



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 7, 2026 – 10:31 PM JST

PDB ID : 9VSK / pdb_00009vsk
Title : Crystal structure of anthocyanin 4'-O-methyltransferase from Vitis vinifera L.
Authors : Lin, W.
Deposited on : 2025-07-09
Resolution : 2.78 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

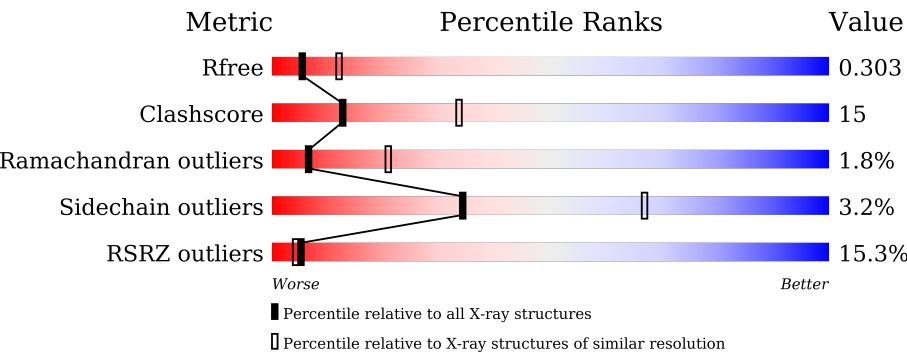
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	235	
1	B	235	
1	C	235	
1	D	235	
1	E	235	
1	F	235	

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Mol	Chain	Length	Quality of chain
1	G	235	19% 63% 31%
1	H	235	20% 64% 29%

2 Entry composition

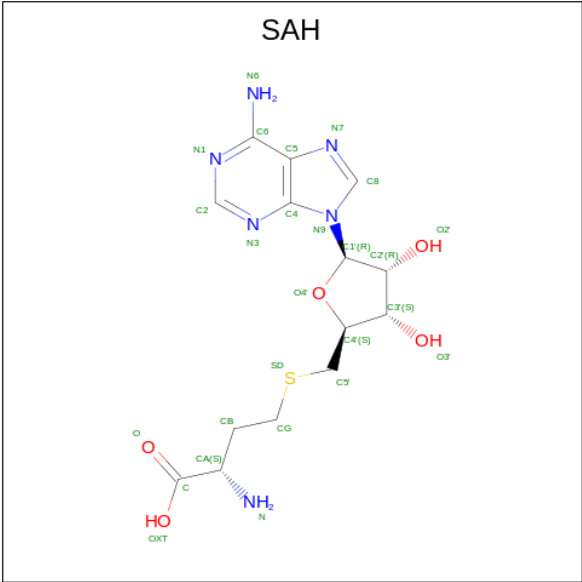
There are 3 unique types of molecules in this entry. The entry contains 14576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Flavonoid 3',5'-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1767	1130	296	332	9			
1	B	230	Total	C	N	O	S	0	0	0
			1820	1165	306	341	8			
1	C	226	Total	C	N	O	S	0	0	0
			1756	1120	295	332	9			
1	D	231	Total	C	N	O	S	0	0	0
			1811	1155	304	343	9			
1	E	226	Total	C	N	O	S	0	0	0
			1769	1131	296	334	8			
1	F	226	Total	C	N	O	S	0	0	0
			1777	1137	295	336	9			
1	G	228	Total	C	N	O	S	0	0	0
			1793	1148	298	339	8			
1	H	226	Total	C	N	O	S	0	0	0
			1771	1134	296	332	9			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	16	Total	O	0	0
			16	16		
3	C	18	Total	O	0	0
			18	18		
3	D	17	Total	O	0	0
			17	17		

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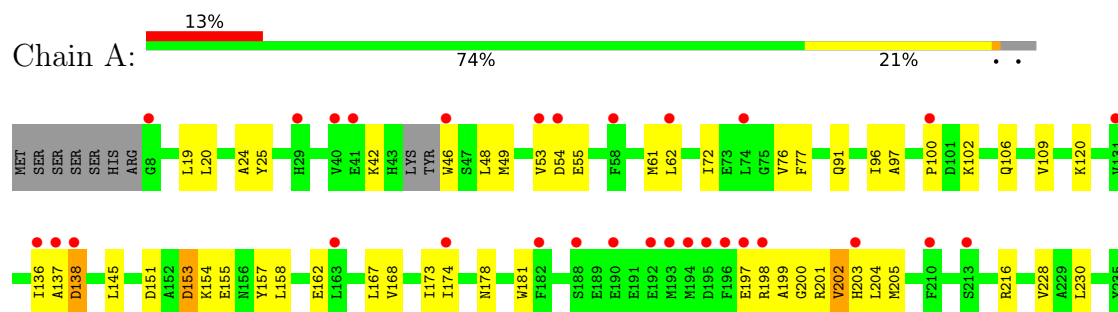
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	7	Total 7	O 7	0	0
3	F	15	Total 15	O 15	0	0
3	G	14	Total 14	O 14	0	0
3	H	5	Total 5	O 5	0	0

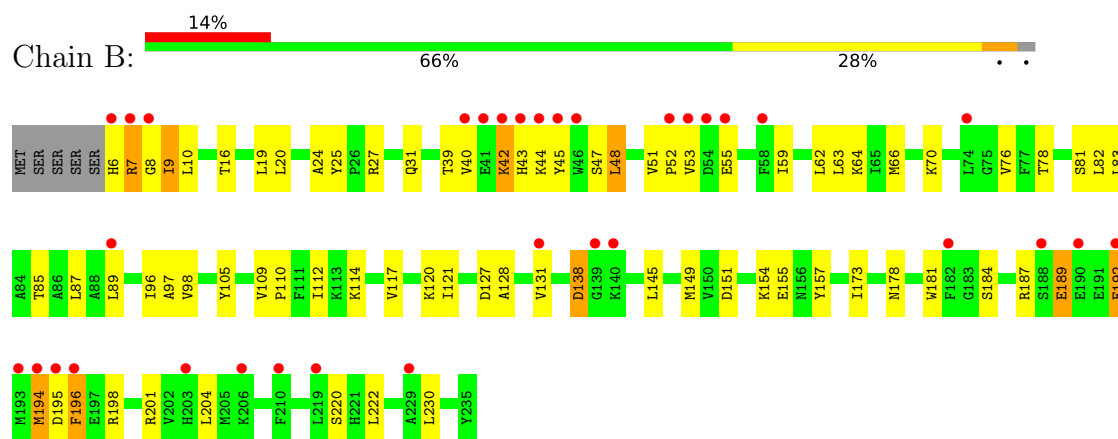
3 Residue-property plots [i](#)

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.

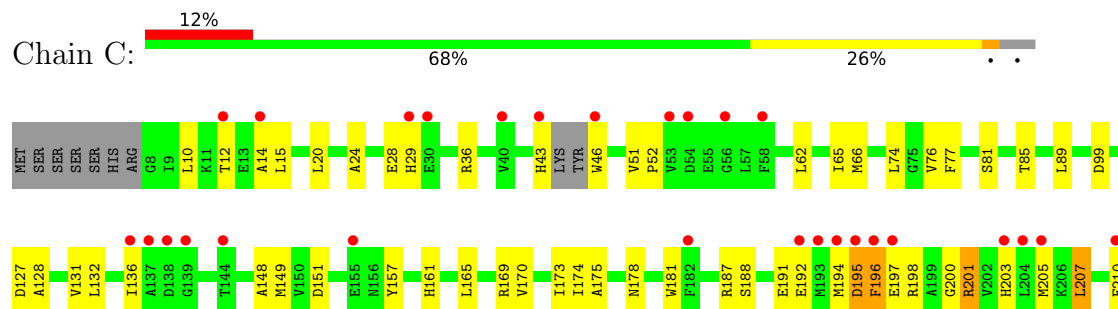
• Molecule 1: Flavonoid 3',5'-methyltransferase

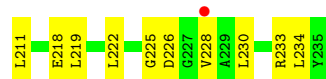


• Molecule 1: Flavonoid 3',5'-methyltransferase

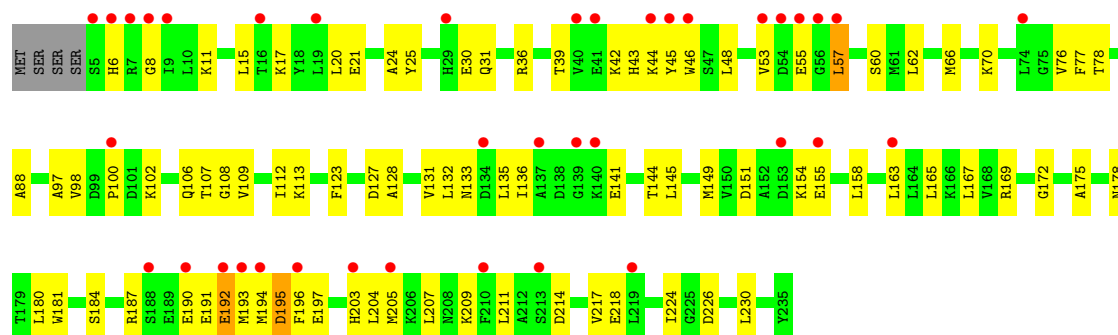


• Molecule 1: Flavonoid 3',5'-methyltransferase

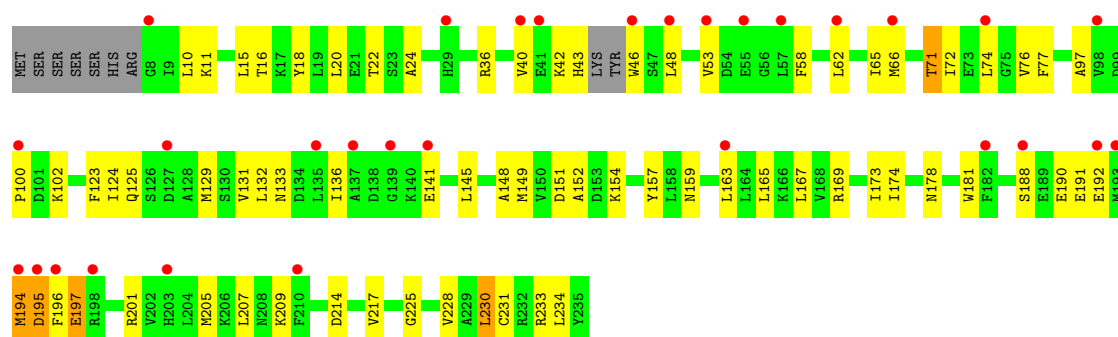




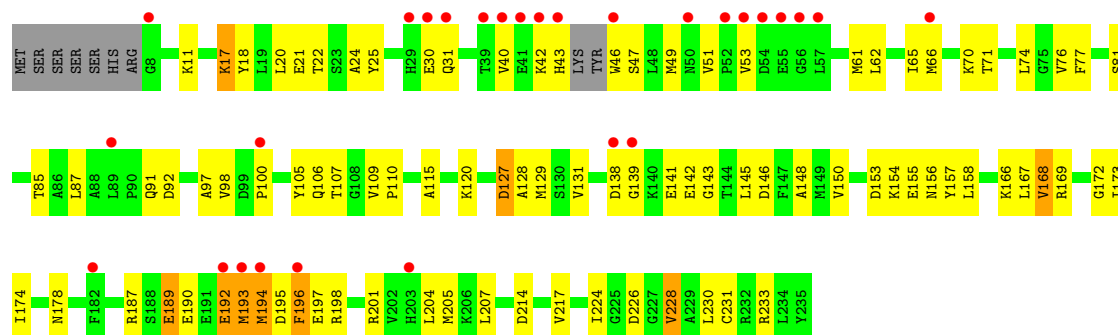
• Molecule 1: Flavonoid 3',5'-methyltransferase



• Molecule 1: Flavonoid 3',5'-methyltransferase

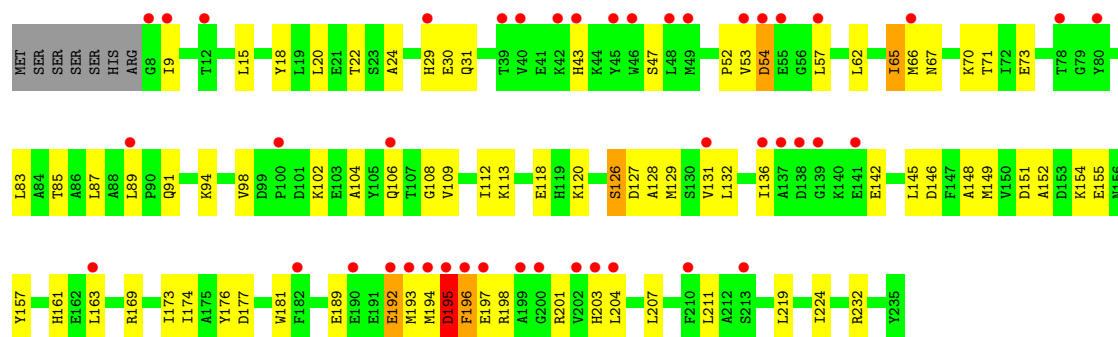


• Molecule 1: Flavonoid 3',5'-methyltransferase

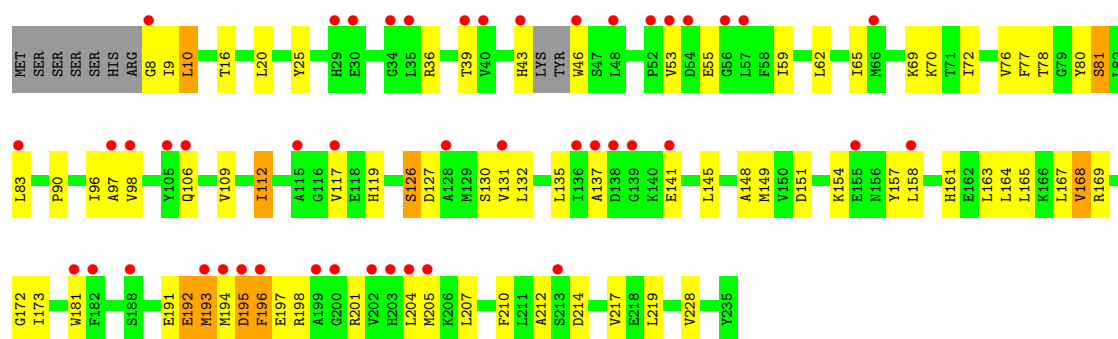


• Molecule 1: Flavonoid 3',5'-methyltransferase





● Molecule 1: Flavonoid 3',5'-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.59Å 199.16Å 95.33Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	46.68 – 2.78 46.68 – 2.78	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.68-2.78) 96.4 (46.68-2.78)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.247 , 0.306 0.246 , 0.303	Depositor DCC
R_{free} test set	2980 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.5	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	0.88	EDS
Total number of atoms	14576	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.16	0/1796	0.36	0/2421
1	B	0.22	0/1853	0.42	0/2498
1	C	0.20	0/1782	0.42	0/2400
1	D	0.23	0/1842	0.47	0/2484
1	E	0.22	0/1798	0.43	0/2424
1	F	0.24	0/1807	0.47	0/2436
1	G	0.24	0/1824	0.47	0/2460
1	H	0.21	0/1800	0.42	0/2425
All	All	0.22	0/14502	0.43	0/19548

