



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:19 PM BST

PDB ID : 5CVJ
Title : Monolignol 4-O-methyltransferase 5 - coniferyl alcohol
Authors : Cai, Y.; Liu, C.-J.
Deposited on : 2015-07-27
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

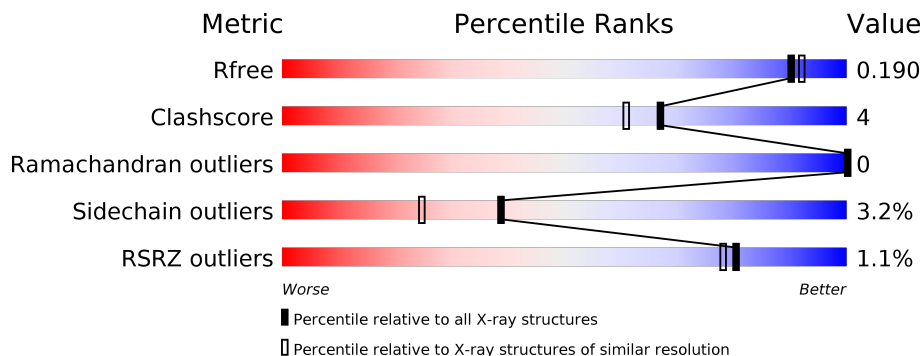
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	368	 87% 10% ..
1	B	368	 88% 8% ..
1	C	368	 88% 8% ..
1	D	368	 86% 11% ..

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	N7I	D	402	-	X	-	-
4	NO3	A	405	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12039 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.

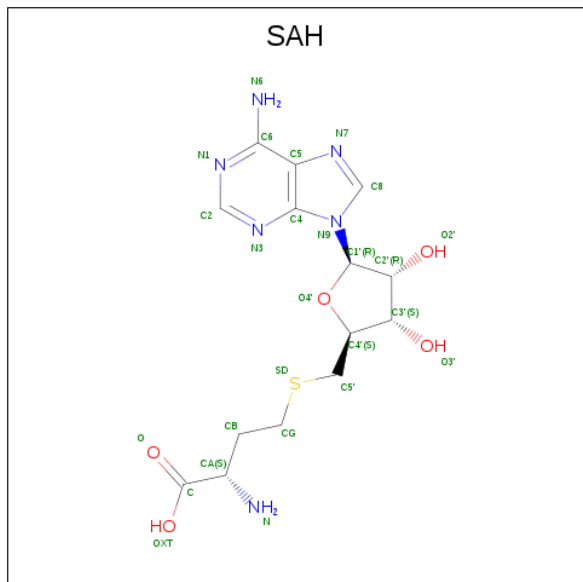
- Molecule 1 is a protein called (Iso)eugenol O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	361	2770	1795	444	513	18	0	0	0
1	A	361	2768	1795	444	511	18	0	0	0
1	B	354	2714	1758	436	502	18	0	0	0
1	C	356	2728	1767	438	505	18	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

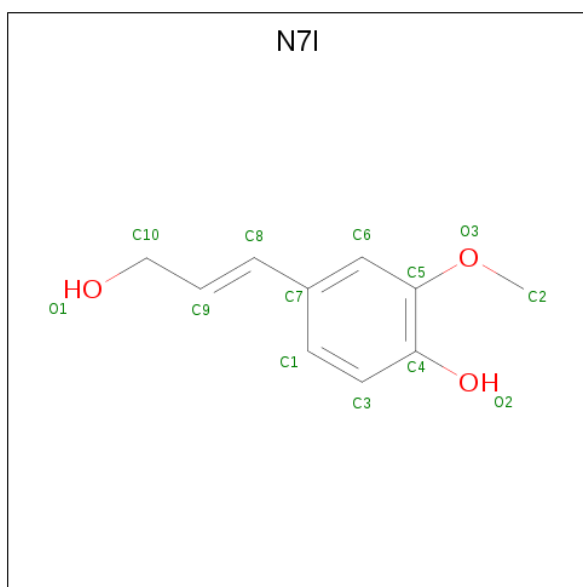
Chain	Residue	Modelled	Actual	Comment	Reference
D	133	LEU	THR	engineered mutation	UNP 004385
D	165	ILE	GLU	engineered mutation	UNP 004385
D	166	TRP	PHE	engineered mutation	UNP 004385
D	169	PHE	HIS	engineered mutation	UNP 004385
D	175	ILE	PHE	engineered mutation	UNP 004385
A	133	LEU	THR	engineered mutation	UNP 004385
A	165	ILE	GLU	engineered mutation	UNP 004385
A	166	TRP	PHE	engineered mutation	UNP 004385
A	169	PHE	HIS	engineered mutation	UNP 004385
A	175	ILE	PHE	engineered mutation	UNP 004385
B	133	LEU	THR	engineered mutation	UNP 004385
B	165	ILE	GLU	engineered mutation	UNP 004385
B	166	TRP	PHE	engineered mutation	UNP 004385
B	169	PHE	HIS	engineered mutation	UNP 004385
B	175	ILE	PHE	engineered mutation	UNP 004385
C	133	LEU	THR	engineered mutation	UNP 004385
C	165	ILE	GLU	engineered mutation	UNP 004385
C	166	TRP	PHE	engineered mutation	UNP 004385
C	169	PHE	HIS	engineered mutation	UNP 004385
C	175	ILE	PHE	engineered mutation	UNP 004385

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



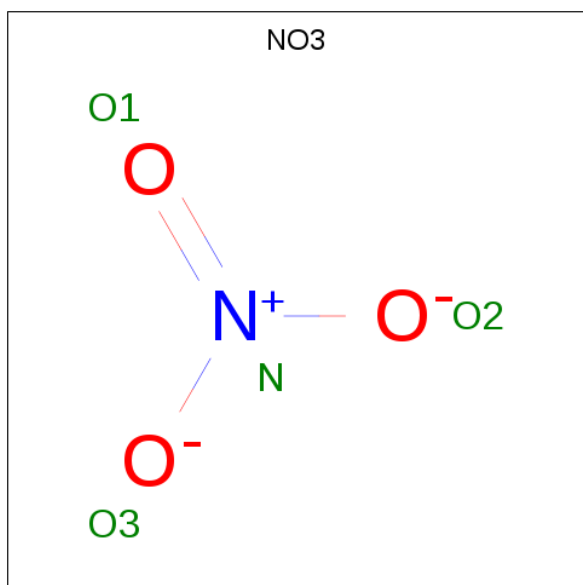
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 4-[(1E)-3-hydroxyprop-1-en-1-yl]-2-methoxyphenol (three-letter code: N7I) (formula: $C_{10}H_{12}O_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	C O	0	0
			13	10 3		
3	A	1	Total	C O	0	0
			13	10 3		
3	B	1	Total	C O	0	0
			13	10 3		
3	C	1	Total	C O	0	0
			13	10 3		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	195	Total O 195 195	0	0
5	A	198	Total O 198 198	0	0

