



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:07 pm BST

PDB ID : 3VSE
Title : Crystal structure of methyltransferase
Authors : Kita, S.; Tanaka, Y.; Yao, M.; Tanaka, I.
Deposited on : 2012-04-25
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

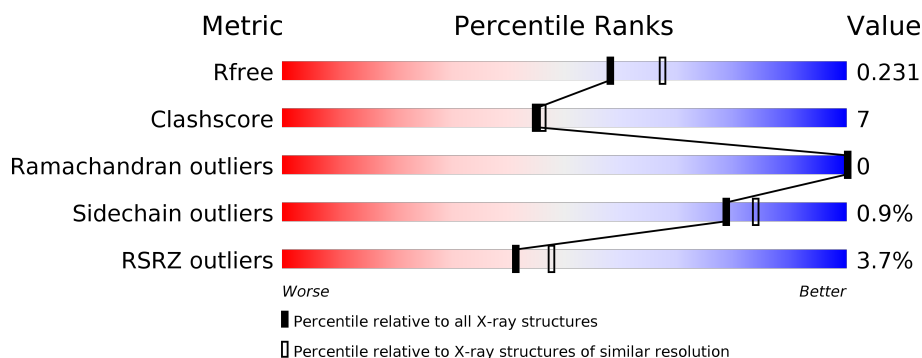
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	398	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>
1	B	398	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	C	398	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	D	398	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>••</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13330 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	2	0
			3178	2051	519	603	5			
1	B	390	Total	C	N	O	S	0	1	0
			3175	2050	523	597	5			
1	C	384	Total	C	N	O	S	0	0	0
			3117	2014	511	588	4			
1	D	390	Total	C	N	O	S	0	0	0
			3176	2049	529	594	4			

There are 32 discrepancies between the modelled and reference sequences:

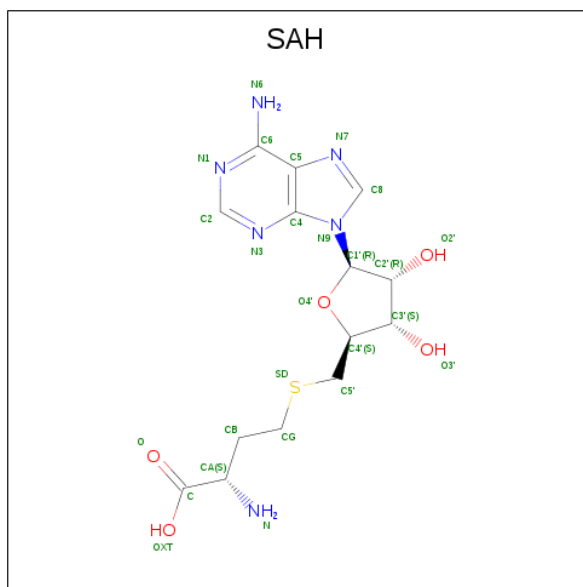
Chain	Residue	Modelled	Actual	Comment	Reference
A	391	LEU	-	EXPRESSION TAG	UNP Q99V16
A	392	GLU	-	EXPRESSION TAG	UNP Q99V16
A	393	HIS	-	EXPRESSION TAG	UNP Q99V16
A	394	HIS	-	EXPRESSION TAG	UNP Q99V16
A	395	HIS	-	EXPRESSION TAG	UNP Q99V16
A	396	HIS	-	EXPRESSION TAG	UNP Q99V16
A	397	HIS	-	EXPRESSION TAG	UNP Q99V16
A	398	HIS	-	EXPRESSION TAG	UNP Q99V16
B	391	LEU	-	EXPRESSION TAG	UNP Q99V16
B	392	GLU	-	EXPRESSION TAG	UNP Q99V16
B	393	HIS	-	EXPRESSION TAG	UNP Q99V16
B	394	HIS	-	EXPRESSION TAG	UNP Q99V16
B	395	HIS	-	EXPRESSION TAG	UNP Q99V16
B	396	HIS	-	EXPRESSION TAG	UNP Q99V16
B	397	HIS	-	EXPRESSION TAG	UNP Q99V16
B	398	HIS	-	EXPRESSION TAG	UNP Q99V16
C	391	LEU	-	EXPRESSION TAG	UNP Q99V16
C	392	GLU	-	EXPRESSION TAG	UNP Q99V16
C	393	HIS	-	EXPRESSION TAG	UNP Q99V16
C	394	HIS	-	EXPRESSION TAG	UNP Q99V16
C	395	HIS	-	EXPRESSION TAG	UNP Q99V16

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Chain	Residue	Modelled	Actual	Comment	Reference
C	396	HIS	-	EXPRESSION TAG	UNP Q99V16
C	397	HIS	-	EXPRESSION TAG	UNP Q99V16
C	398	HIS	-	EXPRESSION TAG	UNP Q99V16
D	391	LEU	-	EXPRESSION TAG	UNP Q99V16
D	392	GLU	-	EXPRESSION TAG	UNP Q99V16
D	393	HIS	-	EXPRESSION TAG	UNP Q99V16
D	394	HIS	-	EXPRESSION TAG	UNP Q99V16
D	395	HIS	-	EXPRESSION TAG	UNP Q99V16
D	396	HIS	-	EXPRESSION TAG	UNP Q99V16
D	397	HIS	-	EXPRESSION TAG	UNP Q99V16
D	398	HIS	-	EXPRESSION TAG	UNP Q99V16

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

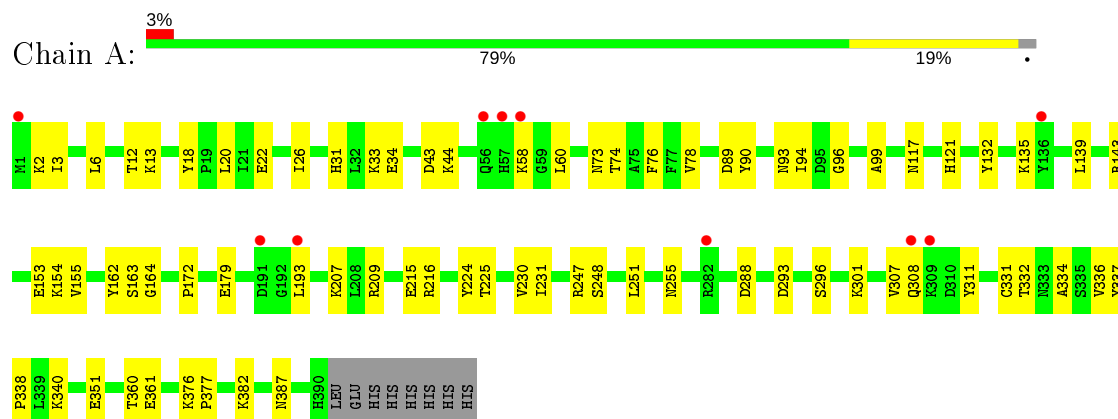
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total 177	O 177	0	0
3	B	133	Total 133	O 133	0	0
3	C	137	Total 137	O 137	0	0
3	D	133	Total 133	O 133	0	0