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 [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	1767	0	1789	35	0
1	B	1820	0	1840	56	0
1	C	1756	0	1775	43	0
1	D	1811	0	1827	70	0
1	E	1769	0	1788	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1777	0	1793	66	0
1	G	1793	0	1803	57	0
1	H	1771	0	1790	66	0
2	A	26	0	19	3	0
2	B	26	0	19	2	0
2	C	26	0	19	3	0
2	D	26	0	19	4	0
2	E	26	0	19	4	0
2	F	26	0	19	3	0
2	G	26	0	19	1	0
2	H	26	0	19	4	0
3	A	12	0	0	1	0
3	B	16	0	0	0	0
3	C	18	0	0	0	0
3	D	17	0	0	2	0
3	E	7	0	0	1	0
3	F	15	0	0	0	0
3	G	14	0	0	2	0
3	H	5	0	0	1	0
All	All	14576	0	14557	440	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 15.

All (440) 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:H:191:GLU:HG3	1:H:192:GLU:H	1.40	0.86
1:H:8:GLY:N	1:H:16:THR:HG1	1.73	0.86
1:H:195:ASP:C	1:H:197:GLU:H	1.80	0.86
1:H:36:ARG:HH11	1:H:53:VAL:HG11	1.40	0.86
1:B:181:TRP:HB2	1:B:204:LEU:HD22	1.61	0.82
1:A:154:LYS:HB3	1:A:204:LEU:HD21	1.65	0.79
1:B:194:MET:HA	1:B:198:ARG:HH21	1.50	0.76
1:H:195:ASP:HA	1:H:198:ARG:HB3	1.66	0.76
1:A:181:TRP:HB2	1:A:204:LEU:HD12	1.68	0.75
1:H:195:ASP:C	1:H:197:GLU:N	2.42	0.75
1:E:148:ALA:HB3	1:E:174:ILE:HD12	1.68	0.75
1:A:102:LYS:NZ	3:A:401:HOH:O	2.20	0.74
1:C:10:LEU:HB3	1:C:15:LEU:HD23	1.70	0.73
1:B:9:ILE:HA	1:D:11:LYS:HD3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:MET:HE2	1:D:169:ARG:HH21	1.53	0.73
1:E:132:LEU:HB3	1:E:163:LEU:HD22	1.70	0.72
1:F:71:THR:HG21	1:F:85:THR:HG21	1.72	0.72
1:F:190:GLU:N	1:F:190:GLU:OE2	2.22	0.70
1:H:62:LEU:HD21	1:H:173:ILE:HD13	1.74	0.70
1:G:195:ASP:C	1:G:197:GLU:H	2.00	0.69
1:D:100:PRO:HD3	2:D:301:SAH:N3	2.08	0.69
1:E:11:LYS:HG2	1:H:9:ILE:CG2	2.22	0.69
1:F:148:ALA:HB3	1:F:174:ILE:HG12	1.74	0.68
1:F:31:GLN:HG3	1:F:115:ALA:HB2	1.75	0.67
1:C:12:THR:HG22	1:C:14:ALA:H	1.59	0.67
1:D:181:TRP:HB2	1:D:204:LEU:HD12	1.76	0.67
1:F:30:GLU:OE2	1:F:31:GLN:NE2	2.28	0.67
1:F:192:GLU:O	1:F:194:MET:N	2.28	0.66
1:B:155:GLU:OE1	1:B:155:GLU:N	2.27	0.66
1:E:165:LEU:O	1:E:233:ARG:NH1	2.28	0.66
1:G:155:GLU:OE2	1:G:155:GLU:N	2.28	0.66
1:H:195:ASP:O	1:H:197:GLU:N	2.27	0.66
1:D:155:GLU:OE2	1:D:155:GLU:N	2.28	0.65
1:F:139:GLY:HA2	1:F:142:GLU:HG3	1.78	0.65
1:D:70:LYS:HG2	1:D:145:LEU:HD13	1.79	0.65
1:G:20:LEU:HA	1:G:24:ALA:HB3	1.79	0.65
1:H:194:MET:HA	1:H:198:ARG:NH1	2.10	0.65
1:D:43:HIS:O	1:D:45:TYR:N	2.30	0.65
1:B:222:LEU:HD22	1:D:224:ILE:HD11	1.79	0.64
1:C:194:MET:O	1:C:196:PHE:N	2.30	0.64
1:E:195:ASP:C	1:E:197:GLU:H	2.05	0.64
1:E:124:ILE:HG21	1:E:131:VAL:HG11	1.79	0.64
1:E:195:ASP:C	1:E:197:GLU:N	2.55	0.64
1:A:181:TRP:HE1	1:A:197:GLU:HA	1.63	0.64
1:F:201:ARG:HG2	1:F:205:MET:HE1	1.80	0.63
1:A:136:ILE:O	1:A:138:ASP:N	2.31	0.63
1:H:76:VAL:HG21	1:H:97:ALA:HB1	1.81	0.63
1:E:43:HIS:O	1:E:46:TRP:N	2.31	0.63
1:H:169:ARG:NH1	3:H:402:HOH:O	2.31	0.63
1:C:194:MET:HG3	1:C:198:ARG:HD2	1.81	0.63
1:D:24:ALA:HA	1:D:57:LEU:HD13	1.80	0.62
1:F:51:VAL:HG21	1:F:81:SER:HB3	1.81	0.62
1:E:196:PHE:O	1:E:197:GLU:HG2	1.98	0.62
1:B:195:ASP:O	1:B:196:PHE:HB3	1.97	0.62
1:F:100:PRO:HD2	2:F:301:SAH:N3	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ASP:OD1	1:G:54:ASP:N	2.32	0.62
1:F:187:ARG:O	1:F:201:ARG:NH2	2.32	0.61
1:E:149:MET:HE3	1:E:151:ASP:HB2	1.82	0.61
1:B:96:ILE:HD12	1:B:145:LEU:HD21	1.81	0.61
1:D:195:ASP:C	1:D:197:GLU:H	2.07	0.61
1:A:76:VAL:HG21	1:A:97:ALA:HB1	1.81	0.61
1:H:145:LEU:HD12	1:H:167:LEU:HB3	1.82	0.61
1:B:194:MET:O	1:B:198:ARG:HB2	2.00	0.61
1:G:169:ARG:HH11	1:G:169:ARG:HG3	1.65	0.61
1:H:194:MET:HA	1:H:198:ARG:CZ	2.30	0.61
1:B:25:TYR:HE1	1:B:53:VAL:HG21	1.65	0.60
1:F:25:TYR:HE1	1:F:53:VAL:HG21	1.66	0.60
1:E:11:LYS:HG2	1:H:9:ILE:HG23	1.83	0.60
1:B:9:ILE:HG23	1:D:15:LEU:HD21	1.83	0.60
1:E:194:MET:C	1:E:196:PHE:N	2.58	0.60
1:F:192:GLU:O	1:F:193:MET:C	2.45	0.60
1:D:62:LEU:HD22	1:D:230:LEU:HD22	1.82	0.60
1:C:211:LEU:HB3	1:C:219:LEU:HD11	1.83	0.59
1:C:157:TYR:HB3	1:C:207:LEU:HD13	1.84	0.59
1:E:194:MET:O	1:E:197:GLU:N	2.32	0.59
1:G:91:GLN:HA	1:G:120:LYS:HE2	1.84	0.59
1:A:62:LEU:HD21	1:A:173:ILE:HD13	1.83	0.59
1:A:201:ARG:O	1:A:205:MET:HG3	2.02	0.59
1:B:52:PRO:HD2	1:B:55:GLU:OE2	2.03	0.59
1:H:77:PHE:HB2	2:H:301:SAH:HG2	1.84	0.59
1:A:200:GLY:O	1:A:204:LEU:HG	2.02	0.59
1:H:69:LYS:NZ	1:H:90:PRO:HG3	2.18	0.59
1:A:155:GLU:N	1:A:155:GLU:OE1	2.36	0.59
1:A:158:LEU:H	1:A:158:LEU:HD12	1.68	0.59
1:B:64:LYS:NZ	1:D:218:GLU:OE2	2.33	0.59
1:F:187:ARG:HB2	1:F:192:GLU:OE2	2.03	0.59
1:C:66:MET:HE2	1:C:169:ARG:HH21	1.68	0.59
1:F:62:LEU:HD13	1:F:230:LEU:HD22	1.84	0.59
1:G:126:SER:OG	1:G:127:ASP:N	2.36	0.58
1:G:148:ALA:HB3	1:G:174:ILE:HG12	1.85	0.58
1:E:10:LEU:HD13	1:E:15:LEU:HD23	1.85	0.58
1:B:39:THR:HG23	1:B:78:THR:HG21	1.84	0.58
1:B:20:LEU:HA	1:B:24:ALA:HB3	1.85	0.58
1:B:220:SER:HA	1:D:57:LEU:HD21	1.85	0.58
1:C:194:MET:HA	1:C:198:ARG:HG3	1.86	0.58
1:F:145:LEU:HD23	1:F:167:LEU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ILE:HD11	1:G:65:ILE:HD11	1.86	0.57
1:C:181:TRP:HE1	1:C:197:GLU:HA	1.68	0.57
1:F:77:PHE:HB2	2:F:301:SAH:HG2	1.85	0.57
1:B:55:GLU:O	1:B:59:ILE:HG13	2.05	0.56
1:G:154:LYS:HB3	1:G:204:LEU:HD21	1.87	0.56
1:D:192:GLU:O	1:D:194:MET:N	2.37	0.56
1:B:189:GLU:O	1:B:198:ARG:NH1	2.39	0.56
1:H:83:LEU:HD13	1:H:112:ILE:HG13	1.86	0.56
1:H:168:VAL:HG22	1:H:172:GLY:HA3	1.87	0.56
1:F:127:ASP:O	1:F:131:VAL:HG23	2.06	0.56
1:D:141:GLU:OE1	1:D:144:THR:OG1	2.20	0.56
1:H:191:GLU:HG3	1:H:192:GLU:N	2.18	0.56
1:B:76:VAL:HG21	1:B:97:ALA:HB1	1.86	0.55
1:B:62:LEU:HD13	1:B:230:LEU:HD22	1.88	0.55
1:C:178:ASN:ND2	1:C:226:ASP:OD2	2.39	0.55
1:G:211:LEU:HB3	1:G:219:LEU:HD13	1.88	0.55
1:E:194:MET:O	1:E:196:PHE:N	2.40	0.55
1:G:161:HIS:ND1	1:G:176:TYR:OH	2.35	0.55
1:F:189:GLU:HG2	1:F:198:ARG:HH11	1.72	0.55
1:E:58:PHE:CE2	1:E:230:LEU:HD11	2.42	0.55
1:G:118:GLU:N	3:G:401:HOH:O	2.39	0.55
1:H:36:ARG:NH1	1:H:53:VAL:HG11	2.18	0.55
1:H:195:ASP:HA	1:H:198:ARG:CB	2.36	0.55
1:B:194:MET:SD	1:B:194:MET:N	2.70	0.55
1:C:201:ARG:O	1:C:205:MET:HG3	2.07	0.55
1:D:20:LEU:HA	1:D:24:ALA:HB3	1.88	0.54
1:C:43:HIS:O	1:C:46:TRP:N	2.39	0.54
1:G:155:GLU:HG3	1:G:203:HIS:ND1	2.23	0.54
1:A:155:GLU:CD	1:A:155:GLU:H	2.15	0.54
1:D:43:HIS:O	1:D:46:TRP:N	2.39	0.54
1:A:199:ALA:O	1:A:202:VAL:HG23	2.07	0.54
1:B:42:LYS:C	1:B:44:LYS:H	2.15	0.54
1:D:76:VAL:HG21	1:D:97:ALA:HB1	1.90	0.54
1:G:195:ASP:C	1:G:197:GLU:N	2.61	0.54
1:C:194:MET:O	1:C:195:ASP:C	2.50	0.53
1:C:194:MET:C	1:C:196:PHE:N	2.64	0.53
1:E:194:MET:CG	1:E:195:ASP:H	2.21	0.53
1:H:201:ARG:O	1:H:205:MET:HG3	2.08	0.53
1:E:159:ASN:O	1:E:163:LEU:HD12	2.07	0.53
1:F:178:ASN:HA	1:F:226:ASP:HB3	1.89	0.53
1:A:96:ILE:HD12	1:A:145:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD21	1:D:180:LEU:HD21	1.89	0.53
1:D:154:LYS:N	1:D:154:LYS:HD2	2.23	0.53
1:F:192:GLU:HG3	1:F:201:ARG:HD2	1.90	0.53
1:F:196:PHE:CE1	1:F:197:GLU:HG2	2.44	0.53
1:B:187:ARG:NH2	1:B:192:GLU:H	2.06	0.53
1:F:195:ASP:O	1:F:196:PHE:CD2	2.62	0.53
1:F:20:LEU:HA	1:F:24:ALA:HB3	1.90	0.53
1:D:154:LYS:HD2	1:D:154:LYS:H	1.73	0.53
1:D:66:MET:HE2	1:D:169:ARG:NH2	2.22	0.53
1:D:106:GLN:HA	1:D:109:VAL:HG23	1.91	0.52
1:E:145:LEU:HD23	1:E:167:LEU:HB3	1.91	0.52
1:E:192:GLU:OE1	1:E:201:ARG:HD2	2.09	0.52
1:C:149:MET:HE3	1:C:151:ASP:HB2	1.90	0.52
1:D:30:GLU:CD	1:D:30:GLU:H	2.17	0.52
1:E:194:MET:HG2	1:E:195:ASP:H	1.75	0.52
1:G:181:TRP:HB2	1:G:204:LEU:HD12	1.92	0.52
1:D:98:VAL:HG11	1:D:128:ALA:HA	1.92	0.52
1:D:190:GLU:OE1	1:D:190:GLU:N	2.42	0.52
1:G:193:MET:HG3	1:G:196:PHE:HE2	1.74	0.52
1:H:135:LEU:HD22	1:H:141:GLU:HG3	1.92	0.52
1:F:62:LEU:HD21	1:F:173:ILE:HD13	1.91	0.52
1:D:149:MET:HE3	1:D:151:ASP:HB2	1.92	0.51
1:E:10:LEU:HB3	1:E:15:LEU:HD23	1.92	0.51
1:F:40:VAL:HA	1:F:47:SER:HB3	1.92	0.51
1:F:168:VAL:HG13	1:F:172:GLY:HA3	1.91	0.51
1:H:43:HIS:HB3	1:H:46:TRP:HB2	1.91	0.51
1:B:63:LEU:HD22	1:B:89:LEU:HD21	1.91	0.51
1:D:42:LYS:NZ	3:D:408:HOH:O	2.41	0.51
1:D:145:LEU:HD23	1:D:167:LEU:HB3	1.92	0.51
1:B:6:HIS:O	1:B:16:THR:HG21	2.11	0.51
1:B:44:LYS:HA	1:B:47:SER:HB3	1.92	0.51
1:E:71:THR:OG1	1:E:72:ILE:N	2.42	0.51
1:G:102:LYS:NZ	3:G:404:HOH:O	2.36	0.51
1:D:25:TYR:HE1	1:D:53:VAL:HG21	1.75	0.51
1:G:136:ILE:HD11	1:G:163:LEU:HB3	1.92	0.51
1:F:66:MET:HE1	1:F:172:GLY:HA2	1.93	0.51
1:H:98:VAL:HG11	1:H:131:VAL:HG21	1.92	0.51
1:C:194:MET:N	1:E:46:TRP:HE1	2.09	0.51
1:G:128:ALA:O	1:G:132:LEU:HG	2.11	0.50
1:G:149:MET:HE1	1:G:177:ASP:HB2	1.92	0.50
1:H:69:LYS:HZ2	1:H:90:PRO:HG3	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:LYS:HG2	1:H:9:ILE:HG22	1.92	0.50
1:F:42:LYS:HD3	1:F:107:THR:HG23	1.92	0.50
1:D:151:ASP:O	2:D:301:SAH:H5'2	2.11	0.50
1:G:195:ASP:O	1:G:197:GLU:N	2.42	0.50
1:H:126:SER:OG	1:H:127:ASP:N	2.44	0.50
1:H:193:MET:HB3	1:H:196:PHE:HE2	1.75	0.50
1:F:192:GLU:CG	1:F:201:ARG:HD2	2.41	0.50
1:D:187:ARG:NH2	1:D:191:GLU:OE1	2.45	0.50
1:E:100:PRO:HD3	2:E:301:SAH:C2	2.42	0.50
1:E:129:MET:HE1	1:E:159:ASN:HB3	1.93	0.50
1:E:77:PHE:HB2	2:E:301:SAH:HG2	1.94	0.50
1:F:153:ASP:OD1	1:F:153:ASP:N	2.37	0.50
1:G:62:LEU:HD21	1:G:173:ILE:HG21	1.93	0.50
1:D:158:LEU:HD12	1:D:158:LEU:H	1.76	0.50
1:G:83:LEU:O	1:G:87:LEU:HG	2.11	0.50
1:H:81:SER:OG	2:H:301:SAH:OXT	2.30	0.50
1:C:170:VAL:HA	1:C:233:ARG:HD3	1.94	0.49
1:F:155:GLU:H	1:F:155:GLU:CD	2.20	0.49
1:H:161:HIS:CD2	1:H:210:PHE:HE2	2.30	0.49
1:C:194:MET:H	1:E:46:TRP:NE1	2.10	0.49
1:F:43:HIS:HB3	1:F:46:TRP:HB2	1.93	0.49
1:G:24:ALA:HA	1:G:57:LEU:HD13	1.95	0.49
1:B:149:MET:HE3	1:B:151:ASP:HB2	1.94	0.49
1:C:200:GLY:O	1:C:203:HIS:N	2.41	0.49
1:H:192:GLU:O	1:H:193:MET:C	2.55	0.49
1:F:49:MET:HB3	2:F:301:SAH:SD	2.52	0.49
1:A:91:GLN:HA	1:A:120:LYS:HE2	1.94	0.49
1:A:106:GLN:HA	1:A:109:VAL:HG23	1.93	0.49
1:C:175:ALA:HB2	1:C:230:LEU:HD13	1.93	0.49
1:F:17:LYS:O	1:F:21:GLU:HG3	2.12	0.49
1:C:77:PHE:HB2	2:C:301:SAH:HG2	1.93	0.49
1:D:195:ASP:C	1:D:197:GLU:N	2.71	0.49
1:G:52:PRO:HB2	1:G:54:ASP:OD1	2.13	0.49
1:B:192:GLU:OE1	1:B:201:ARG:HD2	2.13	0.49
1:D:127:ASP:OD1	1:D:128:ALA:N	2.46	0.49
1:A:20:LEU:HA	1:A:24:ALA:HB3	1.95	0.48
1:B:7:ARG:O	1:B:9:ILE:N	2.41	0.48
1:F:193:MET:O	1:F:194:MET:C	2.56	0.48
1:H:55:GLU:O	1:H:59:ILE:N	2.41	0.48
1:C:194:MET:CG	1:C:198:ARG:HD2	2.42	0.48
