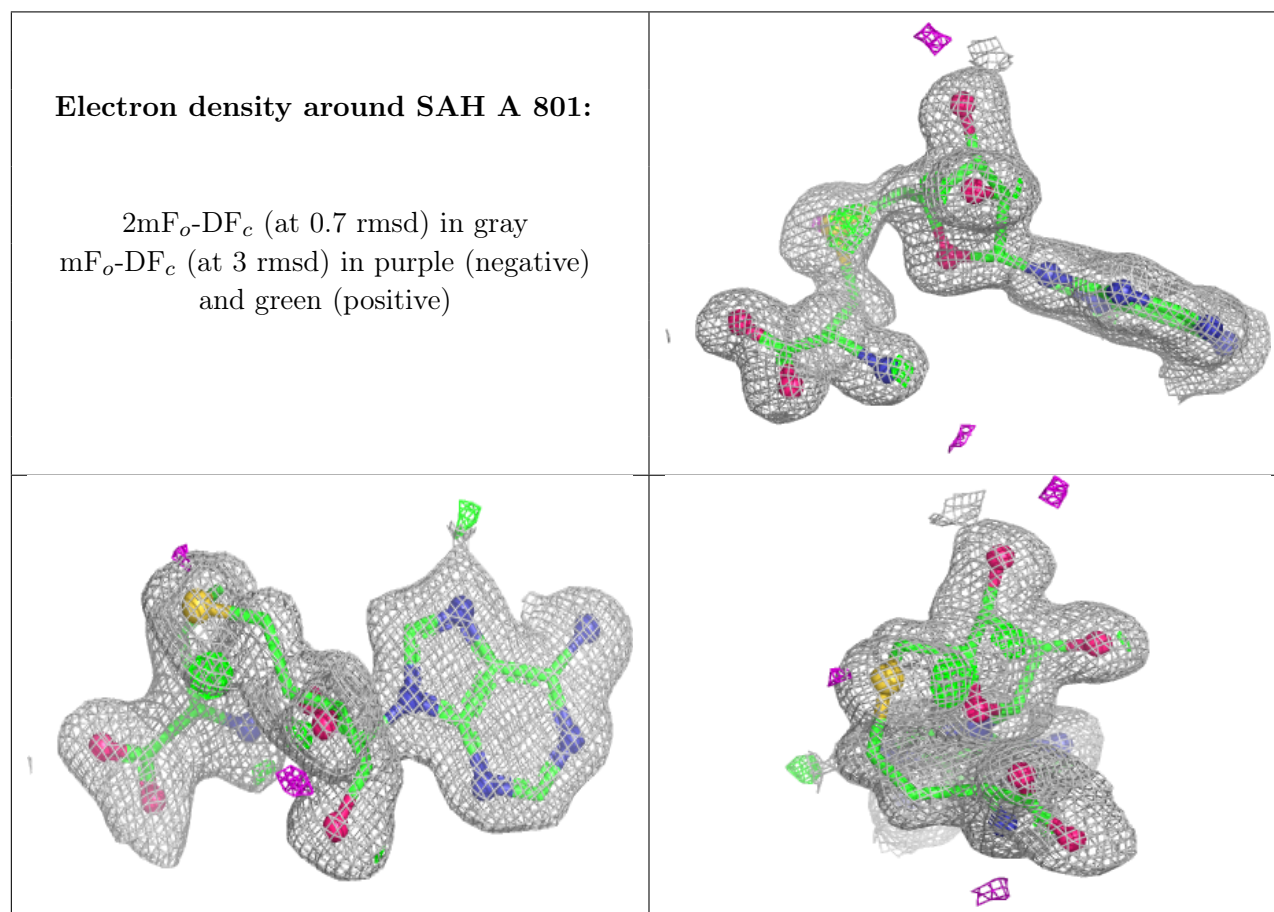
There are no oligosaccharides in this entry.

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.