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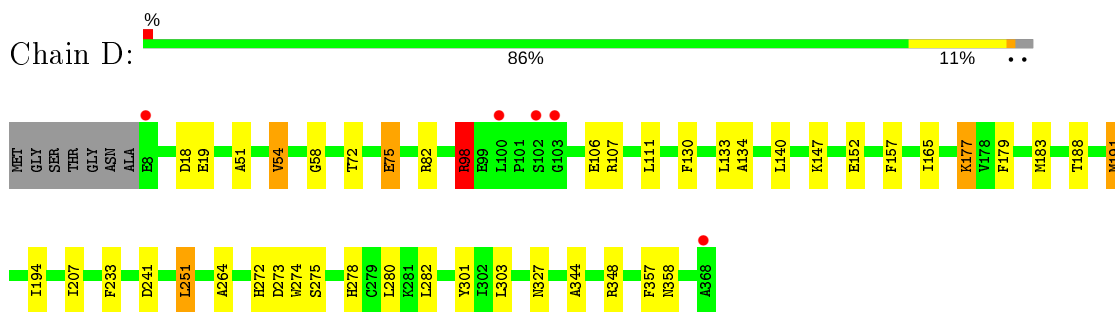
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	248	Total 248	O 248	0	0
5	C	190	Total 190	O 190	0	0

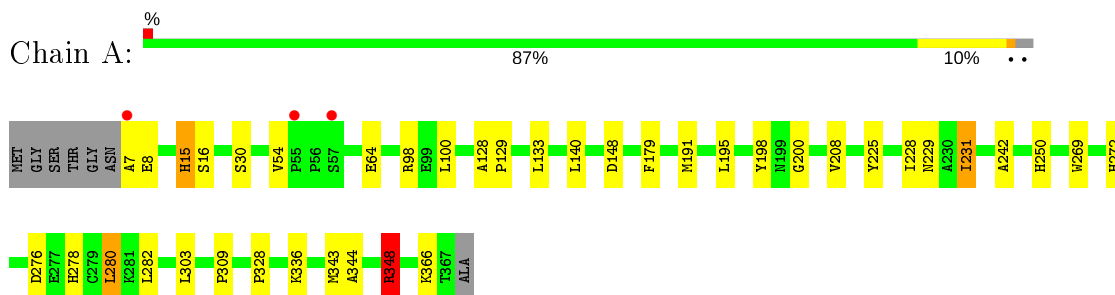
3 Residue-property plots i

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.

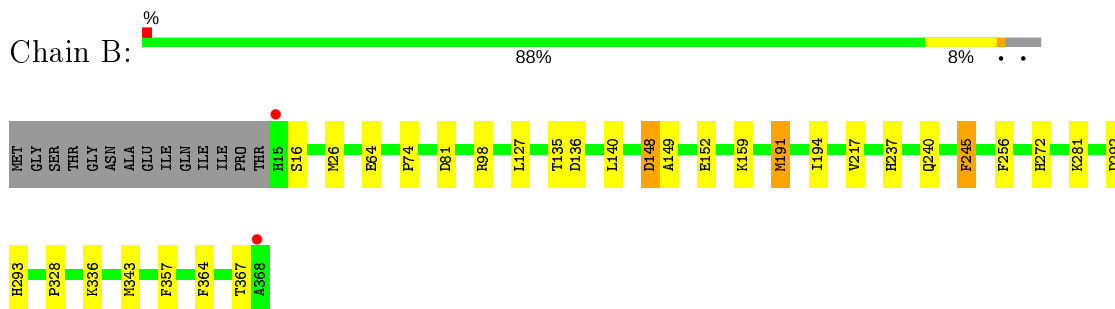
- Molecule 1: (Iso)eugenol O-methyltransferase



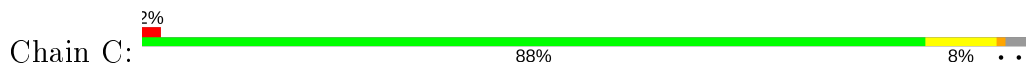
- Molecule 1: (Iso)eugenol O-methyltransferase

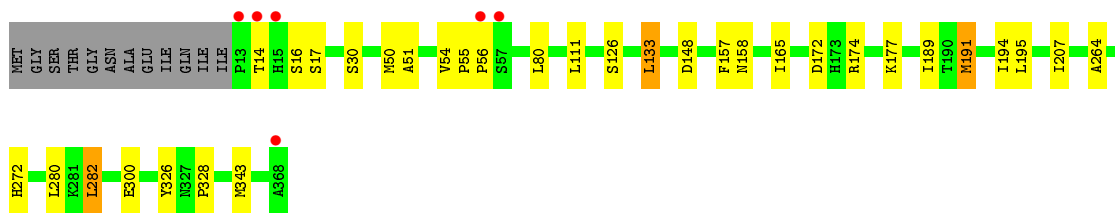


- Molecule 1: (Iso)eugenol O-methyltransferase



- Molecule 1: (Iso)eugenol O-methyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.07Å 150.36Å 67.93Å 90.00° 93.19° 90.00°	Depositor
Resolution (Å)	75.18 – 1.80 65.97 – 1.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.18-1.80) 97.8 (65.97-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.68Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.151 , 0.180 0.161 , 0.190	Depositor DCC
R_{free} test set	7376 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtrriage
Anisotropy	0.153	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.022 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12039	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, N7I, NO3

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	1.02	2/2836 (0.1%)	1.09	11/3857 (0.3%)
1	B	1.13	2/2781 (0.1%)	1.12	10/3779 (0.3%)
1	C	1.08	3/2796 (0.1%)	1.03	7/3800 (0.2%)
1	D	1.09	0/2838	1.05	8/3858 (0.2%)
All	All	1.08	7/11251 (0.1%)	1.07	36/15294 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CD-OE1	10.86	1.37	1.25
1	A	64	GLU	CD-OE1	6.83	1.33	1.25
1	C	300	GLU	CD-OE2	-6.44	1.18	1.25
1	C	174	ARG	N-CA	-6.04	1.34	1.46
1	B	245	PHE	CG-CD2	5.46	1.47	1.38
1	A	30	SER	CA-CB	5.34	1.60	1.52
1	C	30	SER	CA-CB	5.03	1.60	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	MET	CG-SD-CE	-14.91	76.35	100.20
1	B	98	ARG	NE-CZ-NH1	14.70	127.65	120.30
1	B	98	ARG	NE-CZ-NH2	-12.39	114.10	120.30
1	A	348	ARG	NE-CZ-NH1	11.33	125.97	120.30
1	C	177	LYS	CD-CE-NZ	10.13	135.01	111.70
1	A	98	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	B	343	MET	CG-SD-CE	-7.81	87.71	100.20
1	A	348	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	191	MET	CG-SD-CE	-7.42	88.33	100.20
1	D	98	ARG	NE-CZ-NH1	7.39	123.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	MET	CG-SD-CE	-6.89	89.17	100.20
1	A	303	LEU	CA-CB-CG	6.88	131.13	115.30
1	D	18	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	C	172	ASP	CB-CG-OD1	6.78	124.40	118.30
1	D	183	MET	CG-SD-CE	-6.74	89.41	100.20
1	A	148	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	18	ASP	CB-CG-OD1	6.60	124.24	118.30
1	C	148	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	191	MET	CG-SD-CE	-6.33	90.07	100.20
1	B	81	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	107	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	191	MET	CG-SD-CE	6.14	110.03	100.20
1	B	148	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	D	177	LYS	CD-CE-NZ	6.00	125.49	111.70
1	B	148	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	98	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	80	LEU	CB-CG-CD1	-5.86	101.04	111.00
1	B	364	PHE	CB-CG-CD1	5.59	124.72	120.80
1	A	148	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	276	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	D	82	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	282	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	292	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	303	LEU	CB-CG-CD1	5.16	119.77	111.00
1	B	127	LEU	CB-CG-CD2	5.16	119.77	111.00
1	C	282	LEU	CB-CG-CD1	5.08	119.64	111.00

