Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:03 AM EDT

PDB ID	:	3TOS
Title	:	Crystal Structure of CalS11, Calicheamicin Methyltransferase
Authors	:	Chang, A.; Aceti, D.J.; Beebe, E.T.; Makino, S.-I.; Wrobel, R.L.; Bingman, C.A.; Thorson, J.S.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on	:	2011-09-06
Resolution	:	1.55 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 (i) 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 (i)) were used in the production of this report:

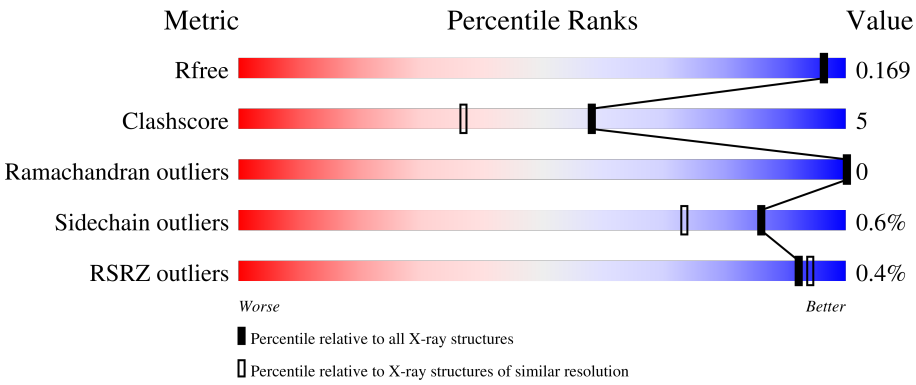
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	257	% 90% 7% •
1	B	257	% 90% 9%
1	C	257	87% 11% •
1	D	257	88% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	257	92% 6%
1	F	257	88% 9%
1	G	257	% 90% 7%
1	H	257	91% 6%
1	I	257	88% 9%
1	J	257	91% 7%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26923 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 CalS11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	251	2127	1355	375	389	3	5	0	13	0
1	B	257	2173	1380	384	401	3	5	0	14	0
1	C	251	2136	1360	376	392	3	5	0	14	0
1	D	251	2125	1355	374	388	3	5	0	13	0
1	E	251	2118	1350	373	387	3	5	0	12	0
1	F	251	2136	1360	376	392	3	5	0	14	0
1	G	252	2131	1357	376	390	3	5	0	13	0
1	H	251	2109	1345	371	385	3	5	0	11	0
1	I	251	2118	1349	373	388	3	5	0	12	0
1	J	251	2118	1349	373	388	3	5	0	12	0

There are 10 discrepancies between the modelled and reference sequences:

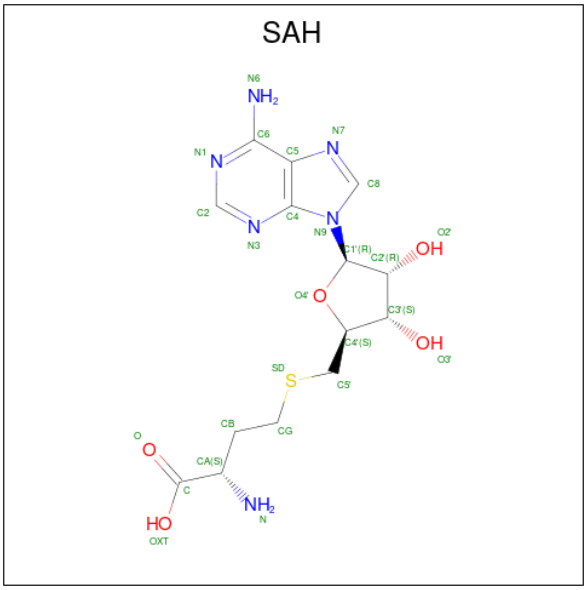
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
B	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
C	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
D	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
E	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
F	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
G	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
H	1	SER	-	EXPRESSION TAG	UNP Q8KNF1
I	1	SER	-	EXPRESSION TAG	UNP Q8KNF1

Continued on next page...

Continued from previous page...

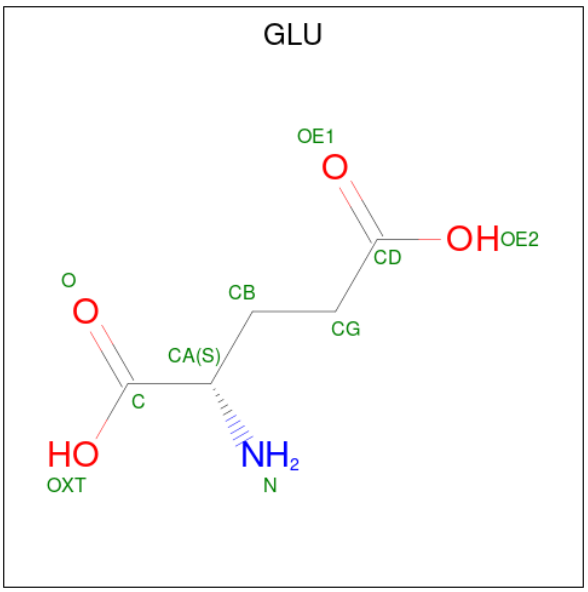
Chain	Residue	Modelled	Actual	Comment	Reference
J	1	SER	-	EXPRESSION TAG	UNP Q8KNF1

- 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	A	1	26	14	6	5	1	0	0
2	B	1	26	14	6	5	1	0	0
2	C	1	26	14	6	5	1	0	0
2	D	1	26	14	6	5	1	0	0
2	E	1	26	14	6	5	1	0	0
2	F	1	26	14	6	5	1	0	0
2	G	1	26	14	6	5	1	0	0
2	H	1	26	14	6	5	1	0	0
2	I	1	26	14	6	5	1	0	0
2	J	1	26	14	6	5	1	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	10	5	1	4	0	0
3	B	1	10	5	1	4	0	0
3	C	1	10	5	1	4	0	0
3	D	1	10	5	1	4	0	0
3	E	1	10	5	1	4	0	0
3	F	1	10	5	1	4	0	0
3	G	1	10	5	1	4	0	0
3	H	1	10	5	1	4	0	0
3	I	1	10	5	1	4	0	0
3	J	1	10	5	1	4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

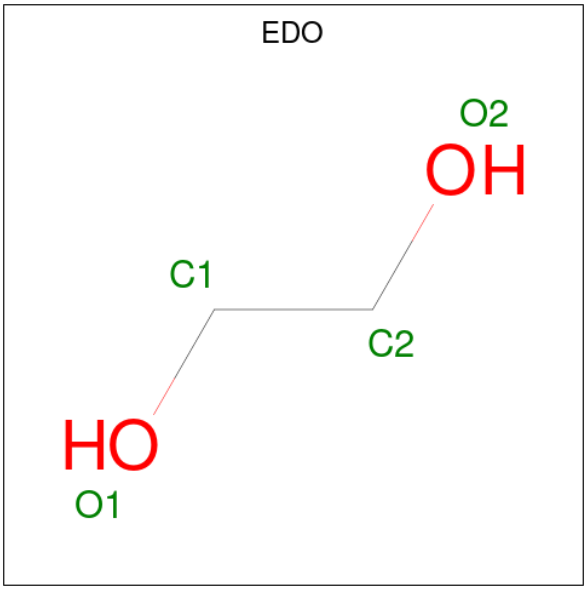
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	F	1	Total Na 1 1	0	0
4	G	1	Total Na 1 1	0	0
4	H	1	Total Na 1 1	0	0
4	I	1	Total Na 1 1	0	0
4	J	1	Total Na 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	D	1	4	2	2	0	0
			Total	C	O		
5	D	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0
			Total	C	O		
5	G	1	4	2	2	0	0
			Total	C	O		
5	H	1	4	2	2	0	0
			Total	C	O		
5	I	1	4	2	2	0	0
			Total	C	O		
5	I	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0
			Total	C	O		
5	J	1	4	2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	551	551	551	0	0
			Total	O		
6	B	494	494	494	0	0
			Total	O		
6	C	516	516	516	0	0
			Total	O		
6	D	495	495	495	0	0
			Total	O		
6	E	477	477	477	0	0
			Total	O		
6	F	512	512	512	0	0

Continued on next page...

Continued from previous page...

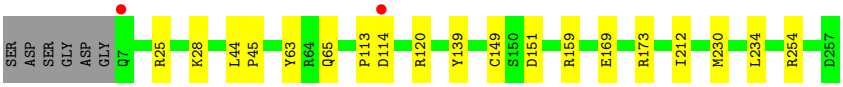
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	G	514	514	514	0	0
			Total	O		
6	H	565	565	565	0	0
			Total	O		
6	I	540	540	540	0	0
			Total	O		
6	J	538	538	538	0	0

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.

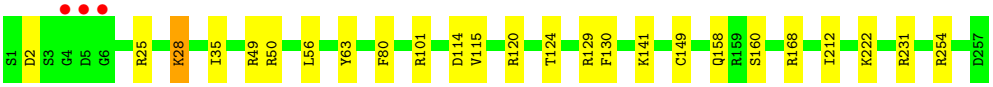
- Molecule 1: CalS11

Chain A:



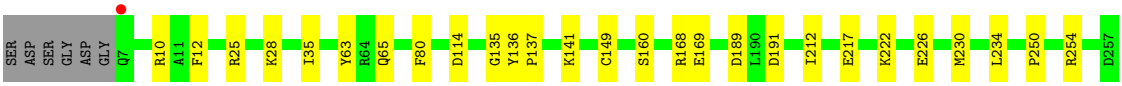
- Molecule 1: CalS11

Chain B:



- Molecule 1: CalS11

Chain C:



- Molecule 1: CalS11

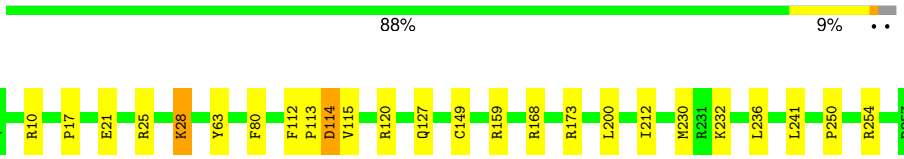
Chain D:

- Molecule 1: CalS11

Chain E:

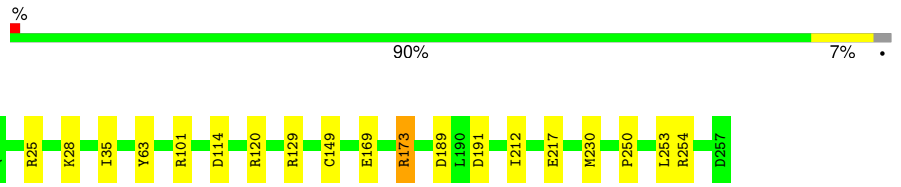
- Molecule 1: CalS11

Chain F:



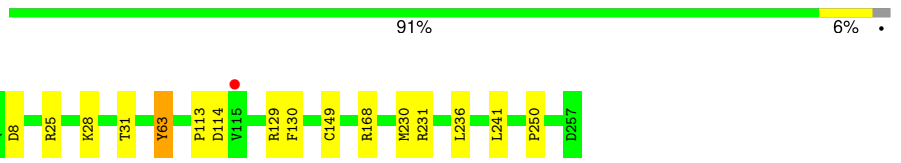
• Molecule 1: CalS11

Chain G:



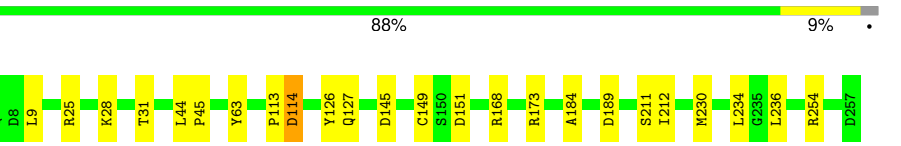
• Molecule 1: CalS11

Chain H:



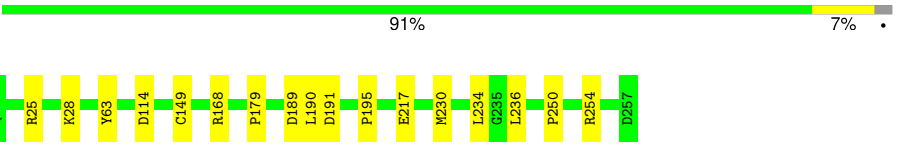
• Molecule 1: CalS11

Chain I:



• Molecule 1: CalS11

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.32Å 106.08Å 106.33Å 68.69° 69.63° 88.56°	Depositor
Resolution (Å)	43.10 – 1.55 43.10 – 1.55	Depositor EDS
% Data completeness (in resolution range)	95.5 (43.10-1.55) 95.6 (43.10-1.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.146 , 0.173 0.142 , 0.169	Depositor DCC
R_{free} test set	1875 reflections (0.45%)	wwPDB-VP
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26923	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.90	0/2178	0.85	3/2956 (0.1%)
1	B	0.91	0/2224	0.87	4/3018 (0.1%)
1	C	0.95	0/2187	0.87	0/2968
1	D	0.91	0/2176	0.82	2/2954 (0.1%)
1	E	0.89	0/2169	0.82	1/2944 (0.0%)
1	F	0.92	0/2187	0.87	1/2968 (0.0%)
1	G	0.94	0/2182	0.87	6/2961 (0.2%)
1	H	0.95	1/2160 (0.0%)	0.85	2/2932 (0.1%)
1	I	0.91	1/2169 (0.0%)	0.88	3/2945 (0.1%)
1	J	0.93	0/2169	0.85	0/2945
All	All	0.92	2/21801 (0.0%)	0.86	22/29591 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	63	TYR	CG-CD1	-5.18	1.32	1.39
1	I	126	TYR	CD1-CE1	-5.12	1.31	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	173[A]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	G	173[B]	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	159[A]	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	159[B]	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	173[A]	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	G	173[B]	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	2	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	231	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	G	129	ARG	NE-CZ-NH2	5.31	122.96	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	H	8	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	H	231	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	I	9	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	D	173[A]	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	173[B]	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	E	231	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	G	101	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	I	145	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	101	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	I	151	ASP	CB-CG-OD1	5.11	122.90	118.30
1	F	112	PHE	CB-CG-CD1	5.06	124.34	120.80
1	A	151	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2127	0	2089	20	0
1	B	2173	0	2132	23	0
1	C	2136	0	2094	33	0
1	D	2125	0	2089	27	0
1	E	2118	0	2082	19	0
1	F	2136	0	2094	24	0
1	G	2131	0	2092	25	0
1	H	2109	0	2074	16	0
1	I	2118	0	2077	22	0
1	J	2118	0	2077	20	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	1	0
2	D	26	0	19	0	0
2	E	26	0	19	1	0
2	F	26	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	26	0	18	1	0
2	H	26	0	19	0	0
2	I	26	0	19	1	0
2	J	26	0	19	1	0
3	A	10	0	5	0	0
3	B	10	0	5	0	0
3	C	10	0	5	0	0
3	D	10	0	5	0	0
3	E	10	0	5	0	0
3	F	10	0	5	0	0
3	G	10	0	5	0	0
3	H	10	0	5	0	0
3	I	10	0	5	0	0
3	J	10	0	5	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	8	0	12	1	0
5	D	8	0	12	0	0
5	E	4	0	6	1	0
5	F	8	0	12	1	0
5	G	4	0	6	1	0
5	H	4	0	6	1	0
5	I	8	0	12	3	0
5	J	8	0	12	2	0
6	A	551	0	0	10	0
6	B	494	0	0	6	0
6	C	516	0	0	15	0
6	D	495	0	0	10	0
6	E	477	0	0	7	0
6	F	512	0	0	10	0
6	G	514	0	0	14	0
6	H	565	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	540	0	0	9	0
6	J	538	0	0	4	0
All	All	26923	0	21229	205	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (205) 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:E:7:GLN:HG3	1:E:8:ASP:H	1.17	1.04
1:F:80:PHE:CG	6:G:5934:HOH:O	2.21	0.93
1:D:28[B]:LYS:HE3	6:D:5445:HOH:O	1.70	0.92
1:C:12:PHE:HB3	6:C:5960:HOH:O	1.72	0.89
1:A:28[A]:LYS:HE2	6:A:4790:HOH:O	1.74	0.85
1:J:230[B]:MSE:HE1	1:J:234:LEU:HD12	1.57	0.85
1:F:28[B]:LYS:HE3	6:F:5775:HOH:O	1.80	0.81
1:B:35[B]:ILE:HD12	1:C:80:PHE:CD1	2.15	0.81
1:G:35:ILE:HG12	6:G:5934:HOH:O	1.80	0.80
1:G:114[A]:ASP:HB3	6:G:5956:HOH:O	1.82	0.79
1:C:135:GLY:HA3	6:C:6020:HOH:O	1.81	0.79
1:E:7:GLN:HG3	1:E:8:ASP:N	1.98	0.75
1:I:28:LYS:HD2	6:I:994:HOH:O	1.87	0.75
1:F:200:LEU:HD13	6:F:4894:HOH:O	1.89	0.73
1:H:28[B]:LYS:HG2	6:H:3926:HOH:O	1.87	0.72
1:B:35[B]:ILE:CD1	1:C:80:PHE:CD1	2.72	0.72
1:G:35:ILE:HG23	6:G:5934:HOH:O	1.89	0.72
1:B:158[A]:GLN:NE2	6:B:662:HOH:O	2.23	0.71
1:D:114[B]:ASP:HB3	6:D:640:HOH:O	1.91	0.71
1:H:31:THR:HG22	5:J:261:EDO:H22	1.73	0.70
1:G:169:GLU:CD	1:G:173[A]:ARG:HH22	1.93	0.70
1:F:230[B]:MSE:HG2	1:F:236:LEU:HD23	1.71	0.70
1:F:17:PRO:O	1:F:21[B]:GLU:HG3	1.93	0.69
1:H:230[A]:MSE:HE3	1:H:241:LEU:HD11	1.74	0.68
1:D:28[B]:LYS:HD2	6:D:3919:HOH:O	1.94	0.68
1:A:113[A]:PRO:HG2	6:A:2349:HOH:O	1.91	0.68
1:J:230[B]:MSE:CE	1:J:234:LEU:HD12	2.24	0.68
1:G:6:GLY:HA3	6:G:392:HOH:O	1.93	0.68
1:F:232:LYS:HD3	6:F:5542:HOH:O	1.92	0.68
1:C:28[A]:LYS:HG2	6:C:3744:HOH:O	1.95	0.67
1:F:80:PHE:CD1	6:G:5934:HOH:O	2.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:GLU:HG2	1:G:173[A]:ARG:NH2	2.10	0.66
1:D:230[B]:MSE:HG2	1:D:236:LEU:HD23	1.77	0.66
1:F:25:ARG:NH1	1:G:149[B]:CYS:SG	2.68	0.66
1:C:230[B]:MSE:HE3	1:C:234:LEU:HD12	1.78	0.66
1:J:230[B]:MSE:HG2	1:J:236:LEU:HD23	1.78	0.66
1:B:28[A]:LYS:HE2	6:B:465:HOH:O	1.95	0.65
1:A:120[B]:ARG:NH1	6:A:3978:HOH:O	2.28	0.64
1:E:28[B]:LYS:HD2	6:E:3604:HOH:O	1.97	0.64
1:C:169:GLU:HG3	6:C:682:HOH:O	1.99	0.63
1:A:28[B]:LYS:HG2	6:A:3783:HOH:O	1.97	0.62
1:E:8:ASP:HB2	6:E:271:HOH:O	1.99	0.62
1:F:113[B]:PRO:HG2	6:F:461:HOH:O	2.00	0.62
1:C:222:LYS:HB2	6:C:5960:HOH:O	2.00	0.61
1:D:232:LYS:HG2	6:D:1781:HOH:O	1.99	0.61
1:H:114[B]:ASP:HB3	6:H:272:HOH:O	2.00	0.61
1:C:114[A]:ASP:OD2	1:C:168:ARG:NH2	2.33	0.60
1:J:28:LYS:HE3	6:J:5235:HOH:O	2.00	0.60
1:C:65:GLN:OE1	1:C:254[B]:ARG:NH2	2.35	0.59
1:D:230[B]:MSE:HE1	1:D:241:LEU:HD21	1.85	0.59
1:C:12:PHE:CB	6:C:5960:HOH:O	2.41	0.59
1:E:7:GLN:CG	1:E:8:ASP:H	2.02	0.58
1:D:28[B]:LYS:HE2	6:D:2316:HOH:O	2.03	0.58
1:J:250:PRO:HD3	5:J:262:EDO:H22	1.86	0.58
1:J:114[B]:ASP:OD1	1:J:168:ARG:NH2	2.34	0.57
1:E:113[B]:PRO:HB3	6:E:918:HOH:O	2.05	0.57
1:G:35:ILE:CG2	6:G:5934:HOH:O	2.50	0.57
1:I:113[B]:PRO:HG2	6:I:283:HOH:O	2.04	0.57
1:B:25:ARG:NH1	1:C:149[B]:CYS:SG	2.79	0.56
1:H:114[A]:ASP:OD2	1:H:168:ARG:NH2	2.38	0.56
1:C:114[B]:ASP:HB3	6:C:274:HOH:O	2.05	0.56
1:H:114[A]:ASP:CG	1:H:168:ARG:HH22	2.09	0.56
1:D:115:VAL:HG22	6:D:279:HOH:O	2.05	0.56
1:F:25:ARG:CZ	1:G:149[B]:CYS:SG	2.95	0.55
1:G:28[A]:LYS:HE2	6:G:5181:HOH:O	2.07	0.55
1:E:108:THR:HG21	1:E:113[B]:PRO:HG3	1.87	0.55
1:H:113[B]:PRO:HG2	6:H:2434:HOH:O	2.06	0.54
1:E:230[B]:MSE:HE1	1:E:253:LEU:CD2	2.38	0.54
1:I:31:THR:HG22	5:I:262:EDO:C1	2.38	0.54
1:A:120[B]:ARG:NH2	6:A:848:HOH:O	2.40	0.54
1:E:25:ARG:CZ	1:I:149[C]:CYS:SG	2.96	0.54
1:A:212:ILE:CD1	1:A:254[B]:ARG:HG2	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127[A]:GLN:NE2	6:I:268:HOH:O	2.42	0.53
1:I:113[A]:PRO:HB3	6:I:5671:HOH:O	2.09	0.52
1:J:114[B]:ASP:CG	1:J:168:ARG:HH22	2.13	0.52
1:D:114[A]:ASP:CG	1:D:168:ARG:HH22	2.12	0.52
1:A:149[C]:CYS:SG	1:D:25:ARG:CZ	2.98	0.52
1:A:65:GLN:OE1	1:A:254[B]:ARG:CZ	2.58	0.52
1:G:169:GLU:CG	1:G:173[A]:ARG:HH22	2.23	0.52
1:B:222:LYS:HD2	6:B:3080:HOH:O	2.10	0.52
1:B:254[A]:ARG:CZ	6:B:3728:HOH:O	2.57	0.52
1:A:25:ARG:CZ	1:D:149[B]:CYS:SG	2.98	0.51
1:D:28[B]:LYS:HG2	6:D:2316:HOH:O	2.10	0.51
1:B:129[B]:ARG:HD3	1:B:130:PHE:N	2.25	0.51
1:C:35:ILE:CG2	6:C:5938:HOH:O	2.59	0.51
1:H:25:ARG:CZ	1:J:149[B]:CYS:SG	2.98	0.51
1:E:149[B]:CYS:SG	1:I:25:ARG:CZ	2.99	0.51
1:A:28[B]:LYS:HG3	6:A:2863:HOH:O	2.10	0.50
1:F:250:PRO:HD3	5:F:261:EDO:H22	1.92	0.50
1:H:230[A]:MSE:HG2	1:H:236:LEU:HD23	1.93	0.50
1:C:28[B]:LYS:HE3	6:C:3272:HOH:O	2.10	0.50
1:J:114[A]:ASP:HB3	6:J:4693:HOH:O	2.10	0.50
1:C:191:ASP:OD1	1:C:217[B]:GLU:CD	2.50	0.50
1:C:217[B]:GLU:HG2	1:C:226:GLU:CD	2.32	0.50
1:I:230[B]:MSE:HG2	1:I:236:LEU:HD23	1.94	0.50
1:C:114[B]:ASP:CB	6:C:274:HOH:O	2.60	0.49
1:H:25:ARG:NH1	1:J:149[B]:CYS:SG	2.85	0.49
1:I:114[A]:ASP:OD1	6:I:2956:HOH:O	2.20	0.49
1:I:211:SER:HB3	6:I:383:HOH:O	2.13	0.49
1:B:35[B]:ILE:HD11	1:C:136:TYR:CE1	2.47	0.49
1:D:159[B]:ARG:NH1	6:D:5975:HOH:O	2.30	0.49
1:F:212:ILE:CD1	1:F:254[B]:ARG:HG2	2.43	0.49
1:H:28[B]:LYS:HG3	6:H:3116:HOH:O	2.12	0.49
1:H:114[B]:ASP:CB	6:H:272:HOH:O	2.59	0.49
1:D:217[B]:GLU:HG2	1:D:226:GLU:CD	2.33	0.49
1:C:114[A]:ASP:CG	1:C:168:ARG:HH22	2.14	0.48
1:D:217[B]:GLU:HG2	1:D:226:GLU:OE1	2.13	0.48
1:G:173[A]:ARG:HD2	6:G:3471:HOH:O	2.14	0.48
1:I:31:THR:HG22	5:I:262:EDO:H12	1.95	0.48
1:B:141:LYS:NZ	1:B:160[A]:SER:O	2.45	0.48
1:B:35[B]:ILE:HD11	1:C:136:TYR:OH	2.14	0.48
1:G:230[B]:MSE:HE2	6:G:2362:HOH:O	2.14	0.48
1:E:25:ARG:NH1	1:I:149[C]:CYS:SG	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ILE:CD1	1:E:254[A]:ARG:HG2	2.45	0.47
1:G:120[A]:ARG:CZ	6:G:765:HOH:O	2.62	0.47
1:F:10:ARG:HD2	6:F:4615:HOH:O	2.13	0.47
1:F:115:VAL:CG2	1:F:120[A]:ARG:HE	2.27	0.47
1:G:169:GLU:HG2	1:G:173[A]:ARG:HH22	1.78	0.47
1:G:212:ILE:CD1	1:G:254[B]:ARG:HG2	2.45	0.47
1:B:25:ARG:CZ	1:C:149[B]:CYS:SG	3.03	0.47
1:F:254[B]:ARG:HD3	6:F:2843:HOH:O	2.15	0.47
1:A:114[A]:ASP:HB3	6:A:4835:HOH:O	2.15	0.46