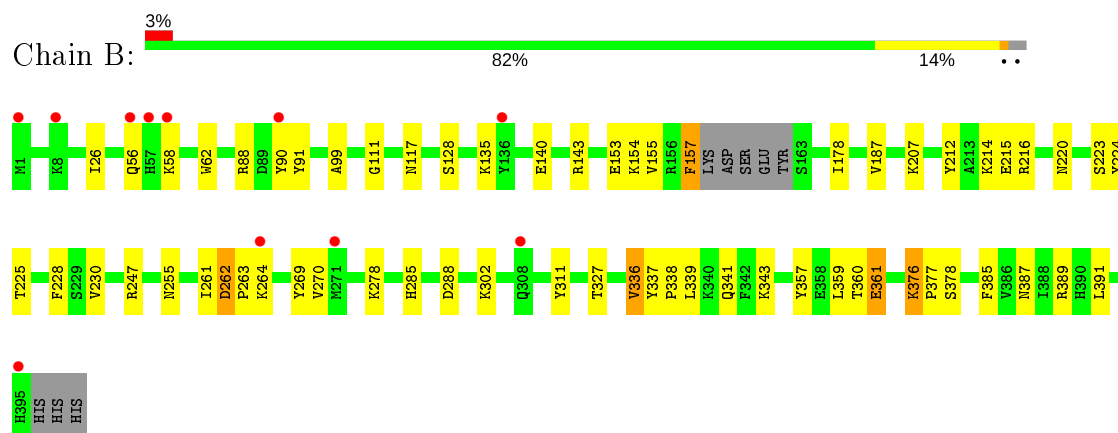
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

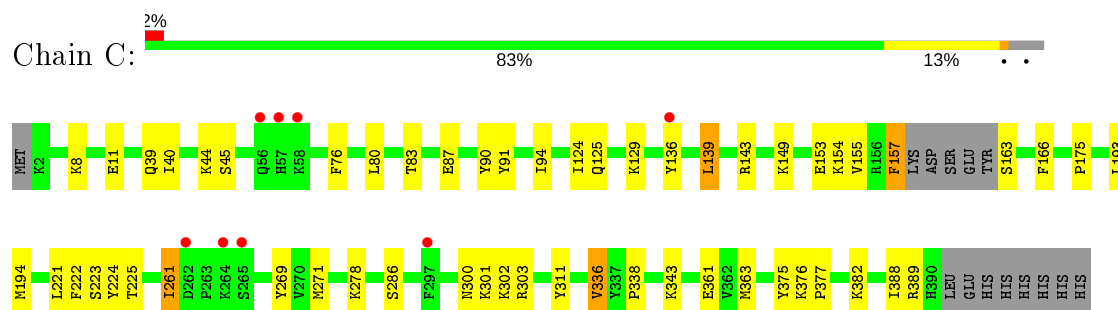
• Molecule 1: Putative uncharacterized protein



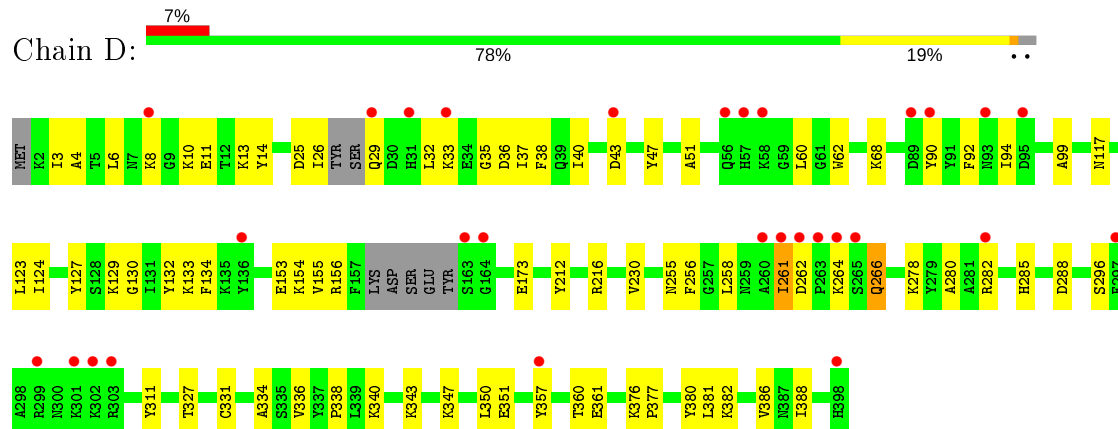
• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein



● Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.48Å 91.57Å 102.63Å 90.00° 94.03° 90.00°	Depositor
Resolution (Å)	34.13 – 2.10 41.80 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.13-2.10) 99.7 (41.80-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1021)	Depositor
R, R_{free}	0.203 , 0.230 0.204 , 0.231	Depositor DCC
R_{free} test set	5145 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13330	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.17 % 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 3.8394e-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: 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	0.85	8/3257 (0.2%)	0.71	2/4398 (0.0%)
1	B	0.91	12/3255 (0.4%)	0.72	3/4395 (0.1%)
1	C	0.96	16/3191 (0.5%)	0.68	3/4309 (0.1%)
1	D	0.92	10/3254 (0.3%)	0.73	6/4393 (0.1%)
All	All	0.91	46/12957 (0.4%)	0.71	14/17495 (0.1%)

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLU	CB-CG	-5.87	1.41	1.52
1	C	343	LYS	CB-CG	-5.86	1.36	1.52
1	B	302	LYS	CE-NZ	-5.83	1.34	1.49
1	C	286	SER	CB-OG	-5.82	1.34	1.42
1	B	357	TYR	CD1-CE1	-5.79	1.30	1.39
1	B	269	TYR	CD2-CE2	-5.76	1.30	1.39
1	A	34	GLU	CB-CG	-5.76	1.41	1.52
1	C	157	PHE	CE2-CZ	-5.74	1.26	1.37
1	C	336	VAL	CB-CG2	-5.72	1.40	1.52
1	D	92	PHE	CD1-CE1	-5.68	1.27	1.39
1	D	261	ILE	CB-CG2	-5.65	1.35	1.52
1	D	132	TYR	CD1-CE1	-5.65	1.30	1.39
1	B	154	LYS	CE-NZ	-5.62	1.34	1.49
1	A	60	LEU	CG-CD2	-5.62	1.31	1.51
1	C	39	GLN	CB-CG	-5.58	1.37	1.52
1	D	381	LEU	C-O	-5.54	1.12	1.23
1	B	357	TYR	CE2-CZ	-5.53	1.31	1.38
1	D	173	GLU	CB-CG	-5.48	1.41	1.52
1	D	132	TYR	CE1-CZ	-5.46	1.31	1.38
1	D	380	TYR	C-O	-5.44	1.13	1.23
1	C	157	PHE	CE1-CZ	-5.38	1.27	1.37
1	C	40	ILE	CB-CG2	-5.37	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	136	TYR	CD2-CE2	-5.36	1.31	1.39
1	B	269	TYR	CE1-CZ	-5.35	1.31	1.38
1	B	278	LYS	CE-NZ	-5.34	1.35	1.49
1	A	340	LYS	CD-CE	5.33	1.64	1.51
1	C	302	LYS	CE-NZ	-5.33	1.35	1.49
1	B	157	PHE	CE1-CZ	-5.29	1.27	1.37
1	B	269	TYR	CG-CD2	-5.29	1.32	1.39
1	D	132	TYR	CE2-CZ	-5.28	1.31	1.38
1	A	340	LYS	CE-NZ	5.27	1.62	1.49
1	C	261	ILE	CB-CG2	-5.25	1.36	1.52
1	C	193	LEU	CG-CD1	-5.20	1.32	1.51
1	B	357	TYR	CD2-CE2	-5.20	1.31	1.39
1	A	332	THR	CB-CG2	-5.17	1.35	1.52
1	C	343	LYS	CD-CE	-5.17	1.38	1.51
1	B	336	VAL	CB-CG2	-5.16	1.42	1.52
1	D	343	LYS	CB-CG	-5.15	1.38	1.52
1	C	163	SER	CA-CB	-5.12	1.45	1.52
1	B	157	PHE	CE2-CZ	-5.12	1.27	1.37
1	C	139	LEU	CG-CD2	-5.12	1.32	1.51
1	C	149	LYS	CB-CG	-5.11	1.38	1.52
1	D	340	LYS	CD-CE	-5.10	1.38	1.51
1	A	301	LYS	CE-NZ	-5.10	1.36	1.49
1	C	166	PHE	CD2-CE2	-5.08	1.29	1.39
1	A	12	THR	CB-CG2	-5.07	1.35	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	391	LEU	CB-CG-CD2	-5.89	100.98	111.00
1	C	193	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	D	380	TYR	CA-C-N	5.64	129.62	117.20
1	D	258	LEU	CA-CB-CG	5.63	128.26	115.30
1	C	278	LYS	CD-CE-NZ	5.61	124.61	111.70
1	D	381	LEU	O-C-N	5.27	131.14	122.70
1	C	40	ILE	CG1-CB-CG2	-5.24	99.87	111.40
1	A	340	LYS	CD-CE-NZ	5.23	123.74	111.70
1	B	391	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	258	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	D	129	LYS	CD-CE-NZ	-5.10	99.97	111.70
1	A	60	LEU	CB-CG-CD2	-5.06	102.40	111.00
1	D	380	TYR	C-N-CA	5.06	134.35	121.70
1	B	262	ASP	CB-CG-OD1	5.03	122.83	118.30