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	2768	0	2787	26	0
1	B	2714	0	2726	19	0
1	C	2728	0	2741	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2770	0	2787	29	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
2	D	26	0	19	0	0
3	A	13	0	12	2	0
3	B	13	0	12	0	0
3	C	13	0	12	3	0
3	D	13	0	12	3	0
4	A	12	0	0	3	0
4	B	32	0	0	0	0
4	C	16	0	0	0	0
4	D	12	0	0	1	0
5	A	198	0	0	6	0
5	B	248	0	0	4	0
5	C	190	0	0	6	0
5	D	195	0	0	4	0
All	All	12039	0	11165	88	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 4.

All (88) 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:B:191:MET:HE2	1:B:194:ILE:HD12	1.49	0.94
1:A:140:LEU:HB2	4:A:405:NO3:N	1.83	0.92
1:D:75:GLU:HG2	5:D:675:HOH:O	1.78	0.84
1:D:134:ALA:O	5:D:501:HOH:O	2.00	0.79
1:C:326:TYR:HE2	3:C:402:N7I:H10A	1.48	0.78
1:D:191:MET:HE2	1:D:194:ILE:HD12	1.65	0.77
1:D:98:ARG:HD2	1:D:106:GLU:OE1	1.89	0.73
1:B:191:MET:CE	1:B:194:ILE:HD12	2.20	0.71
1:B:136:ASP:O	1:B:140:LEU:HD13	1.91	0.71
1:C:133:LEU:HD23	1:C:133:LEU:C	2.12	0.69
1:D:191:MET:CE	1:D:194:ILE:HD12	2.22	0.69
1:A:278:HIS:HD2	5:A:501:HOH:O	1.75	0.69
1:A:140:LEU:HB2	4:A:405:NO3:O1	1.95	0.67
1:B:191:MET:HG3	1:B:217:VAL:HG22	1.77	0.65
1:B:245:PHE:HB3	5:B:733:HOH:O	1.97	0.65
1:D:327:ASN:HD21	3:D:402:N7I:H2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:SER:OG	1:D:278:HIS:HD2	1.81	0.64
1:D:191:MET:HE2	1:D:191:MET:HA	1.82	0.61
3:A:402:N7I:H1	5:A:685:HOH:O	1.99	0.61
1:A:328:PRO:C	5:A:504:HOH:O	2.39	0.60
1:B:135:THR:HA	1:B:140:LEU:HD11	1.85	0.58
1:A:242:ALA:HB1	1:A:250:HIS:CE1	2.38	0.58
1:B:191:MET:CE	1:B:194:ILE:CD1	2.83	0.57
1:C:328:PRO:HD2	5:C:557:HOH:O	2.07	0.54
1:D:140:LEU:HG	5:D:501:HOH:O	2.07	0.54
1:C:326:TYR:CE2	3:C:402:N7I:H10A	2.35	0.53
1:B:240:GLN:OE1	5:B:501:HOH:O	2.18	0.53
1:D:152:GLU:HB3	5:D:657:HOH:O	2.09	0.52
1:A:198:TYR:CZ	1:A:200:GLY:HA3	2.45	0.52
1:A:133:LEU:HD23	1:A:133:LEU:C	2.31	0.51
1:B:328:PRO:HD2	5:B:666:HOH:O	2.10	0.51
1:C:191:MET:SD	1:C:194:ILE:HD12	2.52	0.50
1:D:280:LEU:HD11	1:D:344:ALA:HB3	1.93	0.50
1:D:357:PHE:O	1:D:358:ASN:HB2	2.12	0.50
1:A:336:LYS:CE	5:C:664:HOH:O	2.59	0.49
1:D:157:PHE:CE1	1:D:165:ILE:HA	2.47	0.49
1:C:133:LEU:CD2	1:C:133:LEU:C	2.80	0.49
1:A:348:ARG:CG	1:A:348:ARG:HH11	2.26	0.49
1:B:293:HIS:HD2	1:B:367:THR:OG1	1.96	0.48
1:A:225:TYR:CB	1:A:228:ILE:HD12	2.43	0.48
1:C:126:SER:HA	1:C:189:ILE:HD11	1.96	0.48
1:A:225:TYR:HB2	1:A:228:ILE:HD12	1.96	0.47
1:C:51:ALA:HA	1:C:111:LEU:HD11	1.96	0.47
1:D:130:PHE:CE2	1:B:26:MET:CE	2.97	0.47
1:A:336:LYS:HG3	5:A:575:HOH:O	2.12	0.47
1:D:54:VAL:HG13	1:D:58:GLY:HA2	1.96	0.47
1:A:15:HIS:CG	1:A:16:SER:N	2.84	0.46
1:A:208:VAL:HG13	1:A:231:ILE:HG13	1.97	0.46
1:A:336:LYS:HE2	5:C:664:HOH:O	2.16	0.46
1:C:133:LEU:CD2	3:C:402:N7I:H10	2.46	0.46
1:A:328:PRO:N	5:A:504:HOH:O	2.49	0.46
1:C:328:PRO:CD	5:C:557:HOH:O	2.64	0.46
1:D:130:PHE:CZ	3:D:402:N7I:C10	2.99	0.46
1:D:207:ILE:HD12	1:D:264:ALA:HB3	1.99	0.45
1:C:158:ASN:H	1:C:158:ASN:HD22	1.64	0.45
1:B:237:HIS:HE1	5:B:649:HOH:O	1.99	0.45
1:C:207:ILE:HD12	1:C:264:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:MET:HE1	1:B:194:ILE:HD13	1.98	0.45
1:D:188:THR:HG22	4:D:404:NO3:O2	2.16	0.45
1:D:274:TRP:HB3	1:D:278:HIS:HB2	1.97	0.45
1:D:301:TYR:CD1	1:D:358:ASN:HB3	2.52	0.44
1:D:327:ASN:HD21	3:D:402:N7I:C2	2.28	0.44
1:D:130:PHE:CE2	1:B:26:MET:HE1	2.53	0.44
1:C:157:PHE:CE1	1:C:165:ILE:HA	2.53	0.44
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.83	0.44
1:A:328:PRO:CA	5:A:504:HOH:O	2.66	0.44
1:B:191:MET:HE2	1:B:191:MET:HA	1.99	0.44
1:C:50:MET:O	1:C:54:VAL:HB	2.18	0.44
1:A:280:LEU:HD11	1:A:344:ALA:HB3	2.00	0.44
1:C:158:ASN:HD22	1:C:158:ASN:N	2.15	0.43
1:D:273:ASP:O	1:D:327:ASN:HB3	2.18	0.43
1:A:269:TRP:CE3	3:A:402:N7I:H3	2.54	0.43
1:B:191:MET:HE1	1:B:194:ILE:CD1	2.48	0.43
1:A:336:LYS:HE3	5:C:664:HOH:O	2.17	0.43
1:D:51:ALA:HA	1:D:111:LEU:HD11	2.00	0.43
1:A:133:LEU:HD12	1:A:179:PHE:HA	2.01	0.42
1:D:275:SER:OG	1:D:278:HIS:CD2	2.67	0.42
1:A:140:LEU:HD13	4:A:405:NO3:O3	2.19	0.42
1:D:301:TYR:CE1	1:D:358:ASN:HB3	2.55	0.42
1:A:7:ALA:O	1:A:8:GLU:HG3	2.20	0.42
1:D:19:GLU:OE2	1:B:357:PHE:HA	2.20	0.41
1:A:128:ALA:HB3	1:A:129:PRO:HD3	2.02	0.41
1:B:149:ALA:HA	1:B:159:LYS:HE3	2.02	0.41
1:D:233:PHE:HA	1:D:251:LEU:O	2.20	0.41
1:A:309:PRO:HB3	5:C:535:HOH:O	2.20	0.41
1:B:256:PHE:HB3	1:B:281:LYS:HE2	2.03	0.41
1:C:55:PRO:HB2	1:C:56:PRO:HD2	2.03	0.41
1:D:133:LEU:HD13	1:D:179:PHE:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/368 (98%)	353 (98%)	6 (2%)	0	100	100
1	B	352/368 (96%)	349 (99%)	3 (1%)	0	100	100
1	C	354/368 (96%)	350 (99%)	4 (1%)	0	100	100
1	D	359/368 (98%)	354 (99%)	5 (1%)	0	100	100
All	All	1424/1472 (97%)	1406 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/302 (99%)	287 (96%)	11 (4%)	34	19
1	B	291/302 (96%)	285 (98%)	6 (2%)	53	42
1	C	293/302 (97%)	284 (97%)	9 (3%)	40	25
1	D	298/302 (99%)	286 (96%)	12 (4%)	31	16
All	All	1180/1208 (98%)	1142 (97%)	38 (3%)	39	25