1:G:169:GLU:CG	1:G:173[A]:ARG:NH2	2.76	0.46
1:D:114[B]:ASP:CB	6:D:640:HOH:O	2.57	0.46
1:C:141:LYS:NZ	1:C:160[B]:SER:O	2.48	0.46
1:J:230[B]:MSE:HE3	1:J:230[B]:MSE:HA	1.97	0.46
1:E:28[B]:LYS:HG2	6:E:4542:HOH:O	2.15	0.46
1:F:149[B]:CYS:SG	1:G:25:ARG:CZ	3.04	0.46
1:B:149[B]:CYS:SG	1:C:25:ARG:CZ	3.04	0.46
1:F:173[B]:ARG:HD2	6:F:458:HOH:O	2.16	0.46
1:A:149[C]:CYS:SG	1:D:25:ARG:NH1	2.90	0.45
1:E:8:ASP:HA	6:E:3869:HOH:O	2.16	0.45
1:F:80:PHE:CB	6:G:5934:HOH:O	2.58	0.45
1:J:254[A]:ARG:NE	6:J:585:HOH:O	2.50	0.45
1:E:149[B]:CYS:SG	1:I:25:ARG:NH1	2.90	0.45
1:B:115:VAL:CG2	1:B:120[A]:ARG:HE	2.30	0.45
1:J:230[B]:MSE:HG2	1:J:236:LEU:CD2	2.45	0.45
1:G:191:ASP:OD1	1:G:217[B]:GLU:CD	2.55	0.44
1:H:149[B]:CYS:SG	1:J:25:ARG:CZ	3.05	0.44
1:D:254[B]:ARG:NH1	6:D:658:HOH:O	2.48	0.44
1:C:217[B]:GLU:HG2	1:C:226:GLU:OE1	2.17	0.44
1:I:31:THR:HG22	5:I:262:EDO:H11	2.00	0.44
1:E:250:PRO:HD3	5:E:261:EDO:H11	1.99	0.44
1:I:173[A]:ARG:HD2	6:I:468:HOH:O	2.18	0.44
1:E:254[B]:ARG:HD3	6:E:1624:HOH:O	2.17	0.44
1:D:230[B]:MSE:HE3	1:D:241:LEU:HD11	1.98	0.44
1:J:179:PRO:HB3	6:J:4450:HOH:O	2.18	0.44
1:A:120[B]:ARG:HD3	6:A:279:HOH:O	2.18	0.43
1:I:114[B]:ASP:HB2	6:I:3443:HOH:O	2.17	0.43
1:C:212:ILE:CD1	1:C:254[A]:ARG:HG2	2.48	0.43
1:G:230[B]:MSE:HE1	1:G:253:LEU:CD2	2.48	0.43
1:A:65:GLN:OE1	1:A:254[B]:ARG:NH1	2.51	0.43
1:F:114[A]:ASP:CG	1:F:168:ARG:HH22	2.21	0.43
1:C:35:ILE:HG23	6:C:5938:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:PRO:HD3	5:C:261:EDO:H22	2.01	0.43
1:G:212:ILE:HD11	1:G:254[B]:ARG:HG2	2.00	0.43
1:B:124:THR:O	1:B:129[B]:ARG:HG3	2.19	0.43
1:B:120[A]:ARG:CZ	6:B:5651:HOH:O	2.67	0.43
1:G:28[A]:LYS:HD3	6:G:646:HOH:O	2.18	0.43
1:D:230[A]:MSE:SE	1:D:234:LEU:HD12	2.69	0.43
1:A:25:ARG:NH1	1:D:149[B]:CYS:SG	2.92	0.42
1:B:80:PHE:CB	6:C:5938:HOH:O	2.67	0.42
1:C:189:ASP:O	2:C:258:SAH:H5'2	2.18	0.42
1:F:114[B]:ASP:HA	1:F:127[B]:GLN:CG	2.49	0.42
1:I:114[A]:ASP:CG	1:I:168:ARG:HH22	2.23	0.42
1:I:212:ILE:CD1	1:I:254[B]:ARG:HG2	2.50	0.42
1:A:173[B]:ARG:CZ	6:A:270:HOH:O	2.67	0.42
1:B:35[B]:ILE:HD11	1:C:136:TYR:CZ	2.55	0.42
1:D:117:ASP:OD1	1:D:120[B]:ARG:NH1	2.52	0.42
1:G:35:ILE:CG1	6:G:5934:HOH:O	2.52	0.42
1:J:189:ASP:O	2:J:258:SAH:H5'2	2.18	0.42
1:I:44:LEU:N	1:I:45:PRO:CD	2.82	0.42
1:J:230[B]:MSE:CE	1:J:230[B]:MSE:HA	2.50	0.42
1:F:159[B]:ARG:NH2	6:F:5989:HOH:O	2.35	0.42
1:B:50:ARG:HD3	6:C:718:HOH:O	2.19	0.42
1:J:191:ASP:OD1	1:J:217[B]:GLU:CD	2.58	0.42
1:C:10:ARG:HD2	6:C:437:HOH:O	2.19	0.42
1:F:10:ARG:NH1	6:F:4615:HOH:O	2.52	0.42
1:G:250:PRO:HD3	5:G:261:EDO:H11	2.02	0.42
1:A:230[A]:MSE:SE	1:A:234:LEU:HD12	2.70	0.41
1:B:254[A]:ARG:NE	6:B:3728:HOH:O	2.53	0.41
1:H:129:ARG:O	1:H:130:PHE:HB2	2.20	0.41
1:C:136:TYR:N	1:C:137:PRO:CD	2.83	0.41
1:D:7:GLN:O	1:D:7:GLN:HG3	2.19	0.41
1:D:56:LEU:HD23	1:D:56:LEU:C	2.39	0.41
1:G:189:ASP:O	2:G:258:SAH:H5'2	2.19	0.41
1:I:230[A]:MSE:SE	1:I:234:LEU:HD12	2.71	0.41
1:I:189:ASP:O	2:I:261:SAH:H5'2	2.21	0.41
1:H:250:PRO:HD3	5:H:261:EDO:H11	2.03	0.41
1:B:56:LEU:C	1:B:56:LEU:HD23	2.41	0.41
1:A:169:GLU:HG2	6:A:5482:HOH:O	2.20	0.41
1:B:114[A]:ASP:CG	1:B:168:ARG:HH22	2.22	0.41
1:C:35:ILE:HD13	6:C:5938:HOH:O	2.21	0.41
1:D:44:LEU:N	1:D:45:PRO:CD	2.83	0.41
1:H:149[B]:CYS:SG	1:J:25:ARG:NH1	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:190:LEU:HD13	1:J:195:PRO:HB2	2.03	0.41
1:E:230[B]:MSE:HE2	6:E:1657:HOH:O	2.20	0.40
1:F:230[B]:MSE:HE1	1:F:241:LEU:HD21	2.03	0.40
1:A:44:LEU:N	1:A:45:PRO:CD	2.84	0.40
1:A:139:TYR:CZ	1:D:34:PRO:HD2	2.57	0.40
1:B:212:ILE:CD1	1:B:254[A]:ARG:HG2	2.52	0.40
1:D:28[B]:LYS:HA	1:D:28[B]:LYS:HD3	1.92	0.40
1:E:189:ASP:O	2:E:258:SAH:H5'2	2.21	0.40
1:F:28[B]:LYS:HG3	6:F:2058:HOH:O	2.22	0.40
1:I:184:ALA:C	6:I:383:HOH:O	2.58	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	263/257 (102%)	258 (98%)	5 (2%)	0	100	100
1	B	270/257 (105%)	260 (96%)	10 (4%)	0	100	100
1	C	264/257 (103%)	253 (96%)	11 (4%)	0	100	100
1	D	263/257 (102%)	255 (97%)	8 (3%)	0	100	100
1	E	262/257 (102%)	258 (98%)	4 (2%)	0	100	100
1	F	264/257 (103%)	254 (96%)	10 (4%)	0	100	100
1	G	264/257 (103%)	256 (97%)	8 (3%)	0	100	100
1	H	261/257 (102%)	251 (96%)	10 (4%)	0	100	100
1	I	262/257 (102%)	254 (97%)	8 (3%)	0	100	100
1	J	262/257 (102%)	254 (97%)	8 (3%)	0	100	100
All	All	2635/2570 (102%)	2553 (97%)	82 (3%)	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	229/215 (106%)	228 (100%)	1 (0%)	91	82
1	B	234/215 (109%)	231 (99%)	3 (1%)	69	44
1	C	230/215 (107%)	229 (100%)	1 (0%)	91	82
1	D	229/215 (106%)	228 (100%)	1 (0%)	91	82
1	E	228/215 (106%)	227 (100%)	1 (0%)	91	82
1	F	230/215 (107%)	225 (98%)	5 (2%)	52	23
1	G	229/215 (106%)	228 (100%)	1 (0%)	91	82
1	H	227/215 (106%)	226 (100%)	1 (0%)	91	82
1	I	228/215 (106%)	225 (99%)	3 (1%)	69	44
1	J	228/215 (106%)	227 (100%)	1 (0%)	91	82
All	All	2292/2150 (107%)	2274 (99%)	18 (1%)	86	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	B	28[A]	LYS
1	B	28[B]	LYS
1	B	63	TYR
1	C	63	TYR
1	D	63	TYR
1	E	63	TYR
1	F	28[A]	LYS
1	F	28[B]	LYS
1	F	63	TYR
1	F	114[A]	ASP
1	F	114[B]	ASP
1	G	63	TYR
1	H	63	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	63	TYR
1	I	114[A]	ASP
1	I	114[B]	ASP
1	J	63	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 45 ligands modelled in this entry, 10 are monoatomic - leaving 35 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLU	H	259	4	8,9,9	1.39	0	8,11,11	0.95	1 (12%)
5	EDO	D	261	4	3,3,3	0.43	0	2,2,2	0.50	0
5	EDO	F	262	-	3,3,3	0.48	0	2,2,2	1.23	0
5	EDO	F	261	4	3,3,3	0.48	0	2,2,2	0.63	0
5	EDO	I	262	-	3,3,3	0.40	0	2,2,2	0.59	0
5	EDO	B	261	4	3,3,3	0.58	0	2,2,2	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	J	262	4	3,3,3	0.47	0	2,2,2	0.83	0
3	GLU	A	259	4	8,9,9	1.28	0	8,11,11	1.45	1 (12%)
2	SAH	F	258	-	23,28,28	1.10	2 (8%)	22,40,40	1.99	5 (22%)
2	SAH	H	258	-	23,28,28	0.97	1 (4%)	22,40,40	1.70	2 (9%)
3	GLU	F	259	4	8,9,9	1.35	0	8,11,11	1.19	1 (12%)
3	GLU	J	259	4	8,9,9	1.17	0	8,11,11	1.37	2 (25%)
3	GLU	I	258	4	8,9,9	1.26	1 (12%)	8,11,11	1.48	1 (12%)
3	GLU	B	259	4	8,9,9	1.36	0	8,11,11	1.20	1 (12%)
3	GLU	G	259	4	8,9,9	1.32	0	8,11,11	0.97	0
5	EDO	E	261	4	3,3,3	0.41	0	2,2,2	0.70	0
5	EDO	D	262	-	3,3,3	0.33	0	2,2,2	0.60	0
5	EDO	H	261	4	3,3,3	0.38	0	2,2,2	1.04	0
3	GLU	C	259	4	8,9,9	1.19	0	8,11,11	0.80	0
5	EDO	A	261	4	3,3,3	0.41	0	2,2,2	0.89	0
5	EDO	G	261	4	3,3,3	0.33	0	2,2,2	0.80	0
2	SAH	E	258	-	23,28,28	1.03	2 (8%)	22,40,40	1.97	4 (18%)
2	SAH	A	258	-	23,28,28	1.11	3 (13%)	22,40,40	1.96	5 (22%)
2	SAH	B	258	-	23,28,28	1.12	3 (13%)	22,40,40	1.77	7 (31%)
3	GLU	D	259	4	8,9,9	1.35	1 (12%)	8,11,11	1.09	1 (12%)
5	EDO	J	261	-	3,3,3	0.49	0	2,2,2	0.47	0
5	EDO	C	262	-	3,3,3	0.31	0	2,2,2	1.16	0
2	SAH	J	258	-	23,28,28	0.88	0	22,40,40	1.89	3 (13%)
3	GLU	E	259	4	8,9,9	1.22	0	8,11,11	1.08	1 (12%)
5	EDO	I	260	4	3,3,3	0.41	0	2,2,2	0.98	0
5	EDO	C	261	4	3,3,3	0.68	0	2,2,2	0.46	0
2	SAH	I	261	-	23,28,28	1.45	3 (13%)	22,40,40	2.12	5 (22%)
2	SAH	G	258	-	23,28,28	1.33	4 (17%)	22,40,40	5.21	9 (40%)
2	SAH	D	258	-	23,28,28	0.84	0	22,40,40	1.72	3 (13%)
2	SAH	C	258	-	23,28,28	1.12	2 (8%)	22,40,40	1.80	5 (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	GLU	H	259	4	-	2/9/9/9	-
5	EDO	D	261	4	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	F	262	-	-	0/1/1/1	-
5	EDO	F	261	4	-	0/1/1/1	-
5	EDO	I	262	-	-	0/1/1/1	-
5	EDO	B	261	4	-	0/1/1/1	-
5	EDO	J	262	4	-	0/1/1/1	-
3	GLU	A	259	4	-	1/9/9/9	-
2	SAH	F	258	-	-	0/11/31/31	0/3/3/3
2	SAH	H	258	-	-	0/11/31/31	0/3/3/3
3	GLU	F	259	4	-	0/9/9/9	-
3	GLU	J	259	4	-	1/9/9/9	-
3	GLU	I	258	4	-	2/9/9/9	-
3	GLU	B	259	4	-	0/9/9/9	-
3	GLU	G	259	4	-	0/9/9/9	-
5	EDO	E	261	4	-	0/1/1/1	-
5	EDO	D	262	-	-	1/1/1/1	-
5	EDO	H	261	4	-	0/1/1/1	-
3	GLU	C	259	4	-	0/9/9/9	-
5	EDO	A	261	4	-	0/1/1/1	-
5	EDO	G	261	4	-	0/1/1/1	-
2	SAH	E	258	-	-	1/11/31/31	0/3/3/3
2	SAH	A	258	-	-	0/11/31/31	0/3/3/3
2	SAH	B	258	-	-	0/11/31/31	0/3/3/3
3	GLU	D	259	4	-	2/9/9/9	-
5	EDO	J	261	-	-	1/1/1/1	-
5	EDO	C	262	-	-	0/1/1/1	-
2	SAH	J	258	-	-	0/11/31/31	0/3/3/3
3	GLU	E	259	4	-	0/9/9/9	-
5	EDO	I	260	4	-	0/1/1/1	-
5	EDO	C	261	4	-	0/1/1/1	-
2	SAH	I	261	-	-	0/11/31/31	0/3/3/3
2	SAH	G	258	-	-	4/11/31/31	0/3/3/3
2	SAH	D	258	-	-	0/11/31/31	0/3/3/3
2	SAH	C	258	-	-	1/11/31/31	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	261	SAH	O4'-C1'	3.98	1.46	1.40
2	I	261	SAH	C2-N3	3.28	1.37	1.32
2	C	258	SAH	C2-N3	3.17	1.37	1.32
2	G	258	SAH	C2-N3	2.91	1.36	1.32
2	I	261	SAH	OXT-C	-2.70	1.22	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	258	SAH	C4-N3	2.54	1.39	1.35
2	F	258	SAH	C2-N3	2.39	1.35	1.32
2	F	258	SAH	C2-N1	2.36	1.38	1.33
2	G	258	SAH	CB-CA	2.33	1.58	1.53
2	B	258	SAH	C2-N3	2.28	1.35	1.32
2	A	258	SAH	OXT-C	-2.27	1.23	1.30
2	E	258	SAH	C2-N3	2.26	1.35	1.32
2	A	258	SAH	O4'-C1'	2.22	1.43	1.40
3	D	259	GLU	OE2-CD	-2.16	1.23	1.30
2	G	258	SAH	O3'-C3'	2.14	1.48	1.43
3	I	258	GLU	CG-CD	2.13	1.55	1.50
2	H	258	SAH	C2-N3	2.10	1.35	1.32
2	B	258	SAH	C4-N3	2.08	1.38	1.35
2	A	258	SAH	C2-N3	2.07	1.35	1.32
2	E	258	SAH	OXT-C	-2.05	1.24	1.30
2	G	258	SAH	C5'-SD	2.02	1.88	1.81
2	B	258	SAH	OXT-C	-2.02	1.24	1.30

