Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 05:34 AM EDT

PDB ID	:	3IEI
Title	:	Crystal structure of human leucine carboxylmethyltransferase-1 in complex with S-adenosyl homocysteine
Authors	:	Xing, Y.; Jeffry, P.D.
Deposited on	:	2009-07-22
Resolution	:	1.90 Å(reported)

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

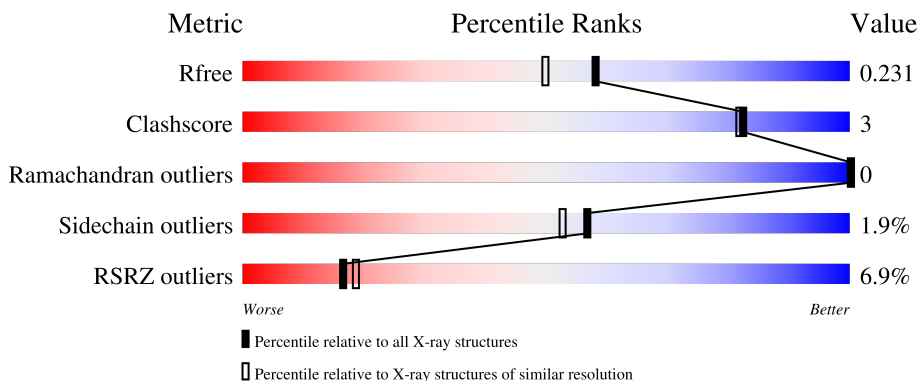|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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.
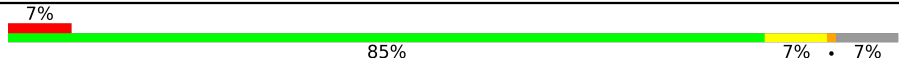
Metric	Percentile Ranks	Value
Rfree		0.231
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.9%
RSRZ outliers		6.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	334	5% / 84% / 8% · 7%
1	B	334	7% / 85% / 7% · 7%
1	C	334	7% / 87% / 5% · 7%
1	D	334	5% / 87% / 5% 7%
1	E	334	3% / 87% / 5% · 7%

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Mol	Chain	Length	Quality of chain
1	F	334	7% 85% 7% · 7%
1	G	334	6% 88% 5% 7%
1	H	334	12% 87% 5% 7%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 22201 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 Leucine carboxyl methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			
1	B	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			
1	C	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			
1	D	310	Total	C	N	O	S	0	1	0
			2511	1584	437	466	24			
1	E	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			
1	F	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			
1	G	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			
1	H	310	Total	C	N	O	S	0	0	0
			2505	1581	436	465	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	CYS	engineered mutation	UNP Q9UIC8
A	21	GLU	ALA	engineered mutation	UNP Q9UIC8
A	22	ASN	ASP	engineered mutation	UNP Q9UIC8
A	115	SER	PRO	engineered mutation	UNP Q9UIC8
B	19	MET	CYS	engineered mutation	UNP Q9UIC8
B	21	GLU	ALA	engineered mutation	UNP Q9UIC8
B	22	ASN	ASP	engineered mutation	UNP Q9UIC8
B	115	SER	PRO	engineered mutation	UNP Q9UIC8
C	19	MET	CYS	engineered mutation	UNP Q9UIC8
C	21	GLU	ALA	engineered mutation	UNP Q9UIC8
C	22	ASN	ASP	engineered mutation	UNP Q9UIC8
C	115	SER	PRO	engineered mutation	UNP Q9UIC8
D	19	MET	CYS	engineered mutation	UNP Q9UIC8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	21	GLU	ALA	engineered mutation	UNP Q9UIC8
D	22	ASN	ASP	engineered mutation	UNP Q9UIC8
D	115	SER	PRO	engineered mutation	UNP Q9UIC8
E	19	MET	CYS	engineered mutation	UNP Q9UIC8
E	21	GLU	ALA	engineered mutation	UNP Q9UIC8
E	22	ASN	ASP	engineered mutation	UNP Q9UIC8
E	115	SER	PRO	engineered mutation	UNP Q9UIC8
F	19	MET	CYS	engineered mutation	UNP Q9UIC8
F	21	GLU	ALA	engineered mutation	UNP Q9UIC8
F	22	ASN	ASP	engineered mutation	UNP Q9UIC8
F	115	SER	PRO	engineered mutation	UNP Q9UIC8
G	19	MET	CYS	engineered mutation	UNP Q9UIC8
G	21	GLU	ALA	engineered mutation	UNP Q9UIC8
G	22	ASN	ASP	engineered mutation	UNP Q9UIC8
G	115	SER	PRO	engineered mutation	UNP Q9UIC8
H	19	MET	CYS	engineered mutation	UNP Q9UIC8
H	21	GLU	ALA	engineered mutation	UNP Q9UIC8
H	22	ASN	ASP	engineered mutation	UNP Q9UIC8
H	115	SER	PRO	engineered mutation	UNP Q9UIC8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).
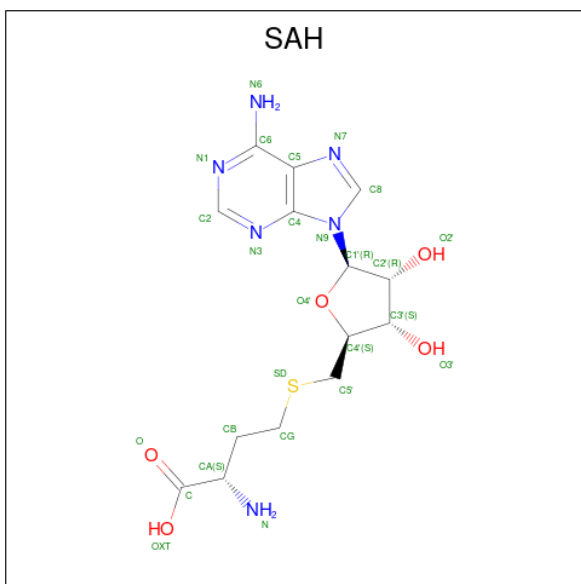
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	H	1	Total 6	C 3	O 3	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
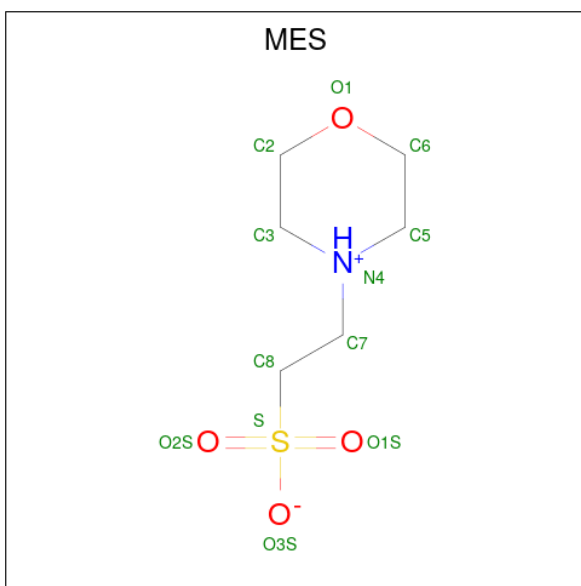
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
4	D	1	Total 12	C 6	N 1	O 4	S 1	0	0
4	E	1	Total 12	C 6	N 1	O 4	S 1	0	0
4	H	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total 239	O 239	0	0

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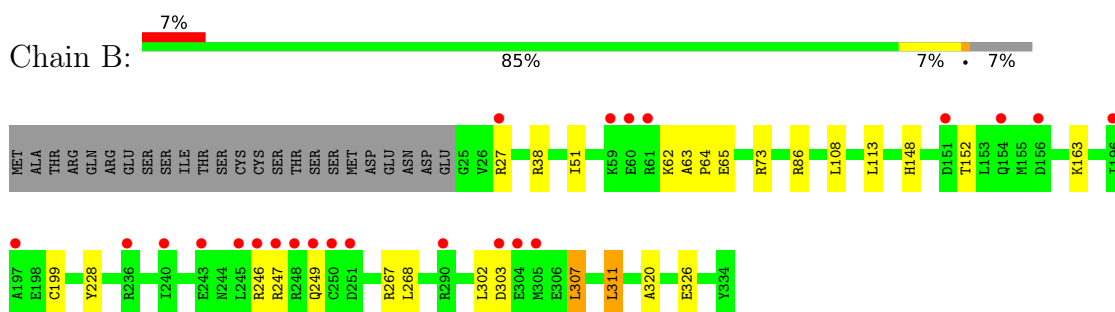| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	197	Total 197	O 197	0	0
5	C	231	Total 231	O 231	0	0
5	D	251	Total 251	O 251	0	0
5	E	283	Total 283	O 283	0	0
5	F	248	Total 248	O 248	0	0
5	G	235	Total 235	O 235	0	0
5	H	167	Total 167	O 167	0	0

