



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:07 AM EDT

PDB ID : 6LYH / pdb_00006lyh
Title : Crystal structure of tea N9-methyltransferase CkTcS in complex with SAH and 1,3,7-trimethyluric acid
Authors : Wang, Y.; Zhang, Z.-M.
Deposited on : 2020-02-14
Resolution : 3.15 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

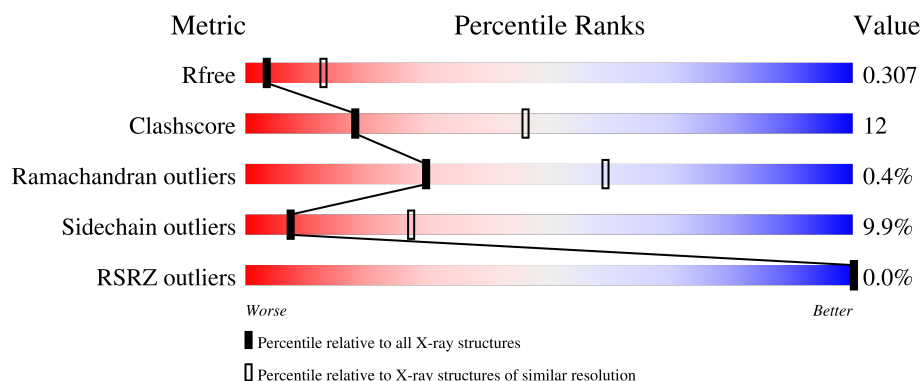
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	363	 66% 31% ..
1	B	363	 66% 27% . .
1	C	363	 70% 22% . .
1	D	363	 69% 26% . .
1	E	363	 66% 30% . .

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Mol	Chain	Length	Quality of chain
1	F	363	73%21%••
1	G	363	66%27%5%•
1	H	363	65%30%••

2 Entry composition

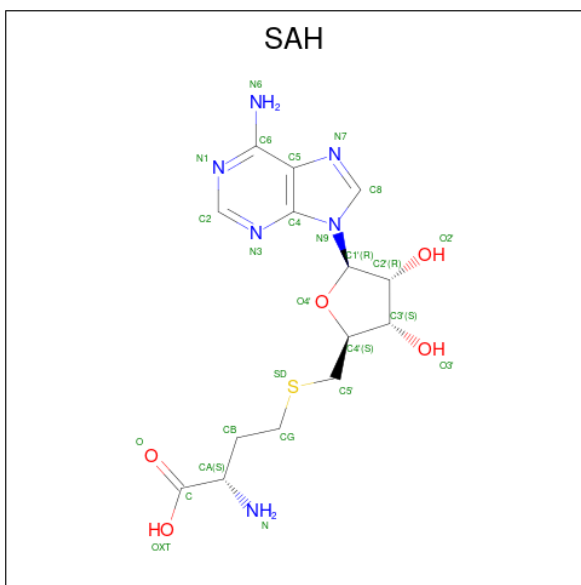
There are 3 unique types of molecules in this entry. The entry contains 20792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-methyltransferase CkTcS.

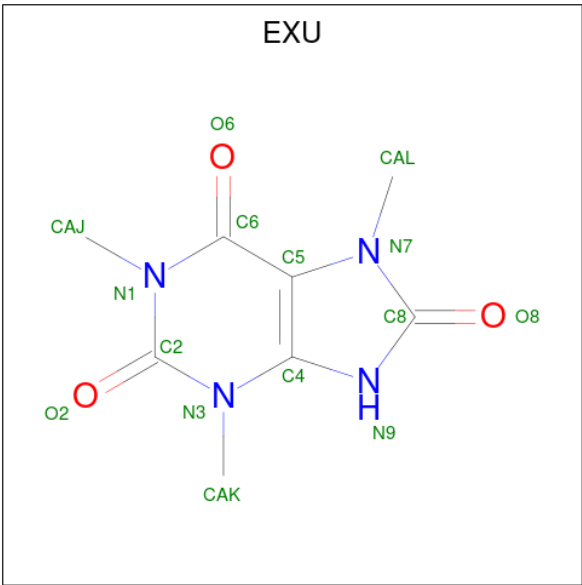
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	350	Total	C	N	O	S	0	0	0
			2517	1605	429	466	17			
1	A	358	Total	C	N	O	S	0	0	0
			2644	1687	444	494	19			
1	C	347	Total	C	N	O	S	0	0	0
			2450	1564	404	466	16			
1	D	358	Total	C	N	O	S	0	0	0
			2662	1698	450	494	20			
1	E	358	Total	C	N	O	S	0	0	0
			2649	1696	444	489	20			
1	F	351	Total	C	N	O	S	0	0	0
			2411	1529	405	462	15			
1	G	357	Total	C	N	O	S	0	0	0
			2652	1692	447	495	18			
1	H	355	Total	C	N	O	S	0	0	0
			2493	1593	420	465	15			

- 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).