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	54	VAL
1	D	72	THR
1	D	75	GLU
1	D	98	ARG
1	D	147	LYS
1	D	177	LYS
1	D	241	ASP
1	D	251	LEU
1	D	272	HIS
1	D	282	LEU

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Mol	Chain	Res	Type
1	D	303	LEU
1	D	348	ARG
1	A	15	HIS
1	A	54	VAL
1	A	100	LEU
1	A	195	LEU
1	A	229	ASN
1	A	231	ILE
1	A	272	HIS
1	A	280	LEU
1	A	282	LEU
1	A	348	ARG
1	A	366	LYS
1	B	16	SER
1	B	74	PRO
1	B	148	ASP
1	B	152	GLU
1	B	272	HIS
1	B	336	LYS
1	C	14	THR
1	C	16	SER
1	C	17	SER
1	C	133	LEU
1	C	195	LEU
1	C	272	HIS
1	C	280	LEU
1	C	282	LEU
1	C	343	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	158	ASN
1	D	173	HIS
1	D	180	ASN
1	D	232	ASN
1	D	237	HIS
1	D	278	HIS
1	D	327	ASN
1	D	339	GLN
1	A	180	ASN
1	A	232	ASN

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Mol	Chain	Res	Type
1	A	237	HIS
1	A	240	GLN
1	A	278	HIS
1	A	293	HIS
1	A	327	ASN
1	B	158	ASN
1	B	173	HIS
1	B	180	ASN
1	B	232	ASN
1	B	237	HIS
1	B	240	GLN
1	B	293	HIS
1	B	327	ASN
1	C	158	ASN
1	C	180	ASN
1	C	232	ASN
1	C	237	HIS
1	C	278	HIS
1	C	327	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NO3	D	403	-	1,3,3	0.62	0	0,3,3	0.00	-
4	NO3	B	406	-	1,3,3	0.51	0	0,3,3	0.00	-
2	SAH	A	401	-	21,28,28	1.32	4 (19%)	20,40,40	1.88	3 (15%)
4	NO3	B	405	-	1,3,3	0.15	0	0,3,3	0.00	-
4	NO3	B	404	-	1,3,3	0.22	0	0,3,3	0.00	-
4	NO3	A	405	-	1,3,3	0.90	0	0,3,3	0.00	-
4	NO3	B	407	-	1,3,3	0.11	0	0,3,3	0.00	-
2	SAH	D	401	-	21,28,28	1.06	3 (14%)	20,40,40	1.14	1 (5%)
2	SAH	C	401	-	21,28,28	1.52	5 (23%)	20,40,40	1.83	5 (25%)
2	SAH	B	401	-	21,28,28	1.14	2 (9%)	20,40,40	1.96	5 (25%)
4	NO3	D	405	-	1,3,3	1.00	0	0,3,3	0.00	-
4	NO3	B	409	-	1,3,3	0.30	0	0,3,3	0.00	-
4	NO3	A	404	-	1,3,3	0.73	0	0,3,3	0.00	-
4	NO3	B	410	-	1,3,3	0.38	0	0,3,3	0.00	-
4	NO3	C	403	-	1,3,3	0.80	0	0,3,3	0.00	-
4	NO3	B	408	-	1,3,3	0.32	0	0,3,3	0.00	-
4	NO3	C	405	-	1,3,3	0.91	0	0,3,3	0.00	-
4	NO3	C	406	-	1,3,3	1.11	0	0,3,3	0.00	-
4	NO3	A	403	-	1,3,3	0.11	0	0,3,3	0.00	-
3	N7I	B	402	-	13,13,13	2.64	4 (30%)	16,16,16	2.40	9 (56%)
4	NO3	D	404	-	1,3,3	0.78	0	0,3,3	0.00	-
3	N7I	A	402	-	13,13,13	2.90	5 (38%)	16,16,16	2.12	6 (37%)
3	N7I	C	402	-	13,13,13	2.99	7 (53%)	16,16,16	1.75	2 (12%)
4	NO3	C	404	-	1,3,3	0.28	0	0,3,3	0.00	-
3	N7I	D	402	-	13,13,13	3.55	7 (53%)	16,16,16	3.19	8 (50%)
4	NO3	B	403	-	1,3,3	1.50	0	0,3,3	0.00	-