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	3178	0	3114	50	0
1	B	3175	0	3110	40	0
1	C	3117	0	3055	29	0
1	D	3176	0	3098	48	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	177	0	0	3	0
3	B	133	0	0	1	0
3	C	137	0	0	1	0
3	D	133	0	0	1	0
All	All	13330	0	12453	164	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 7.

All (164) 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:D:37:ILE:HD11	1:D:134:PHE:CZ	2.30	0.66
1:B:261:ILE:O	1:B:263:PRO:HD3	1.96	0.66
1:A:31:HIS:HB3	1:A:33:LYS:NZ	2.11	0.66
1:B:140:GLU:HG2	1:B:143:ARG:HH21	1.61	0.66
1:D:8:LYS:HD3	1:D:43:ASP:OD2	1.97	0.64
1:A:26:ILE:HD12	1:A:26:ILE:C	2.18	0.64
1:C:76:PHE:CZ	1:C:80:LEU:HD11	2.33	0.64
1:D:37:ILE:HD11	1:D:134:PHE:HZ	1.62	0.64
1:B:360:THR:OG1	1:B:361:GLU:HG2	1.98	0.63
1:A:31:HIS:HB3	1:A:33:LYS:HZ3	1.63	0.62
1:A:336:VAL:HG22	3:A:507:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:OD1	1:A:44:LYS:HG2	2.00	0.61
1:D:35:GLY:HA3	1:D:133:LYS:HD2	1.81	0.61
1:B:339:LEU:HG	1:B:343:LYS:HD2	1.83	0.61
1:D:360:THR:O	1:D:361:GLU:HG2	2.01	0.60
1:A:336:VAL:O	1:A:338:PRO:HD3	2.02	0.60
1:D:10:LYS:HE3	1:D:25:ASP:OD2	2.01	0.60
1:A:230:VAL:HG21	1:A:255:ASN:HB3	1.82	0.60
1:C:83:THR:O	1:C:87:GLU:HG2	2.02	0.59
1:D:26:ILE:HD13	1:D:29:GLN:OE1	2.02	0.58
1:B:247:ARG:NH2	1:C:175:PRO:HG3	2.17	0.58
1:D:13:LYS:HG3	1:D:14:TYR:N	2.19	0.58
1:D:8:LYS:HD2	1:D:11:GLU:OE2	2.03	0.58
1:D:13:LYS:HD2	1:D:14:TYR:CE2	2.37	0.58
1:A:20:LEU:HD23	1:A:22:GLU:OE2	2.04	0.57
1:A:216:ARG:HB3	1:A:288:ASP:HB2	1.85	0.57
1:B:270:VAL:O	1:B:270:VAL:HG12	2.04	0.57
1:A:155:VAL:HG22	1:A:163:SER:HA	1.86	0.57
1:D:90:TYR:CE2	1:D:94:ILE:HD13	2.39	0.57
1:C:44:LYS:O	1:C:45:SER:HB2	2.04	0.56
1:A:13:LYS:HE2	1:A:18:TYR:CD2	2.40	0.56
1:A:376:LYS:N	1:A:377:PRO:CD	2.68	0.56
1:A:155:VAL:CG2	1:A:163:SER:HA	2.37	0.55
1:B:262:ASP:OD2	1:B:264:LYS:HG2	2.06	0.55
1:D:155:VAL:HG23	1:D:155:VAL:O	2.07	0.55
1:A:247:ARG:HD2	1:A:251:LEU:CD1	2.37	0.55
1:A:6:LEU:HD23	1:A:26:ILE:HG22	1.88	0.55
1:B:212:TYR:CD1	1:B:327:THR:HG21	2.41	0.55
1:C:129:LYS:HG2	1:C:157:PHE:CE2	2.42	0.55
1:D:47:TYR:HB2	1:D:68:LYS:HE2	1.89	0.54
1:D:216:ARG:HB3	1:D:288:ASP:HB2	1.89	0.54
1:D:296:SER:OG	1:D:334:ALA:HB2	2.08	0.54
1:D:336:VAL:O	1:D:338:PRO:HD3	2.08	0.54
1:A:155:VAL:HG23	1:A:155:VAL:O	2.08	0.54
1:C:139:LEU:O	1:C:143:ARG:HG3	2.08	0.53
1:B:223:SER:O	1:B:224:TYR:HB3	2.08	0.53
1:D:347:LYS:O	1:D:351:GLU:HG3	2.08	0.53
1:B:216:ARG:HB3	1:B:288:ASP:HB2	1.90	0.53
1:D:6:LEU:HD13	1:D:11:GLU:HA	1.91	0.52
1:A:207:LYS:HD2	1:A:361:GLU:OE2	2.10	0.52
1:D:278:LYS:HB3	1:D:282:ARG:HH21	1.74	0.52
1:D:90:TYR:CZ	1:D:94:ILE:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:HE3	1:A:193:LEU:O	2.09	0.52
1:B:338:PRO:HD2	1:B:341:GLN:OE1	2.10	0.52
1:D:38:PHE:HE2	1:D:40:ILE:HD11	1.75	0.51
1:D:38:PHE:CE2	1:D:40:ILE:HD11	2.46	0.51
1:B:230:VAL:HG21	1:B:255:ASN:HB3	1.93	0.51
1:C:388:ILE:HG22	1:C:389:ARG:N	2.26	0.51
1:A:26:ILE:HD12	1:A:26:ILE:O	2.11	0.50
1:C:361:GLU:HG2	1:C:363:MET:HG3	1.94	0.50
1:D:35:GLY:N	1:D:130:GLY:HA2	2.27	0.50
1:D:278:LYS:HB3	1:D:282:ARG:NH2	2.27	0.50
1:A:247:ARG:HD2	1:A:251:LEU:HD11	1.93	0.50
1:A:22:GLU:OE1	1:A:58:LYS:HG3	2.12	0.49
1:D:230:VAL:HG21	1:D:255:ASN:HB3	1.94	0.49
1:A:351:GLU:CD	1:C:301:LYS:HE2	2.33	0.49
1:D:280:ALA:O	1:D:285:HIS:HB2	2.11	0.49
1:C:90:TYR:O	1:C:94:ILE:HG23	2.12	0.49
1:B:135:LYS:HZ2	1:B:153:GLU:CD	2.17	0.49
1:D:133:LYS:HE2	3:D:633:HOH:O	2.13	0.48
1:A:209:ARG:HD3	1:A:231:ILE:HG12	1.95	0.48
1:D:350:LEU:HB3	1:D:357:TYR:CD2	2.49	0.48
1:A:2:LYS:C	1:A:3:ILE:HD12	2.34	0.48
1:B:262:ASP:CG	1:B:264:LYS:HG2	2.33	0.47
1:D:32:LEU:HD13	1:D:60:LEU:HD21	1.95	0.47
1:D:33:LYS:O	1:D:36:ASP:HB2	2.14	0.47
1:A:207:LYS:HB2	1:A:207:LYS:HE2	1.61	0.47
1:D:51:ALA:HB1	1:D:62:TRP:O	2.15	0.47
1:B:90:TYR:CE2	1:B:91:TYR:CE1	3.03	0.47
1:C:223:SER:O	1:C:224:TYR:HB3	2.15	0.47
1:D:256:PHE:CZ	1:D:266:GLN:HG3	2.50	0.47
1:B:212:TYR:OH	1:B:361:GLU:OE2	2.32	0.47
1:B:389:ARG:HB3	1:B:389:ARG:NH1	2.30	0.47
1:B:360:THR:HG21	1:B:387:ASN:ND2	2.29	0.47
1:A:360:THR:HG21	1:A:387:ASN:ND2	2.30	0.46
