



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 11:32 AM EDT

PDB ID : 8BIG / pdb_00008big
Title : O-Methyltransferase Plu4895 in complex with SAH
Authors : Huber, E.M.; Groll, M.
Deposited on : 2022-11-02
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

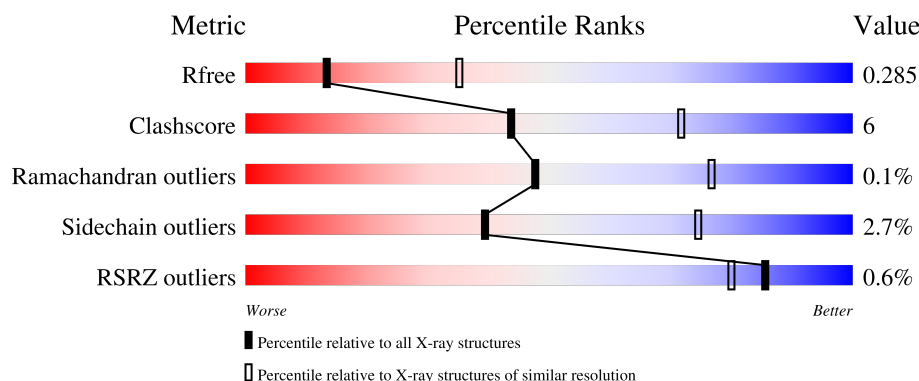
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	318	86%13%.
1	B	318	% 88%11%
1	C	318	85%14%.
1	D	318	% 86%14%.
1	E	318	84%15%

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Mol	Chain	Length	Quality of chain
1	F	318	
1	G	318	
1	H	318	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	H	402	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20724 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.

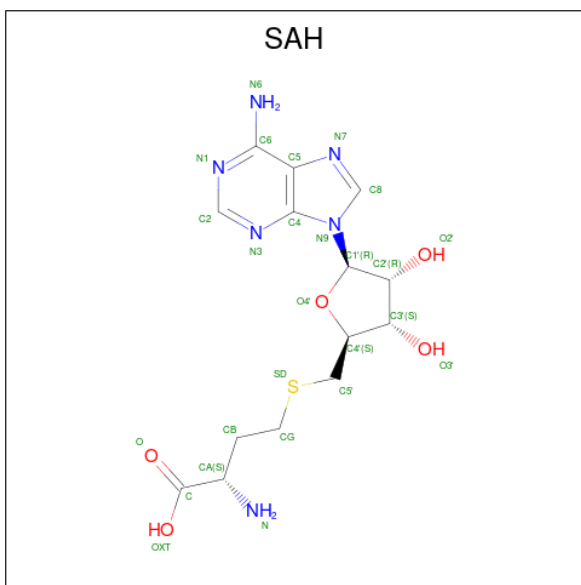
- Molecule 1 is a protein called methyltransferase Plu4895.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			
1	B	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			
1	C	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			
1	D	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			
1	E	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			
1	F	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			
1	G	316	Total	C	N	O	S	0	0	0
			2540	1634	412	483	11			
1	H	318	Total	C	N	O	S	0	0	0
			2556	1644	414	487	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A6L9JQS9
B	0	SER	-	expression tag	UNP A0A6L9JQS9
C	0	SER	-	expression tag	UNP A0A6L9JQS9
D	0	SER	-	expression tag	UNP A0A6L9JQS9
E	0	SER	-	expression tag	UNP A0A6L9JQS9
F	0	SER	-	expression tag	UNP A0A6L9JQS9
G	0	SER	-	expression tag	UNP A0A6L9JQS9
H	0	SER	-	expression tag	UNP A0A6L9JQS9

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).



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

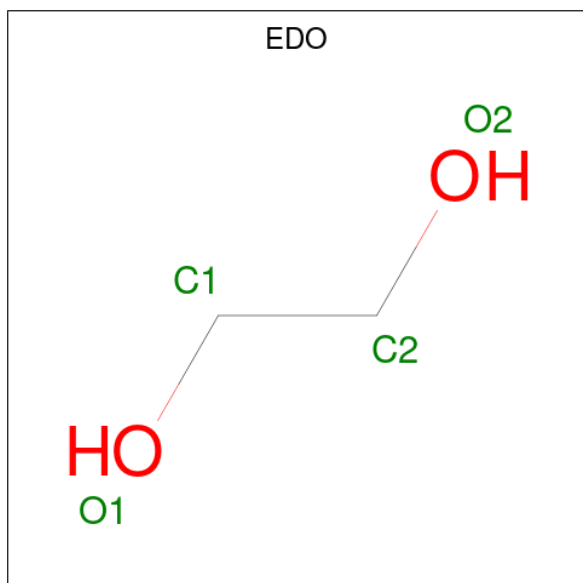
- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	D	2	Total	Ni	0	0
			2	2		
3	E	1	Total	Ni	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	G	1	Total C O 4 2 2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Mg 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	19	Total O 19 19	0	0

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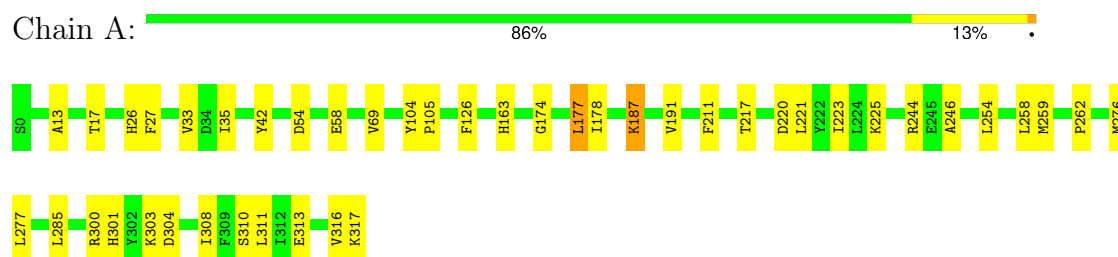
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	11	Total 11	O 11	0	0
7	C	5	Total 5	O 5	0	0
7	D	10	Total 10	O 10	0	0
7	E	4	Total 4	O 4	0	0
7	F	4	Total 4	O 4	0	0
7	G	5	Total 5	O 5	0	0
7	H	10	Total 10	O 10	0	0

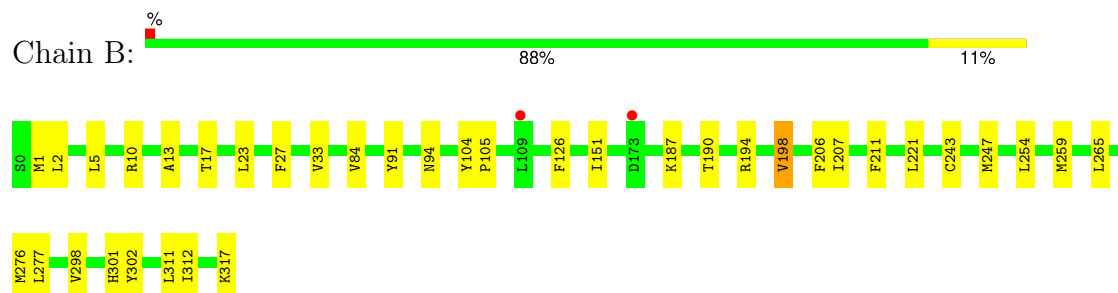
3 Residue-property plots

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.

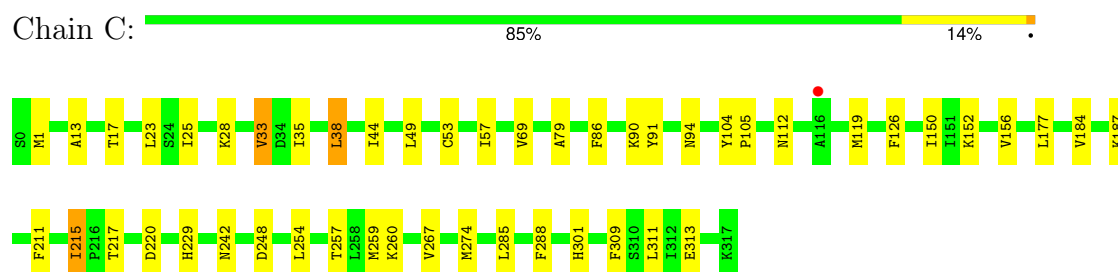
• Molecule 1: methyltransferase Plu4895



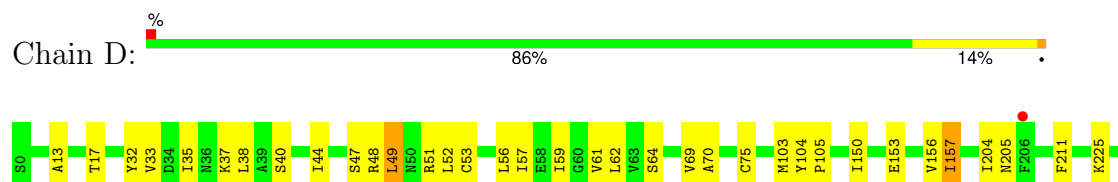
• Molecule 1: methyltransferase Plu4895

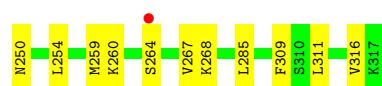


• Molecule 1: methyltransferase Plu4895

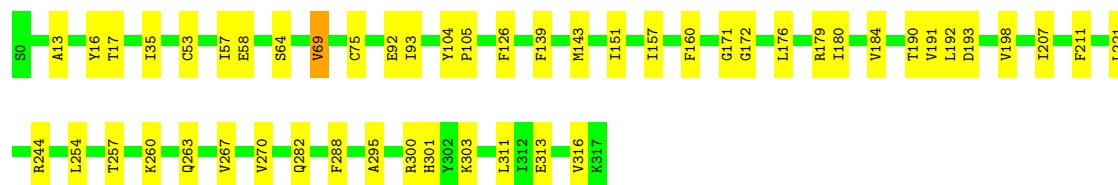
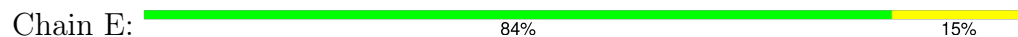