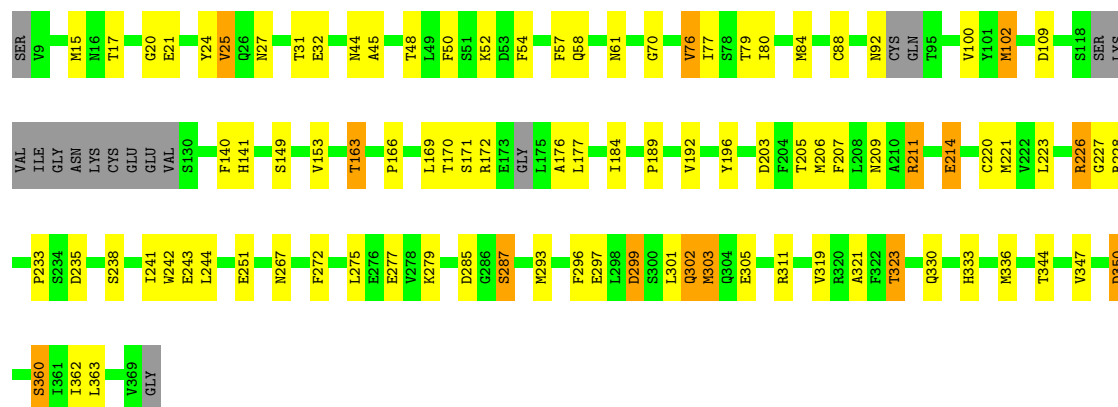


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	A	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	C	1	Total 19	C 10	N 5	O 3	S 1	0	0
2	D	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	E	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	F	1	Total 19	C 10	N 5	O 3	S 1	0	0
2	G	1	Total 26	C 14	N 6	O 5	S 1	0	0
2	H	1	Total 26	C 14	N 6	O 5	S 1	0	0

- Molecule 3 is 1,3,7-trimethyl-9H-purine-2,6,8-trione (CCD ID: EXU) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			15	8	4	3		
3	A	1	Total	C	N	O	0	0
			15	8	4	3		
3	C	1	Total	C	N	O	0	0
			15	8	4	3		
3	D	1	Total	C	N	O	0	0
			15	8	4	3		
3	E	1	Total	C	N	O	0	0
			15	8	4	3		
3	F	1	Total	C	N	O	0	0
			15	8	4	3		
3	G	1	Total	C	N	O	0	0
			15	8	4	3		
3	H	1	Total	C	N	O	0	0
			15	8	4	3		



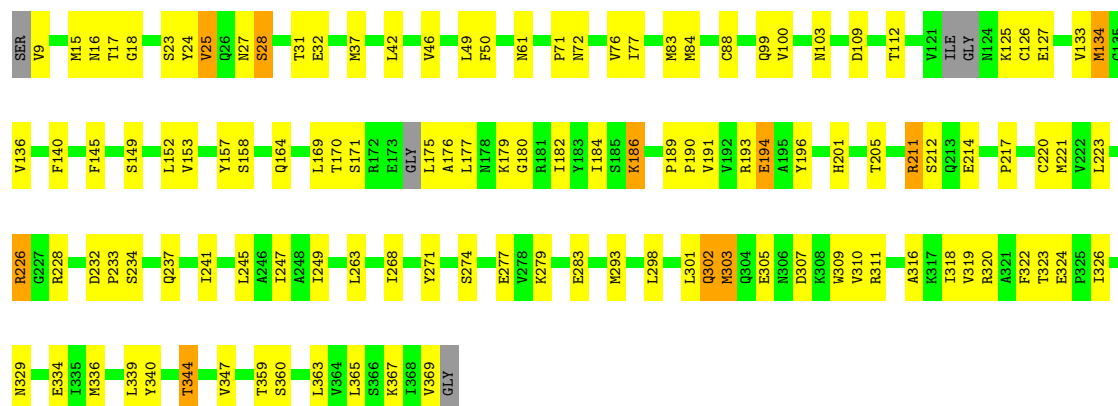
• Molecule 1: N-methyltransferase CkTcS

Chain D: 69% 26% . .