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	258	SAH	CB-CG-SD	16.05	149.29	113.45
2	G	258	SAH	C4'-C5'-SD	-15.31	59.13	113.78
2	F	258	SAH	C4'-O4'-C1'	-6.33	104.13	109.92
2	I	261	SAH	N3-C2-N1	-5.48	121.23	128.67
2	J	258	SAH	N3-C2-N1	-5.37	121.39	128.67
2	E	258	SAH	N3-C2-N1	-5.30	121.48	128.67
2	C	258	SAH	N3-C2-N1	-5.27	121.51	128.67
2	A	258	SAH	N3-C2-N1	-5.26	121.54	128.67
2	J	258	SAH	C4'-O4'-C1'	-5.16	105.20	109.92
2	G	258	SAH	C4'-O4'-C1'	-5.11	105.24	109.92
2	G	258	SAH	N3-C2-N1	-5.09	121.76	128.67
2	E	258	SAH	C4'-O4'-C1'	-4.94	105.40	109.92
2	I	261	SAH	C4'-O4'-C1'	-4.93	105.41	109.92
2	D	258	SAH	N3-C2-N1	-4.84	122.10	128.67
2	A	258	SAH	C4'-O4'-C1'	-4.77	105.56	109.92
2	H	258	SAH	C4'-O4'-C1'	-4.67	105.65	109.92
2	H	258	SAH	N3-C2-N1	-4.20	122.97	128.67
2	D	258	SAH	C4'-O4'-C1'	-4.07	106.20	109.92
2	B	258	SAH	C4'-O4'-C1'	-3.95	106.31	109.92
2	I	261	SAH	N6-C6-N1	3.76	126.36	118.33
2	G	258	SAH	O4'-C4'-C5'	-3.70	99.30	108.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	259	GLU	OXT-C-O	-3.60	115.92	124.08
2	B	258	SAH	C1'-N9-C4	-3.47	120.54	126.64
2	F	258	SAH	N3-C2-N1	-3.27	124.24	128.67
3	I	258	GLU	OXT-C-O	-3.24	116.72	124.08
2	I	261	SAH	C5-C6-N1	-3.24	112.51	120.23
2	B	258	SAH	N3-C2-N1	-3.19	124.34	128.67
2	C	258	SAH	O4'-C1'-N9	3.04	112.77	108.75
2	F	258	SAH	CB-CG-SD	-2.98	106.80	113.45
2	C	258	SAH	C4'-O4'-C1'	-2.89	107.28	109.92
3	B	259	GLU	OXT-C-O	-2.86	117.59	124.08
3	F	259	GLU	OXT-C-O	-2.82	117.69	124.08
2	C	258	SAH	N6-C6-N1	2.78	124.28	118.33
2	A	258	SAH	OXT-C-O	-2.75	117.84	124.08
2	I	261	SAH	C1'-N9-C4	-2.64	122.01	126.64
2	G	258	SAH	N6-C6-N1	2.63	123.96	118.33
2	B	258	SAH	OXT-C-O	-2.51	118.39	124.08
3	J	259	GLU	OXT-C-O	-2.47	118.48	124.08
2	A	258	SAH	N6-C6-N1	2.45	123.57	118.33
2	A	258	SAH	C1'-N9-C4	-2.35	122.52	126.64
2	B	258	SAH	N6-C6-N1	2.33	123.32	118.33
3	D	259	GLU	OXT-C-O	-2.28	118.90	124.08
2	B	258	SAH	C4-C5-N7	-2.28	106.92	109.34
2	F	258	SAH	OXT-C-O	-2.27	118.92	124.08
2	E	258	SAH	C4-C5-N7	-2.24	106.97	109.34
2	D	258	SAH	N6-C6-N1	2.23	123.09	118.33
2	B	258	SAH	C5'-C4'-C3'	-2.20	109.55	115.06
2	J	258	SAH	N6-C6-N1	2.20	123.04	118.33
3	E	259	GLU	OXT-C-O	-2.18	119.13	124.08
2	G	258	SAH	C1'-N9-C4	-2.17	122.82	126.64
2	E	258	SAH	N6-C6-N1	2.15	122.93	118.33
2	G	258	SAH	C5'-C4'-C3'	2.14	120.40	115.06
3	J	259	GLU	OE2-CD-CG	2.11	120.65	114.00
3	H	259	GLU	OXT-C-O	-2.08	119.37	124.08
2	F	258	SAH	N6-C6-N1	2.08	122.77	118.33
2	C	258	SAH	CB-CG-SD	-2.05	108.88	113.45
2	G	258	SAH	C5-C6-N1	-2.02	115.42	120.23

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	258	SAH	O4'-C4'-C5'-SD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	258	SAH	C3'-C4'-C5'-SD
2	G	258	SAH	CA-CB-CG-SD
3	D	259	GLU	OXT-C-CA-CB
3	H	259	GLU	OXT-C-CA-CB
3	H	259	GLU	O-C-CA-CB
2	C	258	SAH	O-C-CA-N
2	E	258	SAH	O-C-CA-N
3	A	259	GLU	O-C-CA-N
3	D	259	GLU	O-C-CA-CB
5	D	262	EDO	O1-C1-C2-O2
5	J	261	EDO	O1-C1-C2-O2
2	G	258	SAH	CB-CG-SD-C5'
3	J	259	GLU	O-C-CA-CB
3	I	258	GLU	OE1-CD-CG-CB
3	I	258	GLU	OE2-CD-CG-CB

There are no ring outliers.

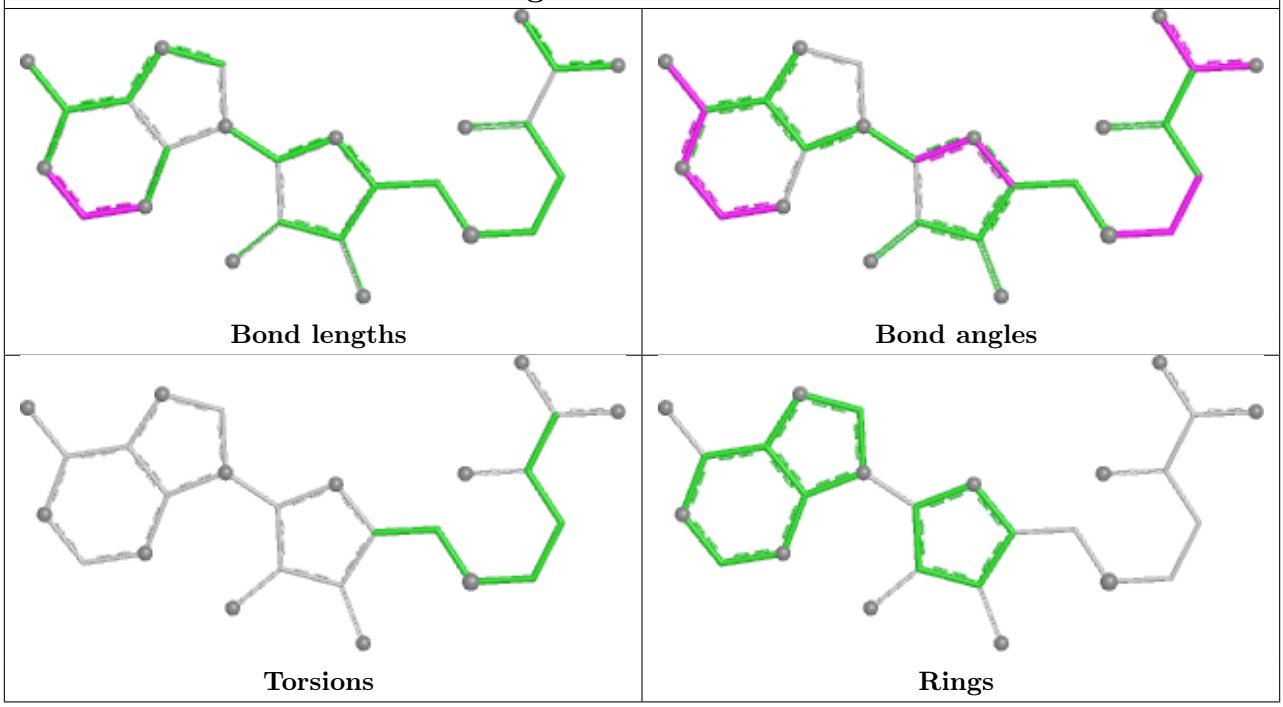
13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	261	EDO	1	0
5	I	262	EDO	3	0
5	J	262	EDO	1	0
5	E	261	EDO	1	0
5	H	261	EDO	1	0
5	G	261	EDO	1	0
2	E	258	SAH	1	0
5	J	261	EDO	1	0
2	J	258	SAH	1	0
5	C	261	EDO	1	0
2	I	261	SAH	1	0
2	G	258	SAH	1	0
2	C	258	SAH	1	0