3 Residue-property plots ⓘ

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.
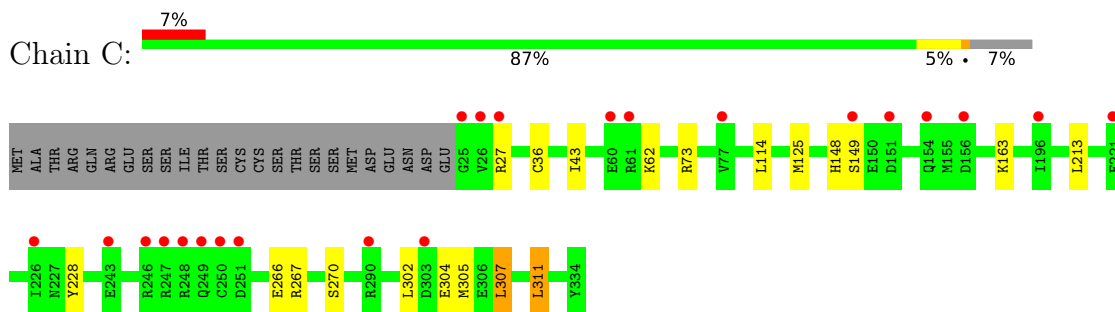
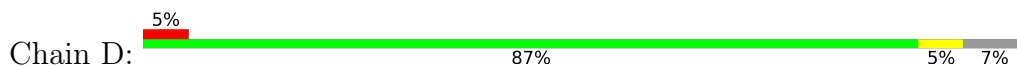• Molecule 1: Leucine carboxyl methyltransferase 1
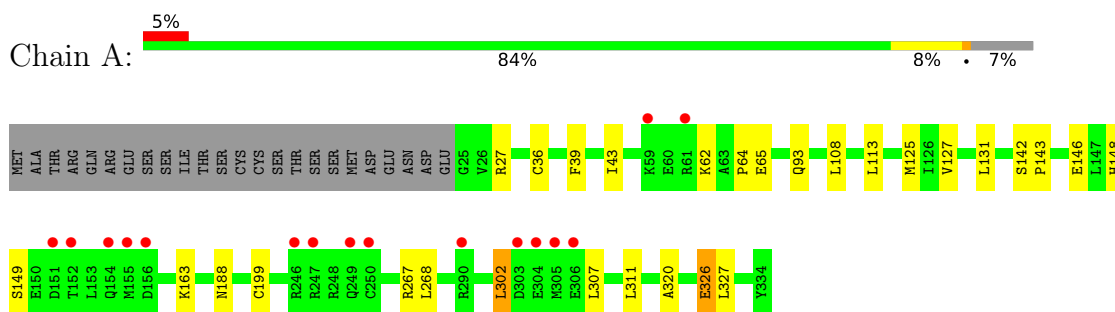
Chain A:

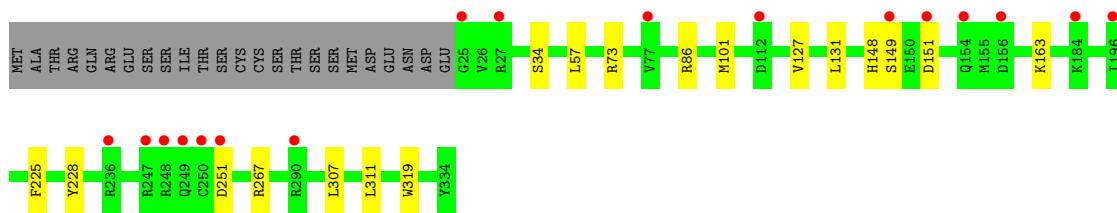• Molecule 1: Leucine carboxyl methyltransferase 1

Chain B:

• Molecule 1: Leucine carboxyl methyltransferase 1

Chain C:

• Molecule 1: Leucine carboxyl methyltransferase 1

Chain D:

• Molecule 1: Leucine carboxyl methyltransferase 1

Chain E:

• Molecule 1: Leucine carboxyl methyltransferase 1

Chain F:

• Molecule 1: Leucine carboxyl methyltransferase 1

Chain G:
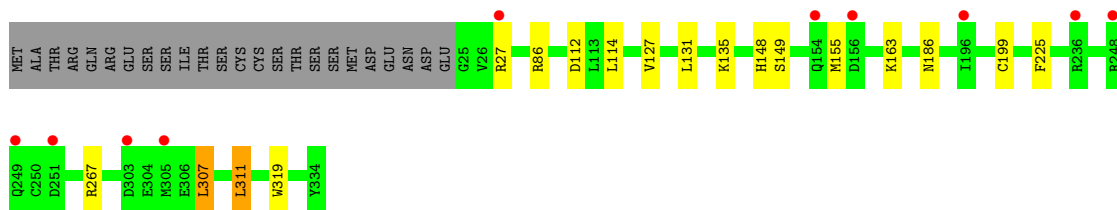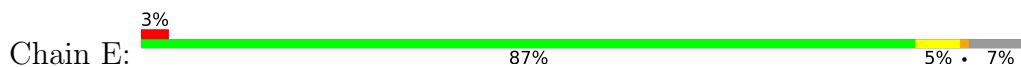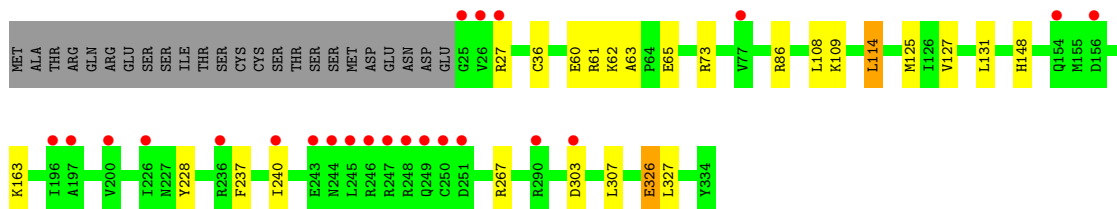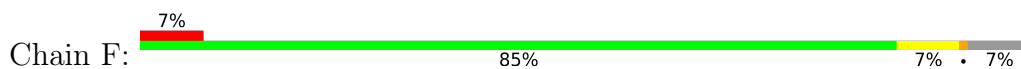

• Molecule 1: Leucine carboxyl methyltransferase 1

Chain H:
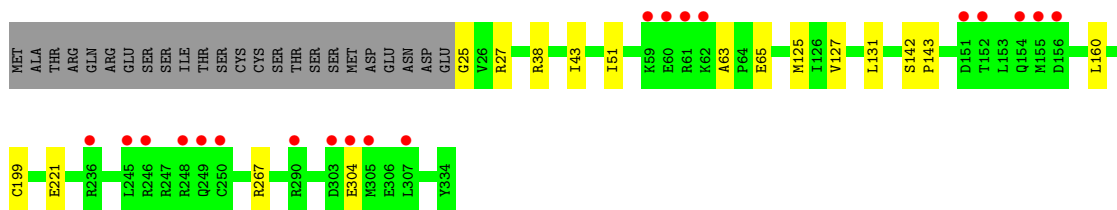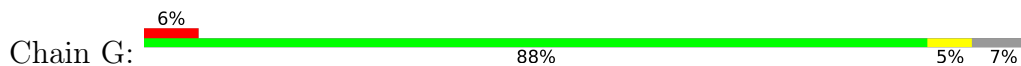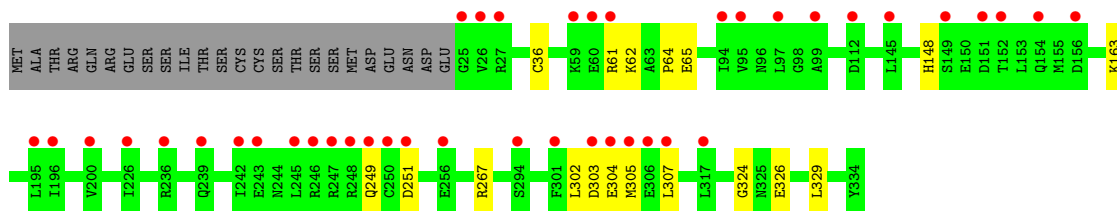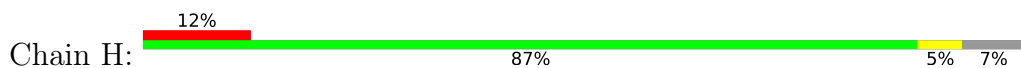
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	106.04Å 81.13Å 82.82Å 105.41° 93.97° 104.29°	Depositor
Resolution (Å)	29.97 – 1.90 29.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (29.97-1.90) 95.3 (29.97-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.184 , 0.232 0.184 , 0.231	Depositor DCC
R_{free} test set	9650 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 51.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22201	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2491e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/2552	0.56	0/3435
1	B	0.43	0/2552	0.54	0/3435
1	C	0.46	0/2552	0.56	0/3435
1	D	0.45	0/2558	0.56	0/3443
1	E	0.46	0/2552	0.57	0/3435
1	F	0.46	0/2552	0.56	0/3435
1	G	0.44	0/2552	0.56	0/3435
1	H	0.41	0/2552	0.53	0/3435
All	All	0.44	0/20422	0.56	0/27488

There are no bond length outliers.

There are no bond angle outliers.