• Molecule 1: methyltransferase Plu4895

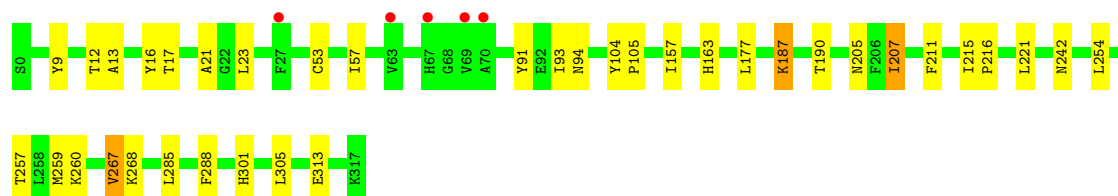
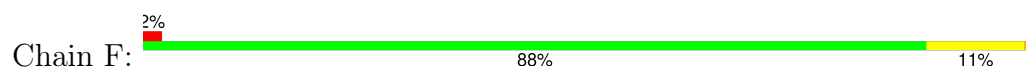




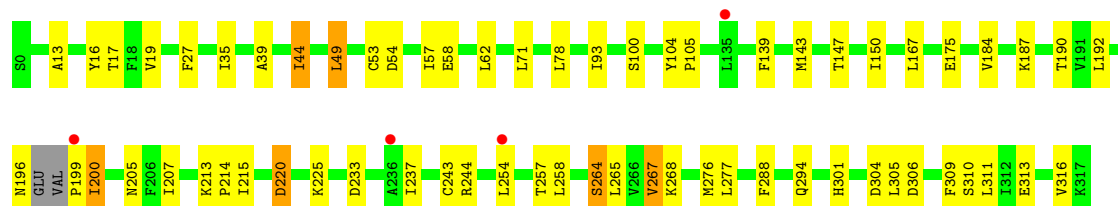
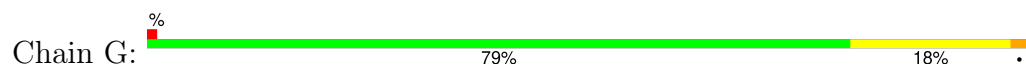
- Molecule 1: methyltransferase Plu4895



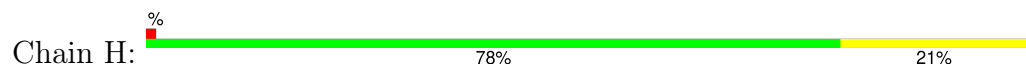
- Molecule 1: methyltransferase Plu4895



- Molecule 1: methyltransferase Plu4895



- Molecule 1: methyltransferase Plu4895



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.06Å 95.90Å 522.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.80) 94.3 (30.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.241 , 0.288 0.242 , 0.285	Depositor DCC
R_{free} test set	3537 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20724	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	0/2606	1.49	0/3517
1	B	1.02	0/2606	1.50	0/3517
1	C	1.02	0/2606	1.51	0/3517
1	D	1.02	0/2606	1.51	0/3517
1	E	1.01	0/2606	1.50	0/3517
1	F	1.02	0/2606	1.51	0/3517
1	G	1.02	0/2589	1.52	0/3491
1	H	1.02	0/2606	1.52	0/3517
All	All	1.02	0/20831	1.51	0/28110

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	2556	0	2558	24	0
1	B	2556	0	2558	28	0
1	C	2556	0	2558	27	0
1	D	2556	0	2558	24	0
1	E	2556	0	2558	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2556	0	2558	21	0
1	G	2540	0	2543	42	0
1	H	2556	0	2558	57	0
2	A	26	0	19	3	0
2	B	26	0	19	1	0
2	C	26	0	19	1	0
2	D	26	0	19	1	0
2	E	26	0	19	2	0
2	F	26	0	19	0	0
2	G	26	0	19	0	0
2	H	26	0	19	0	0
3	A	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	H	1	0	0	2	0
5	D	4	0	6	0	0
5	G	4	0	6	1	0
6	G	1	0	0	0	0
7	A	19	0	0	0	0
7	B	11	0	0	0	0
7	C	5	0	0	0	0
7	D	10	0	0	0	0
7	E	4	0	0	0	0
7	F	4	0	0	0	0
7	G	5	0	0	0	0
7	H	10	0	0	0	0
All	All	20724	0	20613	251	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 6.