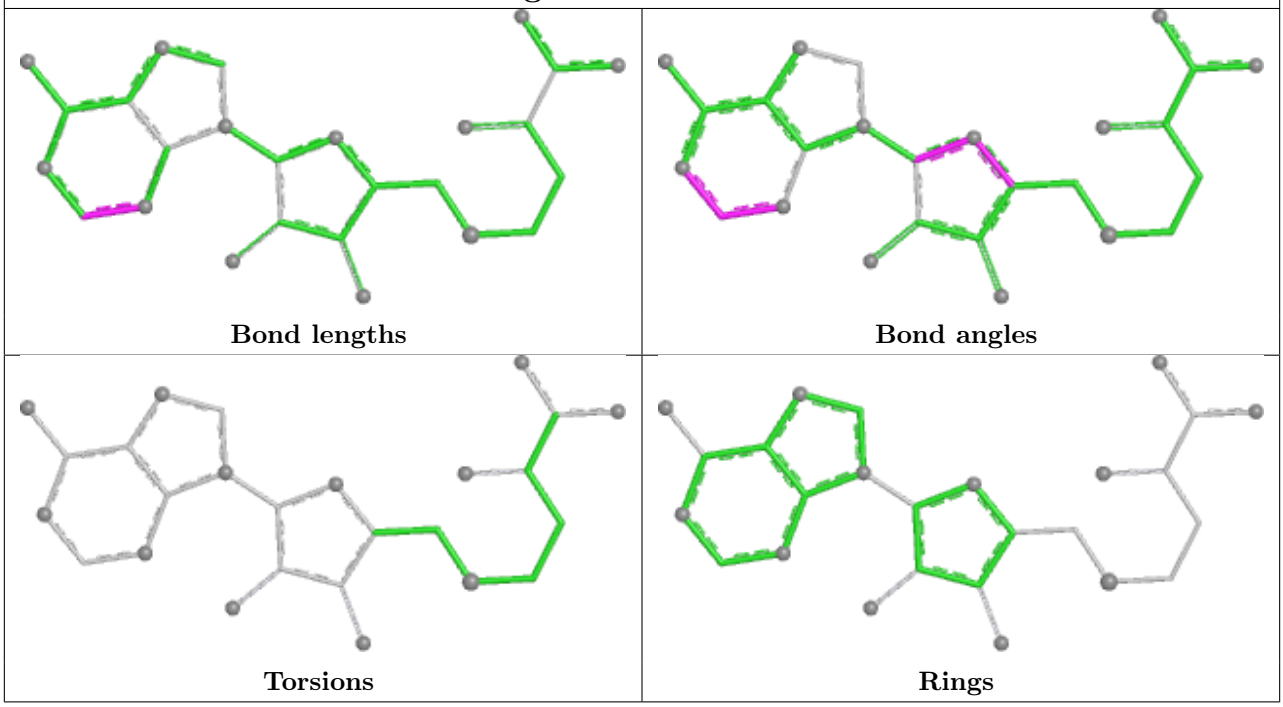
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

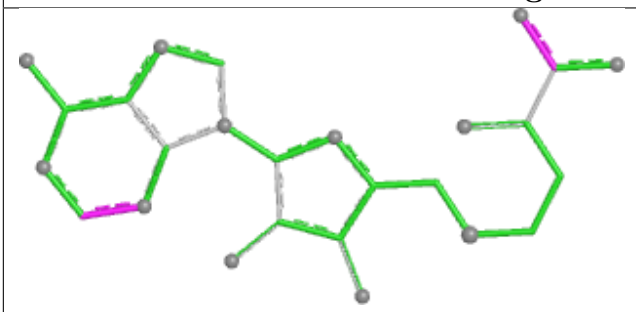
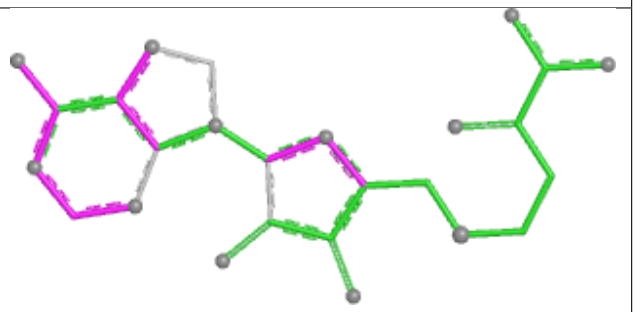
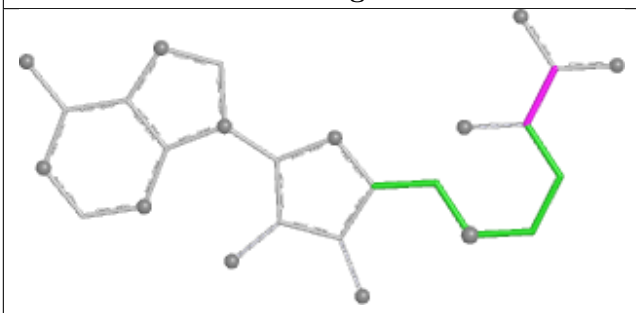
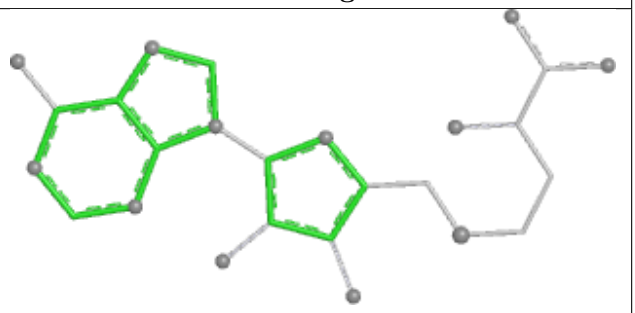
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

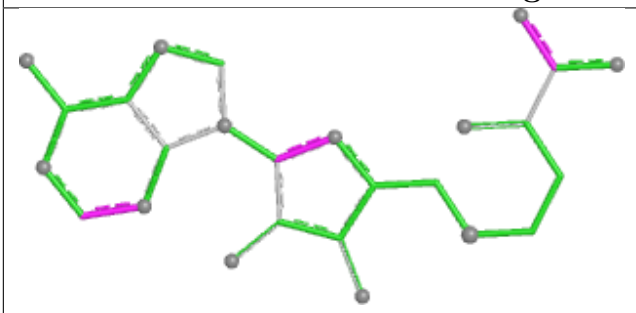
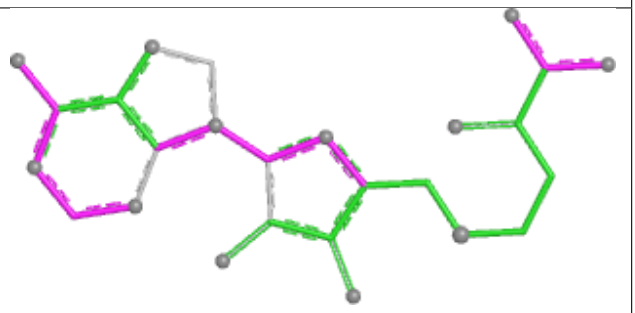
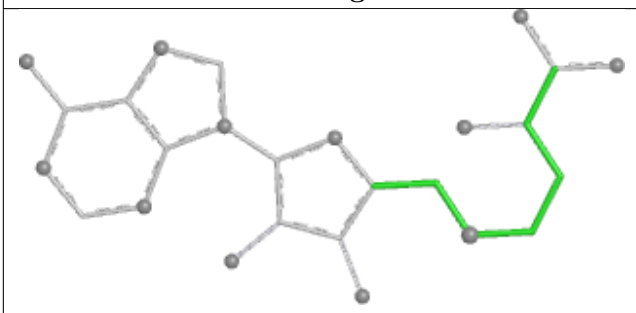
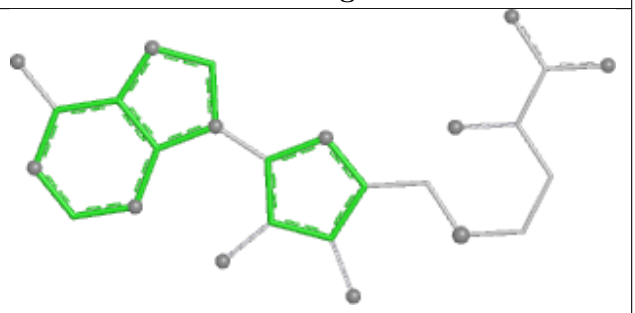
Ligand SAH F 258

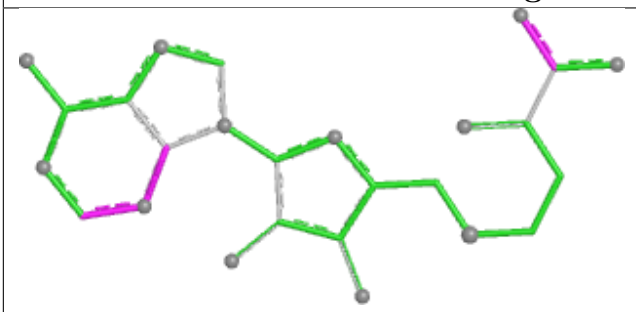
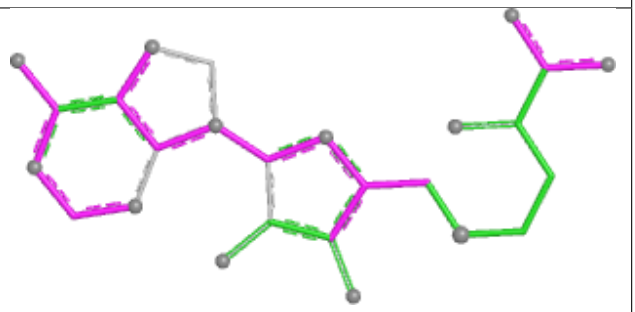
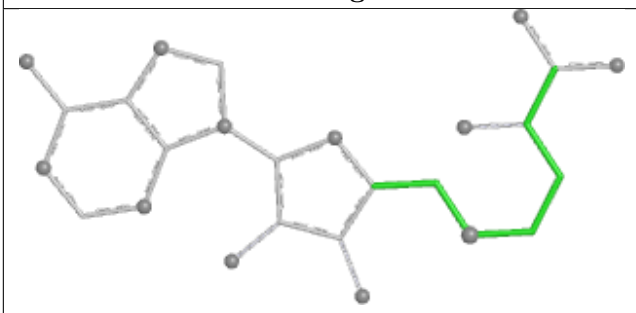
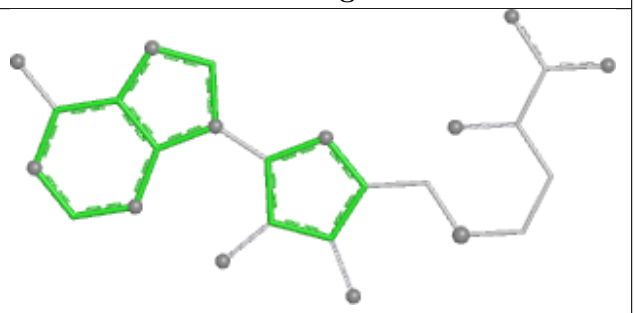


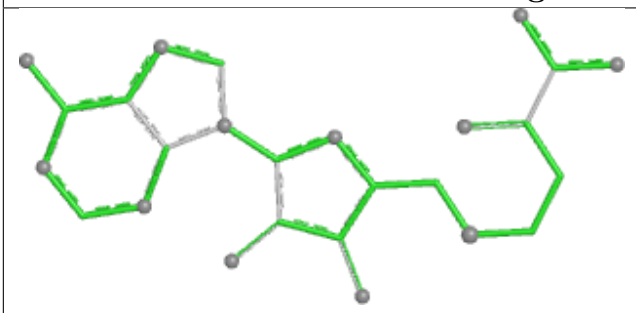
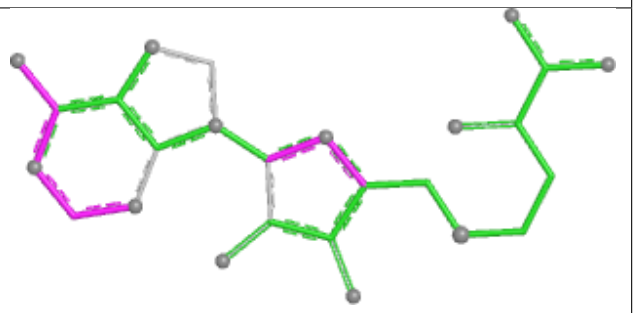
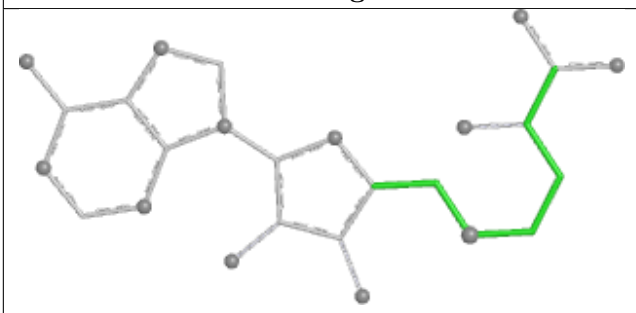
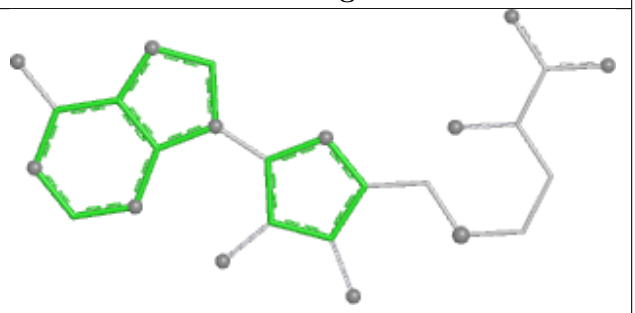
Ligand SAH H 258