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	2505	0	2503	17	0
1	B	2505	0	2503	12	0
1	C	2505	0	2503	14	0
1	D	2511	0	2507	9	0
1	E	2505	0	2503	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2505	0	2503	16	0
1	G	2505	0	2503	10	0
1	H	2505	0	2503	9	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	1	0
2	E	26	0	19	1	0
2	F	26	0	19	0	0
2	G	26	0	19	0	0
2	H	26	0	19	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	B	12	0	12	0	0
4	D	12	0	12	1	0
4	E	12	0	12	0	0
4	H	12	0	12	0	0
5	A	239	0	0	2	0
5	B	197	0	0	2	0
5	C	231	0	0	2	0
5	D	251	0	0	2	0
5	E	283	0	0	4	0
5	F	248	0	0	3	0
5	G	235	0	0	1	0
5	H	167	0	0	0	0
All	All	22201	0	20292	102	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 3.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:HE22	1:A:188:ASN:H	1.05	0.92
1:A:36:CYS:SG	1:A:62:LYS:NZ	2.59	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:LEU:HD13	5:F:448:HOH:O	1.94	0.68
1:E:131:LEU:HB3	1:E:155:MET:HE3	1.78	0.66
1:A:311:LEU:HD23	5:A:821:HOH:O	1.95	0.64
1:E:186:ASN:HB3	5:E:1518:HOH:O	1.98	0.63
1:F:86:ARG:NH2	5:F:375:HOH:O	2.22	0.62
1:F:326:GLU:HG2	1:F:327:LEU:N	2.14	0.61
1:D:73:ARG:HD2	1:D:228:TYR:CE2	2.36	0.60
1:B:108:LEU:HB3	1:B:113:LEU:O	2.03	0.58
1:C:36:CYS:SG	1:C:62:LYS:NZ	2.77	0.58
1:F:109:LYS:HA	1:F:114:LEU:HD22	1.85	0.58
1:A:127:VAL:O	1:A:131:LEU:HG	2.04	0.58
1:A:62:LYS:HE3	5:A:1626:HOH:O	2.03	0.57
1:B:148:HIS:HD2	1:B:163:LYS:H	1.52	0.57
1:E:135:LYS:HB2	1:E:155:MET:HE1	1.85	0.57
4:D:1902:MES:H61	5:D:565:HOH:O	2.04	0.57
1:B:63:ALA:HB1	1:B:65:GLU:OE1	2.06	0.55
1:C:43:ILE:HG22	1:C:43:ILE:O	2.06	0.55
1:D:57:LEU:HD23	1:H:61:ARG:HH21	1.72	0.55
1:H:304:GLU:HG2	1:H:304:GLU:O	2.06	0.55
1:B:148:HIS:CD2	1:B:163:LYS:H	2.25	0.55
1:E:27:ARG:HA	5:E:382:HOH:O	2.05	0.55
1:D:148:HIS:CD2	1:D:163:LYS:H	2.26	0.54
1:B:64:PRO:HB2	1:B:302:LEU:HD13	1.90	0.54
1:E:135:LYS:HD2	1:E:155:MET:HE2	1.89	0.54
1:F:27:ARG:HD2	1:F:125:MET:HE1	1.90	0.54
1:A:65:GLU:HG3	1:A:302:LEU:HD11	1.89	0.53
1:F:148:HIS:CD2	1:F:163:LYS:H	2.28	0.52
1:A:64:PRO:HB2	1:A:302:LEU:HD12	1.90	0.52
1:G:63:ALA:HB1	1:G:65:GLU:OE1	2.09	0.52
1:A:148:HIS:CD2	1:A:163:LYS:H	2.28	0.52
1:F:61:ARG:NH2	1:G:221:GLU:OE2	2.42	0.51
1:C:302:LEU:O	1:C:305:MET:HE3	2.11	0.51
1:E:131:LEU:O	1:E:155:MET:HE1	2.10	0.51
1:C:307:LEU:HD22	1:C:311:LEU:HD22	1.93	0.50
1:H:65:GLU:HG3	1:H:302:LEU:HD21	1.92	0.50
1:C:148:HIS:HD2	1:C:163:LYS:H	1.59	0.50
1:F:148:HIS:HD2	1:F:163:LYS:H	1.57	0.50
1:D:148:HIS:HD2	1:D:163:LYS:H	1.58	0.50
1:F:108:LEU:HB2	5:F:448:HOH:O	2.11	0.50
1:C:73:ARG:HD2	1:C:228:TYR:CE2	2.47	0.50
1:B:307:LEU:HD22	1:B:311:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CE2	1:A:43:ILE:HD11	2.47	0.49
1:C:213:LEU:CD1	1:C:267:ARG:HG2	2.42	0.49
1:A:148:HIS:CD2	1:A:149:SER:H	2.30	0.49
1:F:127:VAL:O	1:F:131:LEU:HG	2.13	0.49
1:E:307:LEU:HD22	1:E:311:LEU:HD22	1.93	0.49
1:D:127:VAL:O	1:D:131:LEU:HG	2.13	0.48
1:C:148:HIS:CD2	1:C:163:LYS:H	2.31	0.48
1:B:73:ARG:HD2	1:B:228:TYR:CE2	2.48	0.48
1:H:36:CYS:SG	1:H:62:LYS:NZ	2.87	0.48
1:D:34:SER:OG	1:D:101:MET:HB2	2.13	0.48
1:F:36:CYS:SG	1:F:62:LYS:NZ	2.87	0.47
2:C:601:SAH:H4'	2:C:601:SAH:HB1	1.96	0.47
1:C:148:HIS:CD2	1:C:149:SER:H	2.33	0.46
1:E:127:VAL:O	1:E:131:LEU:HG	2.15	0.46
1:H:64:PRO:HB2	1:H:302:LEU:HD13	1.96	0.46
1:A:142:SER:HB2	1:A:143:PRO:HD3	1.97	0.46
1:A:268:LEU:HD13	1:A:320:ALA:HB2	1.97	0.46
1:D:86:ARG:NH2	5:D:346:HOH:O	2.49	0.46
1:C:267:ARG:HD3	5:C:1549:HOH:O	2.16	0.46
1:C:304:GLU:HB3	5:C:1622:HOH:O	2.15	0.46
1:G:25:GLY:N	5:G:637:HOH:O	2.48	0.45
1:E:148:HIS:HD2	1:E:163:LYS:H	1.65	0.45
1:H:324:GLY:HA3	1:H:329:LEU:HB2	1.99	0.44
1:A:27:ARG:HD2	1:A:125:MET:CE	2.47	0.44
1:B:38:ARG:HG3	1:B:51:ILE:HG23	1.97	0.44
1:E:148:HIS:CD2	1:E:149:SER:H	2.35	0.44
1:G:160:LEU:C	1:G:160:LEU:HD23	2.39	0.43
1:H:302:LEU:HB3	1:H:305:MET:HE3	2.01	0.43
1:A:326:GLU:HG2	1:A:327:LEU:N	2.34	0.43
1:C:43:ILE:O	1:C:43:ILE:CG2	2.66	0.42
1:G:38:ARG:HG3	1:G:51:ILE:HG23	2.01	0.42
1:A:108:LEU:HB3	1:A:113:LEU:O	2.20	0.42
1:B:247:ARG:C	1:B:249:GLN:H	2.22	0.42
1:F:73:ARG:HD2	1:F:228:TYR:CE2	2.54	0.42
1:G:27:ARG:HE	1:G:125:MET:HE1	1.84	0.42
1:B:62:LYS:HG3	5:B:518:HOH:O	2.17	0.42
1:E:148:HIS:HE1	5:E:403:HOH:O	2.02	0.42
1:C:266:GLU:OE2	1:C:270:SER:HB3	2.20	0.42
1:F:63:ALA:HB1	1:F:65:GLU:OE1	2.20	0.42
1:H:302:LEU:HB3	1:H:305:MET:CE	2.50	0.41
1:F:237:PHE:HA	1:F:240:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:ARG:HH22	1:G:221:GLU:CD	2.23	0.41
1:D:225:PHE:O	1:D:319:TRP:HA	2.20	0.41
1:E:148:HIS:CD2	1:E:163:LYS:H	2.38	0.41
1:G:43:ILE:O	1:G:43:ILE:HG22	2.20	0.41
2:D:601:SAH:HB1	2:D:601:SAH:H4'	2.03	0.41
1:G:142:SER:HB3	1:G:143:PRO:HD3	2.03	0.41
1:H:148:HIS:CD2	1:H:163:LYS:H	2.39	0.41
1:A:142:SER:O	1:A:146:GLU:HG3	2.21	0.41
1:F:303:ASP:O	1:F:303:ASP:OD1	2.38	0.41
1:E:225:PHE:O	1:E:319:TRP:HA	2.21	0.41
1:B:86:ARG:NH2	5:B:350:HOH:O	2.53	0.40
1:B:268:LEU:HD13	1:B:320:ALA:HB2	2.02	0.40
1:E:86:ARG:NH2	5:E:363:HOH:O	2.54	0.40
1:G:127:VAL:O	1:G:131:LEU:HG	2.22	0.40
1:A:43:ILE:O	1:A:43:ILE:HG22	2.22	0.40
2:E:601:SAH:H4'	2:E:601:SAH:HB1	2.04	0.40
1:D:148:HIS:CD2	1:D:149:SER:H	2.38	0.40
1:C:27:ARG:HD2	1:C:125:MET:CE	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/334 (92%)	305 (99%)	3 (1%)	0	100	100
1	B	308/334 (92%)	303 (98%)	5 (2%)	0	100	100
1	C	308/334 (92%)	305 (99%)	3 (1%)	0	100	100
1	D	309/334 (92%)	302 (98%)	7 (2%)	0	100	100
1	E	308/334 (92%)	302 (98%)	6 (2%)	0	100	100
1	F	308/334 (92%)	303 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	308/334 (92%)	302 (98%)	6 (2%)	0	100	100
1	H	308/334 (92%)	300 (97%)	8 (3%)	0	100	100
All	All	2465/2672 (92%)	2422 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/299 (92%)	271 (98%)	5 (2%)	59	55
1	B	276/299 (92%)	267 (97%)	9 (3%)	38	29
1	C	276/299 (92%)	273 (99%)	3 (1%)	73	73
1	D	277/299 (93%)	272 (98%)	5 (2%)	59	55
1	E	276/299 (92%)	270 (98%)	6 (2%)	52	47
1	F	276/299 (92%)	271 (98%)	5 (2%)	59	55
1	G	276/299 (92%)	273 (99%)	3 (1%)	73	73
1	H	276/299 (92%)	270 (98%)	6 (2%)	52	47
All	All	2209/2392 (92%)	2167 (98%)	42 (2%)	57	53

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

Mol	Chain	Res	Type
1	A	199	CYS
1	A	267	ARG
1	A	302	LEU
1	A	307	LEU
1	A	326	GLU
1	B	27	ARG
1	B	152	THR
1	B	199	CYS
1	B	246	ARG

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Mol	Chain	Res	Type
1	B	267	ARG
1	B	303	ASP
1	B	307	LEU
1	B	311	LEU
1	B	326	GLU
1	C	114	LEU
1	C	307	LEU
1	C	311	LEU
1	D	151	ASP
1	D	251	ASP
1	D	267	ARG
1	D	307	LEU
1	D	311	LEU
1	E	112	ASP
1	E	114	LEU
1	E	199	CYS
1	E	267	ARG
1	E	307	LEU
1	E	311	LEU
1	F	60	GLU
1	F	114	LEU
1	F	267	ARG
1	F	307	LEU
1	F	326	GLU
1	G	199	CYS
1	G	267	ARG
1	G	304	GLU
1	H	249	GLN
1	H	251	ASP
1	H	267	ARG
1	H	303	ASP
1	H	307	LEU
1	H	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	75	HIS
1	A	93	GLN
1	A	148	HIS
1	A	186	ASN