All (251) 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:G:213:LYS:HG2	1:G:214:PRO:HD2	1.41	1.00
1:H:228:LEU:HD11	1:H:257:THR:OG1	1.65	0.96
1:A:244:ARG:HG2	1:A:316:VAL:HG22	1.64	0.79
1:F:190:THR:HG22	1:F:207:ILE:HD11	1.64	0.79
1:H:260:LYS:HG3	1:H:282:GLN:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:LYS:HA	1:E:267:VAL:HG11	1.69	0.74
1:C:44:ILE:HD11	1:C:49:LEU:HD22	1.71	0.71
1:C:254:LEU:HD22	1:C:311:LEU:HD11	1.73	0.71
1:H:167:LEU:HD11	1:H:192:LEU:HD13	1.74	0.70
1:G:213:LYS:CG	1:G:214:PRO:HD2	2.22	0.69
1:C:35:ILE:H	1:C:35:ILE:HD12	1.59	0.68
1:G:27:PHE:HB3	1:G:71:LEU:HG	1.76	0.66
1:E:300:ARG:NH1	1:G:304:ASP:HA	2.11	0.66
1:H:258:LEU:HG	1:H:308:ILE:CG2	2.26	0.66
1:H:228:LEU:HG	1:H:229:HIS:N	2.11	0.65
1:H:228:LEU:CD1	1:H:257:THR:OG1	2.44	0.65
1:A:254:LEU:HD22	1:A:311:LEU:HD11	1.80	0.64
1:H:258:LEU:HG	1:H:308:ILE:HG22	1.78	0.64
1:H:259:MET:N	4:H:402:CL:CL	2.63	0.63
1:A:163:HIS:O	1:A:187:LYS:NZ	2.31	0.63
1:H:125:PHE:HB3	1:H:278:PHE:CE1	2.35	0.62
1:F:163:HIS:O	1:F:187:LYS:NZ	2.31	0.62
1:G:254:LEU:HD22	1:G:311:LEU:HD11	1.81	0.62
1:C:33:VAL:HG11	1:C:38:LEU:HD11	1.81	0.61
1:G:276:MET:HE2	1:G:277:LEU:HD23	1.83	0.61
1:H:257:THR:OG1	1:H:258:LEU:N	2.33	0.60
1:E:13:ALA:O	1:E:17:THR:HG23	2.02	0.60
1:C:28:LYS:HG2	1:C:79:ALA:HB1	1.84	0.60
1:D:35:ILE:HD11	1:D:69:VAL:HG11	1.83	0.60
1:H:157:ILE:HD12	1:H:303:LYS:HG2	1.83	0.60
1:E:35:ILE:HD11	1:E:69:VAL:CG1	2.32	0.60
1:H:236:ALA:HB3	1:H:291:ILE:HD11	1.83	0.60
1:G:276:MET:HE2	1:G:277:LEU:CD2	2.33	0.58
1:B:265:LEU:HD23	1:E:58:GLU:HB3	1.86	0.58
1:G:213:LYS:HG2	1:G:214:PRO:CD	2.25	0.58
1:H:258:LEU:N	1:H:258:LEU:HD12	2.19	0.57
1:B:13:ALA:O	1:B:17:THR:HG23	2.04	0.57
1:D:52:LEU:O	1:D:56:LEU:HD12	2.05	0.57
1:G:62:LEU:CD2	1:G:71:LEU:HD23	2.35	0.56
1:E:301:HIS:HB3	1:E:313:GLU:HB3	1.87	0.56
1:C:13:ALA:O	1:C:17:THR:HG23	2.05	0.56
1:A:13:ALA:O	1:A:17:THR:HG23	2.05	0.56
1:F:190:THR:CG2	1:F:207:ILE:HD11	2.33	0.56
1:H:13:ALA:O	1:H:17:THR:HG23	2.06	0.56
1:D:61:VAL:HA	1:D:75:CYS:SG	2.46	0.56
1:E:176:LEU:O	1:E:180:ILE:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:LEU:HD11	1:H:254:LEU:HG	1.89	0.55
1:B:17:THR:HG22	1:E:105:PRO:HD3	1.89	0.55
1:F:259:MET:HE1	1:F:285:LEU:N	2.22	0.55
1:G:13:ALA:O	1:G:17:THR:HG23	2.07	0.55
1:H:104:TYR:N	1:H:105:PRO:HD2	2.22	0.54
1:F:13:ALA:O	1:F:17:THR:HG23	2.07	0.54
1:B:17:THR:HG21	1:E:104:TYR:HD2	1.70	0.54
1:G:264:SER:O	1:G:264:SER:OG	2.18	0.54
1:D:254:LEU:CD2	1:D:311:LEU:HD11	2.38	0.54
1:C:38:LEU:HD23	1:C:38:LEU:N	2.23	0.54
1:E:192:LEU:C	1:E:192:LEU:HD23	2.33	0.54
1:B:104:TYR:N	1:B:105:PRO:HD2	2.23	0.53
1:G:104:TYR:N	1:G:105:PRO:HD2	2.22	0.53
1:H:103:MET:HG3	1:H:120:VAL:CG2	2.39	0.53
1:B:104:TYR:HD2	1:E:17:THR:HG21	1.72	0.53
1:B:126:PHE:CZ	2:B:900:SAH:H5'1	2.44	0.53
1:B:298:VAL:CG2	1:B:317:LYS:HB3	2.39	0.53
1:F:190:THR:HG22	1:F:207:ILE:CD1	2.35	0.53
1:H:228:LEU:HD11	1:H:257:THR:HG1	1.71	0.53
1:H:155:LEU:HD11	1:H:183:GLN:HG2	1.90	0.53
1:B:10:ARG:NH1	1:E:92:GLU:OE1	2.42	0.52
1:G:264:SER:OG	1:G:267:VAL:HG23	2.10	0.52
1:A:177:LEU:HD22	1:A:191:VAL:HG22	1.91	0.52
1:F:53:CYS:O	1:F:57:ILE:HD12	2.09	0.52
1:A:104:TYR:N	1:A:105:PRO:HD2	2.24	0.52
1:D:47:SER:O	1:D:51:ARG:HG3	2.10	0.52
1:G:257:THR:HG21	1:G:288:PHE:CZ	2.45	0.52
1:H:167:LEU:CD1	1:H:192:LEU:HD13	2.39	0.52
1:C:35:ILE:HD11	1:C:69:VAL:HG23	1.92	0.52
1:H:247:MET:HG2	1:H:251:ALA:HB3	1.91	0.51
1:A:26:HIS:NE2	1:A:42:TYR:OH	2.40	0.51
1:C:301:HIS:HB3	1:C:313:GLU:HB3	1.93	0.51
1:D:40:SER:OG	1:H:182:GLU:O	2.29	0.51
1:E:254:LEU:HD22	1:E:311:LEU:HD11	1.93	0.51
1:H:301:HIS:HB3	1:H:313:GLU:HB3	1.92	0.51
1:C:229:HIS:CE1	1:C:274:MET:HE3	2.46	0.50
1:C:260:LYS:HA	1:C:267:VAL:HG11	1.93	0.50
1:G:100:SER:C	1:G:276:MET:HE3	2.36	0.50
1:G:143:MET:HE1	5:G:403:EDO:H21	1.94	0.50
1:G:192:LEU:C	1:G:192:LEU:HD23	2.36	0.50
1:F:215:ILE:HG23	1:F:216:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ARG:HA	1:D:51:ARG:HD3	1.93	0.50
1:G:35:ILE:HG23	1:G:49:LEU:HG	1.93	0.50
1:B:254:LEU:HD22	1:B:311:LEU:HD11	1.92	0.50
1:E:221:LEU:HD11	1:E:254:LEU:HG	1.94	0.50
1:H:281:LYS:HD3	1:H:283:ARG:HA	1.94	0.50
1:A:225:LYS:NZ	2:A:401:SAH:OXT	2.43	0.50
1:B:105:PRO:HD3	1:E:17:THR:HG22	1.92	0.50
1:G:167:LEU:CD1	1:G:190:THR:HG22	2.40	0.50
1:H:228:LEU:HD13	1:H:288:PHE:HZ	1.75	0.50
1:D:57:ILE:HD13	1:D:64:SER:HB2	1.93	0.50
1:E:53:CYS:O	1:E:57:ILE:HG13	2.11	0.50
1:E:244:ARG:HG3	1:E:316:VAL:HG22	1.94	0.49
1:H:153:GLU:O	1:H:156:VAL:N	2.44	0.49
1:C:53:CYS:O	1:C:57:ILE:HG13	2.13	0.49
1:C:215:ILE:HD13	1:C:242:ASN:HB3	1.94	0.49
1:H:103:MET:HG3	1:H:120:VAL:HG22	1.93	0.49
1:B:259:MET:HE3	1:B:302:TYR:CE1	2.48	0.49
1:G:53:CYS:O	1:G:57:ILE:HG13	2.11	0.49
1:D:260:LYS:HA	1:D:267:VAL:HG11	1.95	0.49
1:D:225:LYS:NZ	2:D:401:SAH:OXT	2.37	0.49
1:H:243:CYS:O	1:H:247:MET:HB2	2.12	0.49
1:D:53:CYS:O	1:D:57:ILE:HG13	2.13	0.49
1:E:190:THR:HG21	1:E:207:ILE:HD11	1.95	0.49
1:H:28:LYS:HG2	1:H:79:ALA:HB1	1.94	0.49
1:D:13:ALA:O	1:D:17:THR:HG23	2.13	0.48
1:E:300:ARG:HG3	1:G:304:ASP:HB2	1.94	0.48
1:G:264:SER:O	1:G:268:LYS:HB2	2.12	0.48
1:H:258:LEU:N	1:H:258:LEU:CD1	2.75	0.48
1:H:161:ASP:HA	1:H:187:LYS:HE3	1.95	0.48
1:H:198:VAL:HG23	1:H:206:PHE:HB2	1.95	0.48
1:H:107:SER:HA	1:H:119:MET:HE1	1.95	0.48
1:H:267:VAL:HG22	1:H:308:ILE:HG23	1.95	0.48
1:C:184:VAL:HG12	1:C:187:LYS:HD3	1.95	0.48
1:F:190:THR:HG23	1:F:205:ASN:HB2	1.96	0.48
1:A:217:THR:HG22	1:A:246:ALA:HA	1.94	0.48
1:B:27:PHE:CZ	1:B:33:VAL:HG11	2.48	0.48
1:E:35:ILE:HD11	1:E:69:VAL:HG13	1.95	0.48
1:H:150:ILE:HG23	1:H:305:LEU:HD13	1.96	0.48
1:E:300:ARG:HD2	1:E:300:ARG:HA	1.68	0.48
1:G:264:SER:CB	1:G:267:VAL:HG23	2.44	0.48
1:H:125:PHE:HB3	1:H:278:PHE:HE1	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:MET:HE2	1:H:312:ILE:HD11	1.96	0.47
1:H:289:GLU:HG2	1:H:299:ILE:HD12	1.96	0.47
1:F:260:LYS:HA	1:F:267:VAL:HG11	1.97	0.47
1:H:182:GLU:O	1:H:185:LYS:NZ	2.47	0.47
1:B:221:LEU:HD11	1:B:254:LEU:HG	1.95	0.47
1:D:33:VAL:HG11	1:D:38:LEU:HD21	1.95	0.47
1:H:266:VAL:O	1:H:270:VAL:HG23	2.15	0.47
1:B:298:VAL:HG23	1:B:317:LYS:HB3	1.96	0.47
1:E:104:TYR:N	1:E:105:PRO:HD2	2.30	0.47
1:G:233:ASP:O	1:G:237:ILE:HG13	2.14	0.47
1:A:221:LEU:HD11	1:A:254:LEU:HG	1.95	0.47
1:H:129:LEU:HD11	1:H:136:LYS:N	2.30	0.47
2:E:401:SAH:HG2	2:E:401:SAH:H4'	1.69	0.47
1:F:215:ILE:HD12	1:F:242:ASN:HB3	1.96	0.47
1:F:9:TYR:O	1:F:12:THR:OG1	2.32	0.46
1:G:304:ASP:OD1	1:G:306:ASP:O	2.33	0.46
1:H:105:PRO:O	1:H:109:LEU:HG	2.15	0.46
1:A:300:ARG:NH1	1:A:317:LYS:HE3	2.31	0.46
1:D:44:ILE:HG21	1:D:49:LEU:HD23	1.98	0.46
1:D:153:GLU:O	1:D:157:ILE:HG22	2.15	0.46
1:F:157:ILE:CD1	1:F:305:LEU:HD23	2.46	0.46
1:H:125:PHE:CB	1:H:278:PHE:CE1	2.99	0.46
1:H:260:LYS:CG	1:H:282:GLN:O	2.60	0.46
1:H:125:PHE:HB3	1:H:278:PHE:CD1	2.51	0.46
1:C:104:TYR:N	1:C:105:PRO:CD	2.79	0.46
1:E:151:ILE:HD13	1:E:179:ARG:CB	2.46	0.45
1:G:39:ALA:HA	1:G:44:ILE:HG13	1.98	0.45
1:C:35:ILE:CG2	1:C:49:LEU:HG	2.45	0.45
1:G:54:ASP:O	1:G:58:GLU:HG2	2.16	0.45
1:B:298:VAL:CG2	1:B:317:LYS:HD3	2.46	0.45
1:F:104:TYR:N	1:F:105:PRO:HD2	2.31	0.45
1:E:300:ARG:NH1	1:G:310:SER:OG	2.49	0.45
1:G:27:PHE:CB	1:G:71:LEU:HG	2.45	0.45
1:G:258:LEU:HB3	1:G:267:VAL:HG12	1.97	0.45
1:B:265:LEU:C	1:B:265:LEU:HD13	2.41	0.45
1:C:35:ILE:HD12	1:C:35:ILE:N	2.28	0.45
1:C:184:VAL:CG1	1:C:187:LYS:HD3	2.46	0.45
1:H:258:LEU:HB3	1:H:267:VAL:HG13	1.98	0.45
2:A:401:SAH:H4'	2:A:401:SAH:HG2	1.62	0.45
1:G:16:TYR:HB2	1:G:93:ILE:HG21	1.99	0.45
1:A:27:PHE:CZ	1:A:33:VAL:HG11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:O	1:C:94:ASN:ND2	2.50	0.45
1:A:258:LEU:HD23	1:A:308:ILE:HB	1.98	0.44
1:H:82:ASN:O	1:H:145:LYS:HE3	2.17	0.44
1:G:147:THR:HG22	1:G:225:LYS:HE3	1.98	0.44
1:C:259:MET:HE1	1:C:285:LEU:HB2	1.99	0.44
1:E:151:ILE:HD13	1:E:179:ARG:HB3	1.99	0.44
1:C:257:THR:HG21	1:C:288:PHE:CZ	2.53	0.44
1:D:104:TYR:N	1:D:105:PRO:CD	2.81	0.44
1:G:244:ARG:HG3	1:G:316:VAL:HG13	1.99	0.44
1:H:125:PHE:CB	1:H:278:PHE:CD1	3.01	0.44
1:A:126:PHE:CZ	2:A:401:SAH:H5'1	2.52	0.44
1:A:244:ARG:HD3	1:A:244:ARG:C	2.43	0.44
1:D:259:MET:HE1	1:D:285:LEU:N	2.33	0.44
1:F:53:CYS:C	1:F:57:ILE:HD12	2.42	0.43
1:A:35:ILE:HD11	1:A:69:VAL:CG2	2.48	0.43
1:D:264:SER:O	1:D:268:LYS:HG2	2.17	0.43
1:E:270:VAL:HG12	1:E:282:GLN:HE21	1.83	0.43
1:A:259:MET:HE1	1:A:285:LEU:N	2.33	0.43
1:E:139:PHE:CE1	1:E:143:MET:HE3	2.52	0.43
1:G:301:HIS:HB3	1:G:313:GLU:HB3	2.01	0.43
1:E:57:ILE:HD13	1:E:64:SER:HB2	2.00	0.43
1:H:139:PHE:CE1	1:H:143:MET:HE3	2.54	0.43
1:E:301:HIS:HB3	1:E:313:GLU:CB	2.49	0.43
1:G:200:ILE:C	1:G:200:ILE:HD12	2.44	0.43
1:B:259:MET:HE2	1:B:312:ILE:HD11	2.00	0.43
1:B:276:MET:HE2	1:B:277:LEU:HG	2.01	0.43
1:D:61:VAL:HG12	1:D:62:LEU:HD13	2.01	0.43
1:G:139:PHE:CE1	1:G:143:MET:HE3	2.53	0.43
1:G:215:ILE:HD12	1:G:243:CYS:N	2.34	0.43
1:H:281:LYS:CG	1:H:282:GLN:N	2.82	0.43
1:F:221:LEU:HD11	1:F:254:LEU:HG	2.00	0.43
1:E:157:ILE:HG21	1:E:303:LYS:HG2	2.01	0.42
1:H:176:LEU:O	1:H:180:ILE:HG13	2.19	0.42
1:B:190:THR:HG21	1:B:207:ILE:HD12	2.01	0.42
1:H:247:MET:HE3	1:H:252:THR:C	2.44	0.42
1:G:150:ILE:HG23	1:G:305:LEU:HD13	2.01	0.42
1:A:301:HIS:HB3	1:A:313:GLU:HB2	2.01	0.42
1:E:16:TYR:HB2	1:E:93:ILE:HG21	2.00	0.42
1:A:54:ASP:O	1:A:58:GLU:HG2	2.19	0.42
1:B:1:MET:HE2	1:B:5:LEU:HD11	2.00	0.42
1:E:171:GLY:HA3	1:E:191:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:ALA:HB3	1:F:23:LEU:HD13	2.01	0.42
1:B:198:VAL:HG13	1:B:206:PHE:HB2	2.01	0.42
1:B:265:LEU:HD23	1:E:58:GLU:CB	2.50	0.42
1:C:86:PHE:CE1	1:C:90:LYS:HE3	2.54	0.42
1:G:220:ASP:OD1	1:G:220:ASP:N	2.52	0.42
1:B:91:TYR:O	1:B:94:ASN:ND2	2.50	0.42
1:E:263:GLN:HG3	1:E:263:GLN:O	2.19	0.42
1:H:150:ILE:HD11	1:H:309:PHE:CG	2.55	0.42
1:C:150:ILE:HD11	1:C:309:PHE:CD2	2.55	0.42
1:A:259:MET:HG2	1:A:310:SER:HB2	2.02	0.41
1:E:172:GLY:N	1:E:193:ASP:OD2	2.52	0.41
1:G:184:VAL:HG12	1:G:187:LYS:HD2	2.03	0.41
1:C:126:PHE:CE1	2:C:900:SAH:H2'	2.55	0.41
1:D:44:ILE:HD12	1:D:44:ILE:N	2.35	0.41
1:A:262:PRO:HG2	1:B:317:LYS:HD2	2.03	0.41
1:B:243:CYS:O	1:B:247:MET:HG3	2.20	0.41
1:C:25:ILE:O	1:C:28:LYS:HG3	2.20	0.41
1:D:153:GLU:O	1:D:156:VAL:N	2.54	0.41
1:G:150:ILE:HD11	1:G:309:PHE:CG	2.56	0.41
1:C:86:PHE:CE1	1:C:90:LYS:CE	3.04	0.41
1:D:59:ILE:HG13	1:D:61:VAL:HG23	2.03	0.41
1:E:257:THR:HG21	1:E:288:PHE:CZ	2.55	0.41
1:D:32:TYR:HA	1:D:70:ALA:HB2	2.02	0.41
1:E:244:ARG:HD3	1:E:295:ALA:O	2.21	0.41
1:F:16:TYR:HB2	1:F:93:ILE:HG21	2.03	0.41
1:F:91:TYR:O	1:F:94:ASN:ND2	2.54	0.41
1:F:301:HIS:HB3	1:F:313:GLU:HB3	2.03	0.41
1:G:19:VAL:CG2	1:G:78:LEU:HD22	2.51	0.41
1:H:171:GLY:HA3	1:H:191:VAL:HG13	2.02	0.41
1:D:150:ILE:HD11	1:D:309:PHE:CD2	2.56	0.41
1:H:151:ILE:HG23	1:H:152:LYS:N	2.36	0.40
1:H:152:LYS:O	1:H:156:VAL:HG23	2.20	0.40
1:B:2:LEU:HD22	1:E:75:CYS:HA	2.01	0.40
1:C:152:LYS:O	1:C:156:VAL:HG23	2.21	0.40
1:E:160:PHE:HB2	1:E:184:VAL:HG21	2.04	0.40
1:F:257:THR:HG21	1:F:288:PHE:CZ	2.55	0.40
1:H:308:ILE:O	4:H:402:CL:CL	2.77	0.40
1:A:276:MET:HE2	1:A:277:LEU:HG	2.03	0.40
1:E:126:PHE:CZ	2:E:401:SAH:H5'1	2.56	0.40
1:A:174:GLY:O	1:A:178:ILE:N	2.46	0.40
1:A:303:LYS:HD3	1:B:301:HIS:CD2	2.57	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	316/318 (99%)	307 (97%)	9 (3%)	0	100	100
1	B	316/318 (99%)	308 (98%)	8 (2%)	0	100	100
1	C	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
1	D	316/318 (99%)	306 (97%)	9 (3%)	1 (0%)	36	66
1	E	316/318 (99%)	303 (96%)	13 (4%)	0	100	100
1	F	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
1	G	312/318 (98%)	298 (96%)	13 (4%)	1 (0%)	36	66
1	H	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
All	All	2524/2544 (99%)	2441 (97%)	81 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	175	GLU
1	D	316	VAL