1:B:155:VAL:HG13	1:B:157:PHE:CZ	2.50	0.46
1:D:124:ILE:O	1:D:153:GLU:HA	2.15	0.46
1:C:224:TYR:CG	1:C:225:THR:N	2.82	0.46
1:C:124:ILE:O	1:C:153:GLU:HA	2.15	0.46
1:D:13:LYS:HG3	1:D:14:TYR:CD2	2.51	0.46
1:C:375:TYR:CE2	1:C:377:PRO:HB2	2.50	0.46
1:A:155:VAL:HG21	1:A:162:TYR:O	2.15	0.46
1:A:215:GLU:HG3	1:A:215:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:HA	1:C:94:ILE:CD1	2.46	0.46
1:B:376:LYS:O	1:B:377:PRO:C	2.54	0.46
1:B:155:VAL:HG13	1:B:157:PHE:CE1	2.51	0.46
1:B:214:LYS:HG2	1:B:215:GLU:HG3	1.97	0.45
1:A:139:LEU:O	1:A:143:ARG:HG3	2.17	0.45
1:A:155:VAL:HG22	1:A:163:SER:O	2.17	0.45
1:C:261:ILE:HD12	1:C:261:ILE:HG23	1.48	0.45
1:D:212:TYR:CD1	1:D:327:THR:HG21	2.51	0.45
1:B:336:VAL:O	1:B:338:PRO:HD3	2.17	0.45
1:D:327:THR:HG23	1:D:386:VAL:O	2.16	0.45
1:A:293:ASP:OD2	2:A:401:SAH:N	2.50	0.45
1:B:99:ALA:HA	1:B:117:ASN:O	2.17	0.45
1:B:90:TYR:HE2	1:B:91:TYR:CE1	2.35	0.45
1:D:13:LYS:HD2	1:D:14:TYR:CZ	2.52	0.45
1:A:99:ALA:HA	1:A:117:ASN:O	2.18	0.44
1:A:121:HIS:CE1	1:A:172:PRO:HG3	2.52	0.44
1:A:132:TYR:CE1	1:A:135:LYS:HD2	2.53	0.44
1:B:58:LYS:HB3	3:B:535:HOH:O	2.17	0.44
1:C:221:LEU:O	1:C:222:PHE:HB2	2.17	0.44
1:B:361:GLU:CG	1:B:385:PHE:HB2	2.47	0.44
1:A:155:VAL:HG22	1:A:163:SER:C	2.38	0.44
1:A:90:TYR:CZ	1:A:94:ILE:HG21	2.52	0.44
1:C:194:MET:HE1	1:C:224:TYR:CE1	2.51	0.44
1:A:73:ASN:O	1:A:76:PHE:HB3	2.18	0.44
1:B:26:ILE:C	1:B:26:ILE:HD12	2.38	0.44
1:C:376:LYS:N	1:C:377:PRO:CD	2.81	0.43
1:A:162:TYR:CZ	1:A:164:GLY:HA2	2.53	0.43
1:C:129:LYS:HG3	3:C:610:HOH:O	2.17	0.43
1:B:140:GLU:CG	1:B:143:ARG:HH21	2.26	0.43
1:D:262:ASP:OD1	1:D:264:LYS:HB2	2.17	0.43
1:A:74:THR:O	1:A:78:VAL:HG23	2.18	0.43
1:D:123:LEU:HD11	1:D:154:LYS:HG3	2.00	0.43
1:A:307:VAL:HG13	1:A:308:GLN:N	2.34	0.43
1:A:43:ASP:OD1	1:A:44:LYS:N	2.53	0.42
1:A:89:ASP:OD1	1:A:93:ASN:ND2	2.52	0.42
1:A:224:TYR:CG	1:A:225:THR:N	2.87	0.42
1:D:3:ILE:HD12	1:D:3:ILE:HG23	1.59	0.42
1:B:157:PHE:CD1	1:B:157:PHE:N	2.82	0.42
1:C:125:GLN:HG2	1:C:154:LYS:HB2	2.00	0.42
1:D:376:LYS:N	1:D:377:PRO:CD	2.82	0.42
1:B:359:LEU:HD12	1:B:359:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:VAL:O	1:C:338:PRO:HD3	2.20	0.42
1:A:296:SER:OG	1:A:334:ALA:HB2	2.19	0.42
1:D:38:PHE:HE2	1:D:40:ILE:CD1	2.33	0.42
1:C:155:VAL:O	1:C:155:VAL:HG12	2.19	0.42
1:B:376:LYS:O	1:B:378:SER:N	2.52	0.42
1:B:62:TRP:CD2	1:B:111:GLY:HA3	2.55	0.42
1:C:269:TYR:CD1	1:C:271:MET:HE1	2.54	0.42
1:C:269:TYR:HB3	1:C:271:MET:CE	2.50	0.42
1:D:331:CYS:HA	1:D:382:LYS:O	2.20	0.41
1:A:331:CYS:HA	1:A:382:LYS:O	2.19	0.41
1:B:155:VAL:CG1	1:B:157:PHE:CZ	3.03	0.41
1:B:224:TYR:CG	1:B:225:THR:N	2.88	0.41
1:A:209:ARG:NH2	3:A:537:HOH:O	2.53	0.41
1:C:300:ASN:O	1:C:303:ARG:HB2	2.19	0.41
1:D:99:ALA:HA	1:D:117:ASN:O	2.20	0.41
1:A:58:LYS:HB2	3:A:599:HOH:O	2.20	0.41
1:B:56:GLN:HE21	1:B:128:SER:HB3	1.86	0.41
1:B:376:LYS:C	1:B:378:SER:N	2.74	0.41
1:C:8:LYS:HA	1:C:11:GLU:OE2	2.20	0.41
1:B:178:ILE:HD13	1:B:187:VAL:HG21	2.03	0.41
1:D:4:ALA:HB3	1:D:40:ILE:HD13	2.03	0.41
1:B:247:ARG:HH21	1:C:175:PRO:HG3	1.83	0.41
1:C:382:LYS:HD2	1:C:382:LYS:N	2.36	0.41
1:A:207:LYS:HG2	1:A:361:GLU:OE1	2.21	0.41
1:B:220:ASN:ND2	1:B:228:PHE:HB2	2.37	0.40
1:A:96:GLY:O	1:A:179:GLU:HG2	2.21	0.40
1:A:247:ARG:HG3	1:A:248:SER:N	2.37	0.40
1:D:386:VAL:CG1	1:D:388:ILE:HD11	2.52	0.40
1:D:127:TYR:CZ	1:D:156:ARG:HD3	2.57	0.40
1:D:261:ILE:HD13	1:D:261:ILE:HA	1.79	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	390/398 (98%)	375 (96%)	15 (4%)	0	100	100
1	B	387/398 (97%)	369 (95%)	18 (5%)	0	100	100
1	C	380/398 (96%)	365 (96%)	15 (4%)	0	100	100
1	D	384/398 (96%)	366 (95%)	18 (5%)	0	100	100
All	All	1541/1592 (97%)	1475 (96%)	66 (4%)	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	341/347 (98%)	339 (99%)	2 (1%)	86	90
1	B	340/347 (98%)	333 (98%)	7 (2%)	53	59
1	C	333/347 (96%)	332 (100%)	1 (0%)	92	95
1	D	339/347 (98%)	337 (99%)	2 (1%)	86	90
All	All	1353/1388 (98%)	1341 (99%)	12 (1%)	78	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	TYR
1	A	337	TYR
1	B	88	ARG
1	B	207	LYS
1	B	285	HIS
1	B	311	TYR
1	B	337	TYR
1	B	361	GLU
1	B	376	LYS
1	C	311	TYR