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Mol	Chain	Res	Type
1	B	47	HIS
1	B	75	HIS
1	B	148	HIS
1	C	148	HIS
1	C	310	GLN
1	D	47	HIS
1	D	75	HIS
1	D	148	HIS
1	E	47	HIS
1	E	75	HIS
1	E	148	HIS
1	F	47	HIS
1	F	75	HIS
1	F	148	HIS
1	F	310	GLN
1	H	148	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	MES	B	1903	-	12,12,12	1.99	1 (8%)	14,16,16	2.37	3 (21%)
2	SAH	D	601	-	24,28,28	1.07	3 (12%)	25,40,40	1.58	5 (20%)
4	MES	E	1901	-	12,12,12	1.94	1 (8%)	14,16,16	2.43	3 (21%)
2	SAH	B	601	-	24,28,28	1.01	2 (8%)	25,40,40	1.43	5 (20%)
4	MES	D	1902	-	12,12,12	2.08	1 (8%)	14,16,16	2.51	6 (42%)
3	GOL	C	1914	-	5,5,5	0.40	0	5,5,5	0.26	0
2	SAH	G	601	-	24,28,28	1.05	2 (8%)	25,40,40	1.44	4 (16%)
3	GOL	D	1915	-	5,5,5	0.37	0	5,5,5	0.45	0
2	SAH	E	601	-	24,28,28	1.06	3 (12%)	25,40,40	1.53	7 (28%)
2	SAH	A	601	-	24,28,28	1.06	2 (8%)	25,40,40	1.51	6 (24%)
3	GOL	E	1916	-	5,5,5	0.41	0	5,5,5	0.23	0
4	MES	H	1904	-	12,12,12	2.05	1 (8%)	14,16,16	2.61	6 (42%)
2	SAH	C	601	-	24,28,28	1.05	2 (8%)	25,40,40	1.55	6 (24%)
3	GOL	B	1913	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	H	1918	-	5,5,5	0.38	0	5,5,5	0.31	0
3	GOL	F	1917	-	5,5,5	0.40	0	5,5,5	0.71	0
3	GOL	G	1911	-	5,5,5	0.38	0	5,5,5	0.49	0
3	GOL	A	1912	-	5,5,5	0.41	0	5,5,5	0.26	0
2	SAH	H	601	-	24,28,28	1.02	2 (8%)	25,40,40	1.41	5 (20%)
2	SAH	F	601	-	24,28,28	1.03	3 (12%)	25,40,40	1.43	6 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	B	1903	-	-	1/6/14/14	0/1/1/1
2	SAH	D	601	-	-	0/11/31/31	0/3/3/3
4	MES	E	1901	-	-	1/6/14/14	0/1/1/1
2	SAH	B	601	-	-	0/11/31/31	0/3/3/3
4	MES	D	1902	-	-	1/6/14/14	0/1/1/1
3	GOL	C	1914	-	-	0/4/4/4	-
2	SAH	G	601	-	-	0/11/31/31	0/3/3/3
3	GOL	D	1915	-	-	0/4/4/4	-
2	SAH	E	601	-	-	0/11/31/31	0/3/3/3
2	SAH	A	601	-	-	0/11/31/31	0/3/3/3
3	GOL	E	1916	-	-	0/4/4/4	-
4	MES	H	1904	-	-	1/6/14/14	0/1/1/1
2	SAH	C	601	-	-	0/11/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1913	-	-	0/4/4/4	-
3	GOL	H	1918	-	-	2/4/4/4	-
3	GOL	F	1917	-	-	2/4/4/4	-
3	GOL	G	1911	-	-	2/4/4/4	-
3	GOL	A	1912	-	-	2/4/4/4	-
2	SAH	H	601	-	-	0/11/31/31	0/3/3/3
2	SAH	F	601	-	-	0/11/31/31	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1902	MES	C8-S	-6.93	1.67	1.77
4	H	1904	MES	C8-S	-6.83	1.67	1.77
4	B	1903	MES	C8-S	-6.61	1.68	1.77
4	E	1901	MES	C8-S	-6.38	1.68	1.77
2	A	601	SAH	C5-C4	2.86	1.48	1.40
2	C	601	SAH	C5-C4	2.66	1.48	1.40
2	D	601	SAH	C5-C4	2.63	1.47	1.40
2	E	601	SAH	C5-C4	2.59	1.47	1.40
2	G	601	SAH	C2-N3	2.57	1.36	1.32
2	D	601	SAH	C2-N3	2.48	1.36	1.32
2	F	601	SAH	C5-C4	2.45	1.47	1.40
2	H	601	SAH	C5-C4	2.41	1.47	1.40
2	B	601	SAH	C5-C4	2.39	1.47	1.40
2	G	601	SAH	C5-C4	2.34	1.47	1.40
2	F	601	SAH	C2-N3	2.14	1.35	1.32
2	A	601	SAH	C2-N3	2.13	1.35	1.32
2	F	601	SAH	OXT-C	-2.11	1.23	1.30
2	E	601	SAH	C2-N3	2.10	1.35	1.32
2	B	601	SAH	OXT-C	-2.08	1.23	1.30
2	H	601	SAH	C2-N3	2.04	1.35	1.32
2	E	601	SAH	OXT-C	-2.03	1.23	1.30
2	C	601	SAH	OXT-C	-2.02	1.23	1.30
2	D	601	SAH	OXT-C	-2.01	1.24	1.30

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1903	MES	C5-N4-C3	6.26	122.93	108.83
4	D	1902	MES	C5-N4-C3	5.58	121.38	108.83
4	E	1901	MES	C5-N4-C3	5.51	121.24	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1904	MES	C5-N4-C3	5.42	121.03	108.83
4	H	1904	MES	O1S-S-C8	5.32	113.32	106.92
4	E	1901	MES	O2S-S-C8	4.46	112.28	106.92
4	E	1901	MES	C7-N4-C3	4.46	122.63	111.23
4	D	1902	MES	O2S-S-C8	4.31	112.11	106.92
4	D	1902	MES	C7-N4-C5	4.04	121.57	111.23
4	B	1903	MES	O1S-S-C8	3.92	111.64	106.92
2	C	601	SAH	N3-C2-N1	-3.89	122.59	128.68
4	H	1904	MES	C7-N4-C5	3.79	120.93	111.23
2	D	601	SAH	N3-C2-N1	-3.78	122.77	128.68
2	A	601	SAH	N3-C2-N1	-3.77	122.79	128.68
2	G	601	SAH	N3-C2-N1	-3.77	122.79	128.68
2	B	601	SAH	N3-C2-N1	-3.73	122.85	128.68
4	B	1903	MES	C7-N4-C3	3.72	120.75	111.23
2	H	601	SAH	N3-C2-N1	-3.70	122.90	128.68
2	F	601	SAH	N3-C2-N1	-3.61	123.04	128.68
2	E	601	SAH	N3-C2-N1	-3.47	123.26	128.68
2	D	601	SAH	OXT-C-O	-3.07	117.11	124.09
2	E	601	SAH	OXT-C-O	-2.91	117.49	124.09
2	C	601	SAH	O4'-C1'-C2'	-2.89	102.70	106.93
2	C	601	SAH	OXT-C-O	-2.89	117.54	124.09
2	D	601	SAH	C2-N1-C6	2.78	123.51	118.75
2	A	601	SAH	O4'-C1'-C2'	-2.67	103.02	106.93
4	H	1904	MES	C7-N4-C3	2.65	118.02	111.23
2	C	601	SAH	OXT-C-CA	2.64	122.36	113.38
2	D	601	SAH	OXT-C-CA	2.62	122.30	113.38
2	E	601	SAH	C4-C5-N7	-2.57	106.72	109.40
2	H	601	SAH	OXT-C-O	-2.55	118.29	124.09
2	C	601	SAH	C2-N1-C6	2.52	123.07	118.75
2	B	601	SAH	OXT-C-O	-2.51	118.39	124.09
2	F	601	SAH	O4'-C1'-C2'	-2.48	103.30	106.93
4	D	1902	MES	C2-C3-N4	-2.47	106.35	110.10
2	E	601	SAH	OXT-C-CA	2.44	121.71	113.38
2	A	601	SAH	C2-N1-C6	2.41	122.88	118.75
2	E	601	SAH	C2-N1-C6	2.41	122.88	118.75
2	H	601	SAH	C4-C5-N7	-2.37	106.93	109.40
2	G	601	SAH	OXT-C-CA	2.36	121.42	113.38
2	A	601	SAH	OXT-C-CA	2.34	121.36	113.38
2	E	601	SAH	O4'-C1'-C2'	-2.34	103.51	106.93
2	B	601	SAH	C2-N1-C6	2.32	122.73	118.75
2	D	601	SAH	C4-C5-N7	-2.32	106.98	109.40
2	G	601	SAH	OXT-C-O	-2.31	118.85	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	601	SAH	C4-C5-N7	-2.30	107.00	109.40
2	B	601	SAH	OXT-C-CA	2.28	121.16	113.38
4	D	1902	MES	C7-N4-C3	2.27	117.05	111.23
2	B	601	SAH	C4-C5-N7	-2.25	107.05	109.40
2	F	601	SAH	OXT-C-O	-2.24	119.00	124.09
2	A	601	SAH	OXT-C-O	-2.23	119.02	124.09
4	H	1904	MES	C2-C3-N4	-2.21	106.75	110.10
2	F	601	SAH	OXT-C-CA	2.20	120.89	113.38
2	C	601	SAH	C4-C5-N7	-2.19	107.11	109.40
2	A	601	SAH	C4-C5-N7	-2.17	107.14	109.40
2	H	601	SAH	C2-N1-C6	2.15	122.43	118.75
2	H	601	SAH	OXT-C-CA	2.15	120.70	113.38
4	H	1904	MES	C6-C5-N4	-2.14	106.86	110.10
2	F	601	SAH	C2-N1-C6	2.03	122.23	118.75
2	E	601	SAH	CB-CG-SD	-2.01	108.80	113.31
2	F	601	SAH	CB-CG-SD	-2.01	108.80	113.31
4	D	1902	MES	C6-O1-C2	2.00	116.58	109.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1903	MES	C8-C7-N4-C3
4	D	1902	MES	C8-C7-N4-C5
4	E	1901	MES	C8-C7-N4-C3
4	H	1904	MES	C8-C7-N4-C5
3	A	1912	GOL	O1-C1-C2-C3
3	F	1917	GOL	O1-C1-C2-C3
3	H	1918	GOL	C1-C2-C3-O3
3	F	1917	GOL	O1-C1-C2-O2
3	G	1911	GOL	O1-C1-C2-O2
3	G	1911	GOL	O1-C1-C2-C3
3	H	1918	GOL	O2-C2-C3-O3
3	A	1912	GOL	O1-C1-C2-O2