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	286/286 (100%)	280 (98%)	6 (2%)	47	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	286/286 (100%)	279 (98%)	7 (2%)	43	77
1	C	286/286 (100%)	274 (96%)	12 (4%)	26	61
1	D	286/286 (100%)	278 (97%)	8 (3%)	38	73
1	E	286/286 (100%)	283 (99%)	3 (1%)	68	88
1	F	286/286 (100%)	280 (98%)	6 (2%)	47	79
1	G	284/286 (99%)	272 (96%)	12 (4%)	26	61
1	H	286/286 (100%)	279 (98%)	7 (2%)	43	77
All	All	2286/2288 (100%)	2225 (97%)	61 (3%)	39	74

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	LEU
1	A	187	LYS
1	A	211	PHE
1	A	220	ASP
1	A	223	ILE
1	A	304	ASP
1	B	23	LEU
1	B	84	VAL
1	B	151	ILE
1	B	187	LYS
1	B	194	ARG
1	B	198	VAL
1	B	211	PHE
1	C	1	MET
1	C	23	LEU
1	C	33	VAL
1	C	38	LEU
1	C	112	ASN
1	C	119	MET
1	C	177	LEU
1	C	211	PHE
1	C	215	ILE
1	C	217	THR
1	C	220	ASP
1	C	248	ASP
1	D	37	LYS
1	D	49	LEU
1	D	103	MET

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Mol	Chain	Res	Type
1	D	157	ILE
1	D	204	ILE
1	D	205	ASN
1	D	211	PHE
1	D	250	ASN
1	E	69	VAL
1	E	198	VAL
1	E	211	PHE
1	F	177	LEU
1	F	187	LYS
1	F	207	ILE
1	F	211	PHE
1	F	267	VAL
1	F	268	LYS
1	G	44	ILE
1	G	49	LEU
1	G	196	ASN
1	G	199	PRO
1	G	200	ILE
1	G	205	ASN
1	G	207	ILE
1	G	220	ASP
1	G	264	SER
1	G	265	LEU
1	G	267	VAL
1	G	294	GLN
1	H	157	ILE
1	H	198	VAL
1	H	200	ILE
1	H	258	LEU
1	H	265	LEU
1	H	266	VAL
1	H	278	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	282	GLN
1	B	36	ASN
1	B	148	ASN
1	B	282	GLN