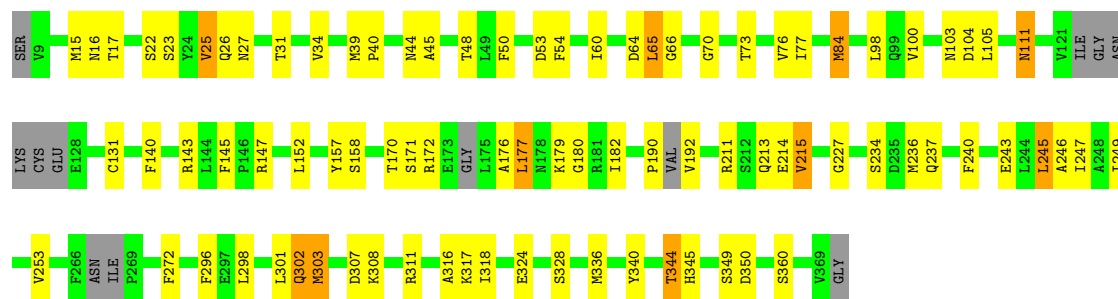
• Molecule 1: N-methyltransferase CkTcS

Chain E: 66% 30% . .



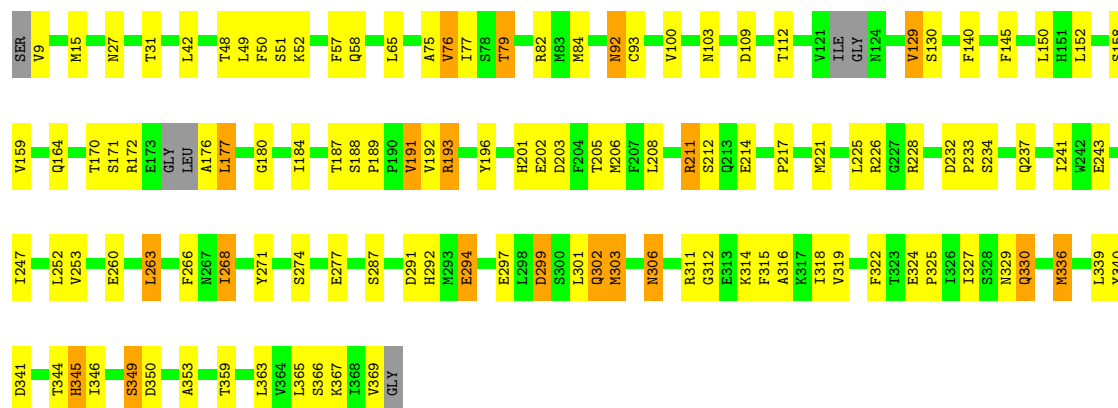
• Molecule 1: N-methyltransferase CkTcS

Chain F: 73% 21% . .