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Mol	Chain	Res	Type
1	D	266	GLN
1	D	311	TYR

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

Mol	Chain	Res	Type
1	A	211	GLN
1	B	56	GLN
1	B	374	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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$
2	SAH	A	401	-	21,28,28	1.64	5 (23%)	20,40,40	1.58	2 (10%)
2	SAH	D	401	-	21,28,28	1.22	2 (9%)	20,40,40	1.76	3 (15%)
2	SAH	B	401	-	21,28,28	1.19	2 (9%)	20,40,40	1.68	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	C	401	-	21,28,28	1.24	2 (9%)	20,40,40	1.70	2 (10%)

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	SAH	A	401	-	-	2/7/31/31	0/3/3/3
2	SAH	D	401	-	-	0/7/31/31	0/3/3/3
2	SAH	B	401	-	-	1/7/31/31	0/3/3/3
2	SAH	C	401	-	-	0/7/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	SAH	C2-N3	4.07	1.38	1.32
2	D	401	SAH	C2-N3	3.98	1.38	1.32
2	B	401	SAH	C2-N3	3.82	1.38	1.32
2	A	401	SAH	C2'-C1'	-3.45	1.48	1.53
2	A	401	SAH	C2-N3	3.00	1.36	1.32
2	A	401	SAH	C6-N6	2.67	1.43	1.34
2	D	401	SAH	C2-N1	2.38	1.38	1.33
2	C	401	SAH	C2-N1	2.38	1.38	1.33
2	B	401	SAH	C2-N1	2.37	1.38	1.33
2	A	401	SAH	C2-N1	2.20	1.38	1.33
2	A	401	SAH	O3'-C3'	-2.01	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	SAH	N3-C2-N1	-5.69	119.78	128.68
2	C	401	SAH	N3-C2-N1	-5.56	119.98	128.68
2	A	401	SAH	N3-C2-N1	-5.55	120.00	128.68
2	B	401	SAH	N3-C2-N1	-5.55	120.01	128.68
2	D	401	SAH	C5'-SD-CG	-3.80	90.86	102.27
2	C	401	SAH	C5'-SD-CG	-3.67	91.27	102.27
2	B	401	SAH	C5'-SD-CG	-3.42	92.01	102.27
2	D	401	SAH	C1'-N9-C4	-2.21	122.75	126.64
2	A	401	SAH	C5'-SD-CG	2.13	108.65	102.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

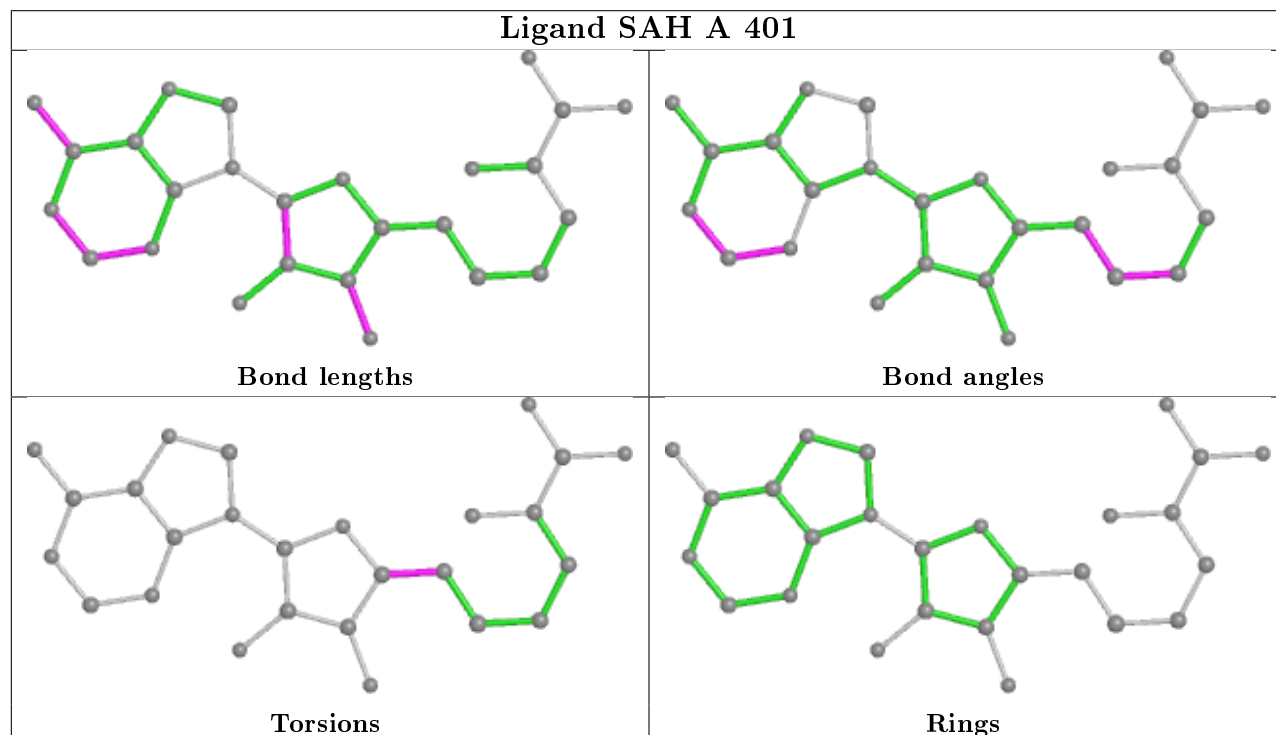
Mol	Chain	Res	Type	Atoms
2	A	401	SAH	O4'-C4'-C5'-SD
2	A	401	SAH	C3'-C4'-C5'-SD
2	B	401	SAH	CA-CB-CG-SD

There are no ring outliers.