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Mol	Chain	Res	Type
1	C	148	ASN
1	D	50	ASN
1	D	250	ASN
1	D	263	GLN
1	D	293	ASN
1	E	164	ASN
1	E	282	GLN
1	F	230	ASN
1	F	250	ASN
1	G	148	ASN
1	G	205	ASN
1	H	282	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
2	SAH	A	401	-	27,28,28	0.51	1 (3%)	36,40,40	0.60	1 (2%)
5	EDO	D	405	-	3,3,3	0.06	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	F	900	-	27,28,28	0.49	1 (3%)	36,40,40	0.58	1 (2%)
2	SAH	H	401	-	27,28,28	0.50	1 (3%)	36,40,40	0.62	1 (2%)
2	SAH	B	900	-	27,28,28	0.50	1 (3%)	36,40,40	0.60	1 (2%)
2	SAH	G	401	-	27,28,28	0.50	1 (3%)	36,40,40	0.61	1 (2%)
2	SAH	E	401	-	27,28,28	0.51	1 (3%)	36,40,40	0.62	1 (2%)
2	SAH	D	401	-	27,28,28	0.51	1 (3%)	36,40,40	0.57	1 (2%)
5	EDO	G	403	-	3,3,3	0.08	0	2,2,2	0.15	0
2	SAH	C	900	-	27,28,28	0.50	1 (3%)	36,40,40	0.62	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	401	-	-	5/15/31/31	0/3/3/3
5	EDO	D	405	-	-	0/1/1/1	-
2	SAH	F	900	-	-	5/15/31/31	0/3/3/3
2	SAH	H	401	-	-	4/15/31/31	0/3/3/3
2	SAH	B	900	-	-	2/15/31/31	0/3/3/3
2	SAH	G	401	-	-	5/15/31/31	0/3/3/3
2	SAH	E	401	-	-	5/15/31/31	0/3/3/3
2	SAH	D	401	-	-	4/15/31/31	0/3/3/3
5	EDO	G	403	-	-	1/1/1/1	-
2	SAH	C	900	-	-	4/15/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	SAH	OXT-C	-2.30	1.23	1.30
2	E	401	SAH	OXT-C	-2.27	1.23	1.30
2	A	401	SAH	OXT-C	-2.25	1.23	1.30
2	H	401	SAH	OXT-C	-2.24	1.23	1.30
2	F	900	SAH	OXT-C	-2.22	1.23	1.30
2	B	900	SAH	OXT-C	-2.22	1.23	1.30
2	G	401	SAH	OXT-C	-2.22	1.23	1.30
2	C	900	SAH	OXT-C	-2.21	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	SAH	OXT-C-O	-2.79	117.76	124.08
2	G	401	SAH	OXT-C-O	-2.74	117.86	124.08
2	F	900	SAH	OXT-C-O	-2.71	117.93	124.08
2	E	401	SAH	OXT-C-O	-2.59	118.21	124.08
2	D	401	SAH	OXT-C-O	-2.57	118.24	124.08
2	A	401	SAH	OXT-C-O	-2.50	118.40	124.08
2	B	900	SAH	OXT-C-O	-2.46	118.51	124.08
2	C	900	SAH	OXT-C-O	-2.35	118.74	124.08

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SAH	N-CA-CB-CG
2	C	900	SAH	C4'-C5'-SD-CG
2	D	401	SAH	O-C-CA-N
2	E	401	SAH	N-CA-CB-CG
2	F	900	SAH	O-C-CA-N
2	G	401	SAH	O-C-CA-N
2	H	401	SAH	O-C-CA-N
2	C	900	SAH	OXT-C-CA-N
2	D	401	SAH	OXT-C-CA-N
2	F	900	SAH	OXT-C-CA-N
2	H	401	SAH	OXT-C-CA-N
2	G	401	SAH	OXT-C-CA-N
2	A	401	SAH	C-CA-CB-CG
2	A	401	SAH	OXT-C-CA-N
2	B	900	SAH	C4'-C5'-SD-CG
2	B	900	SAH	OXT-C-CA-N
2	G	401	SAH	OXT-C-CA-CB
2	H	401	SAH	OXT-C-CA-CB
2	A	401	SAH	O4'-C4'-C5'-SD
2	F	900	SAH	O-C-CA-CB
2	F	900	SAH	OXT-C-CA-CB
2	H	401	SAH	O-C-CA-CB
2	A	401	SAH	C4'-C5'-SD-CG
2	D	401	SAH	C4'-C5'-SD-CG
2	G	401	SAH	C4'-C5'-SD-CG
2	G	401	SAH	O-C-CA-CB
2	E	401	SAH	C-CA-CB-CG
5	G	403	EDO	O1-C1-C2-O2
2	E	401	SAH	C4'-C5'-SD-CG
2	F	900	SAH	C4'-C5'-SD-CG

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Mol	Chain	Res	Type	Atoms
2	D	401	SAH	C2'-C1'-N9-C8
2	C	900	SAH	C2'-C1'-N9-C8
2	C	900	SAH	O-C-CA-N
2	E	401	SAH	O-C-CA-N
2	E	401	SAH	OXT-C-CA-N

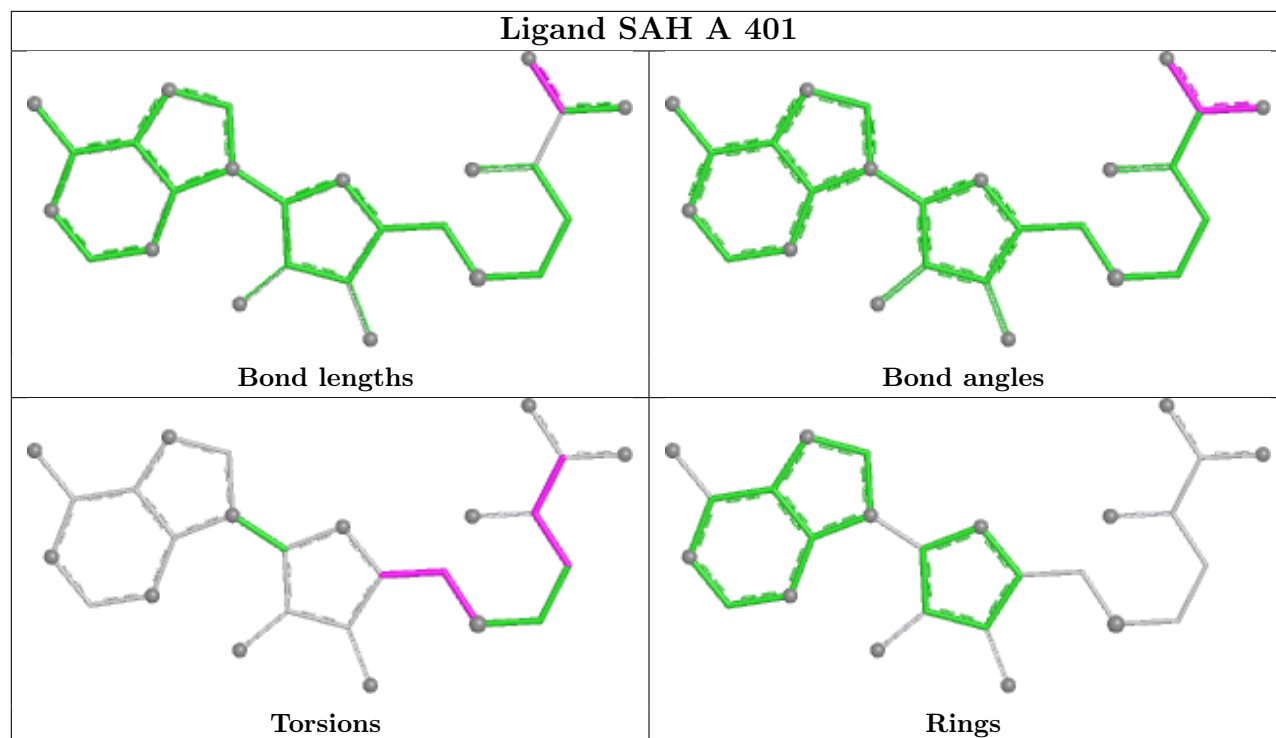
There are no ring outliers.

6 monomers are involved in 9 short contacts:

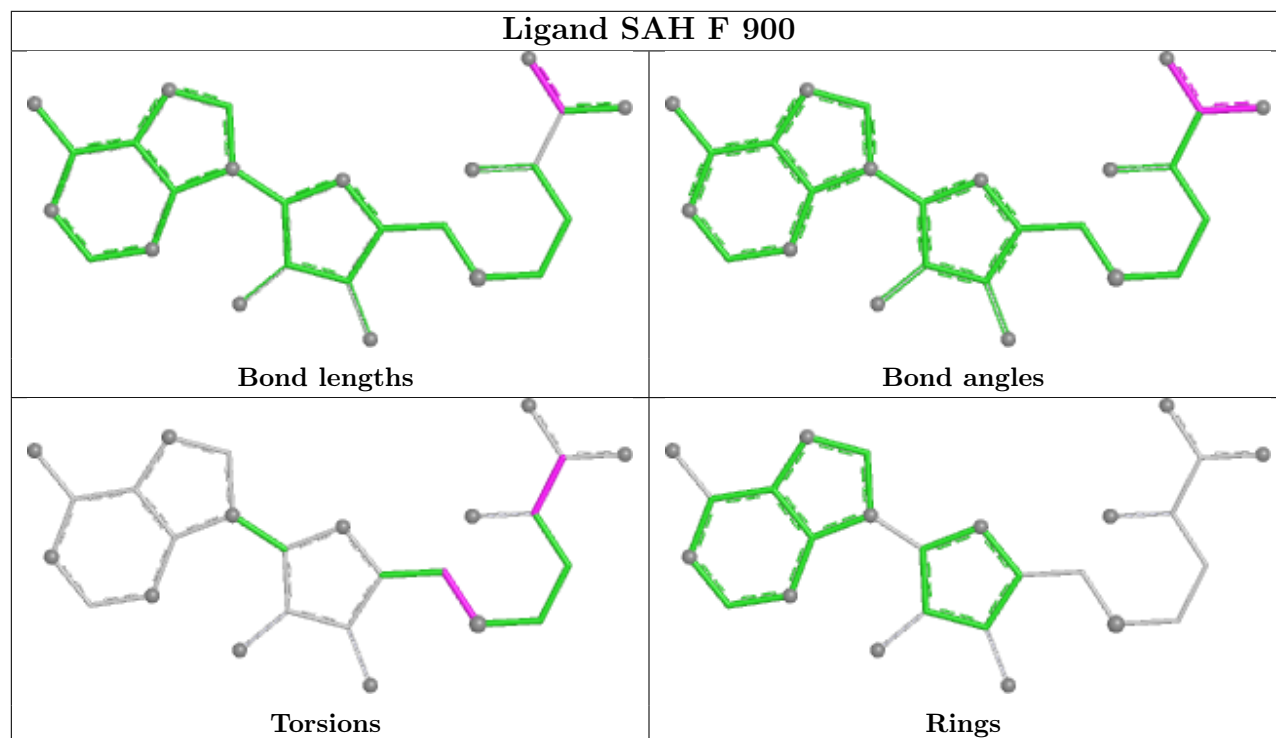
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	SAH	3	0
2	B	900	SAH	1	0
2	E	401	SAH	2	0
2	D	401	SAH	1	0
5	G	403	EDO	1	0
2	C	900	SAH	1	0