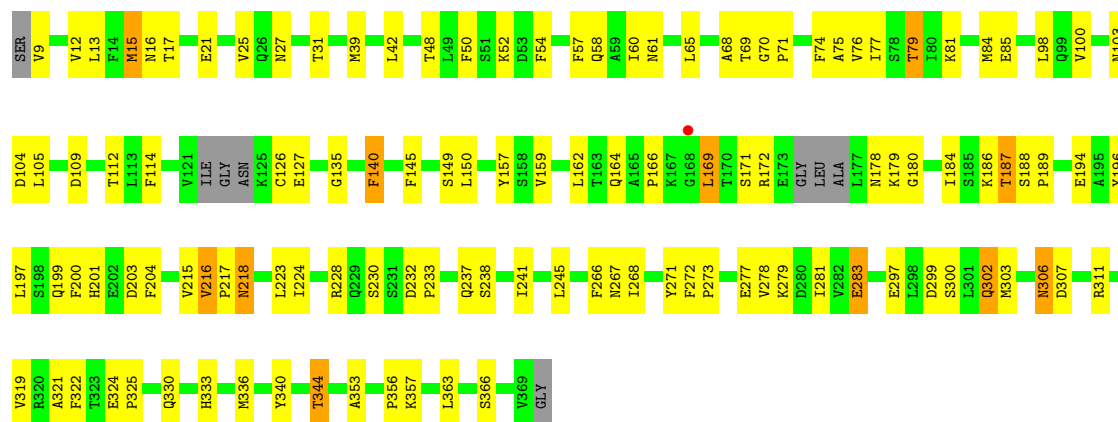
• Molecule 1: N-methyltransferase CkTcS

Chain G: 66% 27% 5%



• Molecule 1: N-methyltransferase CkTcS

Chain H: 65% 30%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	87.74Å 86.81Å 123.26Å 90.21° 90.04° 90.17°	Depositor
Resolution (Å)	43.87 – 3.15 43.87 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.87-3.15) 46.7 (43.87-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN, PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.263 , 0.298 0.263 , 0.307	Depositor DCC
R_{free} test set	1129 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 165.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,h,l 0.000 for k,-h,l 0.307 for -h,k,-l 0.307 for h,-k,-l 0.439 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20792	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4219e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EXU, 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	0.31	0/2696	0.79	4/3665 (0.1%)
1	B	0.34	0/2567	0.83	4/3501 (0.1%)
1	C	0.35	0/2499	0.80	2/3416 (0.1%)
1	D	0.31	0/2714	0.79	7/3684 (0.2%)
1	E	0.32	0/2703	0.80	4/3675 (0.1%)
1	F	0.32	0/2456	0.79	2/3357 (0.1%)
1	G	0.31	0/2704	0.80	2/3674 (0.1%)
1	H	0.32	0/2545	0.82	6/3481 (0.2%)
All	All	0.32	0/20884	0.80	31/28453 (0.1%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	188	SER	CA-C-N	8.62	129.26	120.38
1	H	188	SER	C-N-CA	8.62	129.26	120.38
1	G	302	GLN	CA-C-N	7.75	135.66	121.70
1	G	302	GLN	C-N-CA	7.75	135.66	121.70
1	E	126	CYS	CA-C-N	7.26	134.77	121.70
1	E	126	CYS	C-N-CA	7.26	134.77	121.70
1	D	126	CYS	CA-C-N	7.07	134.42	121.70
1	D	126	CYS	C-N-CA	7.07	134.42	121.70
1	B	302	GLN	CA-C-N	6.53	133.46	121.70
1	B	302	GLN	C-N-CA	6.53	133.46	121.70
1	A	302	GLN	CA-C-N	6.22	132.89	121.70
1	A	302	GLN	C-N-CA	6.22	132.89	121.70
1	D	302	GLN	CA-C-N	6.18	132.83	121.70
1	D	302	GLN	C-N-CA	6.18	132.83	121.70
1	H	302	GLN	CA-C-N	6.17	132.80	121.70
1	H	302	GLN	C-N-CA	6.17	132.80	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	GLN	CA-C-N	6.03	132.55	121.70
1	C	302	GLN	C-N-CA	6.03	132.55	121.70
1	B	121	VAL	CA-C-N	5.87	132.27	121.70
1	B	121	VAL	C-N-CA	5.87	132.27	121.70
1	E	302	GLN	CA-C-N	5.61	131.80	121.70
1	E	302	GLN	C-N-CA	5.61	131.80	121.70
1	D	68	ALA	CB-CA-C	-5.57	110.14	116.54
1	H	69	THR	N-CA-C	-5.55	107.51	114.56
1	H	68	ALA	CB-CA-C	-5.44	110.28	116.54
1	F	302	GLN	CA-C-N	5.22	131.09	121.70
1	F	302	GLN	C-N-CA	5.22	131.09	121.70
1	D	188	SER	CA-C-N	5.20	125.74	120.38
1	D	188	SER	C-N-CA	5.20	125.74	120.38
1	A	126	CYS	CA-C-N	5.04	130.77	121.70
1	A	126	CYS	C-N-CA	5.04	130.77	121.70

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	2644	0	2467	71	0
1	B	2517	0	2277	69	0
1	C	2450	0	2160	54	0
1	D	2662	0	2518	59	0
1	E	2649	0	2481	63	0
1	F	2411	0	2014	47	0
1	G	2652	0	2497	61	0
1	H	2493	0	2154	62	0
2	A	26	0	19	2	0
2	B	26	0	19	4	0
2	C	19	0	12	1	0
2	D	26	0	19	1	0
2	E	26	0	19	4	0
2	F	19	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	26	0	19	0	0
2	H	26	0	19	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
3	E	15	0	0	0	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
3	H	15	0	0	1	0
All	All	20792	0	18706	483	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 12.