1:E:157:TYR:HB3	1:E:207:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:TYR:O	1:F:22:THR:OG1	2.26	0.48
1:H:8:GLY:C	1:H:10:LEU:H	2.20	0.48
1:F:158:LEU:HD21	1:F:207:LEU:HA	1.93	0.48
1:C:194:MET:H	1:E:46:TRP:HE1	1.60	0.48
1:D:17:LYS:O	1:D:21:GLU:HG3	2.13	0.48
1:E:58:PHE:HE2	1:E:230:LEU:HD11	1.78	0.48
1:H:158:LEU:HD23	1:H:158:LEU:H	1.79	0.48
1:G:70:LYS:HD3	1:G:145:LEU:HG	1.95	0.48
1:G:198:ARG:HA	1:G:201:ARG:HB3	1.96	0.48
1:H:39:THR:HG23	1:H:78:THR:HG21	1.94	0.48
1:A:136:ILE:HD11	1:A:167:LEU:HG	1.95	0.48
1:B:110:PRO:O	1:B:114:LYS:HG3	2.13	0.48
1:E:154:LYS:HE3	1:E:181:TRP:CZ3	2.49	0.48
1:B:98:VAL:HG11	1:B:128:ALA:HA	1.96	0.47
1:E:18:TYR:O	1:E:22:THR:HG23	2.14	0.47
1:H:112:ILE:HG23	1:H:117:VAL:HG23	1.96	0.47
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.79	0.47
1:G:151:ASP:O	2:G:301:SAH:H5'2	2.14	0.47
1:H:9:ILE:HG22	1:H:9:ILE:O	2.13	0.47
1:B:184:SER:HA	1:B:187:ARG:HD3	1.96	0.47
1:D:133:ASN:OD1	1:D:163:LEU:HD21	2.14	0.47
1:E:234:LEU:O	3:E:401:HOH:O	2.20	0.47
1:A:153:ASP:OD2	1:A:153:ASP:N	2.44	0.47
1:F:40:VAL:HA	1:F:47:SER:CB	2.45	0.47
1:G:189:GLU:HA	1:G:192:GLU:CD	2.39	0.47
1:D:66:MET:HE1	1:D:172:GLY:HA2	1.96	0.47
1:E:65:ILE:HG22	1:H:65:ILE:HG22	1.96	0.47
1:H:154:LYS:HB3	1:H:204:LEU:HD21	1.97	0.47
1:H:191:GLU:OE2	1:H:191:GLU:HA	2.15	0.47
1:A:62:LEU:HD13	1:A:230:LEU:HD22	1.97	0.47
1:C:127:ASP:O	1:C:131:VAL:HG23	2.16	0.47
1:F:70:LYS:HG2	1:F:145:LEU:HD13	1.96	0.47
1:G:127:ASP:O	1:G:131:VAL:HG23	2.14	0.47
1:F:74:LEU:HD22	1:F:150:VAL:HG22	1.97	0.46
1:H:148:ALA:HB1	1:H:164:LEU:HD23	1.96	0.46
1:A:154:LYS:NZ	1:A:157:TYR:OH	2.43	0.46
1:C:85:THR:O	1:C:89:LEU:HG	2.15	0.46
1:G:129:MET:O	1:G:132:LEU:N	2.48	0.46
1:H:53:VAL:HG12	1:H:80:TYR:CZ	2.51	0.46
1:H:191:GLU:O	1:H:192:GLU:CB	2.62	0.46
1:H:192:GLU:C	1:H:194:MET:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:LEU:HD21	1:F:115:ALA:HB1	1.98	0.46
1:F:195:ASP:O	1:F:197:GLU:N	2.40	0.46
1:H:157:TYR:HD2	1:H:207:LEU:HD22	1.81	0.46
1:B:187:ARG:HH21	1:B:192:GLU:H	1.63	0.46
1:G:136:ILE:CD1	1:G:163:LEU:HB3	2.46	0.46
1:E:194:MET:C	1:E:196:PHE:H	2.23	0.46
1:F:154:LYS:HA	1:F:157:TYR:CD1	2.51	0.46
1:F:224:ILE:HB	1:F:228:VAL:HG23	1.96	0.46
1:D:127:ASP:O	1:D:131:VAL:HG23	2.15	0.46
1:D:194:MET:C	1:D:195:ASP:O	2.57	0.46
1:F:17:LYS:HA	1:F:17:LYS:HD3	1.60	0.46
1:B:44:LYS:HB3	1:B:44:LYS:HE3	1.83	0.45
1:D:155:GLU:HA	1:D:203:HIS:CE1	2.51	0.45
1:G:83:LEU:HD13	1:G:112:ILE:HG12	1.99	0.45
1:G:94:LYS:HB3	1:G:94:LYS:HE3	1.69	0.45
1:E:76:VAL:HG21	1:E:97:ALA:HB1	1.97	0.45
1:F:109:VAL:N	1:F:110:PRO:HD2	2.30	0.45
1:F:155:GLU:OE1	1:F:155:GLU:N	2.37	0.45
1:F:105:TYR:O	1:F:109:VAL:HG23	2.15	0.45
1:F:155:GLU:CD	1:F:155:GLU:N	2.75	0.45
1:B:154:LYS:HA	1:B:157:TYR:CD1	2.52	0.45
1:C:74:LEU:HD12	1:C:128:ALA:HB1	1.97	0.45
1:D:178:ASN:HA	1:D:226:ASP:HB3	1.98	0.45
1:G:67:ASN:O	1:G:67:ASN:ND2	2.50	0.45
1:H:96:ILE:HD12	1:H:145:LEU:HD21	1.98	0.45
1:F:139:GLY:C	1:F:141:GLU:N	2.73	0.45
1:F:143:GLY:N	1:F:166:LYS:O	2.48	0.45
1:F:146:ASP:OD1	1:F:169:ARG:NH2	2.50	0.45
1:H:149:MET:HE3	1:H:151:ASP:HB2	1.97	0.45
1:A:151:ASP:O	2:A:301:SAH:H5'2	2.17	0.45
1:C:28:GLU:OE1	1:C:36:ARG:NH2	2.48	0.45
1:E:20:LEU:HA	1:E:24:ALA:HB3	1.97	0.45
1:E:132:LEU:O	1:E:136:ILE:HD12	2.17	0.45
1:H:181:TRP:HA	1:H:181:TRP:CE3	2.52	0.45
1:D:181:TRP:CD1	1:D:184:SER:HG	2.35	0.45
1:F:76:VAL:HG21	1:F:97:ALA:HB1	1.99	0.45
1:E:10:LEU:HD12	1:E:16:THR:HA	1.97	0.45
1:A:155:GLU:HG3	1:A:203:HIS:CD2	2.52	0.45
1:G:192:GLU:HG2	1:G:198:ARG:HG3	1.98	0.44
1:D:77:PHE:HB2	2:D:301:SAH:HG2	1.99	0.44
1:B:127:ASP:O	1:B:131:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:GLU:HG3	1:C:234:LEU:HD21	1.99	0.44
1:F:214:ASP:HB3	1:F:217:VAL:HG22	1.98	0.44
1:G:152:ALA:O	1:G:154:LYS:NZ	2.48	0.44
1:D:36:ARG:O	1:D:39:THR:HG22	2.18	0.44
1:B:151:ASP:O	2:B:301:SAH:H5'2	2.18	0.44
1:D:195:ASP:O	1:D:196:PHE:CB	2.65	0.44
1:A:198:ARG:NH2	1:A:201:ARG:HE	2.16	0.44
1:B:138:ASP:OD1	1:B:138:ASP:N	2.41	0.44
1:D:181:TRP:HE1	1:D:197:GLU:HA	1.82	0.44
1:E:141:GLU:HB3	1:E:167:LEU:HD22	2.00	0.44
1:E:151:ASP:O	2:E:301:SAH:H5'2	2.18	0.44
1:F:106:GLN:HA	1:F:109:VAL:HG23	2.00	0.44
1:F:204:LEU:HD12	1:F:204:LEU:HA	1.69	0.44
1:A:168:VAL:HG21	1:A:174:ILE:HG13	1.99	0.44
1:F:61:MET:HE3	1:F:65:ILE:HD12	1.99	0.44
1:H:165:LEU:HD23	1:H:165:LEU:HA	1.84	0.44
1:B:70:LYS:HG2	1:B:145:LEU:HD23	1.99	0.44
1:F:91:GLN:HA	1:F:120:LYS:HE2	1.99	0.44
1:A:181:TRP:NE1	1:A:197:GLU:HA	2.29	0.43
1:B:66:MET:HE3	1:B:66:MET:HB2	1.79	0.43
1:E:36:ARG:O	1:E:40:VAL:HG23	2.18	0.43
1:D:113:LYS:HB3	1:G:142:GLU:HB2	1.99	0.43
1:B:117:VAL:HG12	1:B:120:LYS:HE3	2.00	0.43
1:H:70:LYS:HG2	1:H:145:LEU:HD23	2.00	0.43
1:A:42:LYS:HB3	1:A:42:LYS:HE3	1.79	0.43
1:B:62:LEU:HD21	1:B:173:ILE:HG21	2.01	0.43
1:B:83:LEU:HD13	1:B:112:ILE:HG12	1.99	0.43
1:C:51:VAL:HG21	1:C:81:SER:HB3	2.00	0.43
1:E:102:LYS:HD2	1:E:125:GLN:OE1	2.19	0.43
1:H:106:GLN:HA	1:H:109:VAL:HG23	2.00	0.43
1:H:117:VAL:HA	1:H:119:HIS:CE1	2.53	0.43
1:C:151:ASP:O	2:C:301:SAH:H5'2	2.18	0.43
1:G:29:HIS:ND1	1:G:30:GLU:N	2.65	0.43
1:G:31:GLN:H	1:G:31:GLN:HG2	1.66	0.43
1:G:43:HIS:NE2	1:G:104:ALA:HA	2.34	0.43
1:B:48:LEU:HD23	1:B:48:LEU:H	1.83	0.43
1:C:161:HIS:CD2	1:C:210:PHE:HE2	2.36	0.43
1:A:25:TYR:HE1	1:A:53:VAL:HG21	1.82	0.43
1:B:27:ARG:NH2	1:D:211:LEU:O	2.52	0.43
2:B:301:SAH:HG2	2:B:301:SAH:H4'	1.84	0.43
1:D:181:TRP:HD1	1:D:184:SER:OG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:MET:HE1	1:F:156:ASN:HB3	2.00	0.43
1:D:214:ASP:HB3	1:D:217:VAL:HG22	2.01	0.43
1:E:102:LYS:HG3	1:E:123:PHE:CE2	2.54	0.43
1:E:190:GLU:CG	1:E:191:GLU:HG2	2.48	0.43
1:E:195:ASP:O	1:E:197:GLU:N	2.52	0.43
1:D:78:THR:HG22	1:D:107:THR:HB	2.01	0.43
1:D:205:MET:O	1:D:209:LYS:HB2	2.19	0.43
1:E:74:LEU:HD21	1:E:132:LEU:HD11	2.01	0.43
1:H:77:PHE:CD2	1:H:78:THR:HG23	2.54	0.43
1:A:72:ILE:HB	1:A:145:LEU:HD22	2.01	0.42
1:G:66:MET:HE2	1:G:146:ASP:HB3	2.01	0.42
1:H:72:ILE:HG13	1:H:96:ILE:HB	2.01	0.42
1:A:77:PHE:HB2	2:A:301:SAH:HG2	2.00	0.42
1:A:100:PRO:HD3	2:A:301:SAH:C2	2.48	0.42
1:D:154:LYS:N	1:D:155:GLU:OE2	2.52	0.42
1:E:11:LYS:HE3	1:H:9:ILE:HG23	2.01	0.42
1:H:212:ALA:HA	1:H:219:LEU:HD22	2.01	0.42
1:E:66:MET:HE3	1:E:66:MET:HB2	1.75	0.42
1:E:173:ILE:HA	1:E:231:CYS:O	2.18	0.42
1:E:66:MET:SD	1:E:173:ILE:HD12	2.59	0.42
1:H:151:ASP:OD2	2:H:301:SAH:HB2	2.20	0.42
1:C:222:LEU:HD22	1:G:224:ILE:HG13	2.01	0.42
1:D:100:PRO:HD3	2:D:301:SAH:C2	2.49	0.42
1:D:175:ALA:HB2	1:D:230:LEU:HD23	2.00	0.42
1:E:133:ASN:OD1	1:E:163:LEU:HD21	2.20	0.42
1:E:151:ASP:OD2	2:E:301:SAH:HB2	2.20	0.42
1:G:18:TYR:CE1	1:G:22:THR:HG21	2.54	0.42
1:B:31:GLN:H	1:B:31:GLN:HG2	1.64	0.42
1:B:51:VAL:HG13	1:B:55:GLU:HG2	2.02	0.42
1:E:152:ALA:O	1:E:154:LYS:HD2	2.19	0.42
1:B:82:LEU:HD21	1:B:121:ILE:HG21	2.01	0.42
1:E:165:LEU:HD23	1:E:165:LEU:HA	1.92	0.42
1:F:168:VAL:O	1:F:233:ARG:NH1	2.43	0.42
1:H:81:SER:OG	2:H:301:SAH:N	2.53	0.42
1:A:54:ASP:OD2	1:A:55:GLU:N	2.53	0.42
1:C:65:ILE:HG22	1:G:232:ARG:HD3	2.02	0.42
1:C:148:ALA:HB3	1:C:174:ILE:HG23	2.02	0.42
1:E:194:MET:O	1:E:195:ASP:C	2.62	0.42
1:G:154:LYS:H	1:G:154:LYS:HD2	1.85	0.42
1:H:127:ASP:OD1	1:H:130:SER:HB2	2.20	0.42
1:C:62:LEU:HD21	1:C:173:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LEU:HD22	1:C:233:ARG:HG3	2.02	0.42
1:G:73:GLU:HG3	1:G:149:MET:HB3	2.00	0.42
1:H:25:TYR:CE1	1:H:36:ARG:NH1	2.88	0.42
1:D:60:SER:HB2	1:D:88:ALA:HB2	2.02	0.41
1:D:165:LEU:HD23	1:D:165:LEU:HA	1.94	0.41
1:D:204:LEU:HA	1:D:207:LEU:HB3	2.02	0.41
1:G:109:VAL:O	1:G:113:LYS:HG3	2.19	0.41
1:D:31:GLN:H	1:D:31:GLN:HG2	1.62	0.41
1:D:132:LEU:HB3	1:D:163:LEU:HD22	2.02	0.41
1:F:193:MET:HG3	1:F:196:PHE:HE2	1.85	0.41
1:G:127:ASP:OD1	1:G:128:ALA:N	2.52	0.41
1:A:178:ASN:O	1:A:204:LEU:HD13	2.20	0.41
1:B:8:GLY:O	1:B:9:ILE:HB	2.20	0.41
1:D:55:GLU:HB2	1:D:224:ILE:HG22	2.02	0.41
1:E:62:LEU:HD12	1:E:62:LEU:HA	1.81	0.41
1:E:214:ASP:HB3	1:E:217:VAL:HG22	2.01	0.41
1:C:20:LEU:HA	1:C:24:ALA:HB3	2.01	0.41
1:C:66:MET:HE3	1:C:66:MET:HB2	1.91	0.41
1:D:6:HIS:C	1:D:8:GLY:H	2.28	0.41
1:E:36:ARG:HH11	1:E:53:VAL:HG21	1.86	0.41
1:G:85:THR:O	1:G:89:LEU:HG	2.19	0.41
1:A:46:TRP:O	1:A:49:MET:HG3	2.19	0.41
1:C:76:VAL:N	1:C:99:ASP:OD2	2.46	0.41
1:E:136:ILE:HG13	1:E:167:LEU:HD21	2.03	0.41
1:B:25:TYR:CE1	1:B:53:VAL:HG21	2.52	0.41
1:D:131:VAL:O	1:D:135:LEU:HG	2.19	0.41
1:G:108:GLY:O	1:G:112:ILE:HG13	2.20	0.41
1:H:132:LEU:HB2	1:H:163:LEU:HD23	2.03	0.41
1:B:192:GLU:OE2	1:B:201:ARG:NE	2.53	0.41
1:D:108:GLY:O	1:D:112:ILE:HG13	2.21	0.41
1:B:105:TYR:O	1:B:109:VAL:HG23	2.20	0.41
1:G:157:TYR:HD2	1:G:207:LEU:HD22	1.85	0.41
1:A:162:GLU:OE2	1:A:216:ARG:NH2	2.54	0.41
1:B:8:GLY:C	1:B:10:LEU:H	2.28	0.41
1:C:52:PRO:HG3	1:C:225:GLY:HA3	2.03	0.41
1:D:21:GLU:OE2	3:D:401:HOH:O	2.21	0.41
1:D:136:ILE:HD12	1:D:163:LEU:HD23	2.03	0.41
1:G:189:GLU:O	1:G:192:GLU:HB2	2.21	0.41
1:G:192:GLU:C	1:G:194:MET:H	2.29	0.41
1:H:20:LEU:HD23	1:H:20:LEU:HA	1.91	0.41
1:G:98:VAL:HG11	1:G:128:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LEU:O	1:B:87:LEU:HG	2.22	0.40
2:C:301:SAH:HG2	2:C:301:SAH:H4'	1.97	0.40
1:D:191:GLU:HB2	1:D:192:GLU:H	1.72	0.40
1:F:66:MET:SD	1:F:173:ILE:HD12	2.61	0.40
1:H:214:ASP:HB3	1:H:217:VAL:HG22	2.02	0.40
1:G:106:GLN:HA	1:G:109:VAL:HG23	2.03	0.40
1:H:194:MET:HA	1:H:198:ARG:NH2	2.35	0.40
1:B:85:THR:O	1:B:89:LEU:HG	2.21	0.40
1:E:154:LYS:NZ	1:E:178:ASN:HB2	2.37	0.40
1:E:205:MET:HE3	1:E:209:LYS:HG3	2.03	0.40
1:C:132:LEU:O	1:C:136:ILE:HG12	2.22	0.40
1:D:102:LYS:HD2	1:D:123:PHE:CE2	2.56	0.40
1:F:98:VAL:HG11	1:F:128:ALA:HA	2.04	0.40
1:F:138:ASP:CG	1:F:139:GLY:N	2.79	0.40
1:B:178:ASN:O	1:B:204:LEU:HD21	2.21	0.40
1:F:92:ASP:OD1	1:F:92:ASP:N	2.54	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	222/235 (94%)	207 (93%)	13 (6%)	2 (1%)	14	37
1	B	228/235 (97%)	208 (91%)	13 (6%)	7 (3%)	3	10
1	C	222/235 (94%)	204 (92%)	13 (6%)	5 (2%)	5	16
1	D	229/235 (97%)	210 (92%)	15 (7%)	4 (2%)	7	22
1	E	222/235 (94%)	206 (93%)	11 (5%)	5 (2%)	5	16
1	F	222/235 (94%)	204 (92%)	15 (7%)	3 (1%)	9	26
1	G	226/235 (96%)	202 (89%)	23 (10%)	1 (0%)	30	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	222/235 (94%)	198 (89%)	19 (9%)	5 (2%)	5	16
All	All	1793/1880 (95%)	1639 (91%)	122 (7%)	32 (2%)	6	21