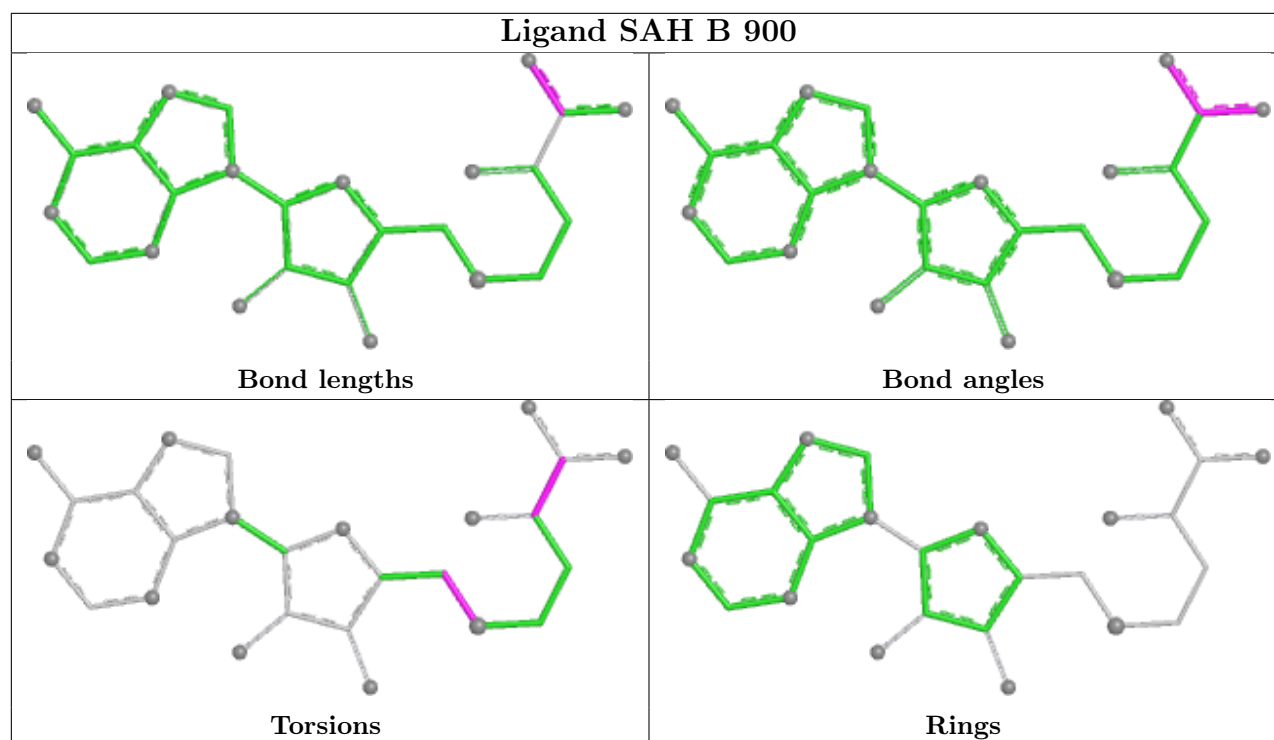
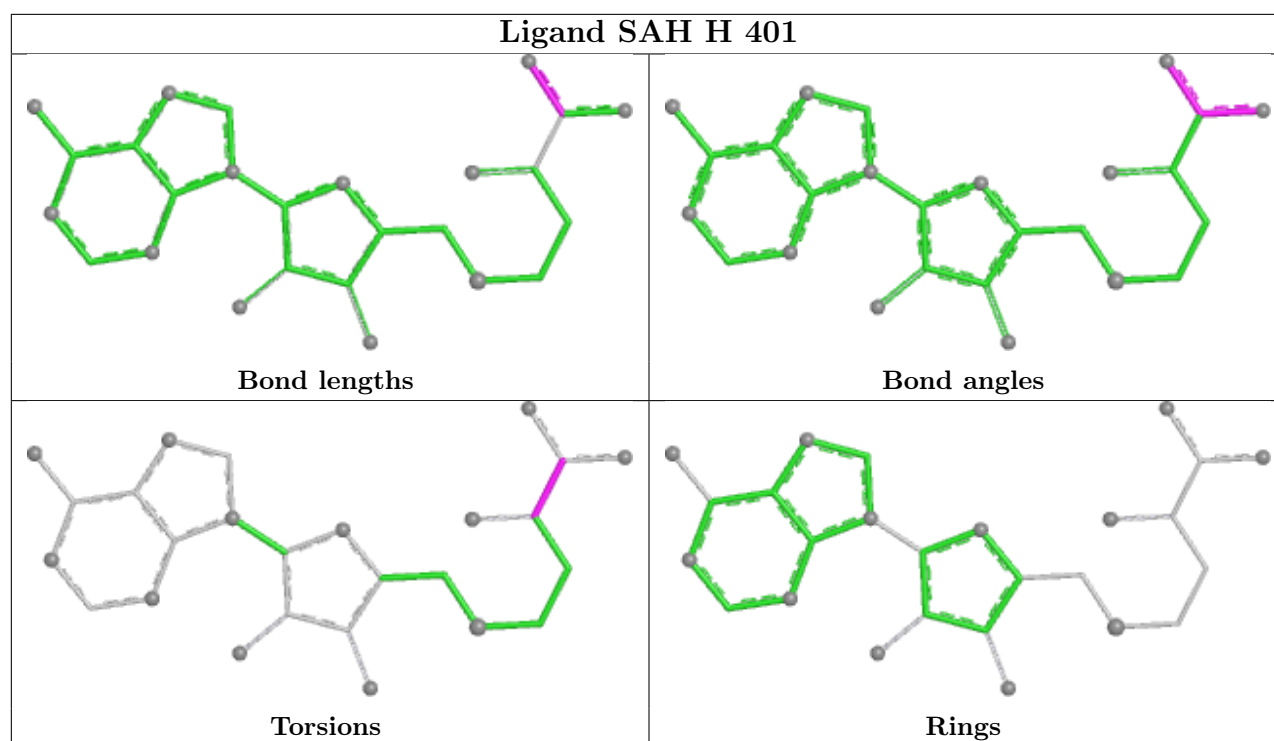
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

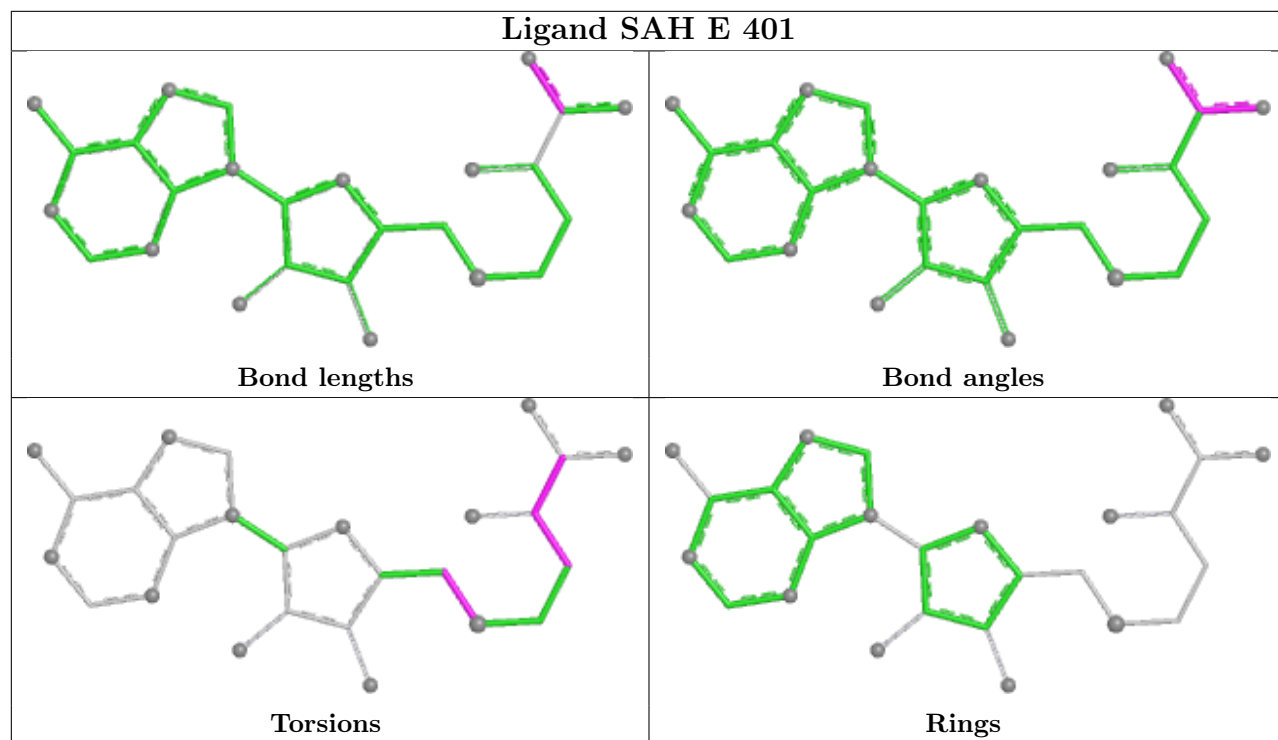
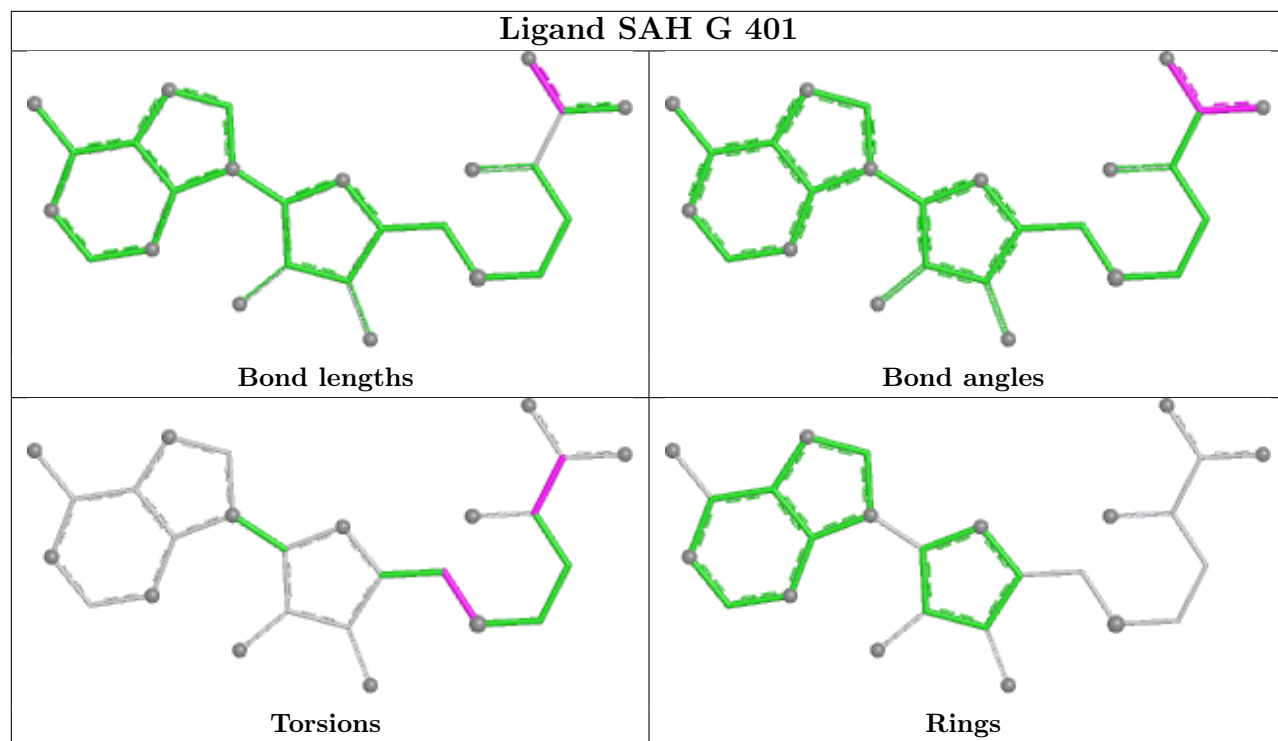
Ligand SAH A 401