There are no ring outliers.
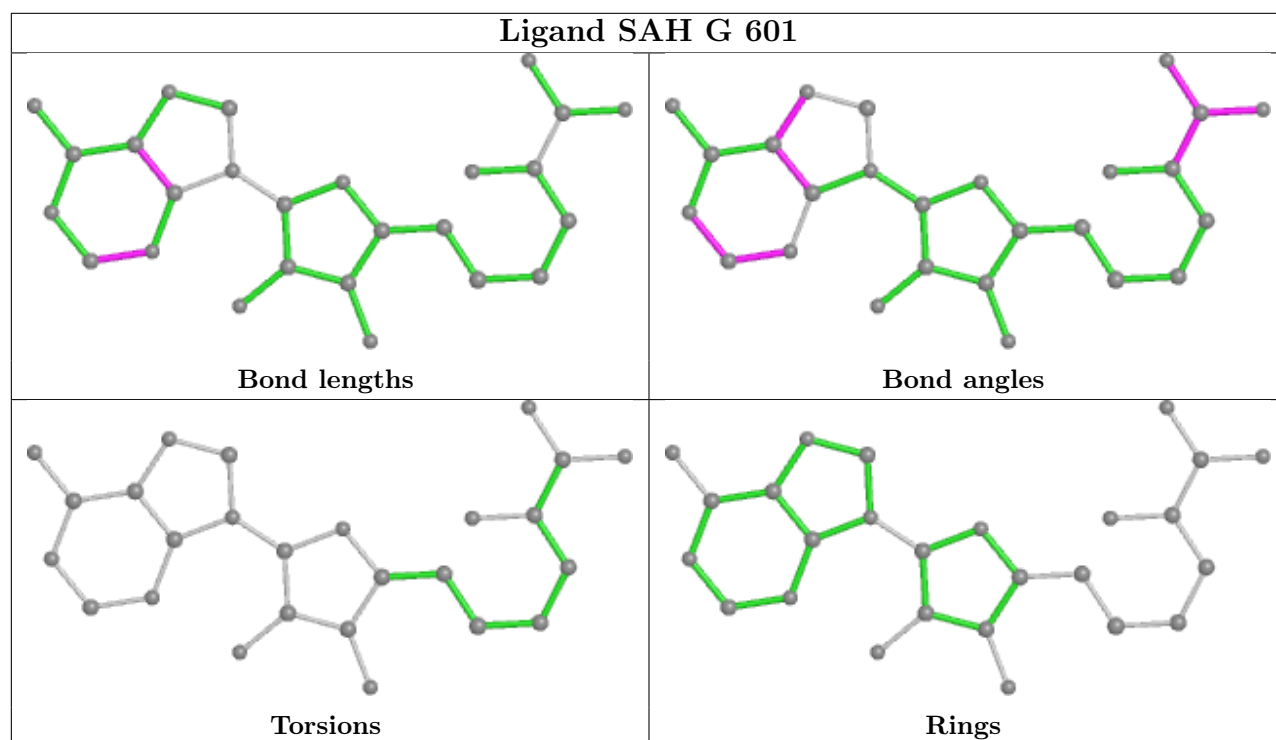
4 monomers are involved in 4 short contacts:

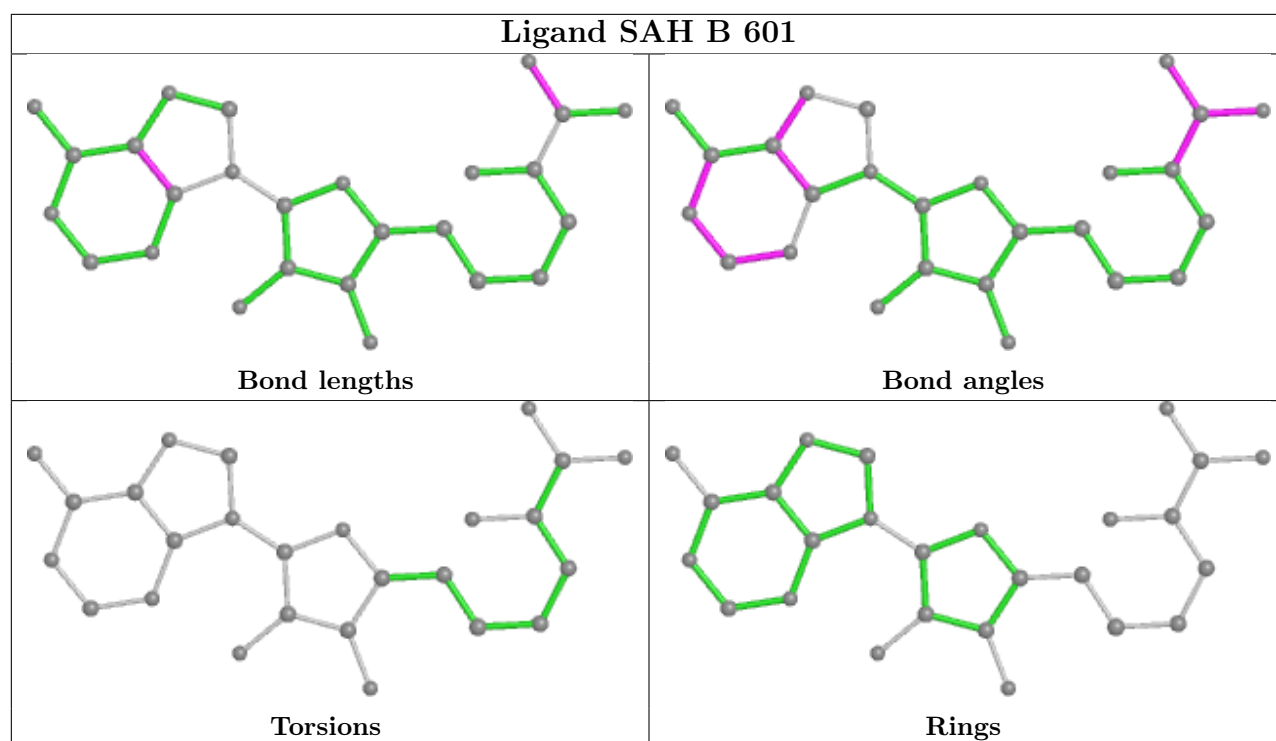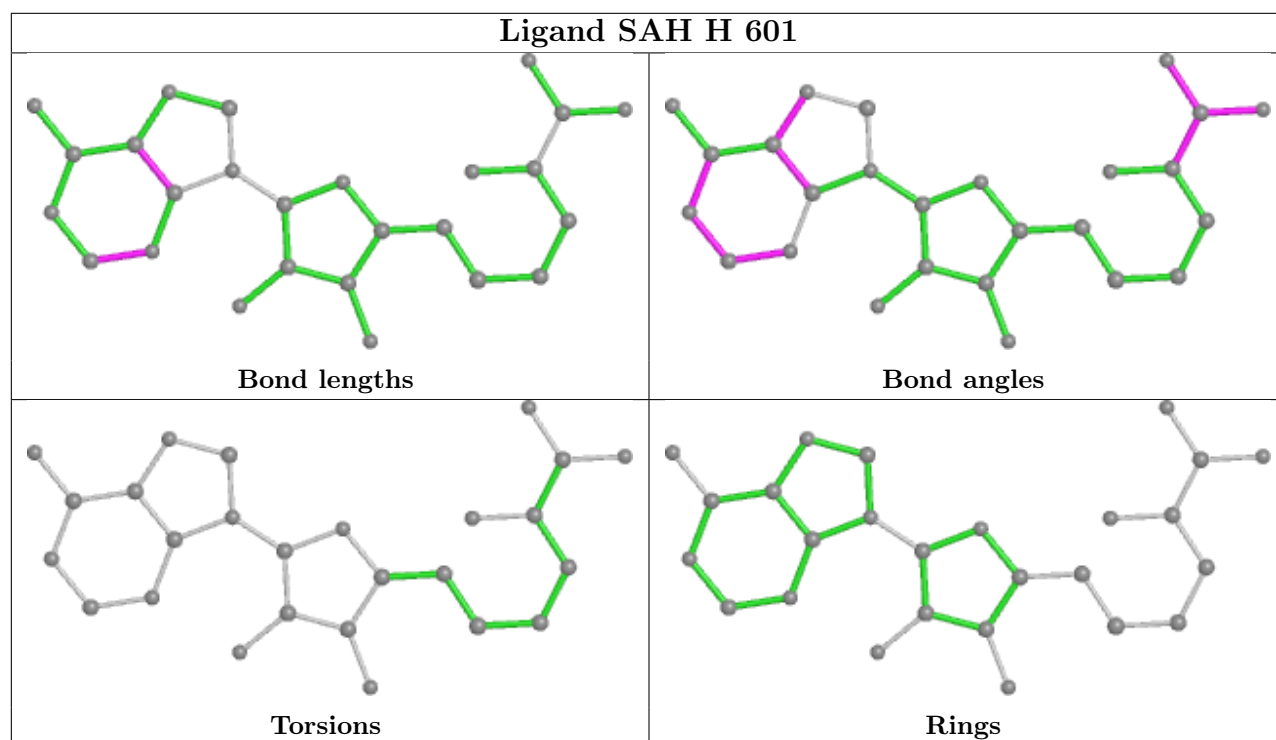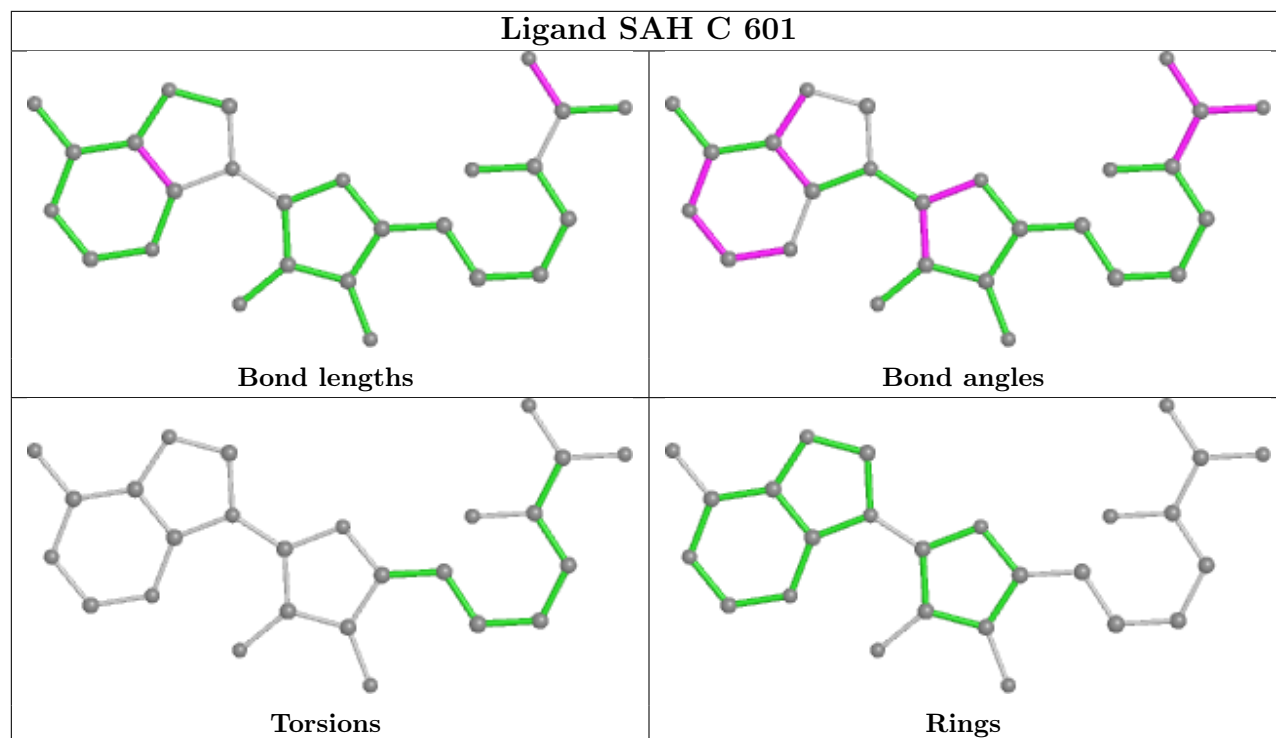| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	SAH	1	0
4	D	1902	MES	1	0