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	D	401	-	-	0/7/31/31	0/3/3/3
2	SAH	C	401	-	-	0/7/31/31	0/3/3/3
2	SAH	B	401	-	-	0/7/31/31	0/3/3/3
2	SAH	A	401	-	-	0/7/31/31	0/3/3/3
3	N7I	B	402	-	-	1/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N7I	A	402	-	-	0/6/6/6	0/1/1/1
3	N7I	C	402	-	-	0/6/6/6	0/1/1/1
3	N7I	D	402	-	-	1/6/6/6	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	N7I	O2-C4	7.65	1.52	1.36
3	C	402	N7I	C8-C9	7.36	1.54	1.31
3	D	402	N7I	C8-C9	6.54	1.52	1.31
3	A	402	N7I	C8-C9	6.34	1.51	1.31
3	B	402	N7I	C8-C9	5.95	1.50	1.31
3	A	402	N7I	O2-C4	5.15	1.46	1.36
3	D	402	N7I	C4-C5	4.44	1.48	1.40
3	B	402	N7I	O2-C4	4.24	1.45	1.36
3	C	402	N7I	O2-C4	3.95	1.44	1.36
3	D	402	N7I	C3-C1	3.90	1.45	1.38
3	A	402	N7I	C4-C5	3.86	1.47	1.40
3	B	402	N7I	C7-C8	-3.74	1.36	1.47
3	A	402	N7I	C7-C8	-3.70	1.36	1.47
2	C	401	SAH	C2-N3	3.59	1.37	1.32
3	B	402	N7I	C4-C5	3.52	1.46	1.40
3	C	402	N7I	C7-C8	-3.50	1.37	1.47
2	A	401	SAH	C2'-C1'	-3.36	1.48	1.53
3	D	402	N7I	C3-C4	3.22	1.45	1.39
3	C	402	N7I	C4-C5	3.19	1.46	1.40
2	C	401	SAH	O3'-C3'	3.03	1.50	1.43
3	D	402	N7I	O3-C2	2.85	1.51	1.42
3	C	402	N7I	C10-C9	2.72	1.55	1.49
3	C	402	N7I	O3-C5	2.51	1.41	1.37
2	C	401	SAH	O4'-C1'	2.41	1.44	1.41
2	D	401	SAH	CA-N	2.40	1.52	1.47
2	B	401	SAH	C5-C4	2.30	1.47	1.40
3	A	402	N7I	C6-C5	2.28	1.42	1.38
2	A	401	SAH	C5-C4	2.22	1.46	1.40
2	A	401	SAH	C8-N7	2.20	1.38	1.34
2	B	401	SAH	CA-N	2.19	1.52	1.47
2	C	401	SAH	CA-N	2.11	1.51	1.47
2	A	401	SAH	O4'-C4'	2.08	1.49	1.45
3	D	402	N7I	C7-C8	-2.08	1.41	1.47
2	D	401	SAH	C2'-C1'	-2.06	1.50	1.53
3	C	402	N7I	O3-C2	2.06	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	SAH	C5-C4	2.04	1.46	1.40
2	C	401	SAH	C5-N7	-2.02	1.32	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	N3-C2-N1	-6.80	118.05	128.68
3	D	402	N7I	C3-C4-C5	-5.77	112.82	119.53
2	C	401	SAH	N3-C2-N1	-5.56	119.99	128.68
3	D	402	N7I	O3-C5-C4	5.27	122.21	114.57
2	B	401	SAH	N3-C2-N1	-4.91	121.00	128.68
3	D	402	N7I	C2-O3-C5	4.37	124.12	117.53
3	D	402	N7I	C7-C6-C5	4.19	125.83	120.17
3	D	402	N7I	O3-C5-C6	-3.89	117.42	124.12
3	A	402	N7I	C3-C4-C5	-3.82	115.09	119.53
3	B	402	N7I	C3-C4-C5	-3.74	115.19	119.53
3	D	402	N7I	C6-C7-C8	-3.71	109.54	120.60
3	D	402	N7I	C1-C3-C4	3.69	124.30	120.50
3	B	402	N7I	C10-C9-C8	-3.65	116.87	124.61
3	C	402	N7I	C10-C9-C8	-3.54	117.09	124.61
3	B	402	N7I	C2-O3-C5	3.48	122.79	117.53
3	A	402	N7I	O3-C5-C4	3.47	119.59	114.57
3	D	402	N7I	C1-C7-C8	3.40	133.52	121.29
3	C	402	N7I	O3-C5-C4	3.34	119.41	114.57
2	B	401	SAH	C2-N1-C6	3.27	124.34	118.75
3	A	402	N7I	O3-C5-C6	-3.26	118.50	124.12
3	A	402	N7I	O2-C4-C5	3.21	127.59	120.09
2	B	401	SAH	N6-C6-N1	3.18	125.18	118.57
3	B	402	N7I	O3-C5-C4	3.07	119.01	114.57
3	B	402	N7I	C1-C3-C4	2.99	123.58	120.50
3	A	402	N7I	C10-C9-C8	-2.94	118.36	124.61
3	B	402	N7I	O2-C4-C5	2.83	126.70	120.09
2	C	401	SAH	O4'-C1'-C2'	-2.81	102.82	106.93
2	A	401	SAH	C2-N1-C6	2.74	123.45	118.75
3	B	402	N7I	C7-C8-C9	-2.61	120.48	126.99
3	B	402	N7I	O1-C10-C9	-2.43	105.24	112.06
2	B	401	SAH	C1'-N9-C4	-2.37	122.48	126.64
3	A	402	N7I	C7-C8-C9	-2.36	121.08	126.99
2	C	401	SAH	N6-C6-N1	2.36	123.46	118.57
2	B	401	SAH	O4'-C1'-C2'	-2.31	103.55	106.93
3	B	402	N7I	O3-C5-C6	-2.29	120.18	124.12
2	C	401	SAH	O2'-C2'-C3'	2.16	118.81	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	SAH	N3-C2-N1	-2.10	125.39	128.68
2	C	401	SAH	C2-N1-C6	2.10	122.35	118.75
2	A	401	SAH	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