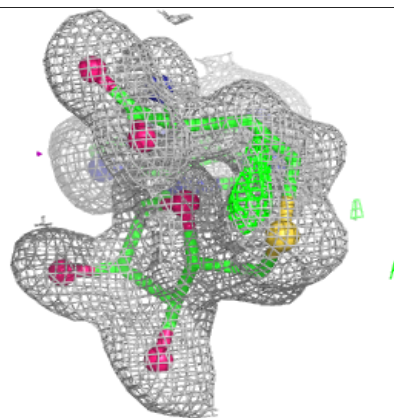
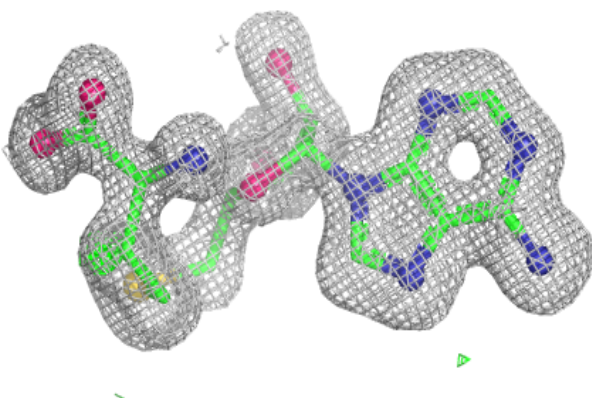
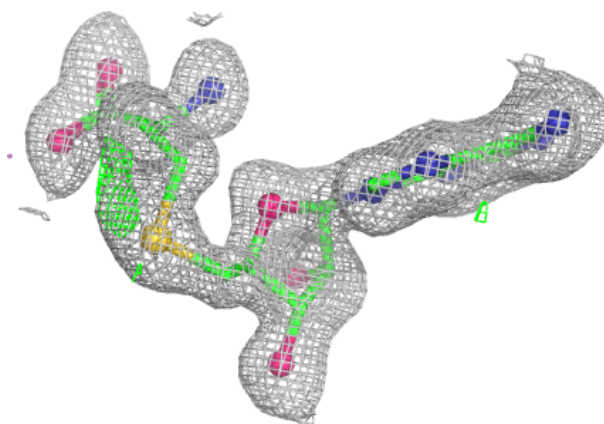
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SAH	A	801	26/26	0.96	0.08	14,18,20,22	0
3	SAH	C	801	26/26	0.98	0.07	15,17,20,23	0
3	SAH	D	801	26/26	0.98	0.06	9,11,12,13	0
3	SAH	B	801	26/26	0.99	0.05	11,13,16,18	0

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.

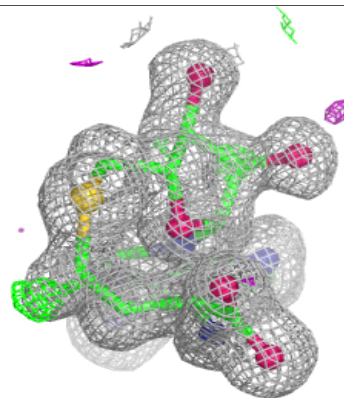
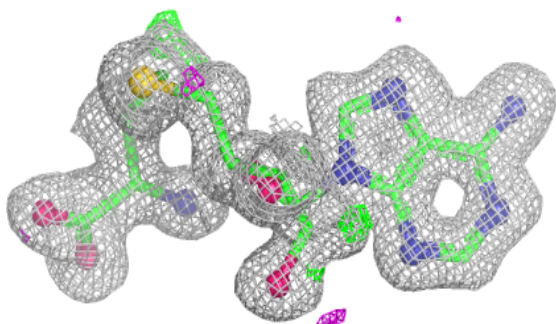
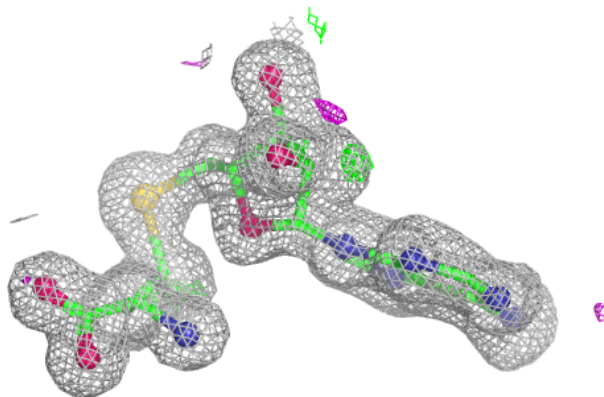