All (483) 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:302:GLN:HA	1:H:303:MET:HB3	1.52	0.89
1:H:171:SER:H	1:H:172:ARG:HA	1.42	0.83
1:B:253:VAL:HG11	1:B:260:GLU:HB3	1.62	0.81
1:A:181:ARG:NH2	1:A:243:GLU:OE2	2.13	0.81
1:A:166:PRO:HA	1:A:199:GLN:HG3	1.62	0.81
1:A:171:SER:H	1:A:172:ARG:HA	1.46	0.80
1:A:303:MET:H	1:A:311:ARG:HD3	1.48	0.79
1:C:15:MET:HE2	2:C:501:SAH:H3'	1.66	0.76
1:G:171:SER:H	1:G:172:ARG:HA	1.49	0.76
1:E:176:ALA:HB3	1:E:177:LEU:HA	1.67	0.76
1:F:302:GLN:HA	1:F:303:MET:HB2	1.69	0.75
1:D:171:SER:H	1:D:172:ARG:HA	1.52	0.74
1:F:171:SER:H	1:F:172:ARG:HA	1.52	0.74
1:B:237:GLN:NE2	1:B:359:THR:OG1	2.20	0.74
1:D:140:PHE:O	1:D:211:ARG:NH2	2.21	0.74
1:H:228:ARG:NH2	1:H:277:GLU:OE2	2.20	0.74
1:D:15:MET:HE2	2:D:501:SAH:H3'	1.70	0.74
1:G:42:LEU:HD11	1:G:76:VAL:HG23	1.68	0.73
1:E:140:PHE:O	1:E:211:ARG:NH2	2.22	0.73
1:A:311:ARG:HE	1:A:353:ALA:HB1	1.54	0.73
1:G:253:VAL:HG11	1:G:260:GLU:HB3	1.70	0.73
1:E:49:LEU:HD11	1:E:152:LEU:HB2	1.71	0.73
1:E:212:SER:O	1:E:367:LYS:NZ	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:LEU:HB3	1:F:103:ASN:HB3	1.71	0.72
1:B:15:MET:HE2	2:B:501:SAH:H3'	1.71	0.71
1:B:228:ARG:NH1	1:B:272:PHE:O	2.24	0.70
1:A:140:PHE:O	1:A:211:ARG:NH2	2.24	0.70
1:D:211:ARG:NH1	1:D:214:GLU:OE1	2.25	0.69
1:A:49:LEU:HD11	1:A:152:LEU:HB2	1.75	0.69
1:G:237:GLN:NE2	1:G:359:THR:OG1	2.25	0.69
1:F:16:ASN:HB3	1:F:23:SER:HA	1.74	0.69
1:B:212:SER:O	1:B:367:LYS:NZ	2.24	0.69
1:A:136:VAL:HG22	1:D:134:MET:HG3	1.75	0.68
1:A:305:GLU:O	1:A:311:ARG:NH2	2.27	0.68
1:C:166:PRO:HG2	1:C:169:LEU:HD11	1.76	0.68
1:E:193:ARG:HG3	1:E:233:PRO:HG2	1.76	0.68
1:E:24:TYR:OH	2:E:501:SAH:N	2.27	0.67
1:E:153:VAL:HB	1:E:221:MET:HG3	1.76	0.67
1:C:319:VAL:O	1:C:323:THR:OG1	2.13	0.67
1:C:153:VAL:HB	1:C:221:MET:HG3	1.77	0.67
1:B:300:SER:OG	1:B:356:PRO:O	2.13	0.66
1:D:9:VAL:HG21	1:D:164:GLN:HA	1.77	0.66
1:E:28:SER:OG	1:E:72:ASN:ND2	2.24	0.66
1:G:9:VAL:HG21	1:G:164:GLN:HA	1.77	0.65
1:H:228:ARG:NH1	1:H:272:PHE:O	2.29	0.65
1:B:367:LYS:HE3	1:B:369:VAL:HB	1.78	0.65
1:A:15:MET:HE2	2:A:501:SAH:H3'	1.77	0.65
1:B:121:VAL:H	1:B:122:ILE:C	2.05	0.65
1:E:15:MET:HE2	2:E:501:SAH:H3'	1.78	0.65
1:H:104:ASP:OD1	1:H:105:LEU:N	2.30	0.65
1:C:211:ARG:NH1	1:C:214:GLU:OE1	2.30	0.65
1:A:40:PRO:O	1:A:44:ASN:ND2	2.30	0.64
1:C:302:GLN:HA	1:C:303:MET:HB3	1.79	0.64
1:E:184:ILE:HG21	1:E:233:PRO:HB2	1.79	0.64
1:A:237:GLN:NE2	1:A:359:THR:OG1	2.29	0.64
1:H:171:SER:N	1:H:172:ARG:HA	2.13	0.64