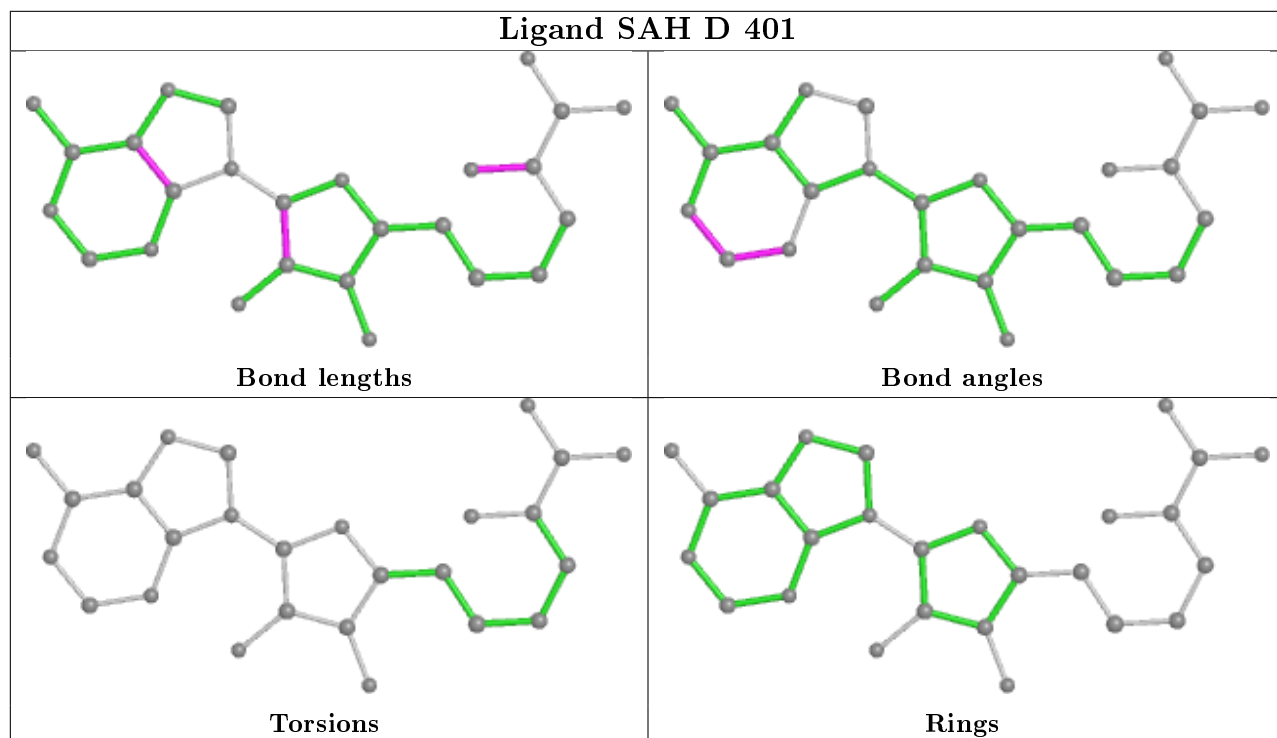
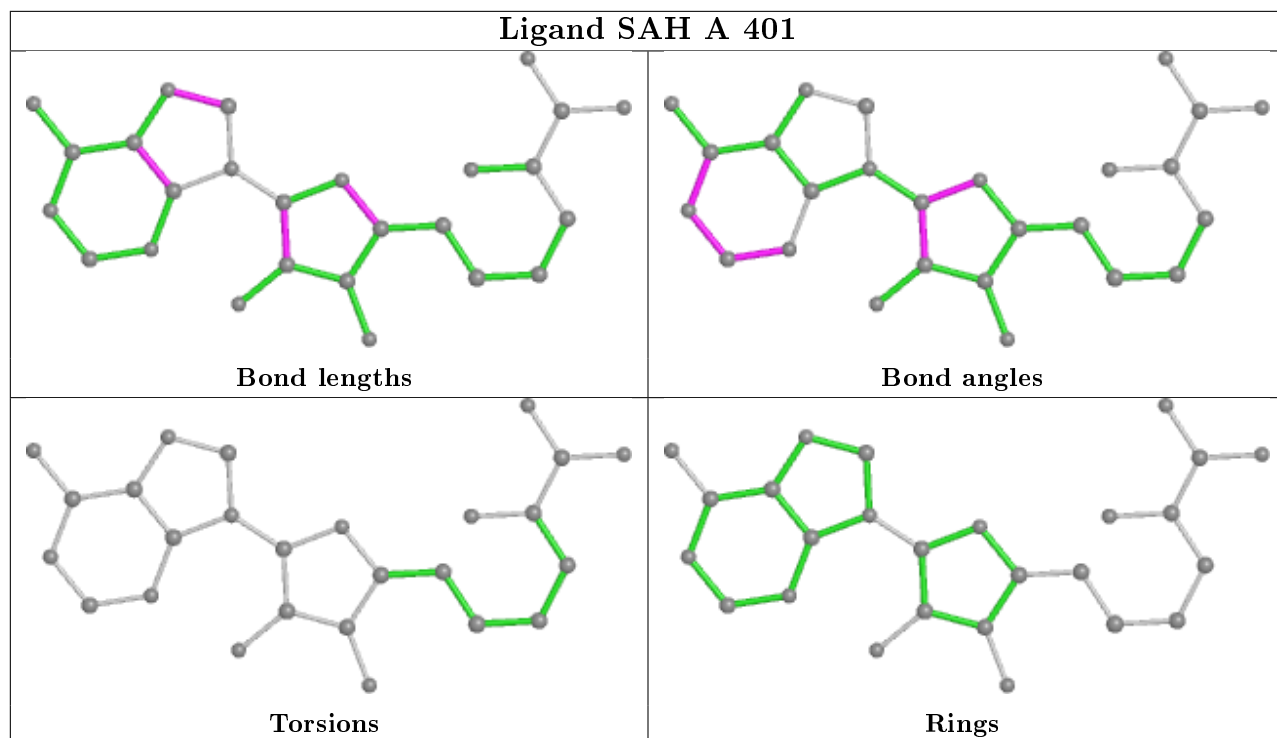
Mol	Chain	Res	Type	Atoms
3	D	402	N7I	C1-C7-C8-C9
3	B	402	N7I	O1-C10-C9-C8