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ALA
1	A	138	ASP
1	B	194	MET
1	C	196	PHE
1	D	44	LYS
1	D	193	MET
1	F	193	MET
1	B	7	ARG
1	B	9	ILE
1	C	192	GLU
1	C	195	ASP
1	D	195	ASP
1	E	195	ASP
1	H	192	GLU
1	B	42	LYS
1	B	192	GLU
1	D	192	GLU
1	E	42	LYS
1	E	194	MET
1	E	197	GLU
1	H	137	ALA
1	H	195	ASP
1	B	43	HIS
1	B	196	PHE
1	C	201	ARG
1	F	192	GLU
1	F	196	PHE
1	G	195	ASP
1	H	10	LEU
1	H	193	MET
1	C	191	GLU
1	E	225	GLY

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	188/200 (94%)	182 (97%)	6 (3%)	34	67
1	B	194/200 (97%)	188 (97%)	6 (3%)	35	68
1	C	186/200 (93%)	182 (98%)	4 (2%)	45	75
1	D	193/200 (96%)	191 (99%)	2 (1%)	68	86
1	E	188/200 (94%)	182 (97%)	6 (3%)	34	67
1	F	190/200 (95%)	182 (96%)	8 (4%)	26	58
1	G	190/200 (95%)	179 (94%)	11 (6%)	18	45
1	H	188/200 (94%)	182 (97%)	6 (3%)	34	67
All	All	1517/1600 (95%)	1468 (97%)	49 (3%)	34	67

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	48	LEU
1	A	61	MET
1	A	153	ASP
1	A	202	VAL
1	A	228	VAL
1	B	40	VAL
1	B	45	TYR
1	B	48	LEU
1	B	81	SER
1	B	138	ASP
1	B	189	GLU
1	C	29	HIS
1	C	188	SER
1	C	207	LEU
1	C	228	VAL
1	D	48	LEU
1	D	57	LEU
1	E	48	LEU

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Mol	Chain	Res	Type
1	E	71	THR
1	E	169	ARG
1	E	188	SER
1	E	228	VAL
1	E	230	LEU
1	F	11	LYS
1	F	17	LYS
1	F	127	ASP
1	F	168	VAL
1	F	189	GLU
1	F	194	MET
1	F	228	VAL
1	F	231	CYS
1	G	9	ILE
1	G	15	LEU
1	G	47	SER
1	G	53	VAL
1	G	54	ASP
1	G	65	ILE
1	G	71	THR
1	G	126	SER
1	G	192	GLU
1	G	195	ASP
1	G	196	PHE
1	H	81	SER
1	H	112	ILE
1	H	126	SER
1	H	168	VAL
1	H	196	PHE
1	H	228	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	203	HIS
1	C	159	ASN
1	D	6	HIS
1	D	91	GLN
1	D	156	ASN
1	D	203	HIS
1	E	43	HIS