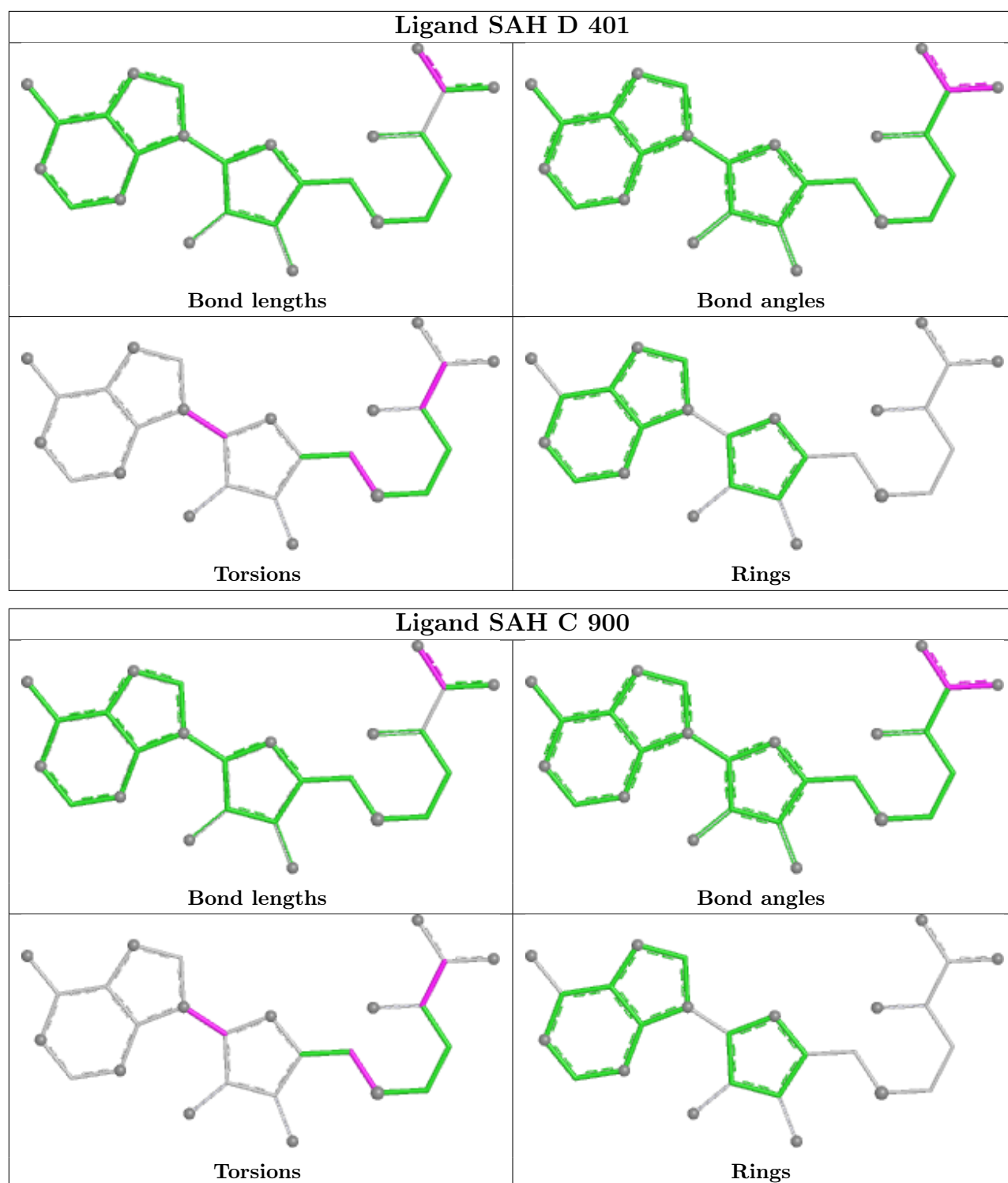


Ligand SAH F 900









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/318 (100%)	-0.07	0 100 100	47, 66, 104, 119	0
1	B	318/318 (100%)	-0.07	2 (0%) 85 80	52, 67, 100, 115	0
1	C	318/318 (100%)	0.05	1 (0%) 90 86	57, 78, 116, 137	0
1	D	318/318 (100%)	0.08	2 (0%) 85 80	53, 78, 148, 168	0
1	E	318/318 (100%)	0.06	0 100 100	56, 84, 116, 137	0
1	F	318/318 (100%)	0.22	5 (1%) 70 61	83, 111, 147, 159	0
1	G	316/318 (99%)	0.38	4 (1%) 75 66	53, 114, 158, 196	0
1	H	318/318 (100%)	0.23	2 (0%) 85 80	53, 99, 124, 135	0
All	All	2542/2544 (99%)	0.11	16 (0%) 85 80	47, 86, 135, 196	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	206	PHE	3.8
1	F	27	PHE	3.5
1	G	199	PRO	3.2
1	F	70	ALA	3.2
1	G	236	ALA	2.9
1	F	69	VAL	2.7
1	C	116	ALA	2.6
1	H	58	GLU	2.5
1	H	210	ASP	2.4
1	G	254	LEU	2.2
1	B	109	LEU	2.2
1	F	67	HIS	2.1
1	F	63	VAL	2.1
1	D	264	SER	2.1
1	B	173	ASP	2.0
1	G	135	LEU	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

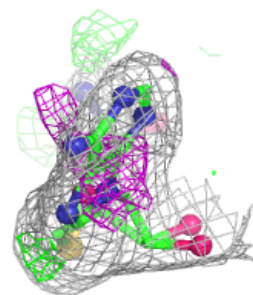
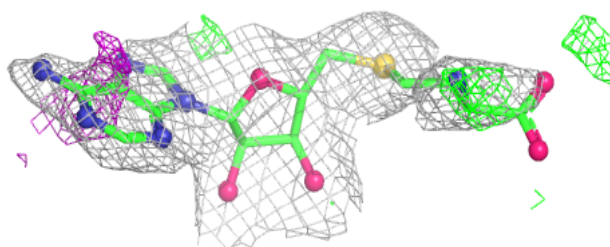
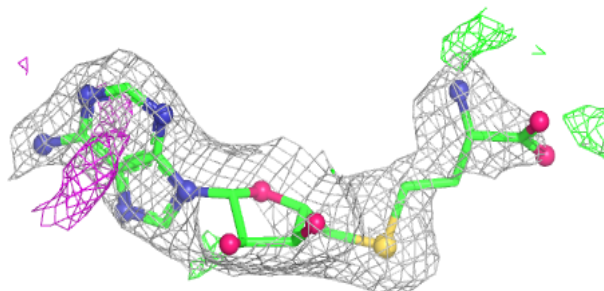
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	G	403	4/4	0.61	0.30	90,90,90,91	0
5	EDO	D	405	4/4	0.62	0.23	68,68,68,68	0
3	NI	A	402	1/1	0.64	0.28	89,89,89,89	0
2	SAH	H	401	26/26	0.74	0.12	104,105,108,110	0
2	SAH	G	401	26/26	0.75	0.12	110,117,123,125	0
2	SAH	F	900	26/26	0.81	0.11	108,108,110,111	0
3	NI	D	403	1/1	0.81	0.17	108,108,108,108	0
3	NI	D	402	1/1	0.86	0.25	96,96,96,96	0
4	CL	H	402	1/1	0.86	0.10	103,103,103,103	0
2	SAH	C	900	26/26	0.89	0.10	68,69,72,73	0
2	SAH	E	401	26/26	0.90	0.09	74,76,81,82	0
3	NI	E	402	1/1	0.91	0.18	93,93,93,93	0
2	SAH	D	401	26/26	0.92	0.09	68,69,71,73	0
2	SAH	A	401	26/26	0.92	0.08	56,56,60,62	0
2	SAH	B	900	26/26	0.93	0.07	58,58,62,63	0
6	MG	G	402	1/1	0.94	0.13	81,81,81,81	0
4	CL	D	404	1/1	0.95	0.07	63,63,63,63	0
4	CL	A	403	1/1	0.96	0.06	65,65,65,65	0