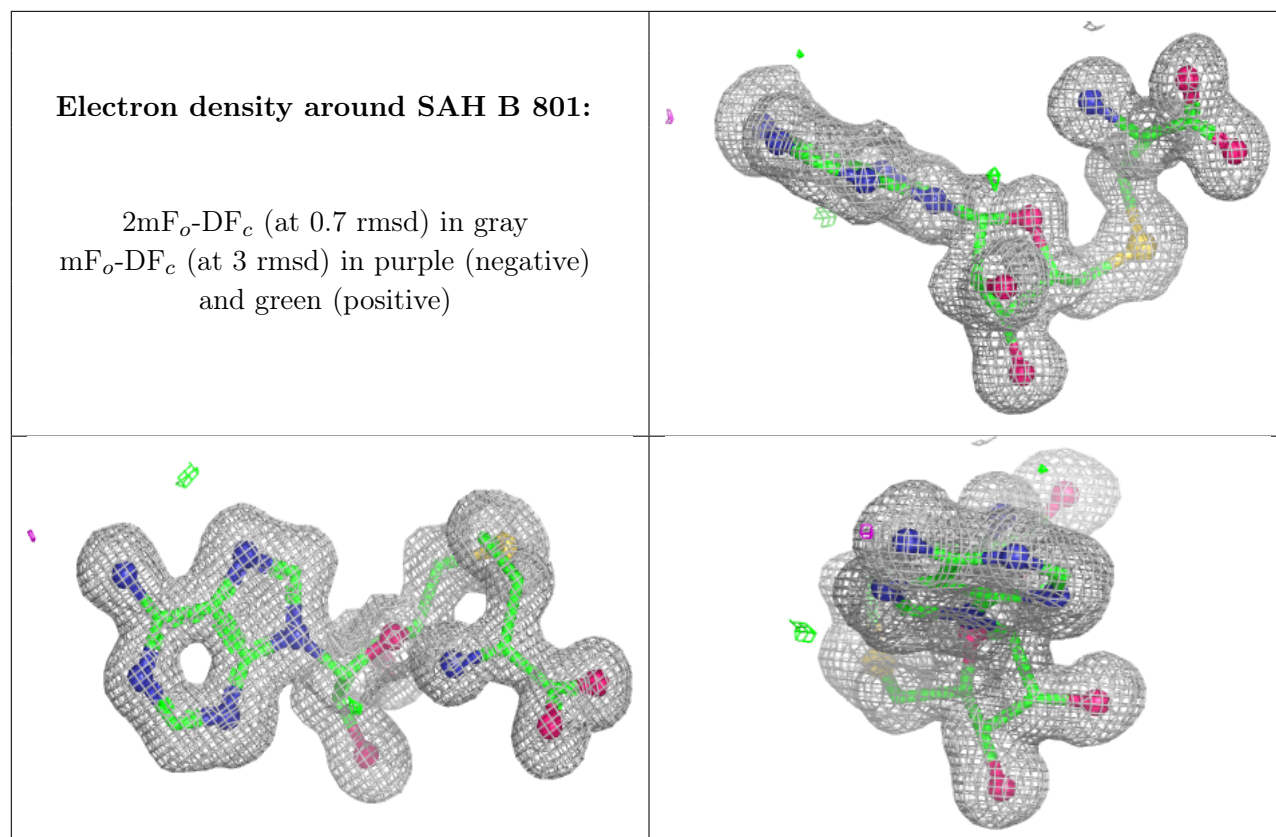
Electron density around SAH C 801:

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

**Electron density around SAH D 801:**

$2mF_o-DF_c$ (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.