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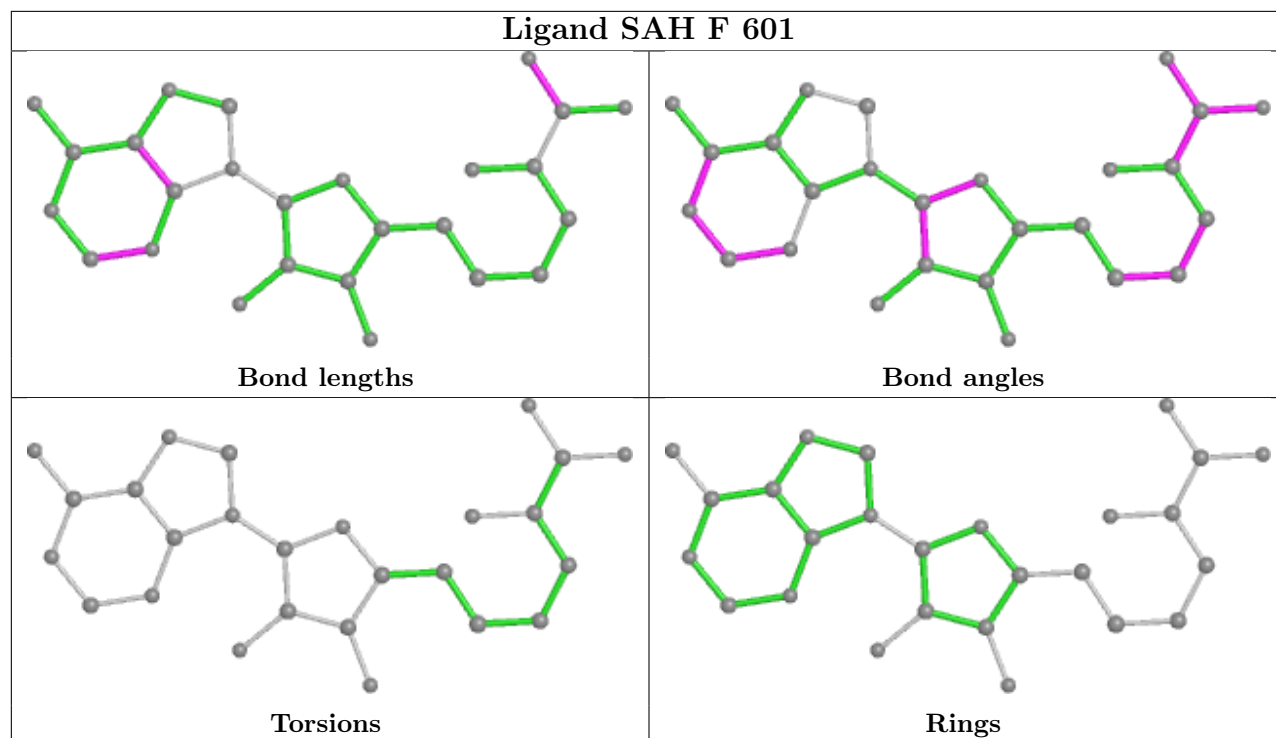| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	SAH	1	0
2	C	601	SAH	1	0

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 D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH H 601