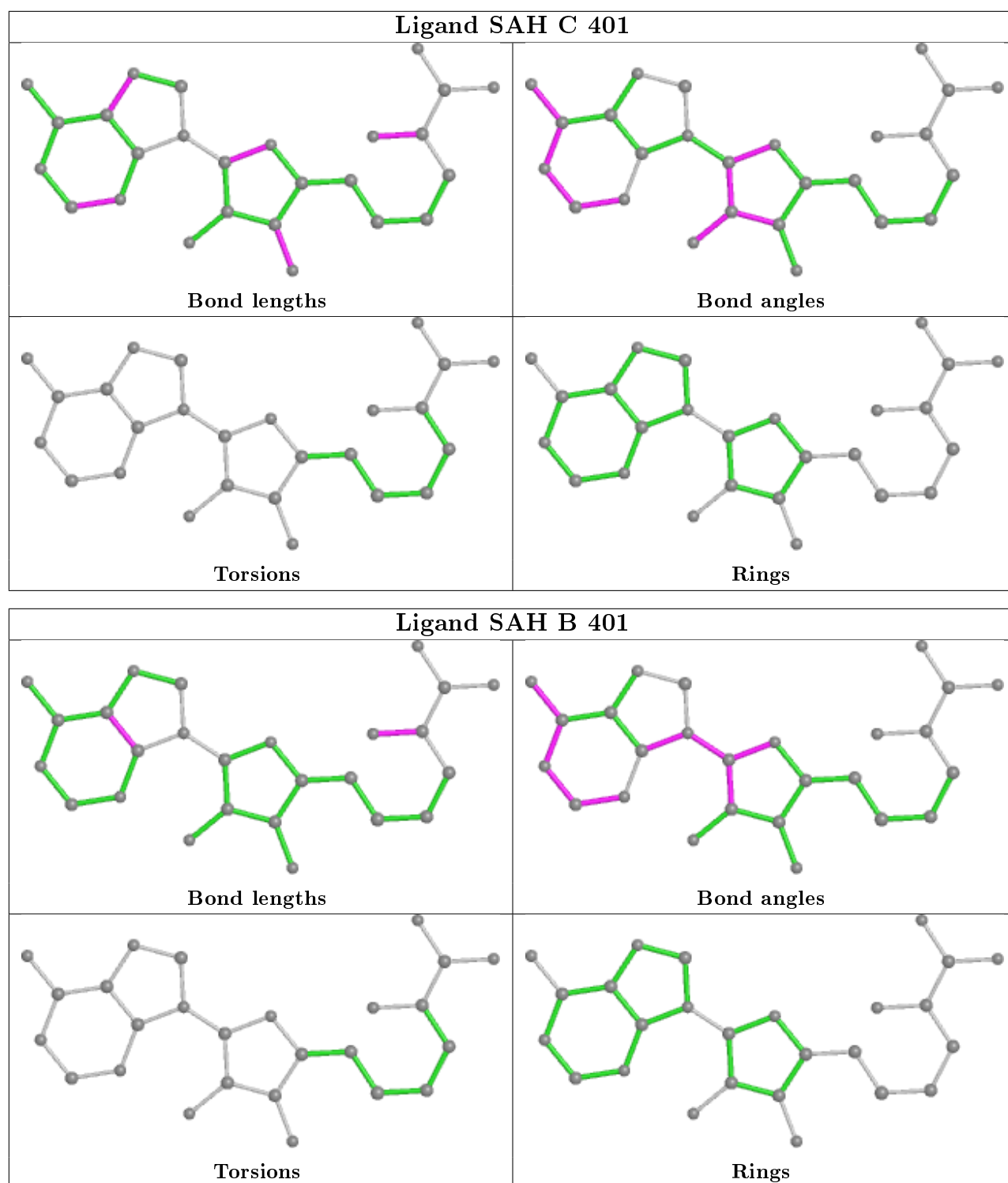
There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	NO3	3	0
4	D	404	NO3	1	0
3	A	402	N7I	2	0
3	C	402	N7I	3	0
3	D	402	N7I	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	361/368 (98%)	-0.56	3 (0%) 86 84	11, 21, 44, 71	0
1	B	354/368 (96%)	-0.67	2 (0%) 89 87	9, 15, 30, 88	0
1	C	356/368 (96%)	-0.55	6 (1%) 70 66	11, 20, 42, 112	0
1	D	361/368 (98%)	-0.57	5 (1%) 75 72	10, 19, 38, 71	0
All	All	1432/1472 (97%)	-0.59	16 (1%) 80 78	9, 19, 40, 112	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	PRO	8.0
1	C	13	PRO	6.3
1	B	15	HIS	4.9
1	D	100	LEU	3.5
1	A	55	PRO	3.5
1	D	103	GLY	3.1
1	C	14	THR	2.9
1	B	368	ALA	2.6
1	C	15	HIS	2.6
1	C	57	SER	2.5
1	A	57	SER	2.5
1	D	8	GLU	2.5
1	D	102	SER	2.3
1	C	368	ALA	2.3
1	D	368	ALA	2.2
1	A	7	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

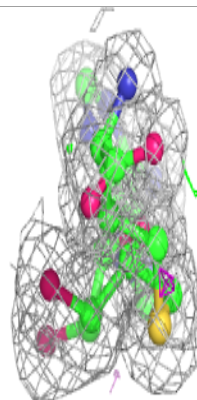
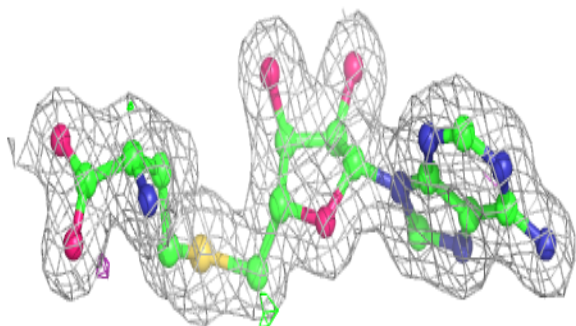
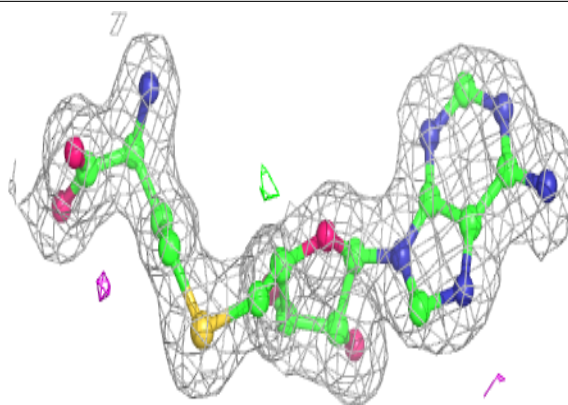
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NO3	A	405	4/4	0.55	0.36	43,51,52,60	0
4	NO3	B	409	4/4	0.76	0.15	38,45,45,49	0
3	N7I	A	402	13/13	0.78	0.26	25,48,57,58	0
3	N7I	B	402	13/13	0.81	0.21	21,41,51,59	0
3	N7I	C	402	13/13	0.82	0.33	23,51,59,69	0
3	N7I	D	402	13/13	0.88	0.35	19,42,93,103	0
4	NO3	D	403	4/4	0.91	0.15	37,39,39,44	0
4	NO3	B	410	4/4	0.92	0.26	46,46,49,57	0
4	NO3	C	406	4/4	0.94	0.15	32,36,44,50	0
4	NO3	B	405	4/4	0.95	0.08	28,32,38,41	0
4	NO3	C	404	4/4	0.95	0.12	29,29,30,32	0
4	NO3	A	404	4/4	0.95	0.22	37,37,41,43	0
4	NO3	A	403	4/4	0.96	0.09	33,37,38,43	0
4	NO3	B	408	4/4	0.96	0.17	24,29,32,38	0
4	NO3	B	407	4/4	0.97	0.11	23,25,26,32	0
4	NO3	D	405	4/4	0.97	0.05	33,40,40,44	0
4	NO3	C	405	4/4	0.97	0.12	41,44,44,47	0
4	NO3	D	404	4/4	0.97	0.19	34,38,39,39	0
2	SAH	A	401	26/26	0.98	0.06	15,18,20,23	0
4	NO3	B	406	4/4	0.98	0.07	21,22,25,29	0
2	SAH	D	401	26/26	0.98	0.06	12,15,17,18	0
4	NO3	C	403	4/4	0.98	0.11	29,30,32,36	0
2	SAH	C	401	26/26	0.98	0.07	13,17,19,20	0
2	SAH	B	401	26/26	0.98	0.07	10,11,12,12	0
4	NO3	B	404	4/4	0.98	0.07	23,26,27,27	0
4	NO3	B	403	4/4	0.98	0.09	25,27,30,32	0