1:H:340:TYR:O	1:H:344:THR:OG1	2.15	0.64
1:D:49:LEU:HD11	1:D:152:LEU:HB2	1.80	0.63
1:E:228:ARG:HE	1:E:274:SER:HB3	1.64	0.63
1:B:50:PHE:HZ	1:B:84:MET:HG3	1.64	0.63
1:B:104:ASP:OD1	1:B:105:LEU:N	2.32	0.63
1:D:261:ASP:O	1:D:265:THR:OG1	2.16	0.63
1:H:65:LEU:HB3	1:H:140:PHE:HD2	1.64	0.63
1:B:23:SER:O	1:B:27:ASN:ND2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:MET:H	1:C:311:ARG:HD3	1.64	0.63
1:D:201:HIS:O	1:D:205:THR:OG1	2.16	0.63
1:H:65:LEU:HA	1:H:103:ASN:HB3	1.81	0.62
1:E:226:ARG:HH12	1:E:241:ILE:HG13	1.64	0.62
1:G:201:HIS:O	1:G:205:THR:OG1	2.16	0.62
1:G:226:ARG:HH12	1:G:241:ILE:HG13	1.65	0.62
1:E:9:VAL:HG21	1:E:164:GLN:HA	1.82	0.62
1:B:300:SER:HB2	1:B:301:LEU:HD13	1.82	0.62
1:C:227:GLY:HA2	1:C:272:PHE:HB3	1.82	0.62
1:A:50:PHE:HZ	1:A:84:MET:HG3	1.65	0.61
1:B:223:LEU:HD12	1:B:363:LEU:HD22	1.81	0.61
1:D:126:CYS:HA	1:D:127:GLU:CB	2.30	0.61
1:E:217:PRO:HA	1:E:367:LYS:HD3	1.81	0.61
1:E:305:GLU:O	1:E:311:ARG:NH2	2.34	0.61
1:A:16:ASN:HB3	1:A:23:SER:HA	1.83	0.61
1:A:302:GLN:HA	1:A:303:MET:HB2	1.83	0.61
1:E:103:ASN:ND2	1:E:136:VAL:O	2.33	0.61
1:H:237:GLN:NE2	1:H:357:LYS:O	2.33	0.61
1:G:140:PHE:O	1:G:211:ARG:NH2	2.33	0.61
1:G:306:ASN:OD1	1:G:306:ASN:N	2.34	0.61
1:E:77:ILE:HG12	1:E:100:VAL:HG11	1.83	0.60
1:G:345:HIS:O	1:G:349:SER:OG	2.19	0.60
1:F:27:ASN:HB3	1:F:318:ILE:HA	1.83	0.60
1:B:268:ILE:HD11	1:B:327:ILE:HD11	1.83	0.60
1:G:208:LEU:O	1:G:212:SER:OG	2.19	0.60
1:B:19:GLU:H	1:B:20:GLY:HA2	1.66	0.60
1:C:61:ASN:ND2	1:C:149:SER:O	2.29	0.60
1:B:215:VAL:HG23	1:B:367:LYS:HD2	1.84	0.59
1:D:237:GLN:NE2	1:D:359:THR:OG1	2.35	0.59
1:C:77:ILE:HG12	1:C:100:VAL:HG11	1.84	0.59
1:B:24:TYR:OH	2:B:501:SAH:N	2.29	0.59
1:F:15:MET:HE2	2:F:501:SAH:H3'	1.84	0.59
1:B:302:GLN:HA	1:B:303:MET:CB	2.32	0.59
1:D:23:SER:O	1:D:27:ASN:ND2	2.35	0.59
1:D:279:LYS:NZ	1:D:283:GLU:OE2	2.36	0.59
1:A:211:ARG:NH1	1:A:214:GLU:OE1	2.34	0.59
1:A:184:ILE:HG21	1:A:233:PRO:HB2	1.85	0.58
1:G:203:ASP:HA	1:G:206:MET:HE3	1.85	0.58
1:F:111:ASN:N	1:F:111:ASN:OD1	2.36	0.58
1:E:50:PHE:HZ	1:E:84:MET:HG3	1.68	0.58
1:E:211:ARG:NH1	1:E:214:GLU:OE1	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:HIS:NE2	1:G:294:GLU:OE1	2.30	0.58
1:F:104:ASP:OD1	1:F:105:LEU:N	2.35	0.58
1:C:285:ASP:OD2	1:C:287:SER:OG	2.22	0.57
1:B:49:LEU:HD11	1:B:152:LEU:HB2	1.86	0.57
1:A:171:SER:N	1:A:172:ARG:HA	2.17	0.57
1:C:17:THR:HB	1:C:109:ASP:HB2	1.87	0.57
1:D:230:SER:O	1:D:232:ASP:N	2.35	0.57