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Mol	Chain	Res	Type
1	E	159	ASN
1	F	159	ASN
1	H	29	HIS
1	H	106	GLN
1	H	203	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SAH	B	301	-	27,28,28	1.05	4 (14%)	38,40,40	2.05	10 (26%)
2	SAH	H	301	-	27,28,28	1.09	4 (14%)	38,40,40	1.95	10 (26%)
2	SAH	D	301	-	27,28,28	1.08	4 (14%)	38,40,40	2.04	10 (26%)
2	SAH	F	301	-	27,28,28	1.09	4 (14%)	38,40,40	2.12	11 (28%)
2	SAH	E	301	-	27,28,28	1.06	4 (14%)	38,40,40	2.05	10 (26%)
2	SAH	G	301	-	27,28,28	1.13	4 (14%)	38,40,40	2.01	12 (31%)
2	SAH	A	301	-	27,28,28	1.05	4 (14%)	38,40,40	2.09	10 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	C	301	-	27,28,28	1.10	4 (14%)	38,40,40	2.03	11 (28%)

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	B	301	-	-	1/15/31/31	0/3/3/3
2	SAH	H	301	-	-	5/15/31/31	0/3/3/3
2	SAH	D	301	-	-	4/15/31/31	0/3/3/3
2	SAH	F	301	-	-	3/15/31/31	0/3/3/3
2	SAH	E	301	-	-	5/15/31/31	0/3/3/3
2	SAH	G	301	-	-	2/15/31/31	0/3/3/3
2	SAH	A	301	-	-	3/15/31/31	0/3/3/3
2	SAH	C	301	-	-	4/15/31/31	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	SAH	C2-N1	2.77	1.39	1.33
2	F	301	SAH	C2-N3	2.73	1.39	1.33
2	G	301	SAH	C2-N3	2.64	1.38	1.33
2	E	301	SAH	C2-N3	2.51	1.38	1.33
2	C	301	SAH	C2-N3	2.50	1.38	1.33
2	D	301	SAH	C2-N3	2.49	1.38	1.33
2	C	301	SAH	C2-N1	2.46	1.38	1.33
2	A	301	SAH	C2-N3	2.42	1.38	1.33
2	D	301	SAH	C2-N1	2.41	1.38	1.33
2	H	301	SAH	C2-N1	2.41	1.38	1.33
2	H	301	SAH	C2-N3	2.38	1.38	1.33
2	E	301	SAH	C2-N1	2.38	1.38	1.33
2	B	301	SAH	C2-N1	2.35	1.38	1.33
2	B	301	SAH	C2-N3	2.35	1.38	1.33
2	A	301	SAH	C2-N1	2.33	1.38	1.33
2	A	301	SAH	C8-N7	2.31	1.36	1.31
2	F	301	SAH	C2-N1	2.29	1.38	1.33
2	D	301	SAH	C8-N7	2.25	1.35	1.31
2	B	301	SAH	C8-N7	2.25	1.35	1.31
2	E	301	SAH	C8-N7	2.20	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	SAH	OXT-C	-2.19	1.23	1.30
2	H	301	SAH	C8-N7	2.18	1.35	1.31
2	F	301	SAH	OXT-C	-2.17	1.23	1.30
2	C	301	SAH	C8-N7	2.16	1.35	1.31
2	H	301	SAH	OXT-C	-2.16	1.23	1.30
2	F	301	SAH	C8-N7	2.14	1.35	1.31
2	C	301	SAH	OXT-C	-2.11	1.23	1.30
2	B	301	SAH	OXT-C	-2.11	1.23	1.30
2	D	301	SAH	OXT-C	-2.10	1.23	1.30
2	G	301	SAH	C8-N7	2.06	1.35	1.31
2	A	301	SAH	OXT-C	-2.01	1.24	1.30
2	E	301	SAH	OXT-C	-2.01	1.24	1.30

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	SAH	N3-C2-N1	-5.60	119.85	128.60
2	B	301	SAH	N3-C2-N1	-5.59	119.86	128.60
2	H	301	SAH	N3-C2-N1	-5.51	119.98	128.60
2	D	301	SAH	N3-C2-N1	-5.48	120.02	128.60
2	F	301	SAH	N3-C2-N1	-5.42	120.12	128.60
2	E	301	SAH	N3-C2-N1	-5.38	120.19	128.60
2	C	301	SAH	N3-C2-N1	-5.28	120.34	128.60
2	F	301	SAH	C5-C4-N3	-5.22	119.94	126.75
2	D	301	SAH	C5-C4-N3	-4.93	120.32	126.75
2	E	301	SAH	C5-C4-N3	-4.86	120.42	126.75
2	G	301	SAH	C5-C4-N3	-4.85	120.42	126.75
2	A	301	SAH	C5-C4-N3	-4.74	120.56	126.75
2	B	301	SAH	C5-C4-N3	-4.51	120.87	126.75
2	C	301	SAH	C5-C4-N3	-4.46	120.93	126.75
2	G	301	SAH	N3-C2-N1	-4.46	121.63	128.60
2	A	301	SAH	N9-C8-N7	-4.22	108.15	113.91
2	H	301	SAH	N9-C8-N7	-4.21	108.16	113.91
2	C	301	SAH	N9-C8-N7	-4.17	108.22	113.91
2	G	301	SAH	N9-C8-N7	-4.14	108.25	113.91
2	B	301	SAH	N9-C8-N7	-4.11	108.29	113.91
2	F	301	SAH	N9-C8-N7	-4.04	108.39	113.91
2	E	301	SAH	N9-C8-N7	-4.03	108.41	113.91
2	D	301	SAH	N9-C8-N7	-3.94	108.53	113.91
2	H	301	SAH	C5-C4-N3	-3.87	121.69	126.75
2	A	301	SAH	C5-N7-C8	3.85	108.97	103.51
2	C	301	SAH	C5'-SD-CG	-3.84	90.74	102.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	SAH	C5-N7-C8	3.81	108.92	103.51
2	C	301	SAH	C5-N7-C8	3.80	108.91	103.51
2	G	301	SAH	C5-N7-C8	3.80	108.90	103.51
2	F	301	SAH	C2-N3-C4	3.74	120.58	111.75
2	D	301	SAH	C2-N3-C4	3.72	120.54	111.75
2	A	301	SAH	C2-N3-C4	3.70	120.50	111.75
2	B	301	SAH	C5-N7-C8	3.66	108.71	103.51
2	D	301	SAH	C5-N7-C8	3.65	108.69	103.51
2	E	301	SAH	C5-N7-C8	3.65	108.69	103.51
2	H	301	SAH	C5'-SD-CG	-3.58	91.51	102.27
2	E	301	SAH	C2-N3-C4	3.58	120.20	111.75
2	B	301	SAH	C2-N3-C4	3.54	120.11	111.75
2	H	301	SAH	C5-N7-C8	3.49	108.47	103.51
2	G	301	SAH	C5'-SD-CG	-3.46	91.87	102.27
2	G	301	SAH	N3-C4-N9	3.46	132.78	127.08
2	A	301	SAH	C5'-SD-CG	-3.44	91.94	102.27
2	F	301	SAH	N3-C4-N9	3.39	132.66	127.08
2	C	301	SAH	C2-N3-C4	3.30	119.55	111.75
2	E	301	SAH	N3-C4-N9	3.28	132.48	127.08
2	F	301	SAH	C5'-SD-CG	-3.23	92.59	102.27
2	D	301	SAH	N3-C4-N9	3.20	132.35	127.08
2	D	301	SAH	C5'-SD-CG	-3.15	92.81	102.27
2	G	301	SAH	C2-N3-C4	3.15	119.19	111.75
2	C	301	SAH	N3-C4-N9	3.12	132.22	127.08
2	A	301	SAH	OXT-C-O	-3.12	117.01	124.09
2	E	301	SAH	OXT-C-O	-3.05	117.16	124.09
2	H	301	SAH	C2-N3-C4	3.03	118.90	111.75
2	B	301	SAH	OXT-C-O	-2.98	117.32	124.09
2	D	301	SAH	OXT-C-O	-2.95	117.39	124.09
2	A	301	SAH	N3-C4-N9	2.95	131.94	127.08
2	F	301	SAH	OXT-C-O	-2.89	117.54	124.09
2	C	301	SAH	OXT-C-O	-2.87	117.57	124.09
2	H	301	SAH	N3-C4-N9	2.85	131.78	127.08
2	G	301	SAH	OXT-C-O	-2.80	117.73	124.09
2	B	301	SAH	N3-C4-N9	2.79	131.67	127.08
2	B	301	SAH	C5'-SD-CG	-2.74	94.06	102.27
2	B	301	SAH	OXT-C-CA	2.71	122.62	113.38
2	A	301	SAH	OXT-C-CA	2.65	122.41	113.38
2	H	301	SAH	OXT-C-O	-2.63	118.11	124.09
2	E	301	SAH	C5'-SD-CG	-2.59	94.50	102.27
2	A	301	SAH	C4-C5-N7	-2.50	107.58	110.62
2	E	301	SAH	OXT-C-CA	2.46	121.76	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	SAH	C4-N9-C8	2.44	108.37	105.73
2	G	301	SAH	OXT-C-CA	2.39	121.54	113.38
2	D	301	SAH	OXT-C-CA	2.38	121.50	113.38
2	F	301	SAH	C4-C5-N7	-2.37	107.73	110.62
2	B	301	SAH	C4-C5-N7	-2.35	107.75	110.62
2	F	301	SAH	OXT-C-CA	2.34	121.36	113.38
2	C	301	SAH	OXT-C-CA	2.28	121.14	113.38
2	D	301	SAH	C4-C5-N7	-2.27	107.85	110.62
2	C	301	SAH	C4-C5-N7	-2.22	107.91	110.62
2	C	301	SAH	C4-N9-C8	2.20	108.12	105.73
2	H	301	SAH	OXT-C-CA	2.19	120.85	113.38
2	G	301	SAH	C6-C5-C4	2.15	120.07	117.18
2	E	301	SAH	C4-C5-N7	-2.15	108.00	110.62
2	F	301	SAH	O4'-C1'-N9	2.15	112.29	108.06
2	G	301	SAH	C4-C5-N7	-2.09	108.08	110.62
2	G	301	SAH	C4-N9-C8	2.07	107.97	105.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SAH	N-CA-CB-CG
2	A	301	SAH	C-CA-CB-CG
2	C	301	SAH	N-CA-CB-CG
2	C	301	SAH	C-CA-CB-CG
2	D	301	SAH	N-CA-CB-CG
2	D	301	SAH	C-CA-CB-CG
2	E	301	SAH	N-CA-CB-CG
2	E	301	SAH	C-CA-CB-CG
2	F	301	SAH	N-CA-CB-CG
2	F	301	SAH	C-CA-CB-CG
2	H	301	SAH	N-CA-CB-CG
2	H	301	SAH	C-CA-CB-CG
2	E	301	SAH	C3'-C4'-C5'-SD
2	G	301	SAH	C-CA-CB-CG
2	E	301	SAH	O4'-C4'-C5'-SD
2	H	301	SAH	O4'-C4'-C5'-SD
2	C	301	SAH	O-C-CA-CB
2	C	301	SAH	OXT-C-CA-CB
2	B	301	SAH	C-CA-CB-CG
2	D	301	SAH	O-C-CA-N
2	G	301	SAH	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	E	301	SAH	C4'-C5'-SD-CG
2	F	301	SAH	C4'-C5'-SD-CG
2	H	301	SAH	C4'-C5'-SD-CG
2	D	301	SAH	C2'-C1'-N9-C8
2	H	301	SAH	C3'-C4'-C5'-SD
2	A	301	SAH	C2'-C1'-N9-C8

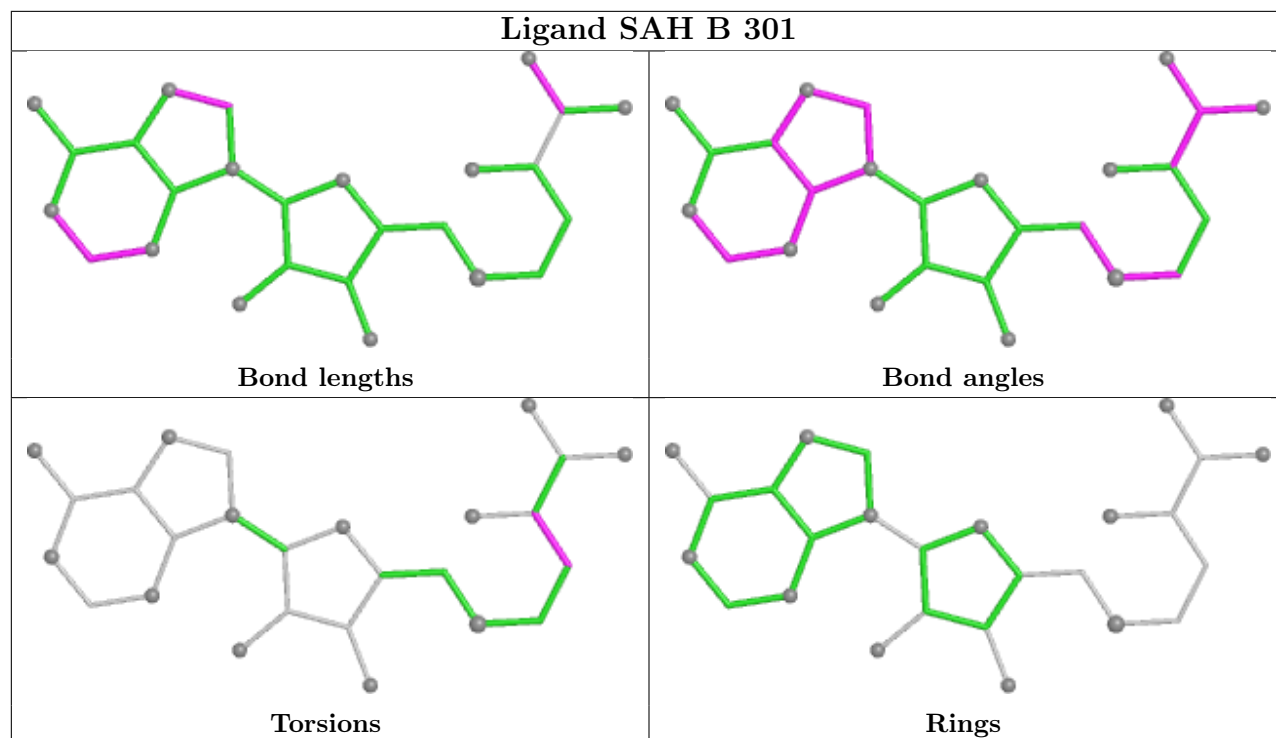
There are no ring outliers.