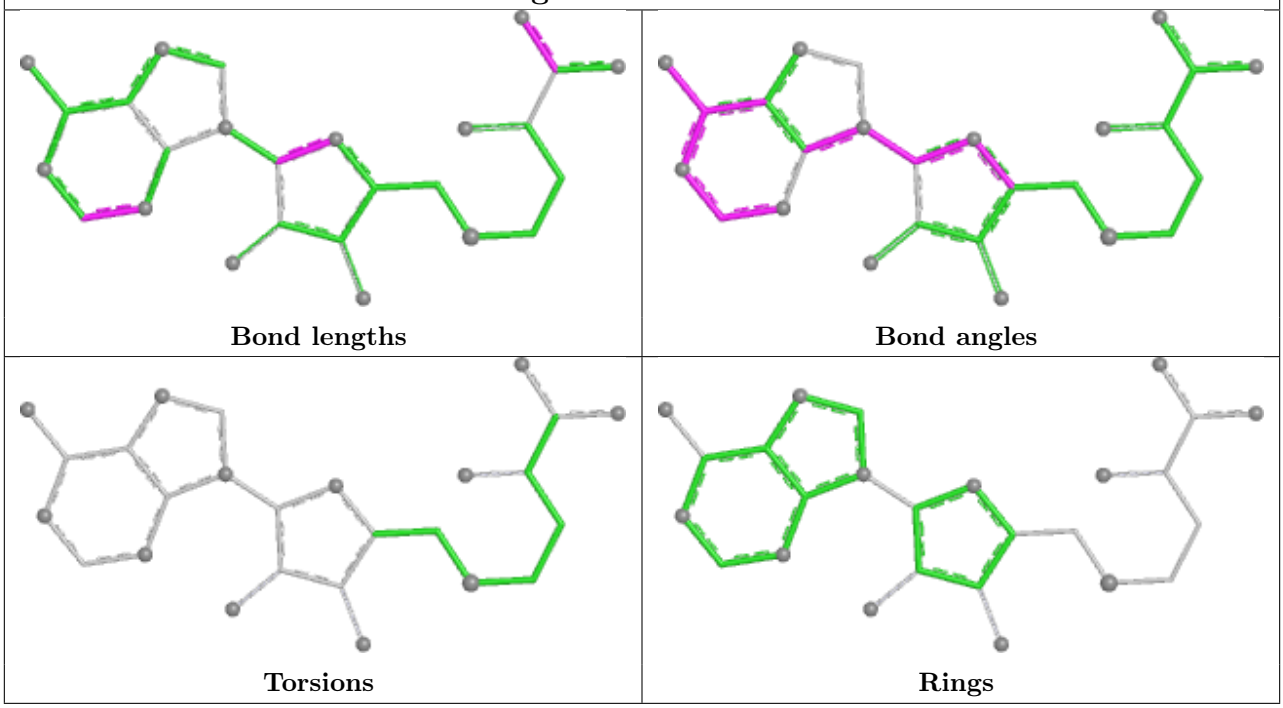
Ligand SAH E 258	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH A 258	
 Bond lengths	 Bond angles
 Torsions	 Rings

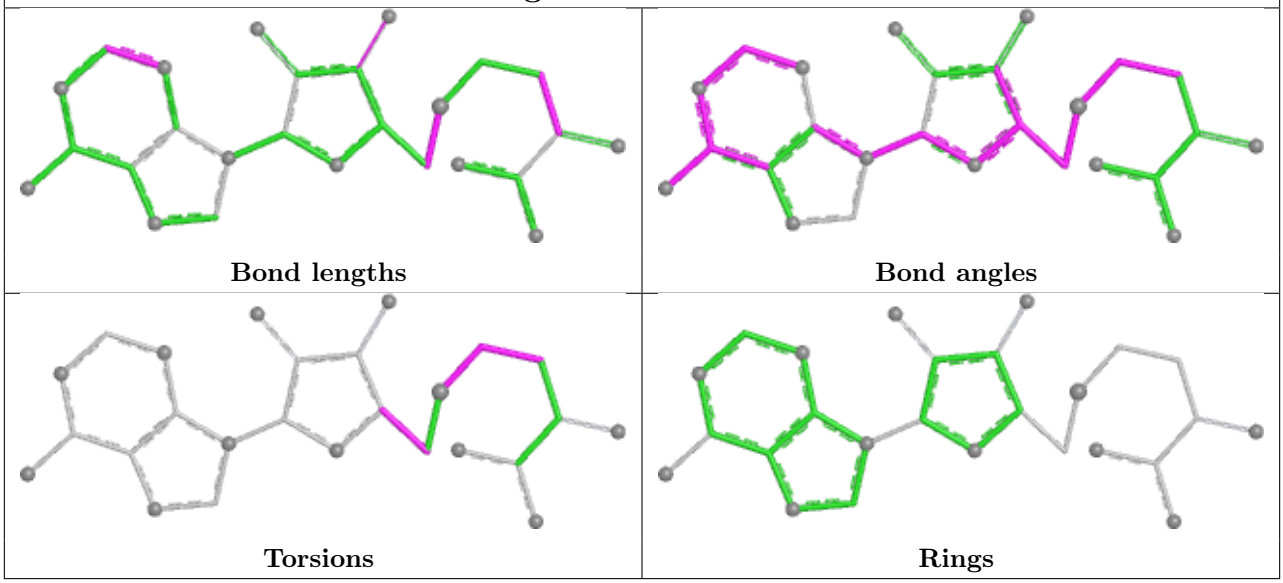
Ligand SAH B 258	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH J 258	
 Bond lengths	 Bond angles
 Torsions	 Rings