1:E:232:ASP:OD2	1:E:234:SER:OG	2.21	0.57
1:H:162:LEU:HD13	1:H:199:GLN:HG2	1.86	0.57
1:B:228:ARG:NH1	1:B:233:PRO:HB3	2.20	0.57
1:E:279:LYS:HB2	1:E:293:MET:HE1	1.86	0.56
1:D:221:MET:HB3	1:D:365:LEU:HB2	1.87	0.56
1:B:71:PRO:HA	1:B:74:PHE:HE1	1.70	0.56
1:D:249:ILE:HG12	1:D:339:LEU:HD21	1.85	0.56
1:H:114:PHE:HZ	1:H:135:GLY:HA3	1.70	0.56
2:E:501:SAH:N	2:E:501:SAH:SD	2.78	0.56
1:C:305:GLU:O	1:C:311:ARG:NH2	2.38	0.56
1:D:217:PRO:HA	1:D:367:LYS:HD2	1.88	0.56
1:A:347:VAL:HG13	1:A:355:LEU:HD11	1.88	0.56
1:D:291:ASP:OD2	1:D:366:SER:OG	2.24	0.56
1:B:96:LEU:HB2	1:B:129:VAL:HG12	1.88	0.55
1:A:208:LEU:O	1:A:212:SER:OG	2.18	0.55
1:G:211:ARG:NH1	1:G:214:GLU:OE1	2.39	0.55
1:C:176:ALA:HB1	1:C:177:LEU:HB2	1.89	0.55
1:C:140:PHE:O	1:C:211:ARG:NH2	2.39	0.55
1:E:237:GLN:NE2	1:E:359:THR:OG1	2.39	0.55
1:A:134:MET:HG2	1:D:136:VAL:HG22	1.89	0.55
1:B:19:GLU:N	1:B:20:GLY:HA2	2.22	0.55
1:C:228:ARG:NH2	1:C:277:GLU:OE2	2.40	0.55
1:H:9:VAL:O	1:H:13:LEU:N	2.38	0.55
1:A:226:ARG:HH12	1:A:241:ILE:HG13	1.72	0.55
1:G:299:ASP:OD1	1:G:299:ASP:N	2.40	0.55
1:B:301:LEU:O	1:B:303:MET:HB2	2.06	0.55
1:G:302:GLN:HA	1:G:303:MET:CB	2.36	0.54
1:E:336:MET:HE3	1:E:340:TYR:HE2	1.73	0.54
1:G:193:ARG:HG3	1:G:233:PRO:HG2	1.90	0.54
1:A:184:ILE:HG12	1:A:192:VAL:HG12	1.90	0.53
1:D:252:LEU:HD12	1:D:339:LEU:HD22	1.89	0.53
1:G:319:VAL:HA	1:G:322:PHE:CE2	2.44	0.53
1:C:169:LEU:HD13	1:C:267:ASN:HD22	1.72	0.53
1:F:40:PRO:O	1:F:44:ASN:ND2	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:HE3	1:A:340:TYR:HE2	1.72	0.53
1:B:266:PHE:CD1	1:B:330:GLN:HG3	2.43	0.53
1:E:226:ARG:NH1	1:E:241:ILE:HG13	2.23	0.53
1:G:77:ILE:HG23	1:G:100:VAL:HG21	1.90	0.53
1:E:279:LYS:NZ	1:E:283:GLU:OE2	2.42	0.53
1:C:203:ASP:HA	1:C:206:MET:HE3	1.90	0.52
1:C:296:PHE:HE1	1:C:362:ILE:HG13	1.74	0.52
1:D:302:GLN:HA	1:D:303:MET:CB	2.39	0.52
1:A:16:ASN:ND2	1:A:22:SER:O	2.35	0.52
1:G:232:ASP:OD2	1:G:234:SER:OG	2.19	0.52
1:B:181:ARG:NH2	1:B:187:THR:OG1	2.42	0.52
1:H:109:ASP:OD2	1:H:112:THR:OG1	2.23	0.52
1:F:16:ASN:ND2	1:F:22:SER:O	2.42	0.52
1:G:176:ALA:HB3	1:G:177:LEU:HA	1.92	0.52
1:A:217:PRO:HA	1:A:367:LYS:HD3	1.91	0.52
1:H:61:ASN:ND2	1:H:149:SER:O	2.39	0.52
1:D:178:ASN:OD1	1:D:188:SER:OG	2.24	0.52
1:E:27:ASN:O	1:E:318:ILE:HG13	2.09	0.52
1:C:25:VAL:HA	1:C:70:GLY:HA2	1.92	0.52
1:B:71:PRO:HA	1:B:74:PHE:CE1	2.45	0.51
1:E:201:HIS:O	1:E:205:THR:OG1	2.19	0.51
1:F:182:ILE:HG12	1:F:246:ALA:HB2	1.92	0.51
1:G:77:ILE:HG12	1:G:100:VAL:HG11	1.92	0.51