8 monomers are involved in 24 short contacts:

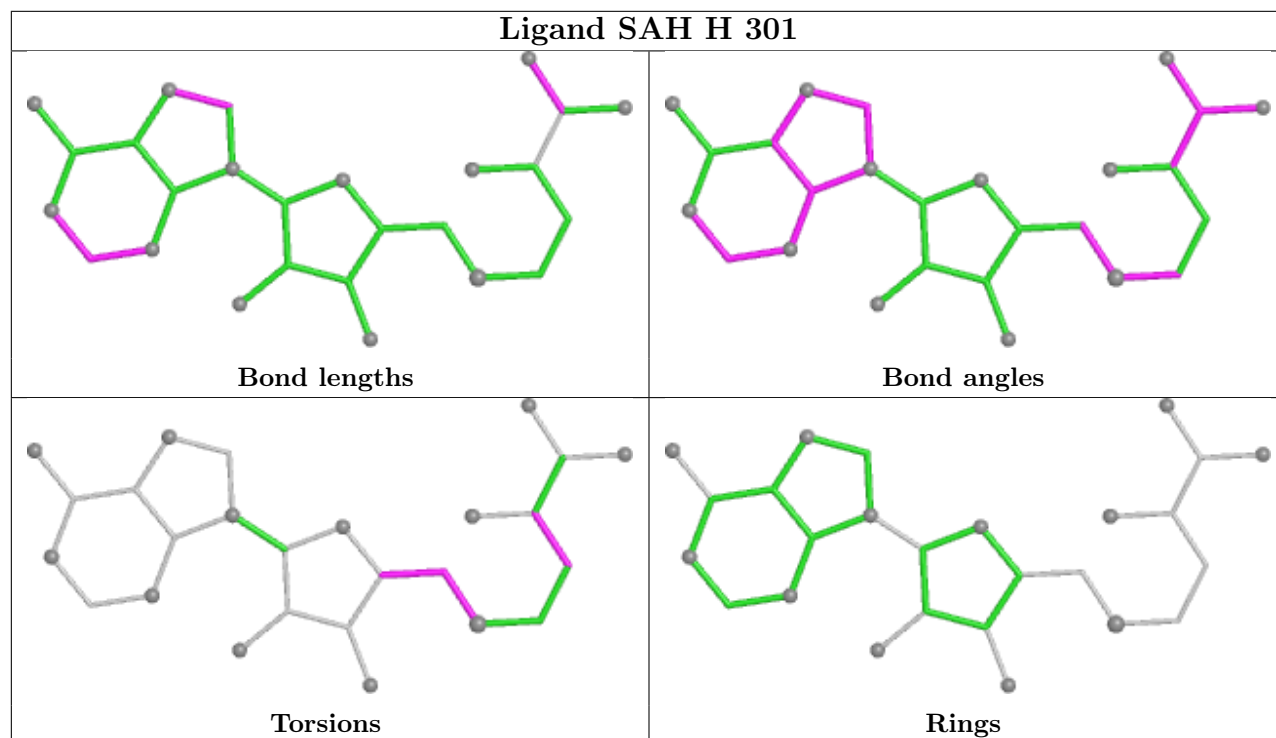
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SAH	2	0
2	H	301	SAH	4	0
2	D	301	SAH	4	0
2	F	301	SAH	3	0
2	E	301	SAH	4	0
2	G	301	SAH	1	0
2	A	301	SAH	3	0
2	C	301	SAH	3	0

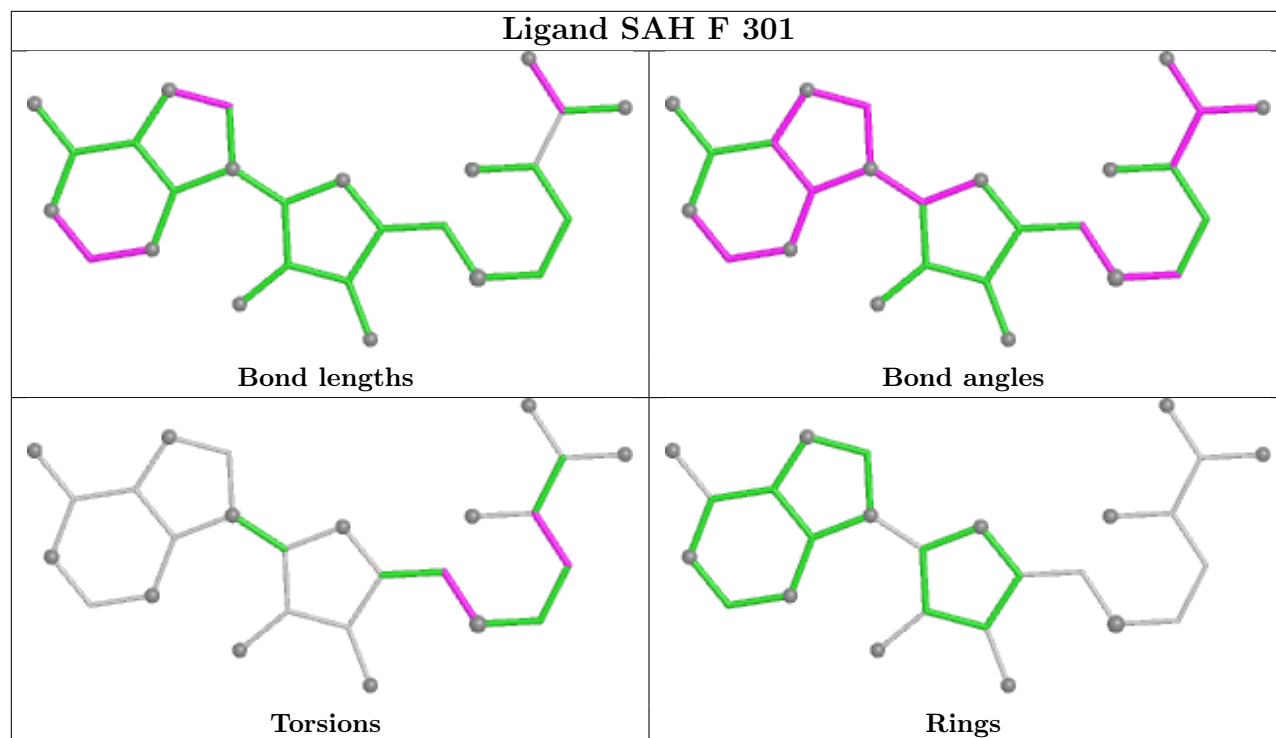
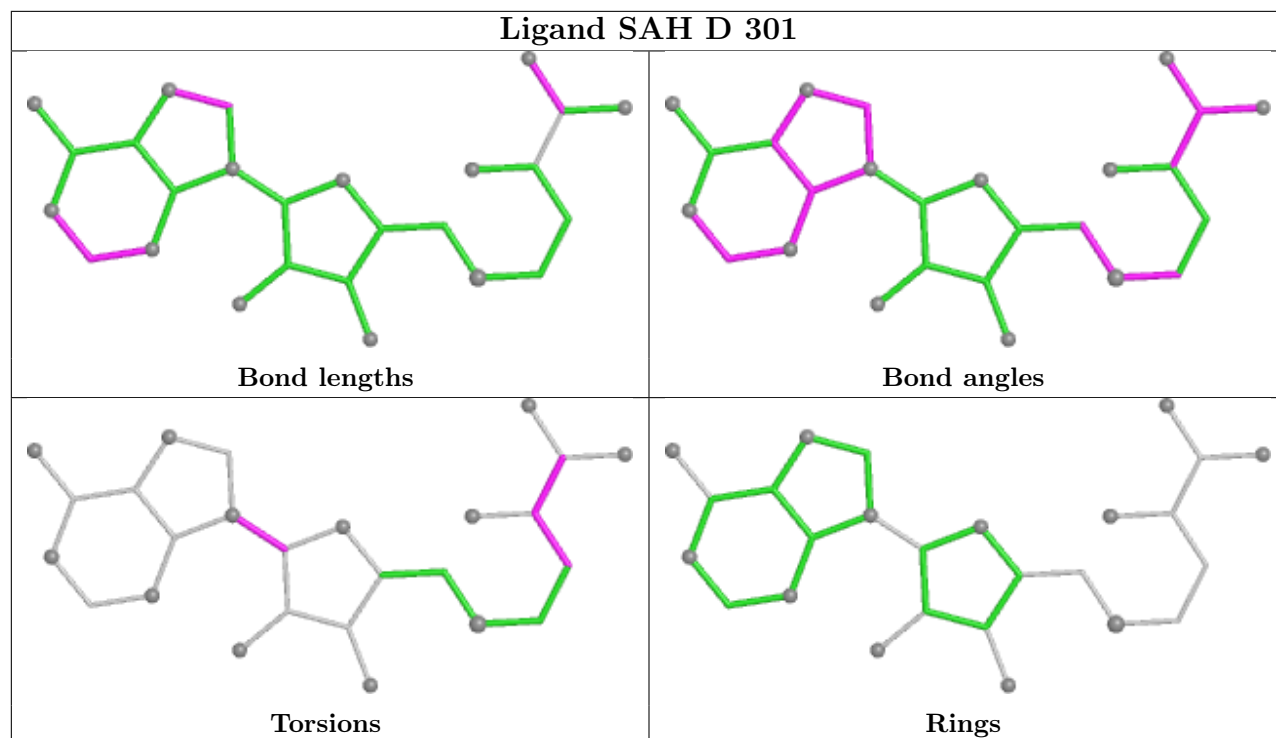
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand SAH B 301