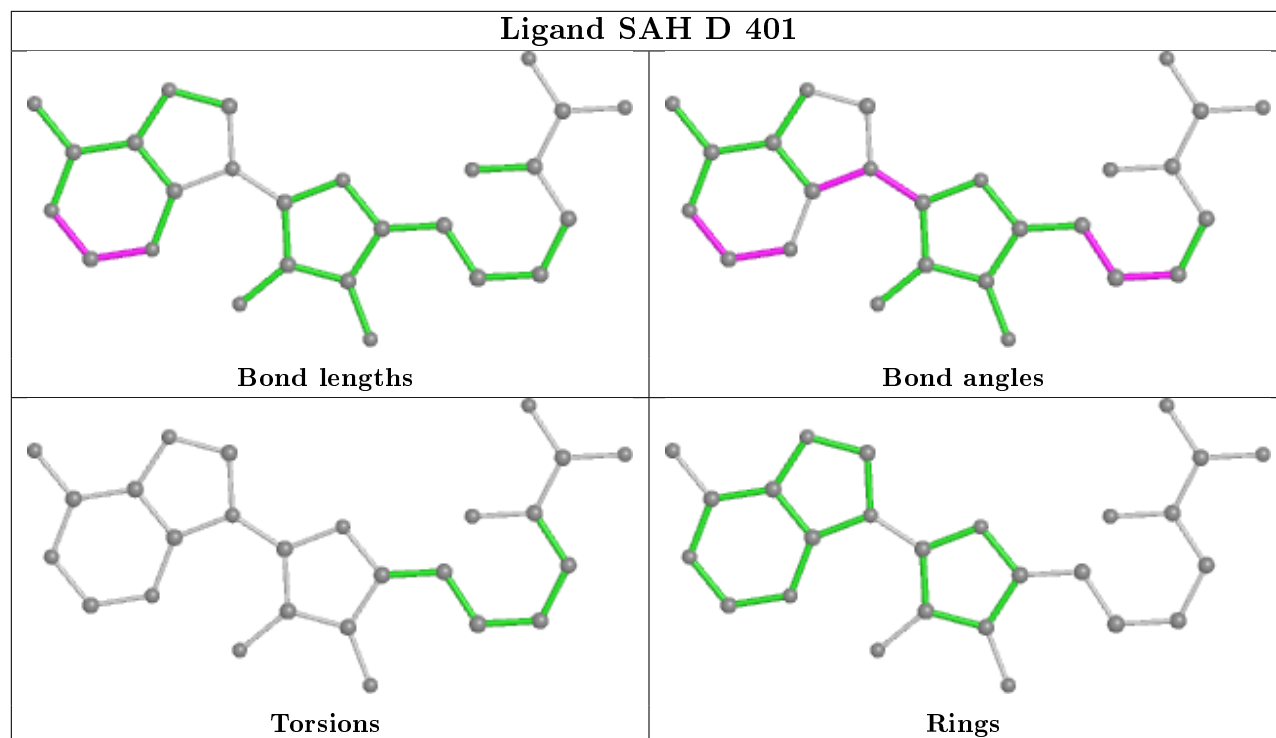
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SAH	1	0

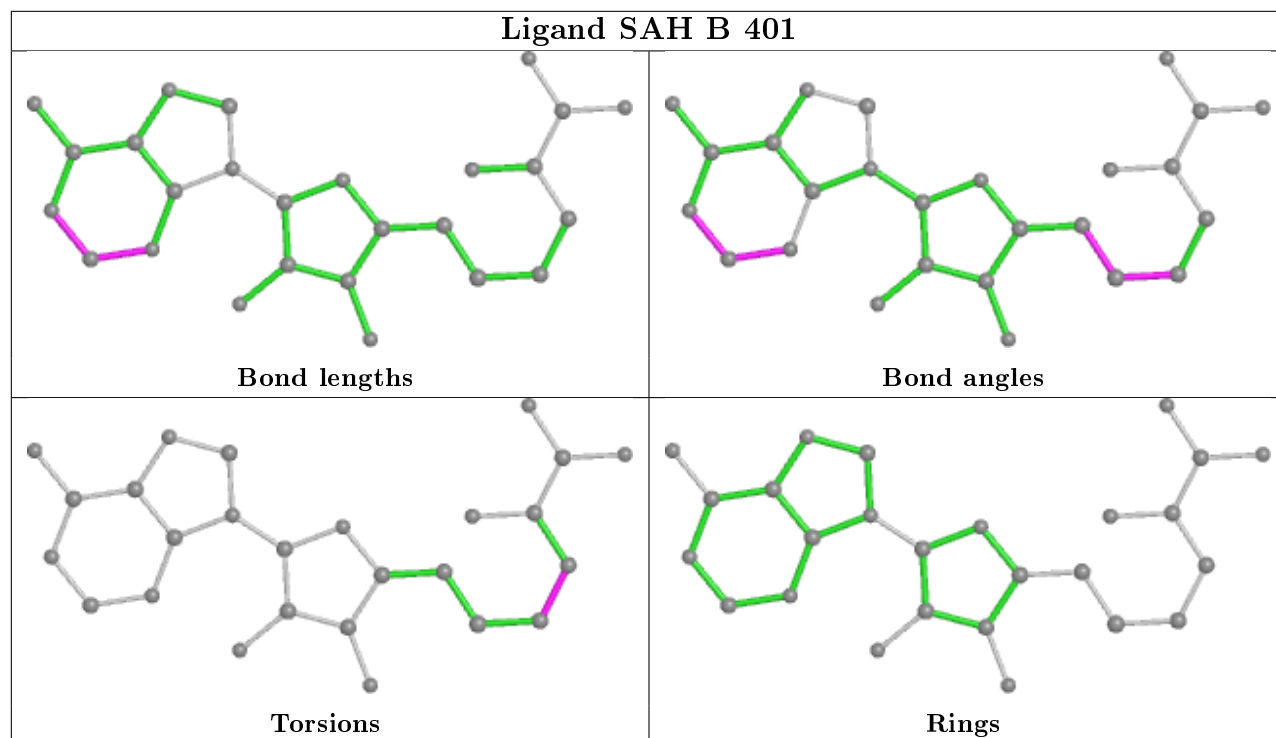
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