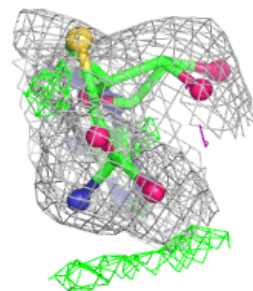
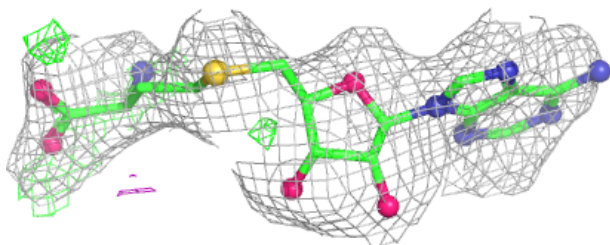
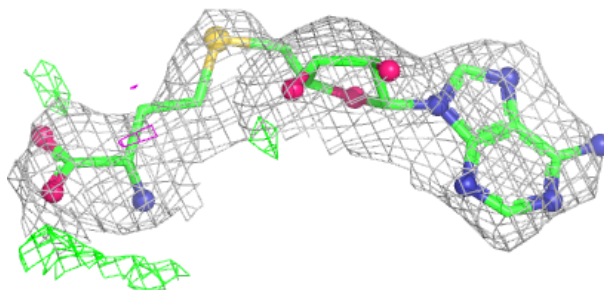
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH H 401:

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

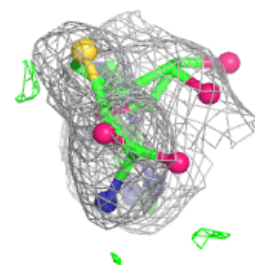
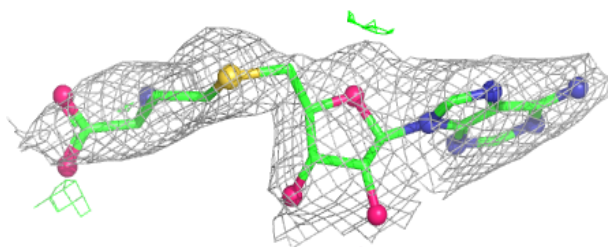
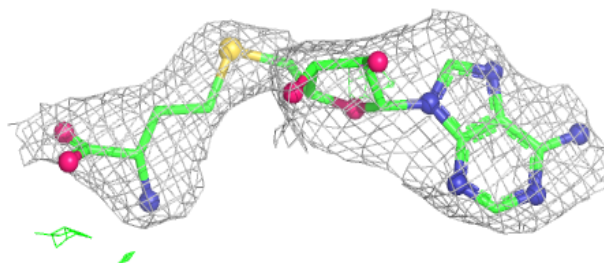
**Electron density around SAH G 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

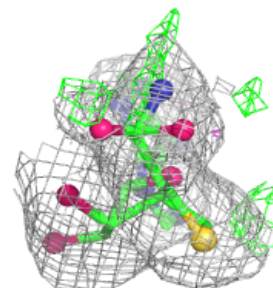
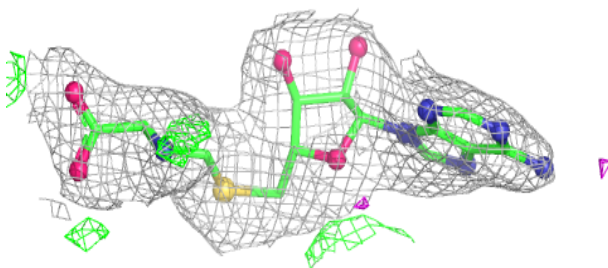
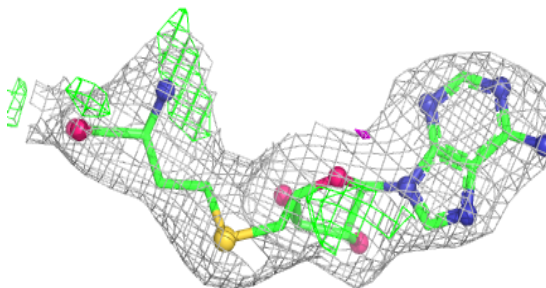


Electron density around SAH F 900:

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

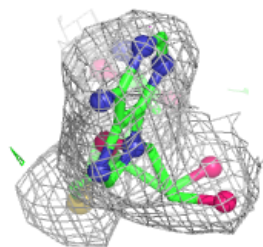
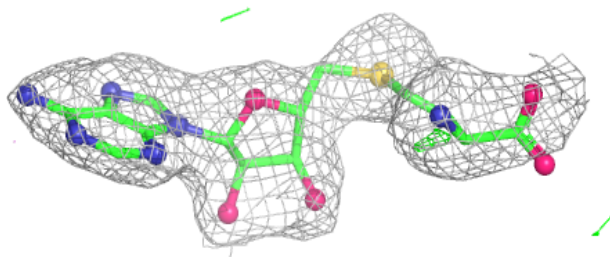
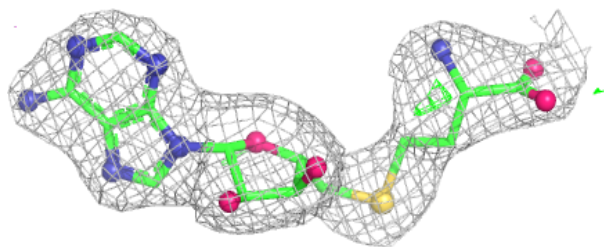
**Electron density around SAH C 900:**

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

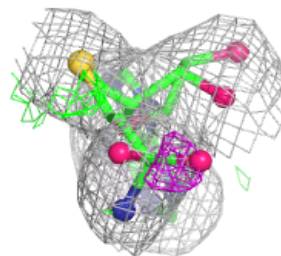
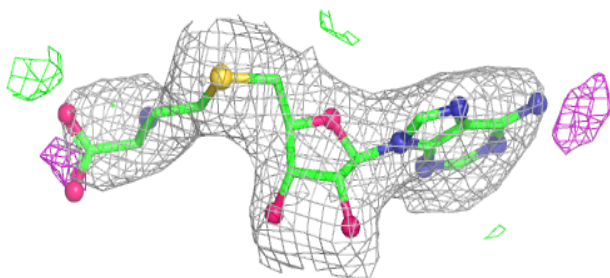
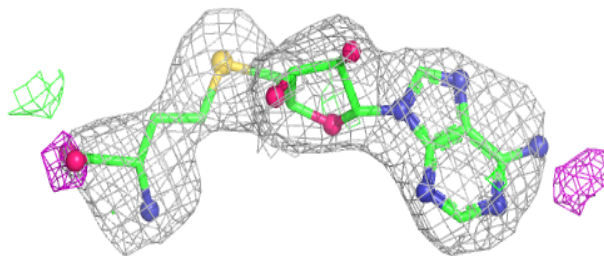


Electron density around SAH E 401:

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and green (positive)

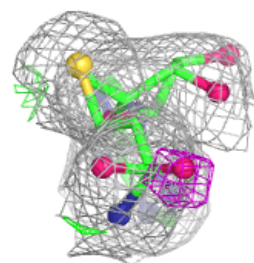
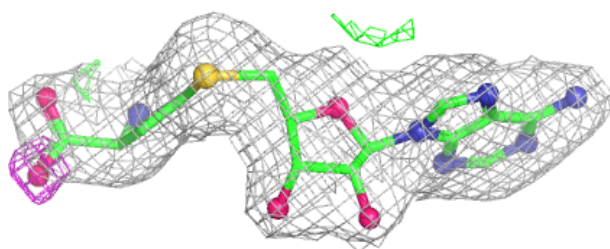
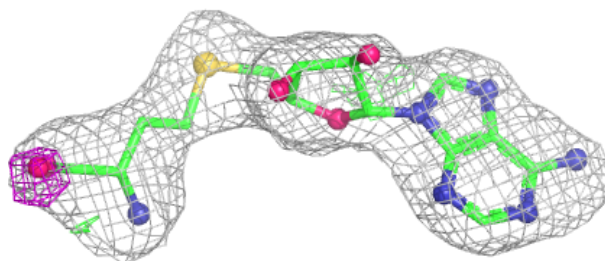
**Electron density around SAH D 401:**

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and green (positive)

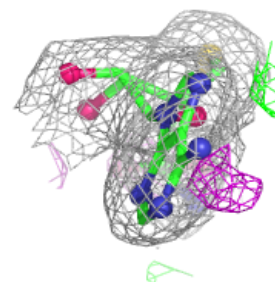
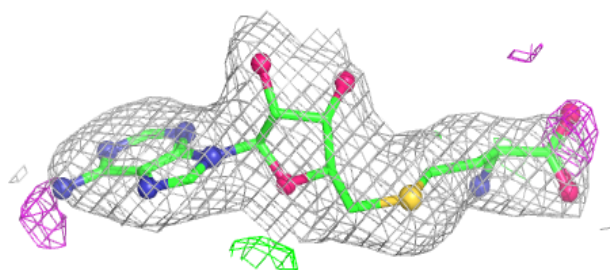
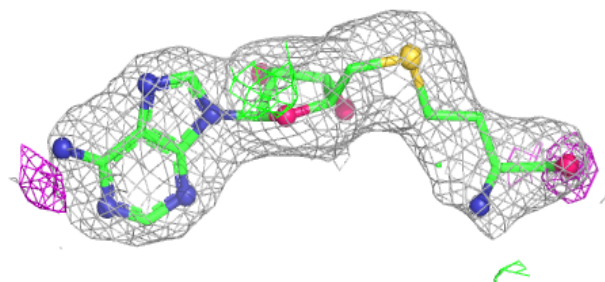


Electron density around SAH A 401:

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

**Electron density around SAH B 900:**

$2mF_o-DF_c$ (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.