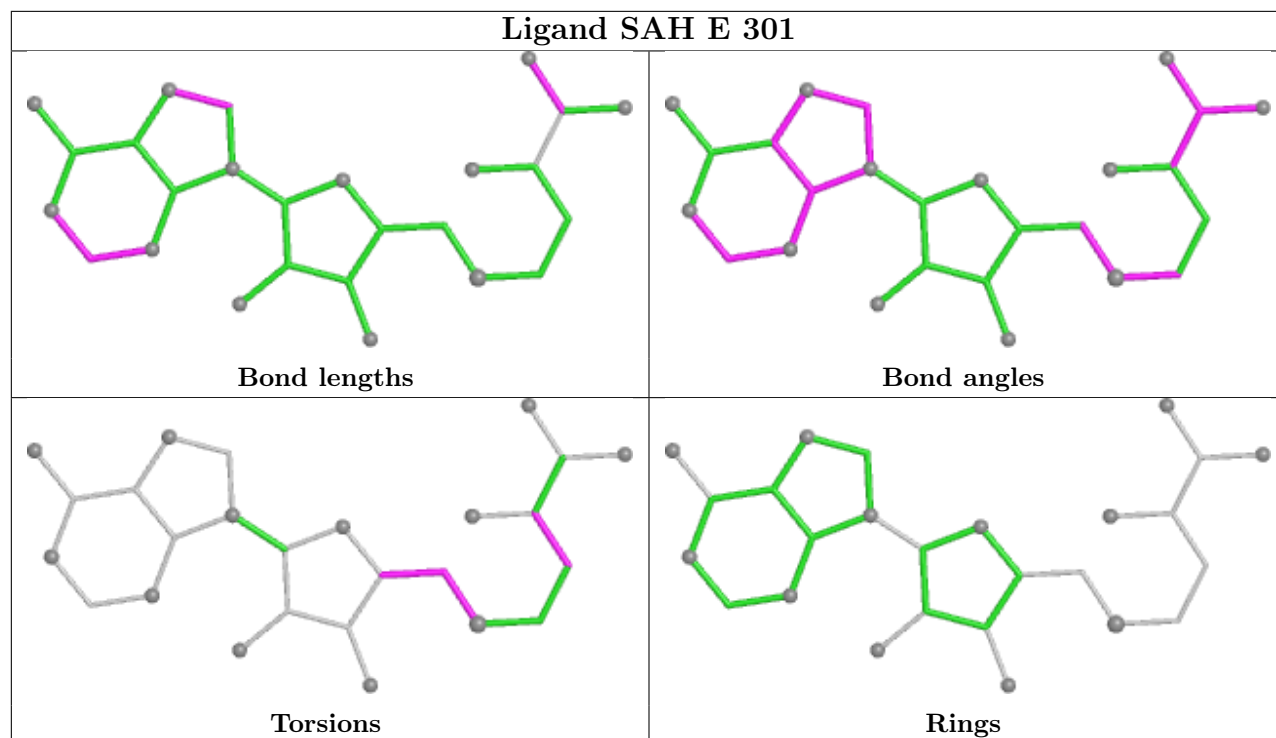


Ligand SAH H 301

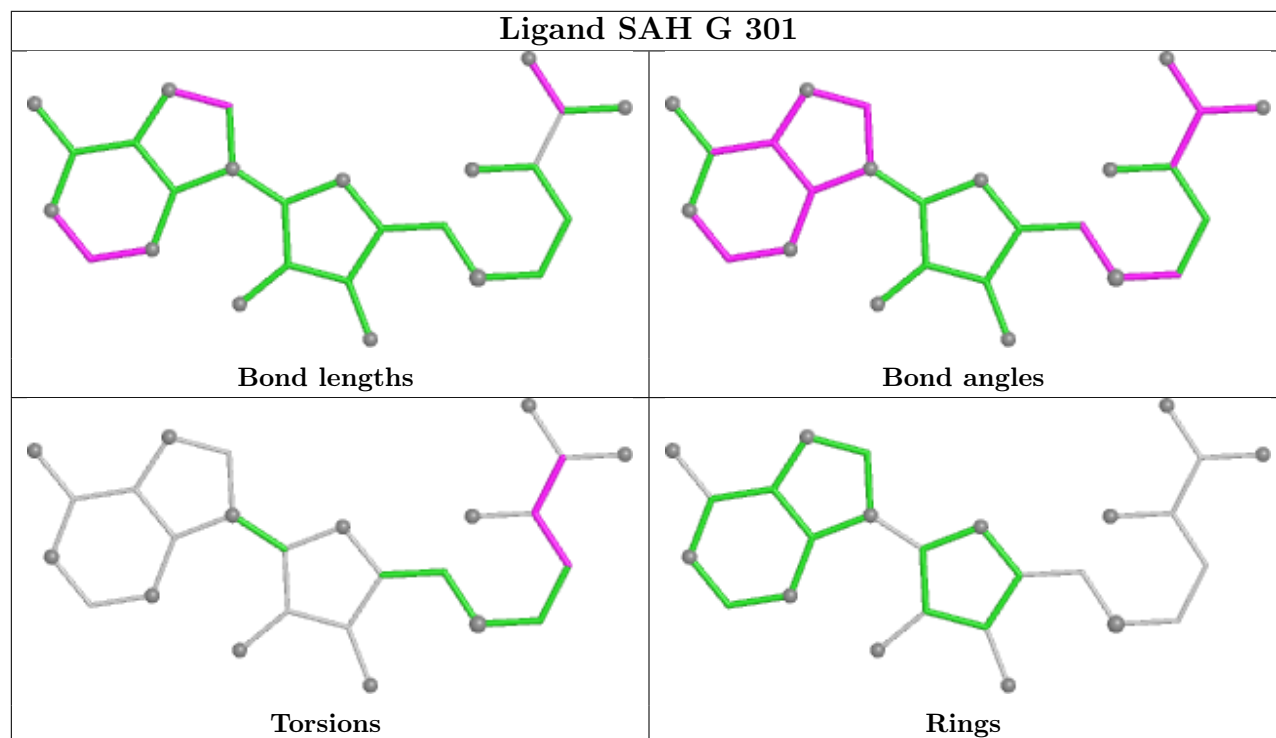


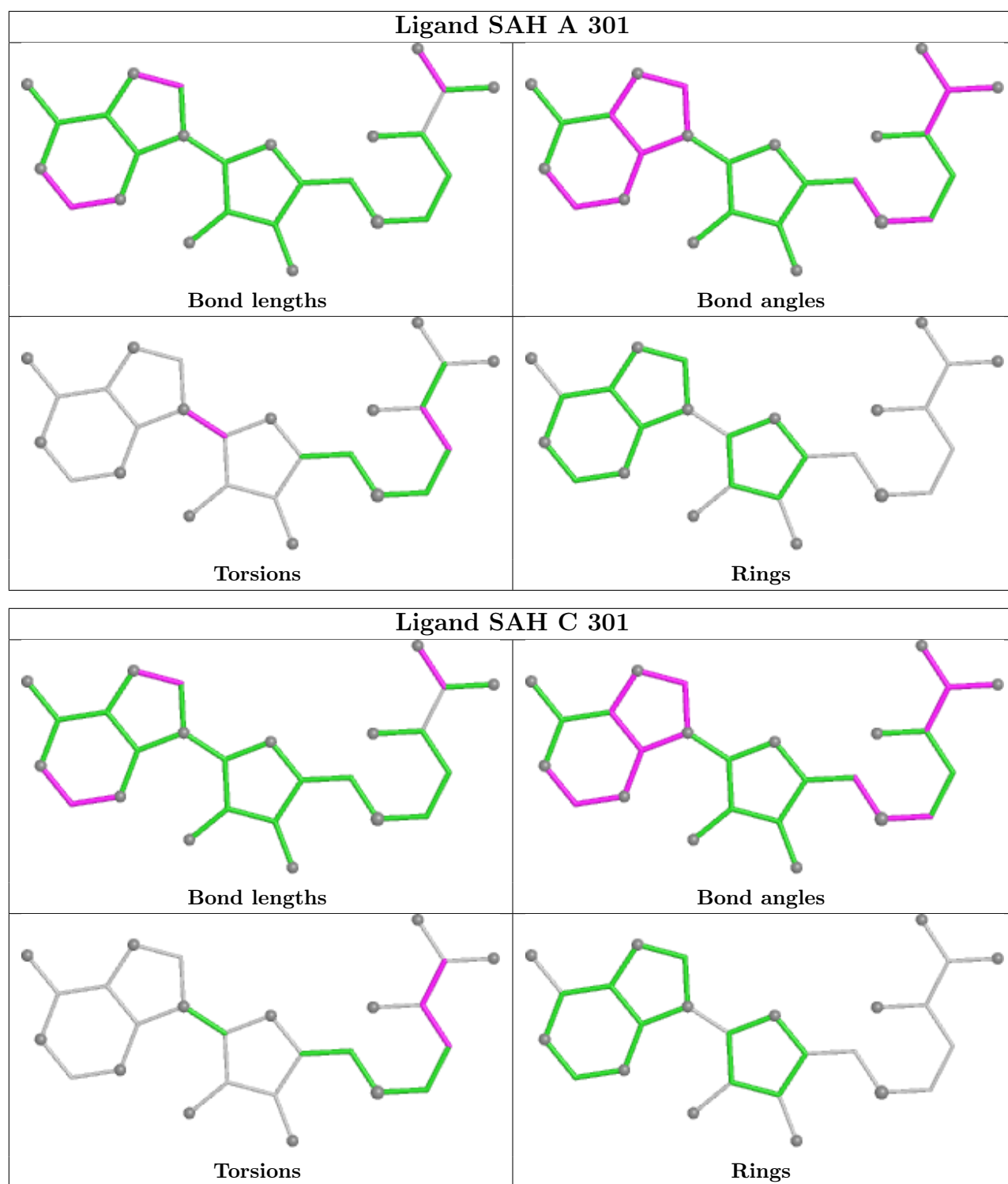


Ligand SAH E 301



Ligand SAH G 301





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	226/235 (96%)	0.62	30 (13%) 7 6	19, 36, 73, 110	0
1	B	230/235 (97%)	0.71	33 (14%) 6 5	20, 36, 75, 92	0
1	C	226/235 (96%)	0.79	29 (12%) 7 6	24, 42, 70, 103	0
1	D	231/235 (98%)	0.93	38 (16%) 4 3	22, 42, 87, 100	0
1	E	226/235 (96%)	0.89	30 (13%) 7 6	28, 48, 74, 99	0
1	F	226/235 (96%)	0.72	28 (12%) 8 6	22, 40, 77, 105	0
1	G	228/235 (97%)	1.22	44 (19%) 3 2	30, 56, 92, 117	0
1	H	226/235 (96%)	1.21	46 (20%) 3 2	27, 58, 94, 121	0
All	All	1819/1880 (96%)	0.89	278 (15%) 5 4	19, 44, 83, 121	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	ARG	7.4
1	E	196	PHE	7.3
1	G	193	MET	6.0
1	E	195	ASP	5.7
1	C	195	ASP	5.3
1	G	8	GLY	5.2
1	D	56	GLY	5.2
1	F	57	LEU	5.1
1	E	55	GLU	4.9
1	H	8	GLY	4.9
1	A	194	MET	4.9
1	B	42	LYS	4.8
1	F	46	TRP	4.8
1	B	196	PHE	4.6
1	B	45	TYR	4.5
1	B	46	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	136	ILE	4.5
1	G	196	PHE	4.5
1	G	138	ASP	4.5
1	C	46	TRP	4.5
1	F	139	GLY	4.4
1	E	40	VAL	4.4
1	G	192	GLU	4.4
1	A	53	VAL	4.4
1	A	29	HIS	4.4
1	D	213	SER	4.4
1	G	55	GLU	4.4
1	B	7	ARG	4.3
1	D	193	MET	4.3
1	B	192	GLU	4.3
1	D	192	GLU	4.3
1	C	194	MET	4.3
1	D	55	GLU	4.2
1	C	29	HIS	4.1
1	B	139	GLY	4.0
1	D	8	GLY	4.0
1	E	182	PHE	4.0
1	C	53	VAL	4.0
1	G	53	VAL	4.0
1	H	131	VAL	4.0
1	G	204	LEU	4.0
1	H	182	PHE	4.0
1	F	193	MET	4.0
1	A	196	PHE	4.0
1	B	53	VAL	4.0
1	B	52	PRO	4.0
1	H	54	ASP	4.0
1	G	163	LEU	3.9
1	B	190	GLU	3.9
1	E	192	GLU	3.9
1	D	196	PHE	3.9
1	B	43	HIS	3.9
1	G	48	LEU	3.9
1	B	194	MET	3.8
1	F	55	GLU	3.8
1	C	139	GLY	3.8
1	E	193	MET	3.8
1	H	203	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	46	TRP	3.8
1	F	182	PHE	3.8
1	D	53	VAL	3.8
1	B	193	MET	3.7
1	B	6	HIS	3.7
1	D	45	TYR	3.7
1	D	219	LEU	3.7
1	D	44	LYS	3.7
1	F	42	LYS	3.7
1	G	45	TYR	3.7
1	H	200	GLY	3.7
1	E	100	PRO	3.7
1	G	46	TRP	3.6
1	A	136	ILE	3.6
1	C	137	ALA	3.6
1	C	203	HIS	3.6
1	B	55	GLU	3.6
1	C	43	HIS	3.5
1	C	193	MET	3.5
1	F	138	ASP	3.5
1	A	182	PHE	3.5
1	F	196	PHE	3.5
1	H	196	PHE	3.5
1	E	53	VAL	3.5
1	F	43	HIS	3.5
1	G	139	GLY	3.4
1	C	196	PHE	3.4
1	F	56	GLY	3.4
1	G	182	PHE	3.4
1	F	192	GLU	3.4
1	H	158	LEU	3.4
1	B	203	HIS	3.4
1	F	203	HIS	3.4
1	H	52	PRO	3.3
1	H	46	TRP	3.3
1	H	205	MET	3.3
1	B	54	ASP	3.3
1	H	57	LEU	3.3
1	A	137	ALA	3.3
1	D	6	HIS	3.2
1	B	182	PHE	3.2
1	G	131	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	54	ASP	3.2
1	H	195	ASP	3.2
1	D	29	HIS	3.2
1	A	203	HIS	3.2
1	F	39	THR	3.2
1	C	58	PHE	3.1
1	A	195	ASP	3.1
1	C	228	VAL	3.1
1	B	41	GLU	3.1
1	G	43	HIS	3.1
1	G	203	HIS	3.1
1	A	54	ASP	3.1
1	C	54	ASP	3.1
1	F	41	GLU	3.1
1	B	40	VAL	3.1
1	C	12	THR	3.0
1	C	182	PHE	3.0
1	F	29	HIS	3.0
1	F	53	VAL	3.0
1	A	46	TRP	3.0
1	D	46	TRP	3.0
1	C	138	ASP	3.0
1	D	153	ASP	3.0
1	A	193	MET	3.0
1	H	115	ALA	3.0
1	E	203	HIS	2.9
1	B	195	ASP	2.9
1	H	128	ALA	2.9
1	D	190	GLU	2.9
1	G	197	GLU	2.9
1	H	105	TYR	2.9
1	H	138	ASP	2.9
1	C	204	LEU	2.9
1	D	40	VAL	2.9
1	H	204	LEU	2.9
1	D	203	HIS	2.9
1	G	29	HIS	2.9
1	G	194	MET	2.8
1	E	8	GLY	2.8
1	D	137	ALA	2.8
1	A	197	GLU	2.8
1	C	197	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLY	2.8
1	H	139	GLY	2.8
1	E	29	HIS	2.8
1	F	194	MET	2.8
1	H	188	SER	2.8
1	C	40	VAL	2.8
1	D	41	GLU	2.8
1	E	141	GLU	2.8
1	C	155	GLU	2.8
1	A	213	SER	2.7
1	A	163	LEU	2.7
1	G	89	LEU	2.7
1	G	12	THR	2.7
1	A	210	PHE	2.7
1	D	139	GLY	2.7
1	E	188	SER	2.7
1	B	44	LYS	2.7
1	G	137	ALA	2.7
1	D	205	MET	2.6
1	E	194	MET	2.6
1	F	30	GLU	2.6
1	G	202	VAL	2.6
1	A	198	ARG	2.6
1	G	42	LYS	2.6
1	G	40	VAL	2.6
1	G	78	THR	2.6
1	A	174	ILE	2.6
1	H	48	LEU	2.6
1	H	83	LEU	2.6
1	G	200	GLY	2.6
1	H	98	VAL	2.6
1	H	193	MET	2.6
1	G	199	ALA	2.6
1	G	39	THR	2.5
1	G	213	SER	2.5
1	F	54	ASP	2.5
1	B	74	LEU	2.5
1	B	140	LYS	2.5
1	F	8	GLY	2.5
1	C	14	ALA	2.5
1	D	54	ASP	2.5
1	G	141	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	100	PRO	2.5
1	D	57	LEU	2.5
1	H	137	ALA	2.5
1	E	74	LEU	2.5
1	E	41	GLU	2.5
1	B	210	PHE	2.5
1	B	229	ALA	2.5
1	G	66	MET	2.4
1	H	29	HIS	2.4
1	D	210	PHE	2.4
1	A	190	GLU	2.4
1	F	40	VAL	2.4
1	H	53	VAL	2.4
1	A	58	PHE	2.4
1	B	58	PHE	2.4
1	G	9	ILE	2.4
1	G	136	ILE	2.4
1	H	39	THR	2.4
1	D	188	SER	2.4
1	G	195	ASP	2.4
1	C	30	GLU	2.3
1	A	188	SER	2.3
1	H	56	GLY	2.3
1	D	9	ILE	2.3
1	C	205	MET	2.3
1	H	66	MET	2.3
1	H	141	GLU	2.3
1	A	100	PRO	2.3
1	E	210	PHE	2.3
1	A	41	GLU	2.3
1	H	155	GLU	2.3
1	H	213	SER	2.3
1	H	35	LEU	2.3
1	E	66	MET	2.3
1	D	5	SER	2.3
1	D	19	LEU	2.3
1	E	48	LEU	2.3
1	E	163	LEU	2.3
1	H	97	ALA	2.2
1	G	190	GLU	2.2
1	H	30	GLU	2.2
1	G	80	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	50	ASN	2.2
1	G	100	PRO	2.2
1	D	134	ASP	2.2
1	D	163	LEU	2.2
1	H	202	VAL	2.2
1	B	206	LYS	2.2
1	C	192	GLU	2.2
1	F	52	PRO	2.2
1	A	138	ASP	2.2
1	B	89	LEU	2.2
1	C	210	PHE	2.2
1	D	194	MET	2.2
1	E	198	ARG	2.2
1	A	8	GLY	2.2
1	G	49	MET	2.2
1	A	192	GLU	2.2
1	D	16	THR	2.2
1	F	31	GLN	2.2
1	A	62	LEU	2.2
1	B	8	GLY	2.2
1	F	89	LEU	2.2
1	B	131	VAL	2.2
1	B	188	SER	2.2
1	H	199	ALA	2.1
1	H	194	MET	2.1
1	E	139	GLY	2.1
1	H	34	GLY	2.1
1	H	117	VAL	2.1
1	D	155	GLU	2.1
1	F	100	PRO	2.1
1	G	106	GLN	2.1
1	E	57	LEU	2.1
1	B	219	LEU	2.1
1	E	135	LEU	2.1
1	H	181	TRP	2.1
1	D	140	LYS	2.1
1	A	74	LEU	2.1
1	G	57	LEU	2.1
1	H	43	HIS	2.1
1	H	40	VAL	2.1
1	G	210	PHE	2.1
1	E	137	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	144	THR	2.0
1	F	66	MET	2.0
1	H	106	GLN	2.0
1	H	136	ILE	2.0
1	A	131	VAL	2.0
1	E	127	ASP	2.0
1	D	74	LEU	2.0
1	E	62	LEU	2.0
1	A	40	VAL	2.0
1	E	98	VAL	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](#)