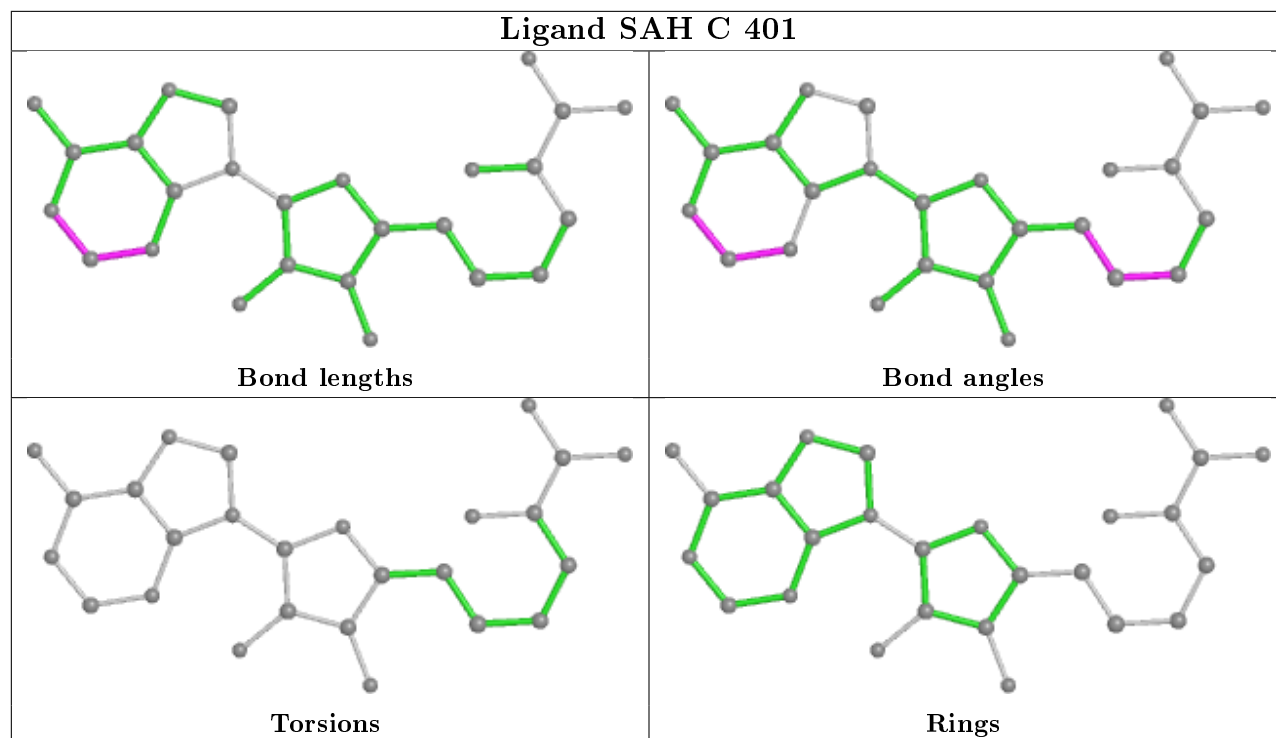


Ligand SAH D 401



Ligand SAH B 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	390/398 (97%)	0.02	10 (2%) 56 61	5, 16, 35, 59	0
1	B	390/398 (97%)	0.11	11 (2%) 53 59	7, 19, 40, 54	0
1	C	384/398 (96%)	0.06	8 (2%) 63 68	8, 19, 37, 66	0
1	D	390/398 (97%)	0.20	29 (7%) 14 18	9, 19, 44, 64	0
All	All	1554/1592 (97%)	0.10	58 (3%) 41 48	5, 18, 40, 66	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	TYR	6.6
1	D	303	ARG	5.5
1	C	262	ASP	5.2
1	A	1	MET	5.0
1	D	31	HIS	4.6
1	D	29	GLN	4.6
1	D	297	PHE	4.4
1	B	136	TYR	4.3
1	D	58	LYS	4.1
1	D	57	HIS	4.1
1	D	264	LYS	4.0
1	A	136	TYR	3.9
1	B	90	TYR	3.9
1	C	58	LYS	3.7
1	C	264	LYS	3.6
1	B	271	MET	3.6
1	D	56	GLN	3.4
1	D	261	ILE	3.3
1	D	301	LYS	3.3
1	D	136	TYR	3.3
1	D	43	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	56	GLN	3.2
1	A	57	HIS	3.2
1	C	57	HIS	3.1
1	D	282	ARG	3.1
1	B	1	MET	3.1
1	D	262	ASP	3.1
1	D	8	LYS	3.0
1	D	263	PRO	3.0
1	D	163	SER	3.0
1	B	57	HIS	3.0
1	A	56	GLN	2.9
1	A	58	LYS	2.8
1	D	299	ARG	2.6
1	A	309	LYS	2.6
1	D	164	GLY	2.6
1	D	357	TYR	2.6
1	B	58	LYS	2.6
1	D	302	LYS	2.6
1	D	95	ASP	2.5
1	D	90	TYR	2.5
1	A	191	ASP	2.5
1	D	260	ALA	2.5
1	C	56	GLN	2.4
1	D	89	ASP	2.4
1	C	265	SER	2.3
1	D	265	SER	2.3
1	B	308	GLN	2.3
1	A	282	ARG	2.2
1	D	33	LYS	2.2
1	D	93	ASN	2.2
1	C	297	PHE	2.2
1	B	395	HIS	2.2
1	A	308	GLN	2.2
1	D	398	HIS	2.1
1	A	193	LEU	2.1
1	B	8	LYS	2.1
1	B	264	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

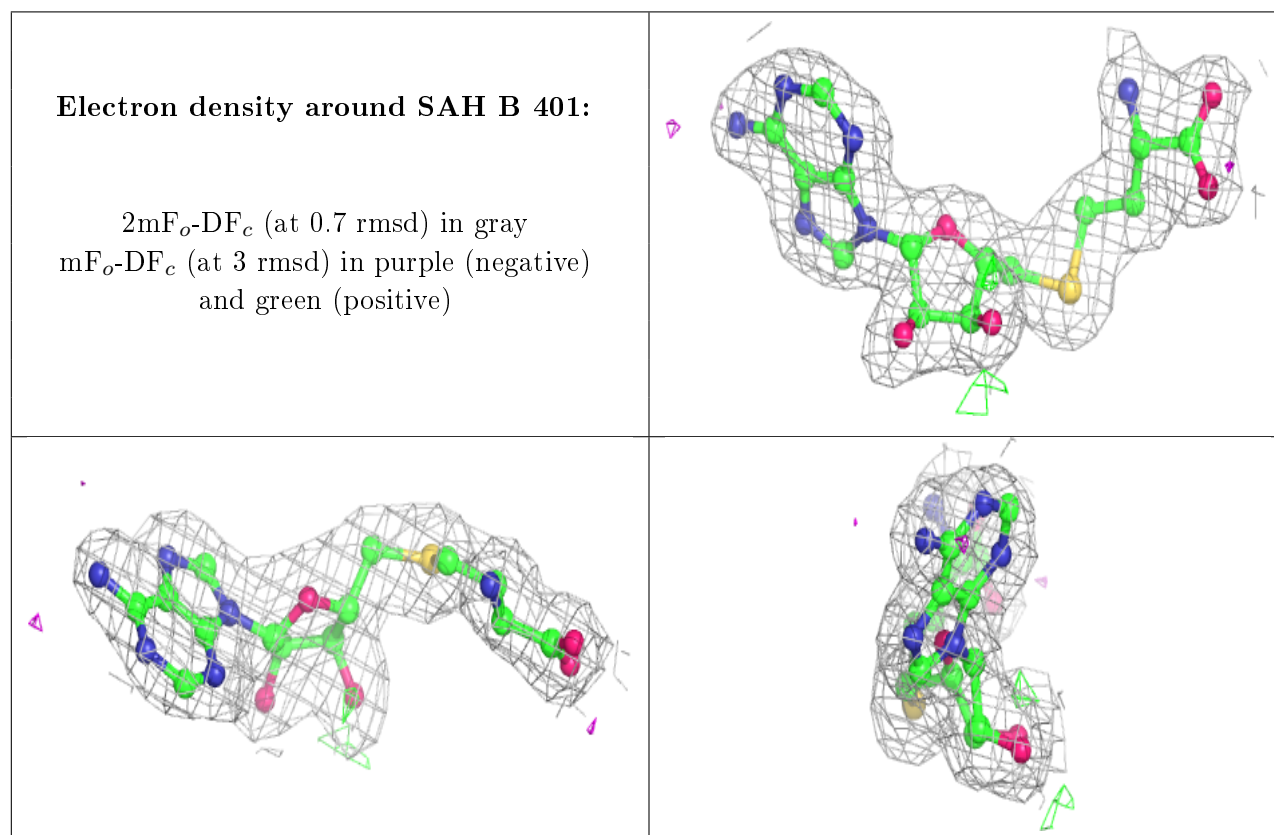
There are no carbohydrates in this entry.