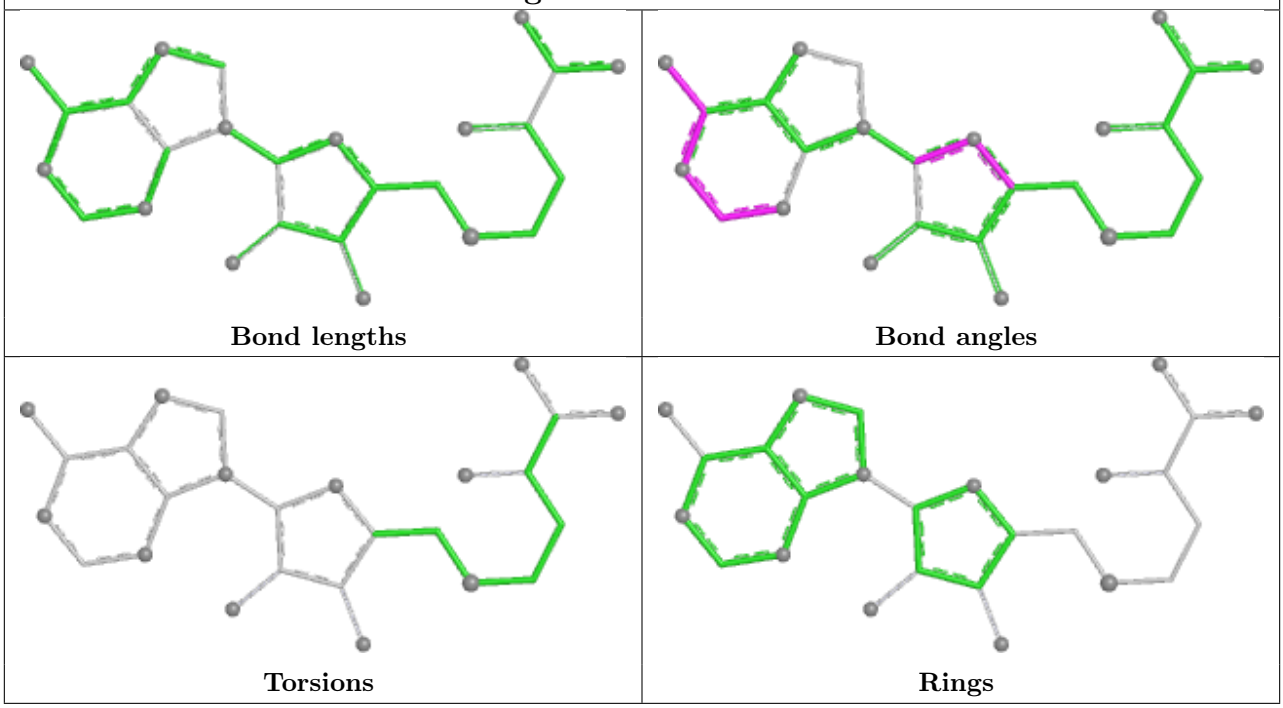
Ligand SAH I 261



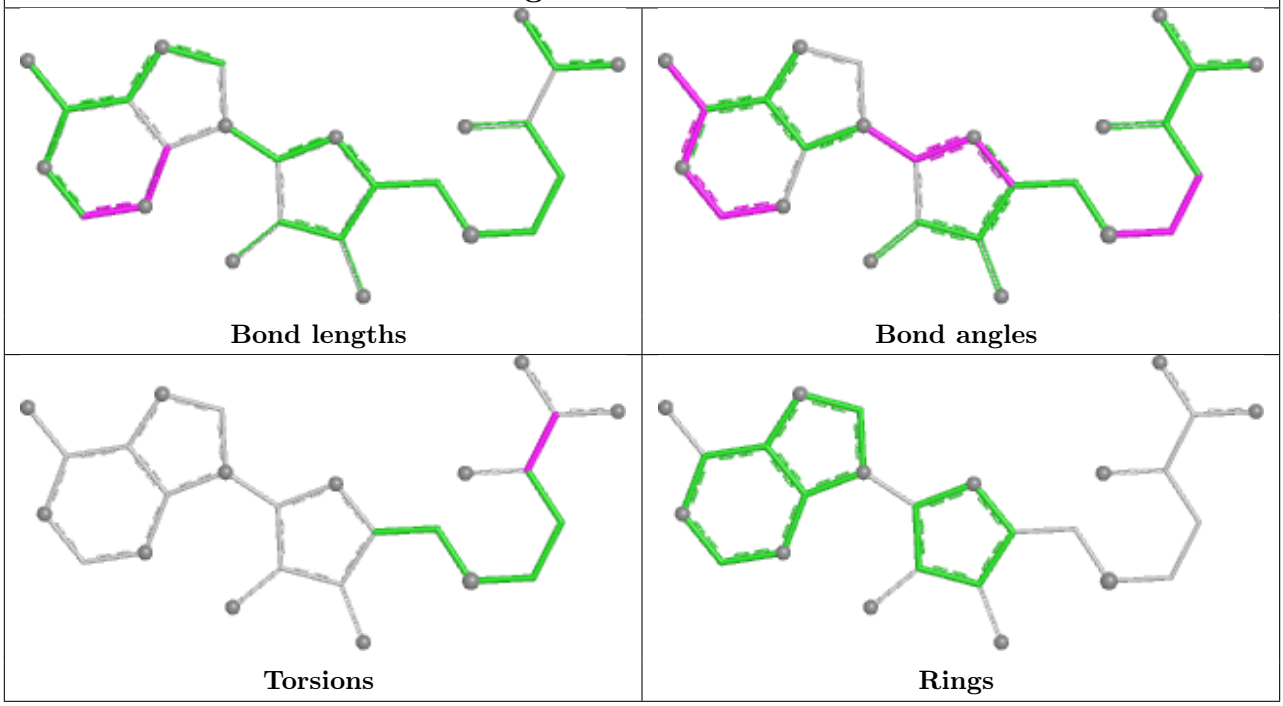
Ligand SAH G 258



Ligand SAH D 258



Ligand SAH C 258



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 (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	247/257 (96%)	-0.54	2 (0%) 86 89	8, 11, 18, 50	1 (0%)
1	B	253/257 (98%)	-0.49	3 (1%) 79 83	8, 11, 19, 60	1 (0%)
1	C	247/257 (96%)	-0.53	1 (0%) 92 94	8, 11, 18, 57	1 (0%)
1	D	247/257 (96%)	-0.56	0 100 100	8, 12, 20, 47	1 (0%)
1	E	247/257 (96%)	-0.59	1 (0%) 92 94	8, 11, 18, 59	2 (0%)
1	F	247/257 (96%)	-0.53	1 (0%) 92 94	8, 11, 18, 53	1 (0%)
1	G	248/257 (96%)	-0.47	2 (0%) 86 89	7, 11, 18, 65	1 (0%)
1	H	247/257 (96%)	-0.29	1 (0%) 92 94	9, 13, 20, 43	1 (0%)
1	I	247/257 (96%)	-0.54	0 100 100	8, 11, 18, 56	1 (0%)
1	J	247/257 (96%)	-0.44	0 100 100	9, 13, 19, 41	1 (0%)
All	All	2477/2570 (96%)	-0.50	11 (0%) 92 94	7, 12, 19, 65	11 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	7	GLN	3.7
1	G	6	GLY	3.6
1	E	7	GLN	3.4
1	B	4	GLY	2.7
1	H	115	VAL	2.6
1	F	7	GLN	2.5
1	B	5	ASP	2.4
1	C	7	GLN	2.3
1	B	6	GLY	2.2
1	A	114[A]	ASP	2.1
1	A	7	GLN	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
5	EDO	F	262	4/4	0.73	0.15	30,31,40,62	0
2	SAH	G	258	26/26	0.77	0.11	8,9,12,18	0
5	EDO	C	262	4/4	0.84	0.11	30,34,42,56	0
3	GLU	E	259	10/10	0.87	0.14	30,33,35,35	0
3	GLU	G	259	10/10	0.89	0.12	21,23,25,26	0
5	EDO	C	261	4/4	0.90	0.11	18,19,20,23	0
3	GLU	A	259	10/10	0.91	0.13	23,26,27,28	0
3	GLU	C	259	10/10	0.91	0.12	21,23,26,27	0
3	GLU	I	258	10/10	0.91	0.12	22,25,26,27	0
5	EDO	J	261	4/4	0.92	0.10	39,39,55,64	0
3	GLU	H	259	10/10	0.93	0.10	23,26,27,27	0
5	EDO	B	261	4/4	0.93	0.11	23,23,24,26	0
3	GLU	J	259	10/10	0.94	0.08	22,25,29,29	0
5	EDO	E	261	4/4	0.94	0.10	18,23,24,25	0
3	GLU	B	259	10/10	0.94	0.09	22,24,25,26	0
3	GLU	D	259	10/10	0.94	0.10	26,28,30,31	0
5	EDO	D	261	4/4	0.95	0.08	22,23,23,27	0
5	EDO	H	261	4/4	0.95	0.12	20,21,25,26	0
5	EDO	A	261	4/4	0.95	0.10	20,20,21,26	0
5	EDO	D	262	4/4	0.96	0.08	24,31,34,51	0
3	GLU	F	259	10/10	0.96	0.08	22,25,26,28	0
5	EDO	I	260	4/4	0.96	0.08	21,23,26,28	0
5	EDO	I	262	4/4	0.96	0.12	23,27,28,85	0
5	EDO	F	261	4/4	0.96	0.09	24,24,26,26	0
5	EDO	J	262	4/4	0.96	0.09	20,23,25,25	0
5	EDO	G	261	4/4	0.97	0.09	20,22,24,26	0
2	SAH	H	258	26/26	0.97	0.07	10,12,14,15	0

Continued on next page...

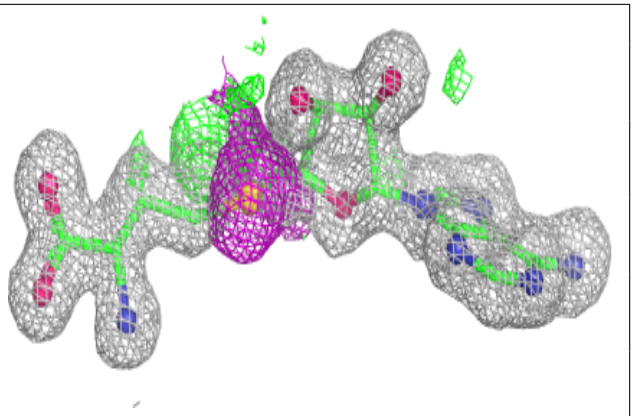
Continued from previous page...

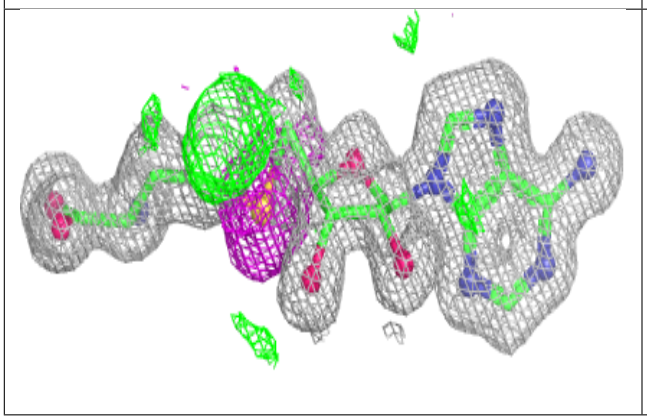
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	F	258	26/26	0.98	0.06	8,10,12,13	0
2	SAH	B	258	26/26	0.98	0.06	9,10,12,12	0
2	SAH	C	258	26/26	0.98	0.06	9,10,11,13	0
2	SAH	I	261	26/26	0.98	0.07	7,10,13,14	0
2	SAH	J	258	26/26	0.98	0.06	11,12,13,15	0
2	SAH	E	258	26/26	0.98	0.06	9,10,12,13	0
2	SAH	D	258	26/26	0.99	0.05	10,12,13,14	0
4	NA	B	260	1/1	0.99	0.14	9,9,9,9	0
4	NA	C	260	1/1	0.99	0.12	9,9,9,9	0
4	NA	E	260	1/1	0.99	0.07	12,12,12,12	0
4	NA	G	260	1/1	0.99	0.14	9,9,9,9	0
4	NA	I	259	1/1	0.99	0.13	9,9,9,9	0
2	SAH	A	258	26/26	0.99	0.05	9,10,12,13	0
4	NA	F	260	1/1	1.00	0.13	8,8,8,8	0
4	NA	D	260	1/1	1.00	0.05	11,11,11,11	0
4	NA	H	260	1/1	1.00	0.11	10,10,10,10	0
4	NA	A	260	1/1	1.00	0.14	10,10,10,10	0
4	NA	J	260	1/1	1.00	0.11	11,11,11,11	0

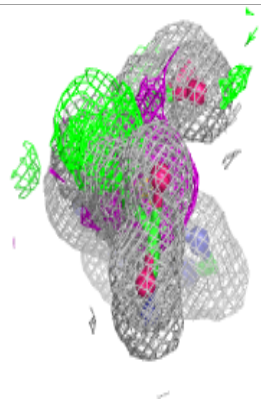
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH G 258:

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

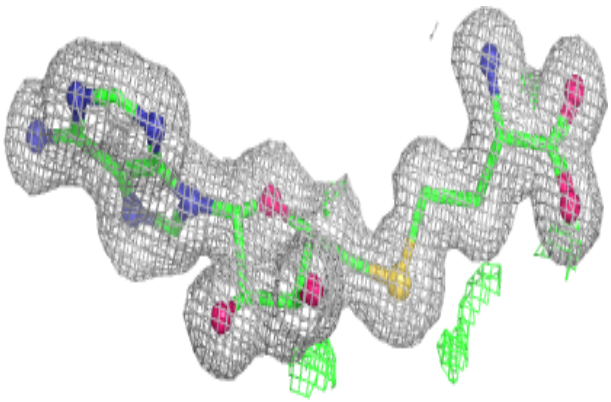


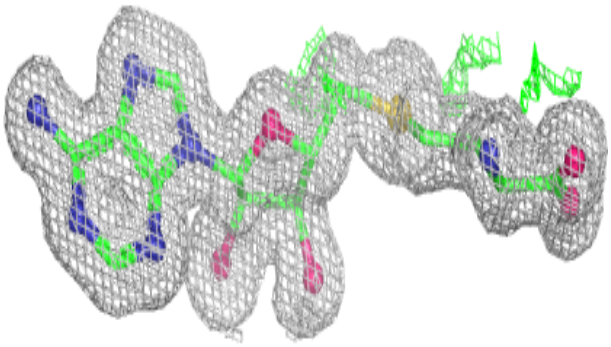


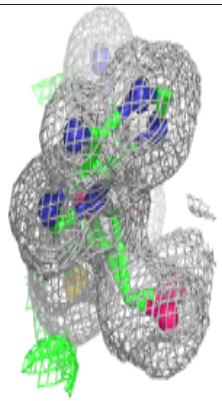


Electron density around SAH H 258:

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

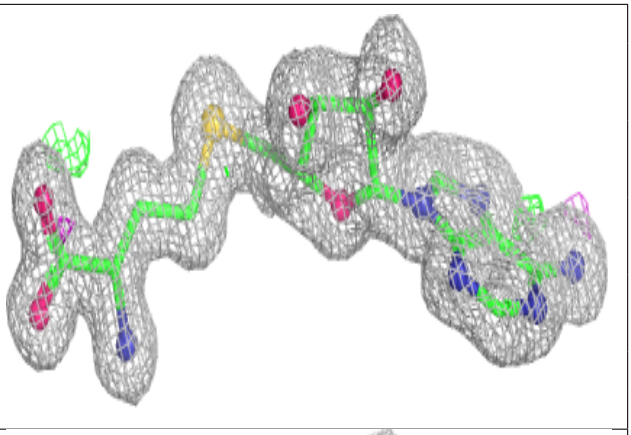


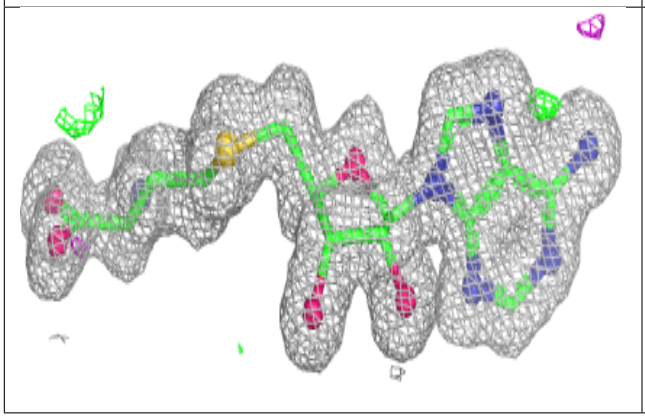




Electron density around SAH F 258:

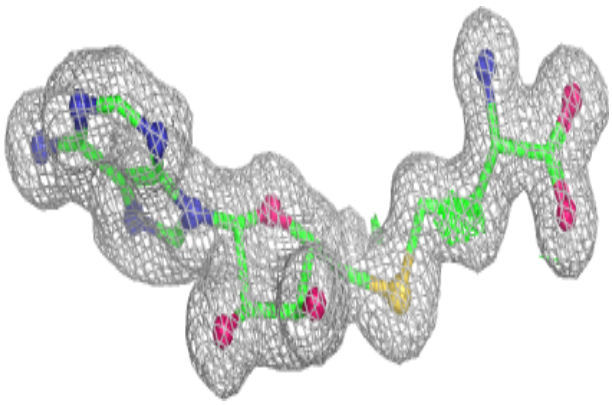
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

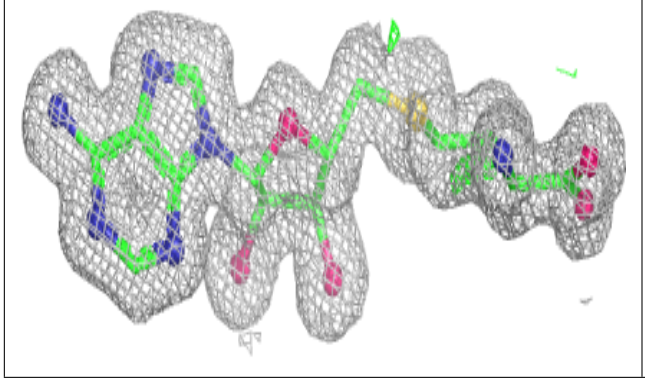


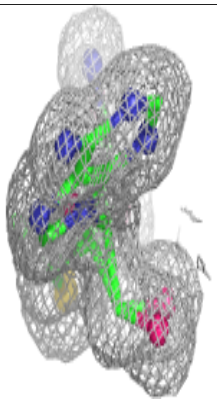


Electron density around SAH B 258:

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

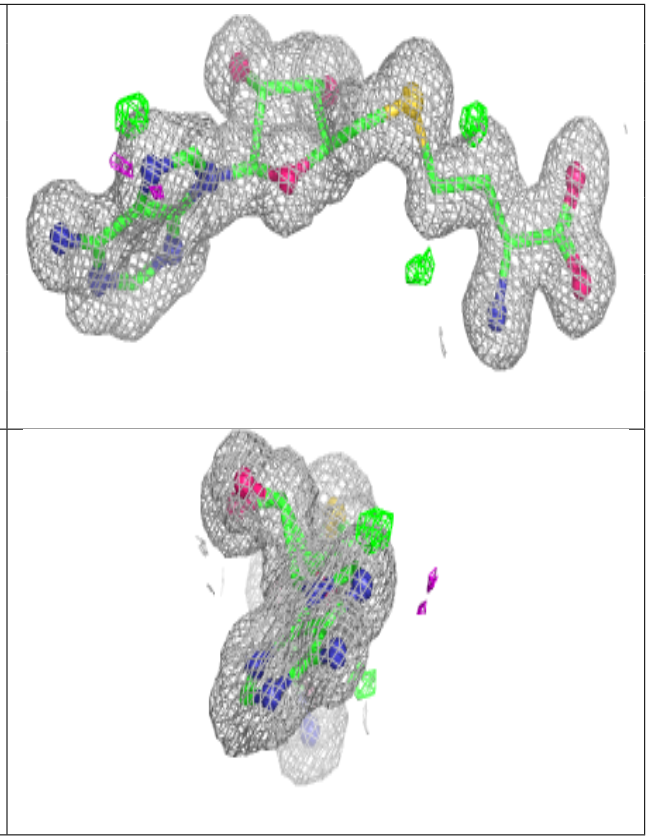






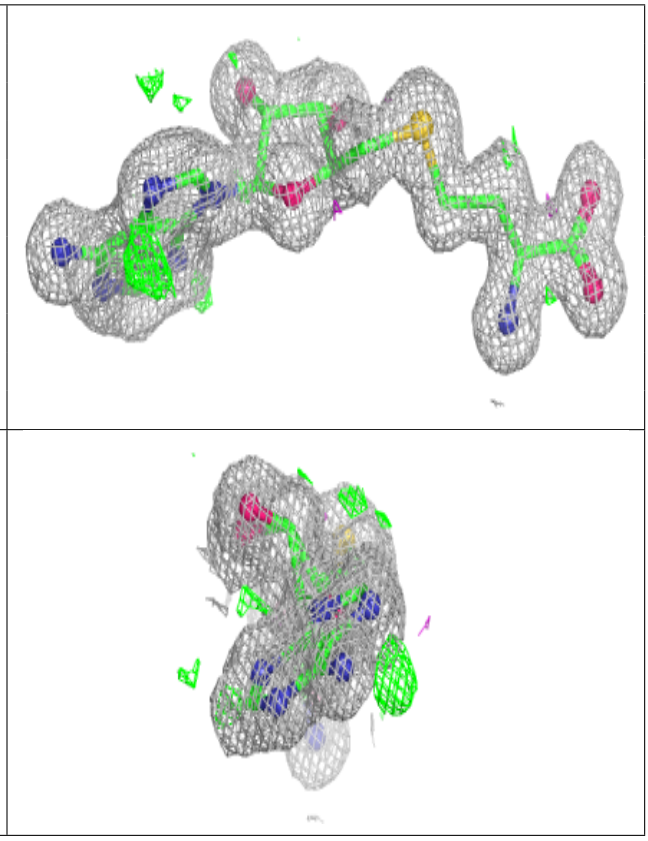
Electron density around SAH C 258:

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



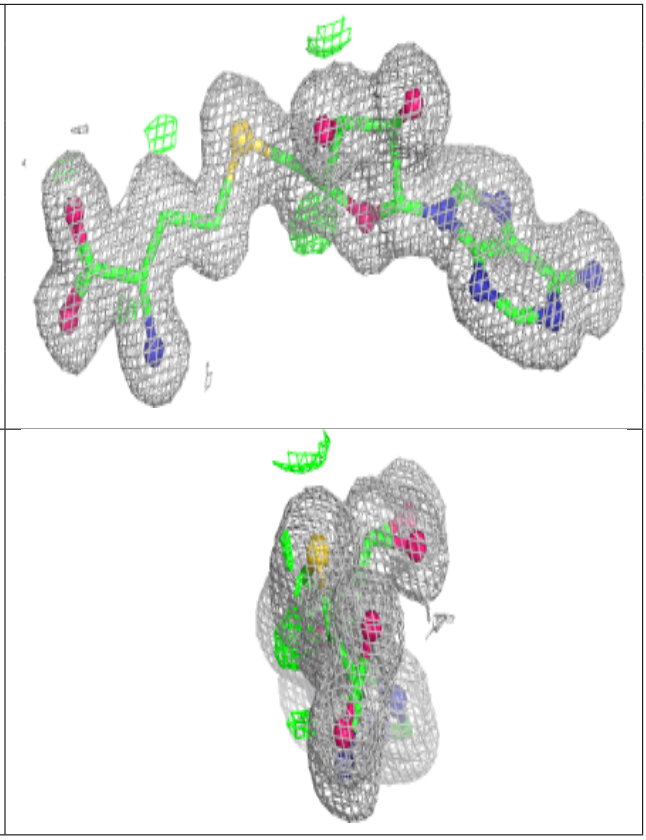
Electron density around SAH I 261:

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



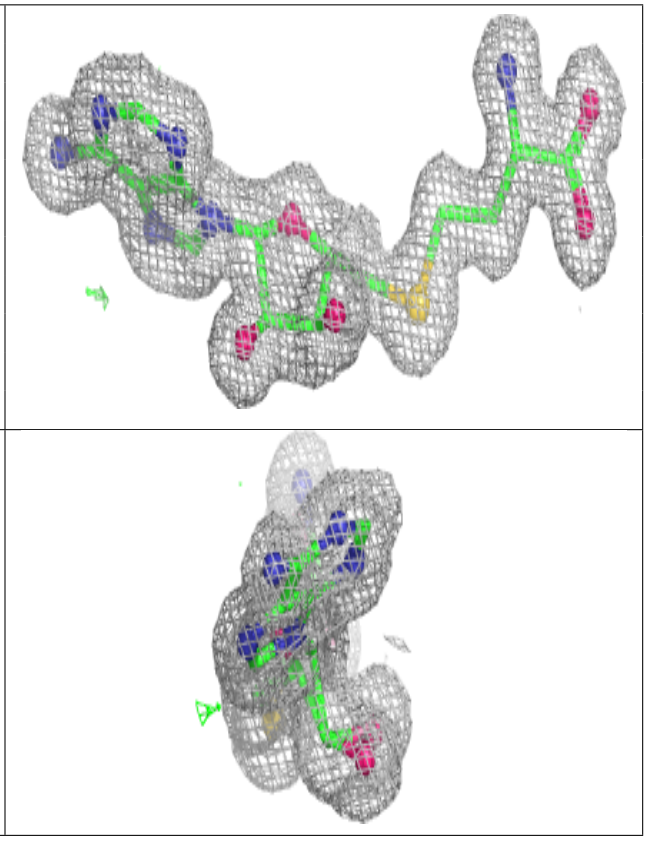
Electron density around SAH J 258:

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



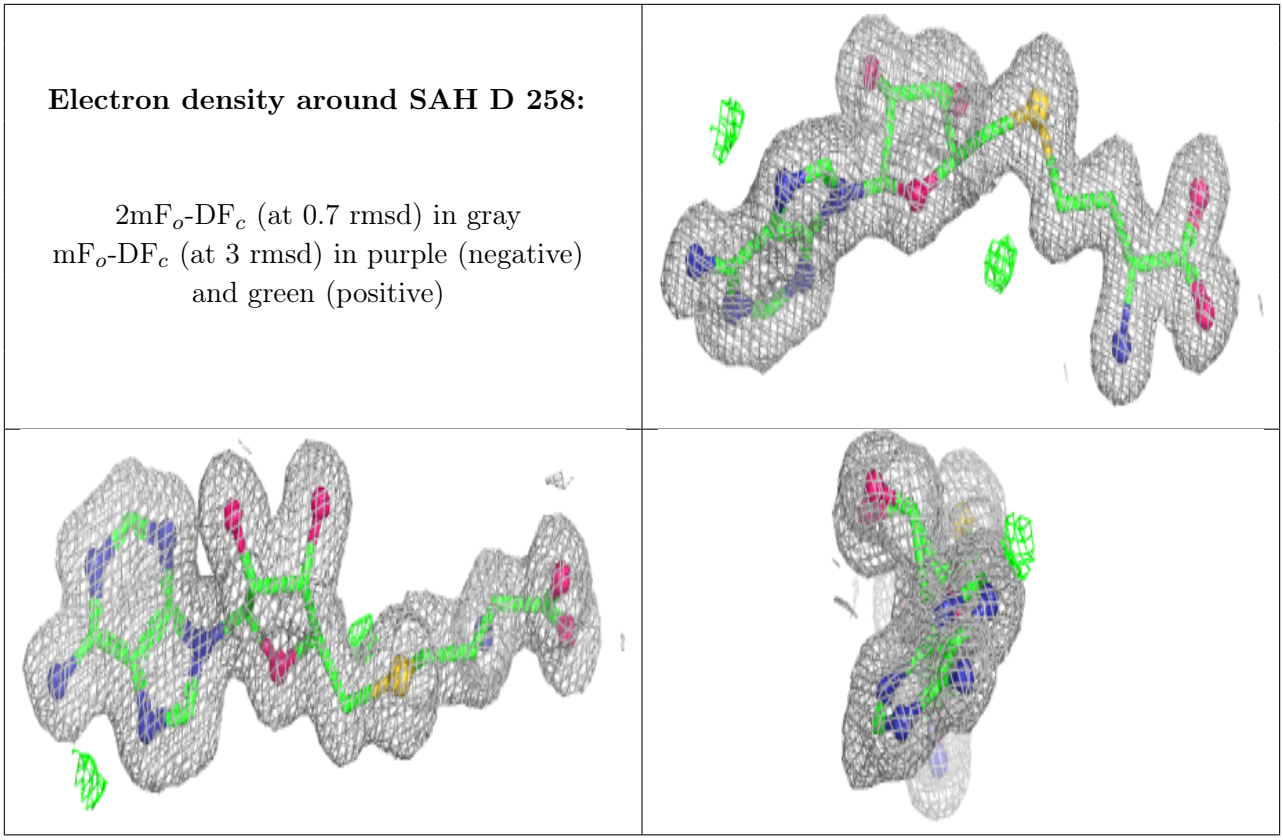
Electron density around SAH E 258:

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



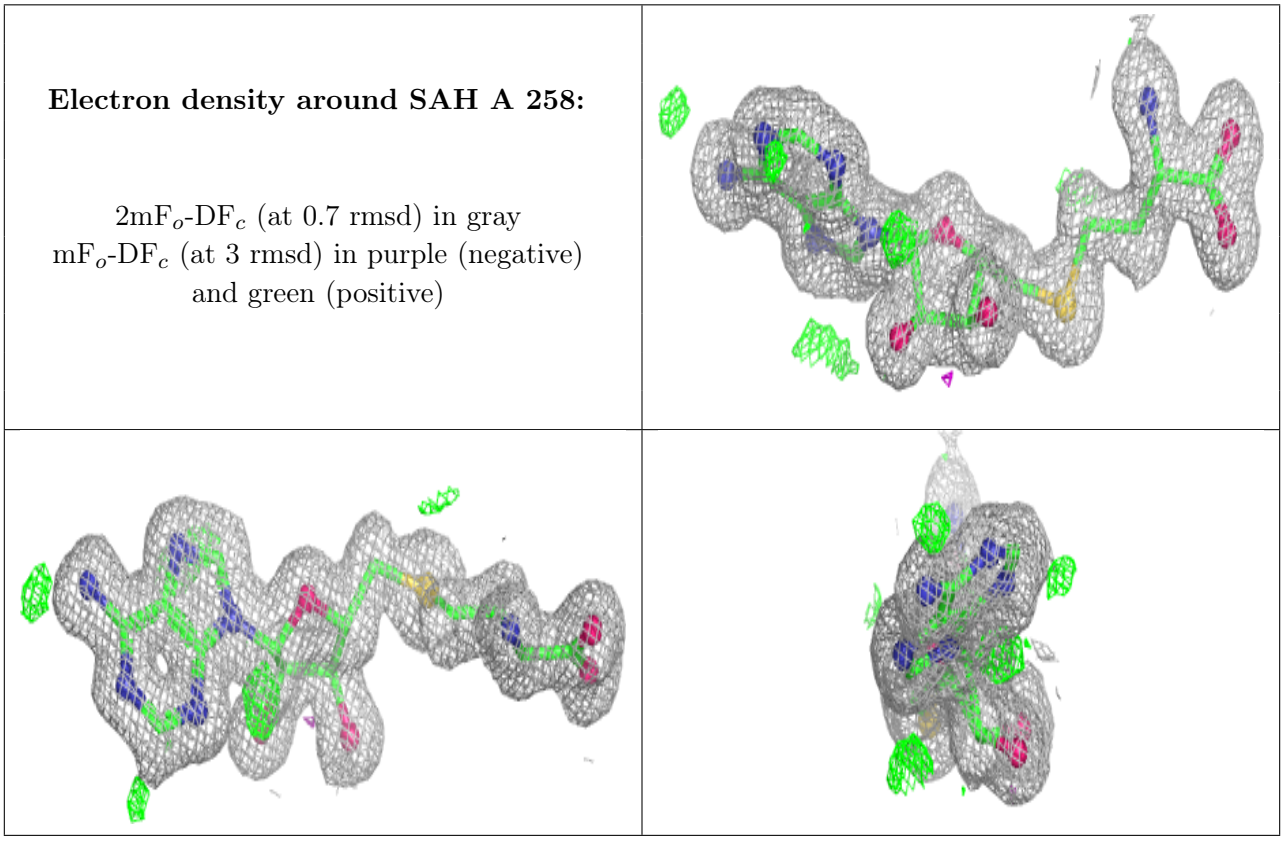
Electron density around SAH D 258:

$2mF_o$-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 258:

$2mF_o$-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.