Bond lengths

Bond angles

Torsions

Rings

Ligand SAH F 601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	310/334 (92%)	0.14	16 (5%)	27	30	15, 24, 44, 54	0
1	B	310/334 (92%)	0.39	23 (7%)	14	16	17, 27, 48, 64	0
1	C	310/334 (92%)	0.28	22 (7%)	16	17	16, 25, 44, 60	0
1	D	310/334 (92%)	0.07	17 (5%)	25	28	17, 24, 43, 53	0
1	E	310/334 (92%)	0.04	10 (3%)	47	50	15, 23, 41, 50	0
1	F	310/334 (92%)	0.22	23 (7%)	14	16	15, 23, 41, 60	0
1	G	310/334 (92%)	0.17	20 (6%)	18	21	15, 25, 45, 56	0
1	H	310/334 (92%)	0.57	41 (13%)	3	3	21, 30, 52, 60	0
All	All	2480/2672 (92%)	0.24	172 (6%)	16	19	15, 25, 46, 64	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	ARG	7.3
1	F	25	GLY	6.9
1	B	250	CYS	6.9
1	H	249	GLN	6.0
1	B	246	ARG	6.0
1	H	61	ARG	6.0
1	F	247	ARG	5.9
1	C	249	GLN	5.9
1	B	249	GLN	5.9
1	C	247	ARG	5.8
1	F	248	ARG	5.8
1	H	248	ARG	5.6
1	H	156	ASP	5.5
1	F	250	CYS	5.3
1	A	61	ARG	5.3
1	F	249	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	61	ARG	5.2
1	B	154	GLN	5.2
1	A	249	GLN	5.0
1	D	156	ASP	5.0
1	B	251	ASP	5.0
1	B	27	ARG	4.9
1	H	154	GLN	4.8
1	B	236	ARG	4.8
1	C	27	ARG	4.8
1	C	246	ARG	4.8
1	D	249	GLN	4.7
1	G	249	GLN	4.6
1	C	248	ARG	4.6
1	C	156	ASP	4.5
1	F	156	ASP	4.4
1	B	61	ARG	4.4
1	H	303	ASP	4.4
1	A	154	GLN	4.4
1	G	156	ASP	4.3
1	F	240	ILE	4.3
1	C	25	GLY	4.3
1	E	156	ASP	4.3
1	A	305	MET	4.3
1	C	250	CYS	4.2
1	B	156	ASP	4.2
1	C	61	ARG	4.2
1	H	27	ARG	4.2
1	H	151	ASP	4.2
1	F	244	ASN	4.1
1	G	250	CYS	4.1
1	C	154	GLN	4.1
1	D	27	ARG	4.0
1	A	156	ASP	4.0
1	E	249	GLN	3.9
1	D	154	GLN	3.9
1	C	26	VAL	3.9
1	F	27	ARG	3.8
1	H	250	CYS	3.8
1	B	59	LYS	3.8
1	F	246	ARG	3.8
1	B	248	ARG	3.8
1	G	154	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	60	GLU	3.7
1	H	251	ASP	3.7
1	E	27	ARG	3.6
1	H	304	GLU	3.6
1	G	304	GLU	3.5
1	H	25	GLY	3.5
1	E	248	ARG	3.5
1	G	305	MET	3.5
1	B	243	GLU	3.4
1	H	59	LYS	3.3
1	H	196	ILE	3.3
1	D	248	ARG	3.3
1	F	243	GLU	3.3
1	E	303	ASP	3.3
1	H	236	ARG	3.2
1	A	246	ARG	3.2
1	A	304	GLU	3.2
1	A	306	GLU	3.2
1	H	112	ASP	3.2
1	G	59	LYS	3.2
1	H	26	VAL	3.2
1	F	251	ASP	3.1
1	D	250	CYS	3.1
1	H	243	GLU	3.1
1	G	62	LYS	3.1
1	E	251	ASP	3.1
1	G	248	ARG	3.1
1	A	247	ARG	3.1
1	D	236	ARG	3.1
1	G	246	ARG	3.1
1	G	60	GLU	3.0
1	C	251	ASP	3.0
1	B	305	MET	3.0
1	B	303	ASP	3.0
1	B	196	ILE	2.9
1	H	256	GLU	2.9
1	C	196	ILE	2.9
1	A	59	LYS	2.9
1	H	152	THR	2.9
1	C	151	ASP	2.9
1	H	247	ARG	2.8
1	F	226	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	99	ALA	2.8
1	E	154	GLN	2.8
1	A	152	THR	2.7
1	H	306	GLU	2.8
1	D	112	ASP	2.7
1	A	151	ASP	2.7
1	D	151	ASP	2.7
1	H	226	ILE	2.7
1	G	236	ARG	2.7
1	F	245	LEU	2.7
1	D	290	ARG	2.7
1	H	246	ARG	2.7
1	A	290	ARG	2.6
1	F	196	ILE	2.6
1	G	245	LEU	2.6
1	B	290	ARG	2.6
1	F	290	ARG	2.6
1	D	247	ARG	2.6
1	D	196	ILE	2.6
1	B	304	GLU	2.6
1	H	60	GLU	2.6
1	A	250	CYS	2.5
1	H	307	LEU	2.5
1	C	243	GLU	2.4
1	H	149	SER	2.4
1	G	151	ASP	2.4
1	F	236	ARG	2.4
1	G	152	THR	2.4
1	E	236	ARG	2.4
1	H	94	ILE	2.4
1	F	26	VAL	2.4
1	C	226	ILE	2.4
1	B	197	ALA	2.3
1	A	303	ASP	2.3
1	H	95	VAL	2.3
1	G	307	LEU	2.3
1	F	303	ASP	2.3
1	H	239	GLN	2.3
1	H	200	VAL	2.3
1	C	290	ARG	2.3
1	F	197	ALA	2.3
1	B	245	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	149	SER	2.3
1	B	240	ILE	2.3
1	G	303	ASP	2.3
1	H	195	LEU	2.2
1	D	25	GLY	2.2
1	H	242	ILE	2.2
1	H	301	PHE	2.2
1	F	77	VAL	2.2
1	H	294	SER	2.2
1	D	77	VAL	2.2
1	C	221	GLU	2.2
1	F	154	GLN	2.1
1	F	200	VAL	2.1
1	D	184	LYS	2.1
1	H	97	LEU	2.1
1	C	60	GLU	2.1
1	H	145	LEU	2.1
1	G	290	ARG	2.1
1	A	155	MET	2.1
1	C	303	ASP	2.1
1	D	251	ASP	2.1
1	H	305	MET	2.0
1	B	151	ASP	2.0
1	E	305	MET	2.0
1	G	155	MET	2.0
1	C	149	SER	2.0
1	C	77	VAL	2.0
1	E	196	ILE	2.0
1	H	245	LEU	2.0
1	H	317	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	G	1911	6/6	0.85	0.17	30,35,37,38	0
3	GOL	B	1913	6/6	0.87	0.14	30,32,34,35	0
3	GOL	A	1912	6/6	0.88	0.18	25,32,32,33	0
3	GOL	F	1917	6/6	0.89	0.15	24,29,31,32	0
3	GOL	H	1918	6/6	0.90	0.12	33,36,37,38	0
4	MES	D	1902	12/12	0.93	0.15	35,40,43,44	0
2	SAH	H	601	26/26	0.94	0.11	21,23,24,24	0
4	MES	E	1901	12/12	0.94	0.13	32,37,42,42	0
3	GOL	C	1914	6/6	0.95	0.10	25,27,27,28	0
4	MES	B	1903	12/12	0.95	0.13	29,34,38,40	0
2	SAH	B	601	26/26	0.95	0.10	20,22,23,23	0
2	SAH	A	601	26/26	0.95	0.10	18,20,21,21	0
4	MES	H	1904	12/12	0.95	0.14	31,37,40,41	0
3	GOL	E	1916	6/6	0.96	0.07	23,25,25,26	0
2	SAH	E	601	26/26	0.96	0.11	15,19,20,20	0
2	SAH	G	601	26/26	0.96	0.09	18,19,21,21	0
2	SAH	D	601	26/26	0.96	0.11	17,20,21,21	0
3	GOL	D	1915	6/6	0.97	0.09	22,24,25,27	0
2	SAH	F	601	26/26	0.97	0.11	18,19,20,21	0
2	SAH	C	601	26/26	0.97	0.10	17,19,21,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
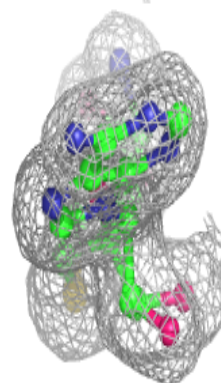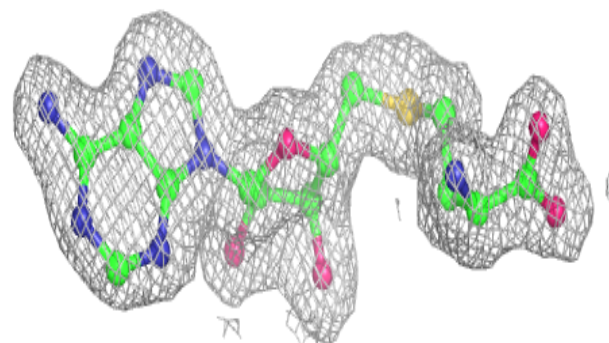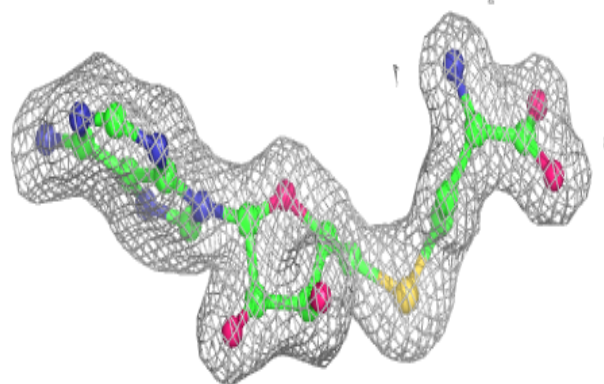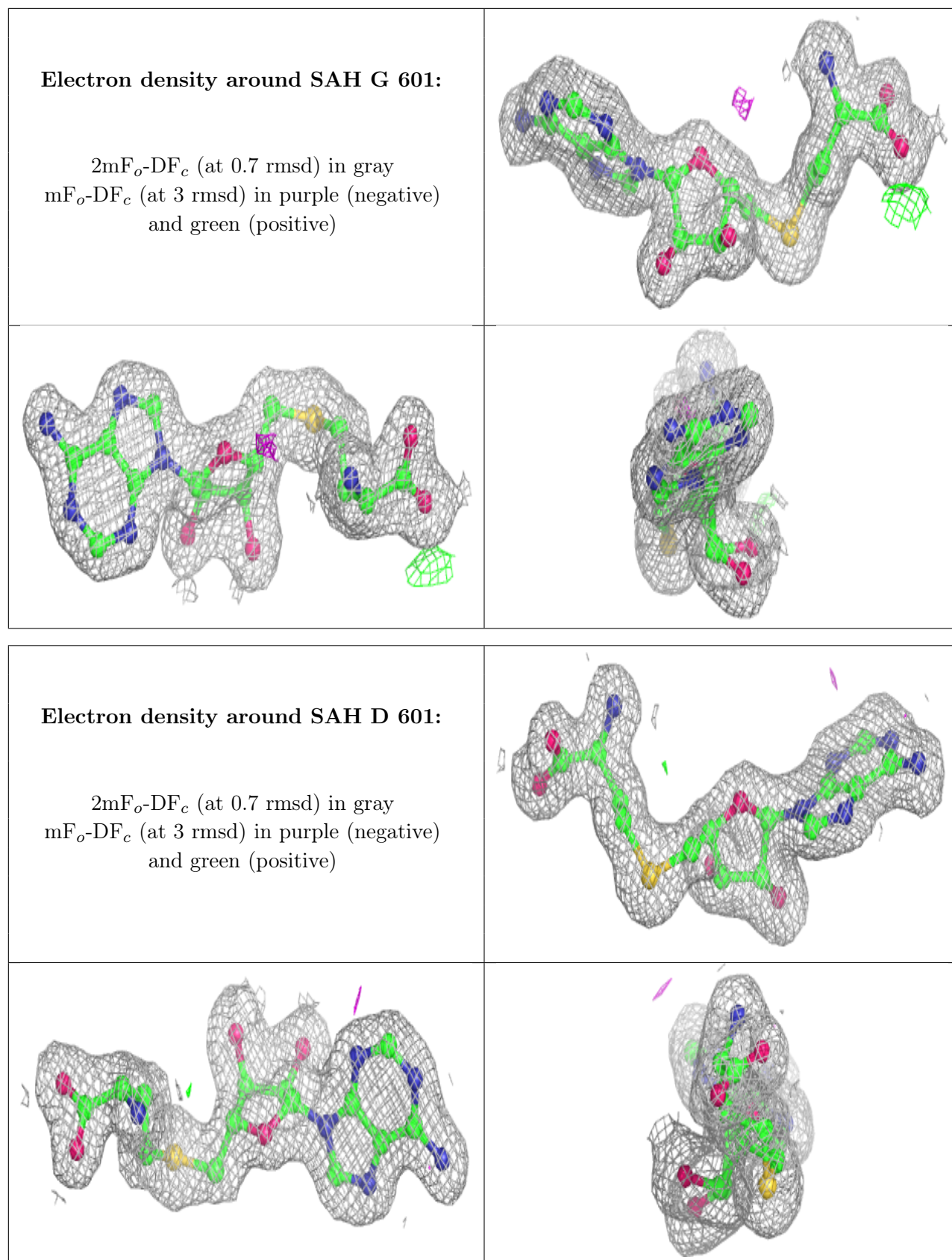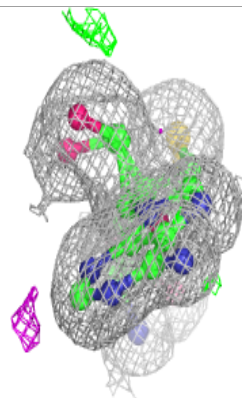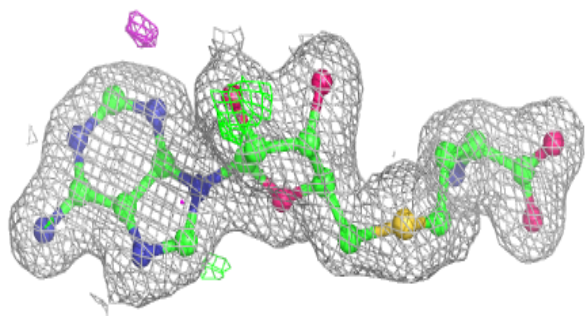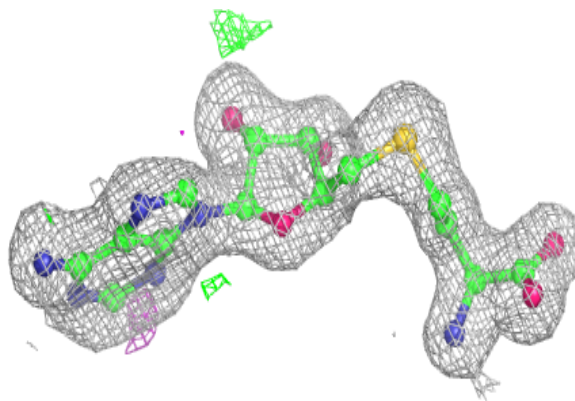
Electron density around SAH H 601:

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 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
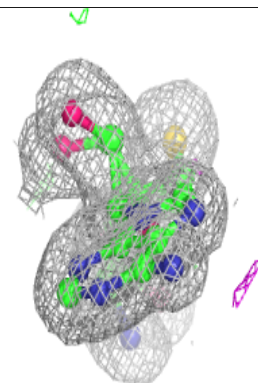and green (positive)
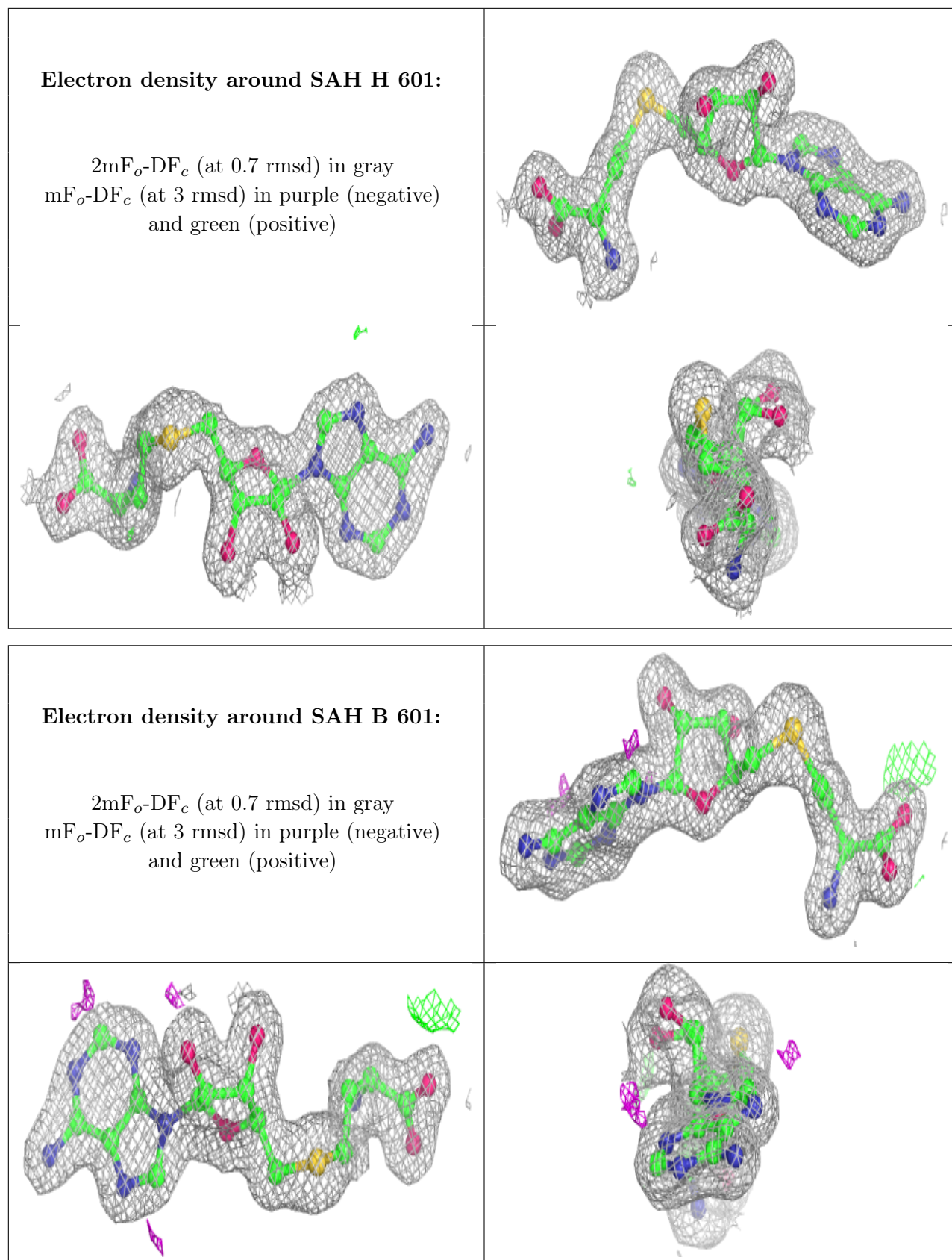
Electron density around SAH A 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
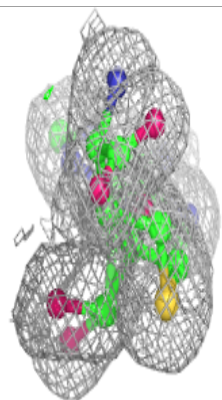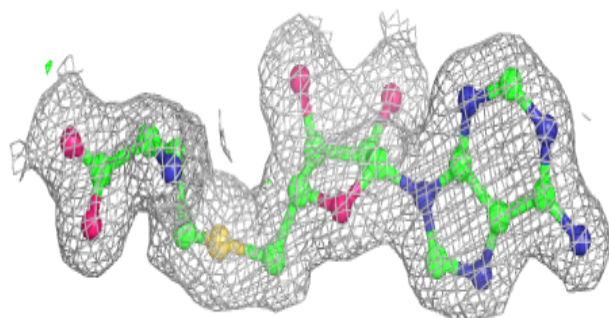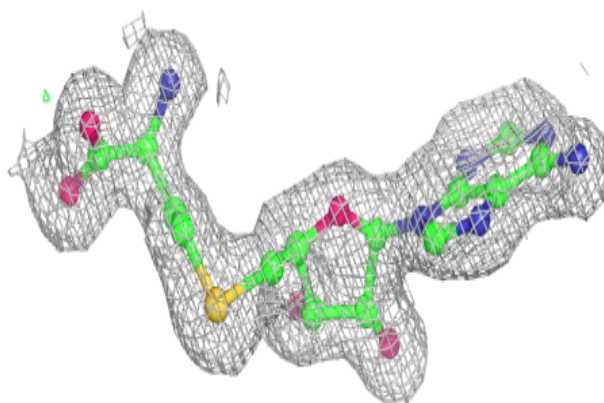
Electron density around SAH E 601:

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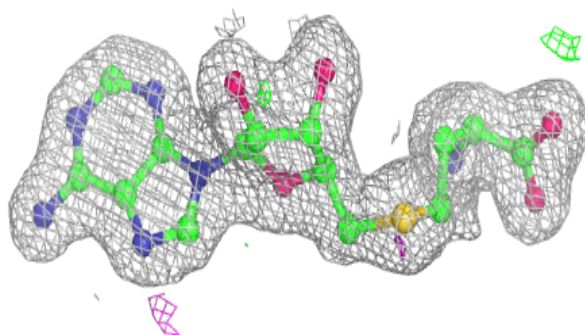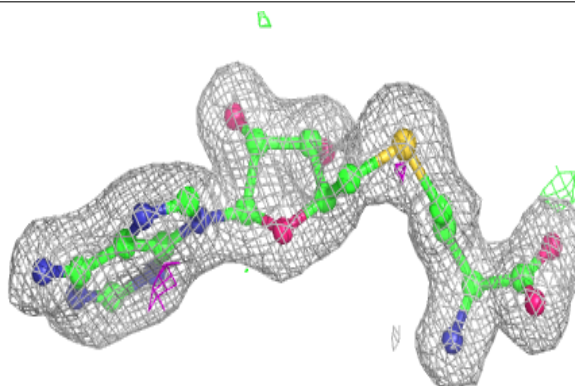and green (positive)

Electron density around SAH G 601:

$2mF_o$-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 601:

$2mF_o$-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 601:

$2mF_o$-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 601:

$2mF_o$-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.