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.

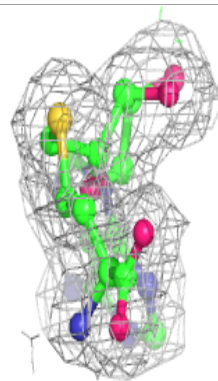
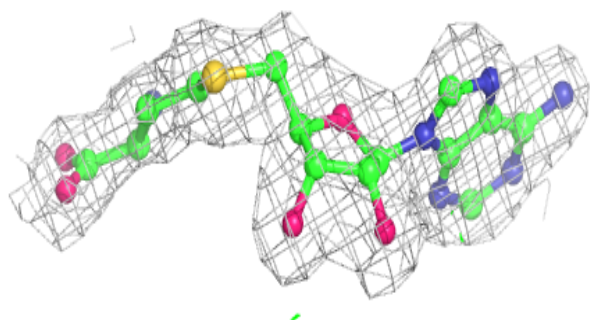
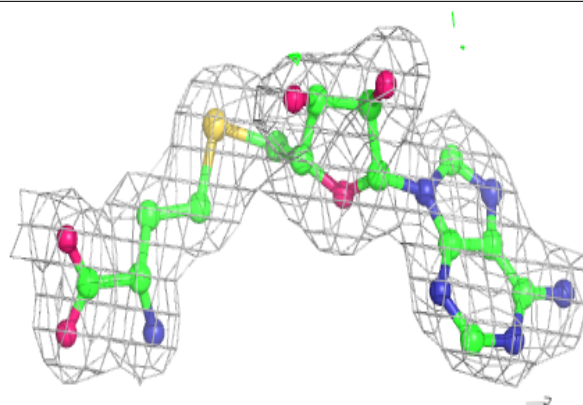
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SAH	B	401	26/26	0.94	0.11	10,15,18,20	0
2	SAH	C	401	26/26	0.95	0.12	13,16,21,22	0
2	SAH	A	401	26/26	0.96	0.11	8,11,15,16	0
2	SAH	D	401	26/26	0.96	0.09	12,16,21,22	0

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.

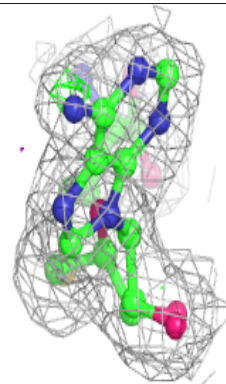
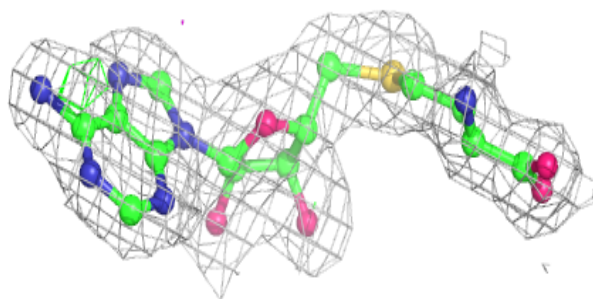
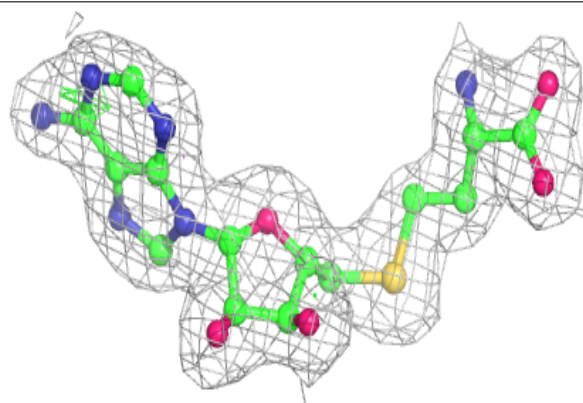


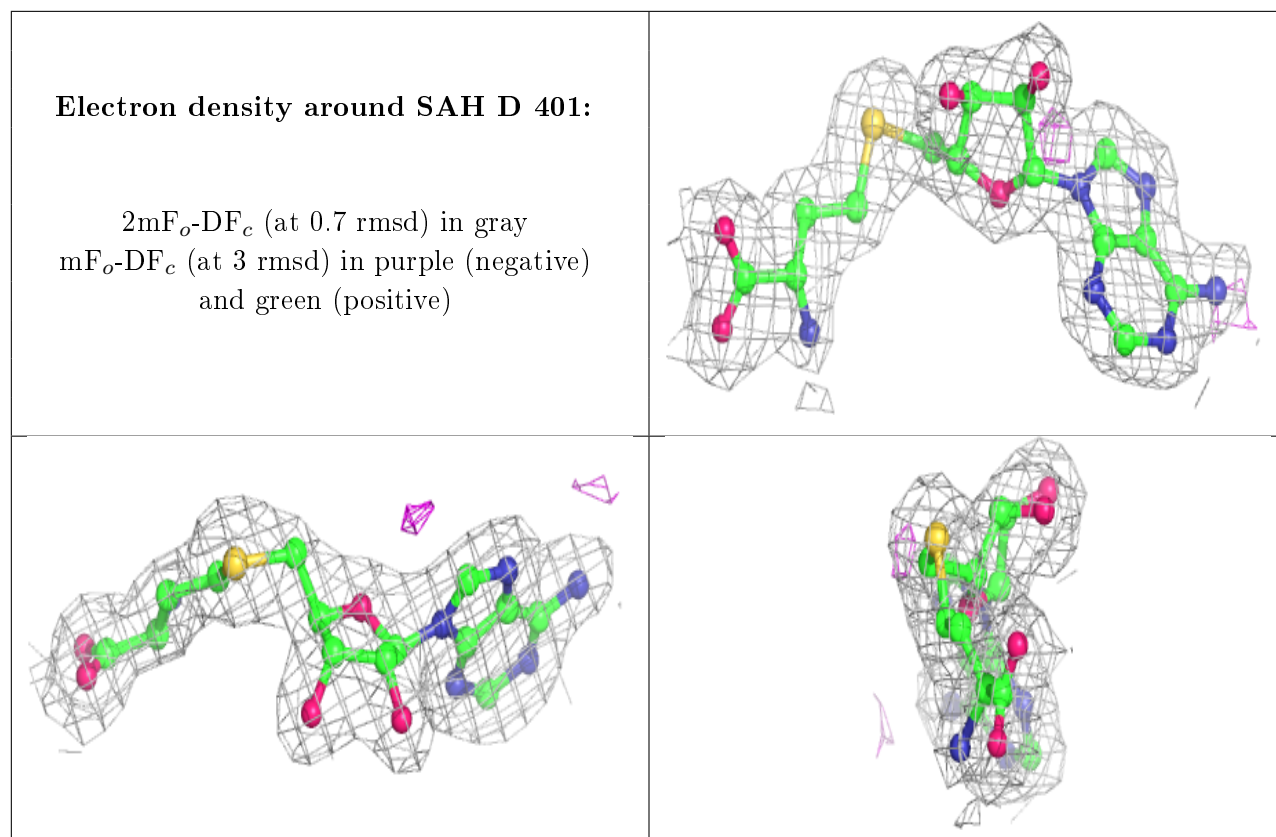
Electron density around SAH C 401:

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

**Electron density around SAH A 401:**

$2mF_o-DF_c$ (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.