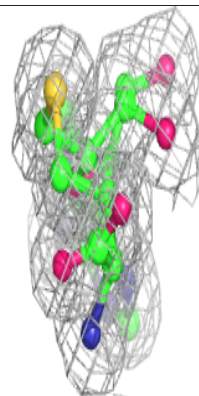
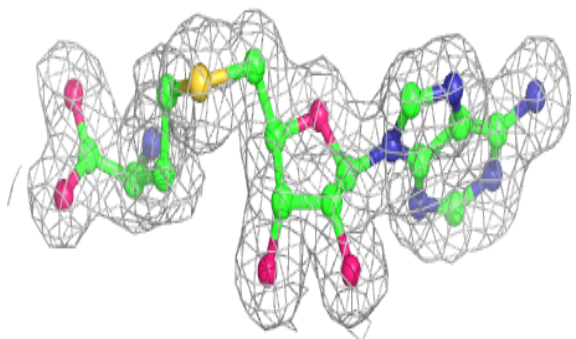
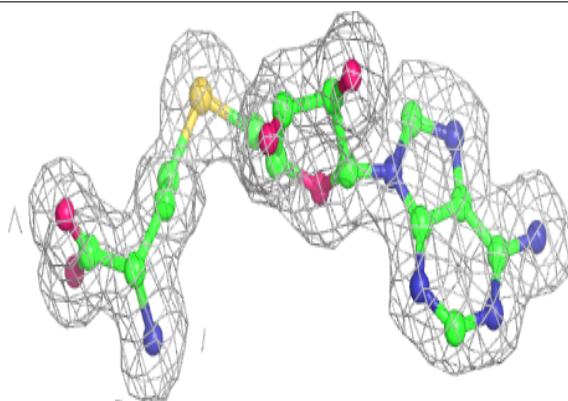
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH 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)

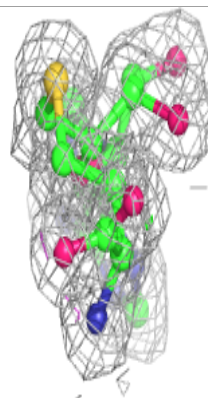
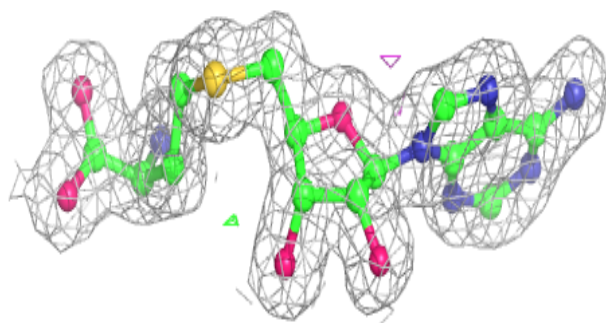
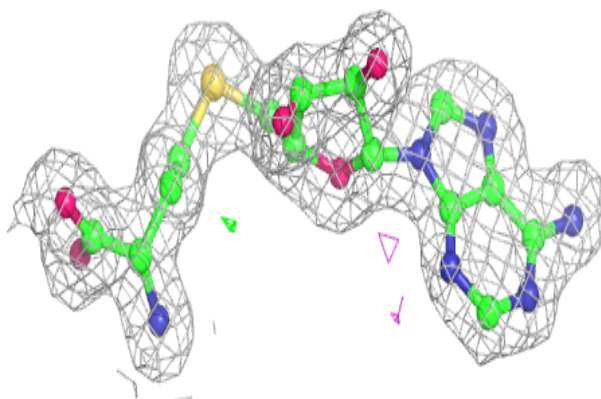
**Electron density around SAH D 401:**

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

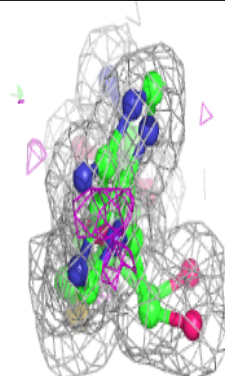
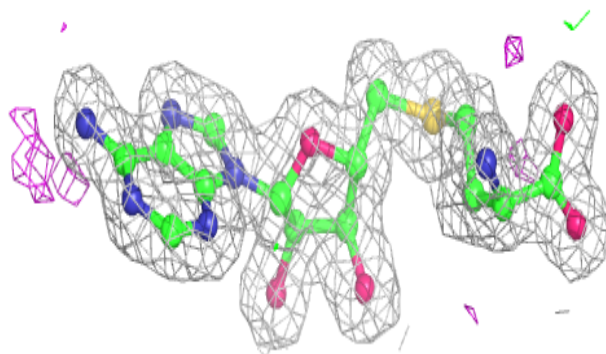
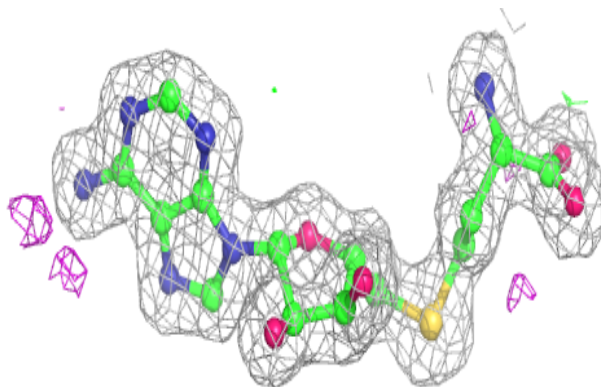


Electron density around SAH C 401:

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

**Electron density around SAH B 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

There are no such residues in this entry.