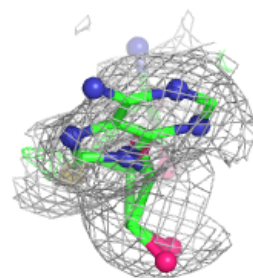
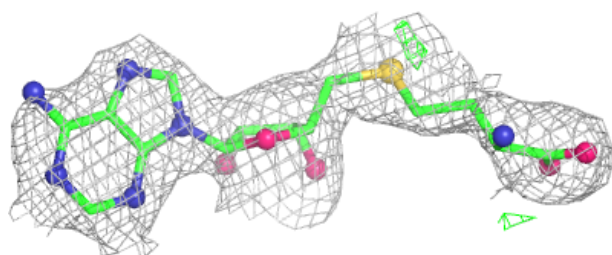
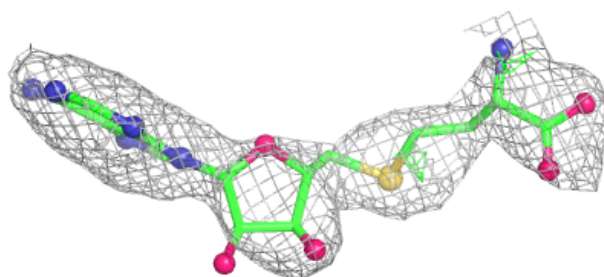
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SAH	G	301	26/26	0.84	0.15	43,56,65,78	26
2	SAH	H	301	26/26	0.86	0.14	48,62,74,89	0
2	SAH	F	301	26/26	0.88	0.13	30,36,49,54	26
2	SAH	A	301	26/26	0.89	0.12	16,33,43,45	0
2	SAH	C	301	26/26	0.89	0.14	25,37,48,49	26
2	SAH	E	301	26/26	0.89	0.13	30,49,61,65	0
2	SAH	D	301	26/26	0.90	0.13	18,38,46,50	26
2	SAH	B	301	26/26	0.91	0.11	19,30,38,45	0

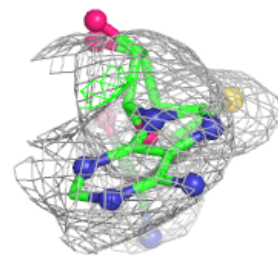
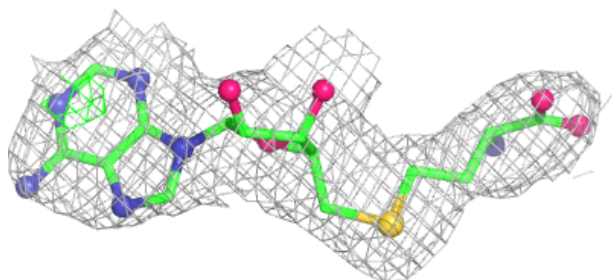
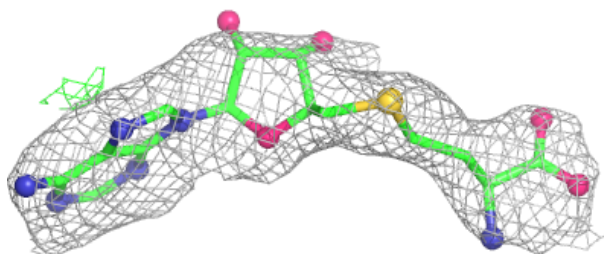
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH G 301:

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

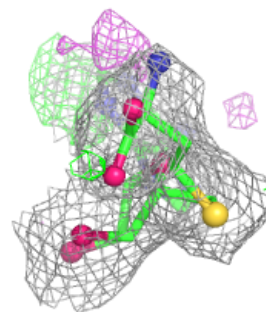
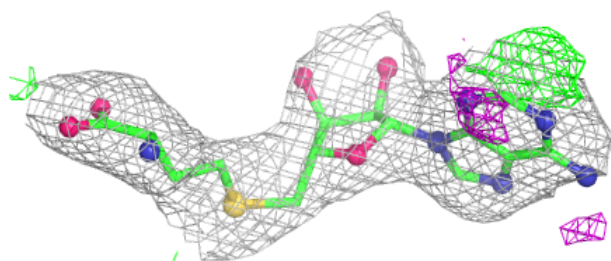
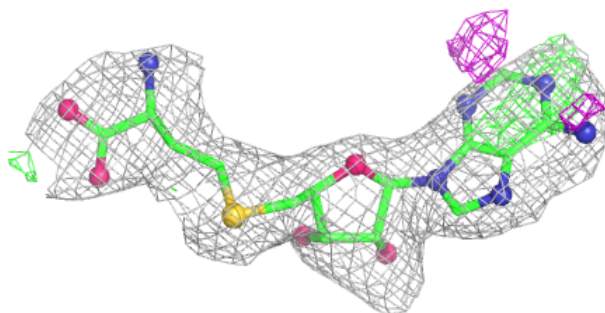
**Electron density around SAH H 301:**

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

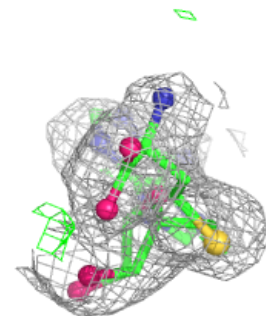
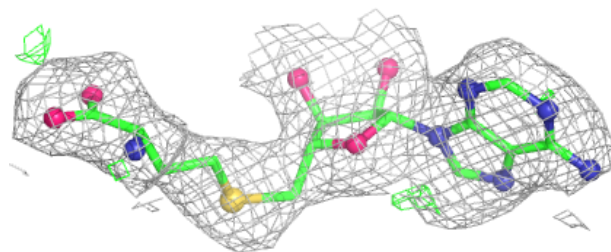
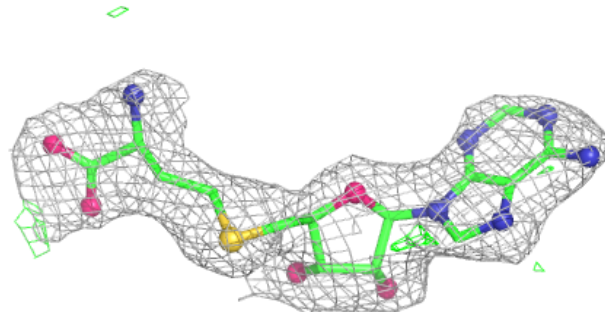


Electron density around SAH F 301:

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

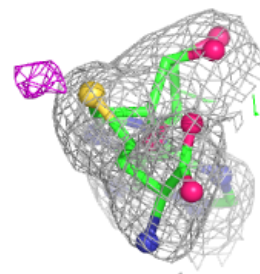
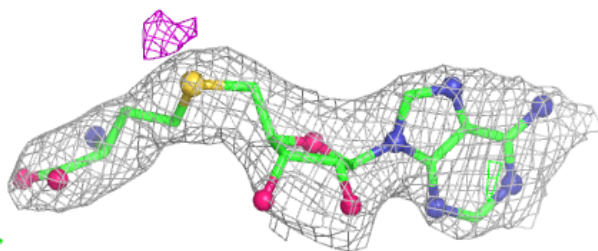
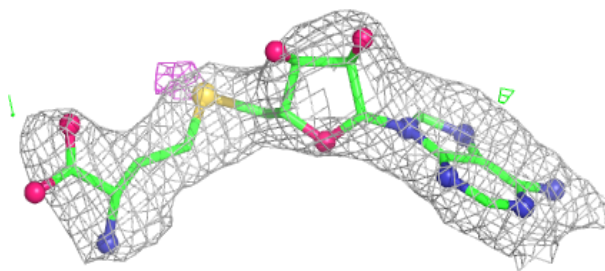
**Electron density around SAH A 301:**

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

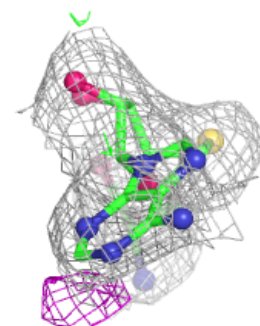
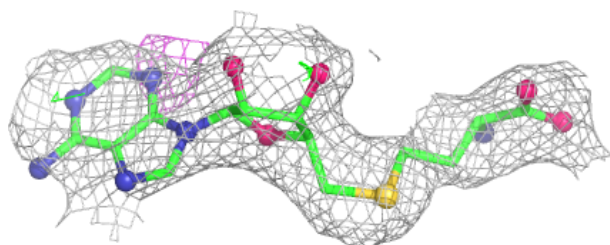
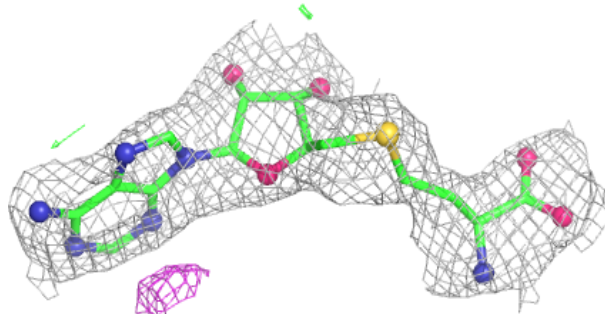


Electron density around SAH C 301:

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

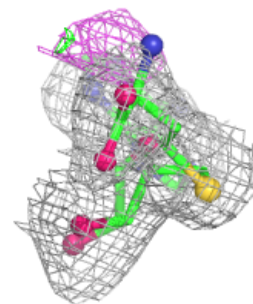
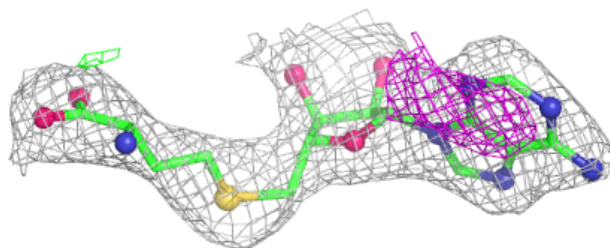
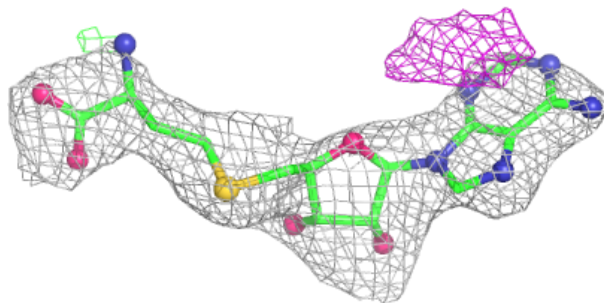
**Electron density around SAH E 301:**

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

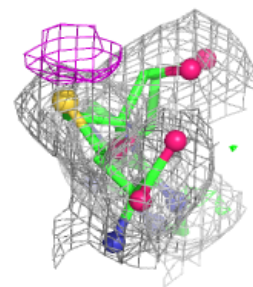
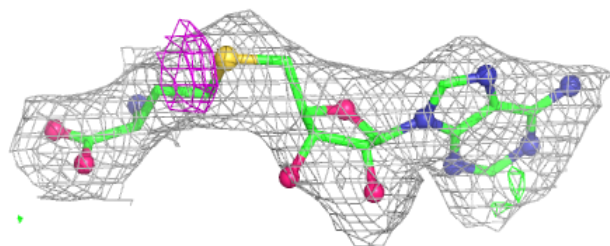
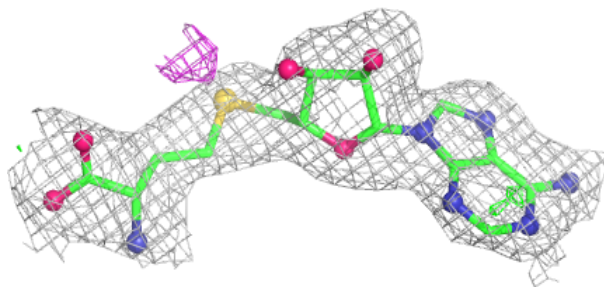


Electron density around SAH D 301:

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

**Electron density around SAH B 301:**

$2mF_o-DF_c$ (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.