1:B:78:SER:HB3	1:H:187:THR:HG22	1.93	0.51
1:D:186:LYS:NZ	1:D:232:ASP:OD2	2.44	0.51
1:F:25:VAL:HA	1:F:70:GLY:HA2	1.92	0.51
1:C:184:ILE:HG21	1:C:233:PRO:HB2	1.91	0.51
1:A:291:ASP:OD2	1:A:366:SER:OG	2.24	0.51
1:G:217:PRO:HA	1:G:367:LYS:HD3	1.93	0.51
1:G:228:ARG:HE	1:G:274:SER:HB3	1.75	0.51
1:B:305:GLU:O	1:B:311:ARG:NH2	2.44	0.51
1:B:288:PHE:HB2	1:B:365:LEU:HB3	1.92	0.50
1:D:333:HIS:HA	1:D:336:MET:HG2	1.93	0.50
1:A:95:THR:O	1:D:147:ARG:NH2	2.43	0.50
1:C:211:ARG:HA	1:C:214:GLU:HG3	1.94	0.50
1:C:221:MET:HE3	1:C:223:LEU:HD11	1.93	0.50
1:G:49:LEU:HD11	1:G:152:LEU:HB2	1.94	0.50
1:H:25:VAL:HA	1:H:70:GLY:HA2	1.93	0.50
1:G:312:GLY:O	1:G:316:ALA:N	2.43	0.50
1:C:77:ILE:HD11	1:C:102:MET:HE3	1.93	0.50
1:C:279:LYS:HG3	1:C:293:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:LEU:HD11	1:H:178:ASN:HB3	1.94	0.49
1:A:201:HIS:CD2	1:A:281:ILE:HG12	2.47	0.49
1:D:43:GLU:HB3	1:D:83:MET:HE2	1.94	0.49
1:E:61:ASN:ND2	1:E:149:SER:O	2.43	0.49
1:G:340:TYR:O	1:G:344:THR:OG1	2.25	0.49
1:A:232:ASP:OD2	1:A:234:SER:OG	2.28	0.49
1:E:15:MET:HE2	2:E:501:SAH:H5'1	1.94	0.49
1:A:153:VAL:HB	1:A:221:MET:HG3	1.94	0.49
1:F:245:LEU:O	1:F:249:ILE:HG13	2.13	0.49
1:H:15:MET:HE2	2:H:501:SAH:H3'	1.94	0.49
1:H:311:ARG:HH11	1:H:353:ALA:HB3	1.78	0.49
1:D:307:ASP:OD1	1:D:308:LYS:N	2.44	0.49
1:A:228:ARG:NH2	1:A:277:GLU:OE2	2.46	0.49
1:G:336:MET:HE3	1:G:339:LEU:HD23	1.94	0.49
1:H:145:PHE:CD2	1:H:150:LEU:HD11	2.48	0.49
1:B:88:CYS:HB2	1:B:96:LEU:HD12	1.95	0.49
1:D:170:THR:HA	1:D:171:SER:HA	1.56	0.49
1:A:77:ILE:HG23	1:A:100:VAL:HG21	1.95	0.48
1:C:88:CYS:O	1:C:92:ASN:N	2.46	0.48
1:D:171:SER:N	1:D:172:ARG:HA	2.23	0.48
1:E:220:CYS:SG	1:E:221:MET:N	2.85	0.48
1:H:230:SER:C	1:H:232:ASP:H	2.21	0.48
1:H:300:SER:OG	1:H:356:PRO:O	2.31	0.48
1:E:307:ASP:HB3	1:E:310:VAL:HB	1.94	0.48
1:D:25:VAL:HG23	1:D:71:PRO:HD3	1.95	0.48
1:E:316:ALA:HB2	1:E:344:THR:HG23	1.96	0.48
1:F:157:TYR:OH	1:F:360:SER:OG	2.23	0.48
1:H:21:GLU:O	1:H:27:ASN:ND2	2.44	0.48
1:H:39:MET:HA	1:H:42:LEU:HD12	1.95	0.48
1:H:164:GLN:HG3	1:H:199:GLN:NE2	2.28	0.48
1:B:153:VAL:HB	1:B:221:MET:HG3	1.96	0.48
1:A:109:ASP:OD2	1:A:112:THR:OG1	2.22	0.48
1:H:77:ILE:HG12	1:H:100:VAL:HG11	1.96	0.48
1:H:164:GLN:HG3	1:H:199:GLN:HE22	1.77	0.48
1:E:179:LYS:HA	1:E:180:GLY:HA2	1.60	0.48
1:A:279:LYS:HB2	1:A:293:MET:HE1	1.95	0.48
1:G:184:ILE:HG12	1:G:192:VAL:HG12	1.95	0.48
1:H:77:ILE:HG23	1:H:100:VAL:HG21	1.96	0.48
1:F:171:SER:N	1:F:172:ARG:HA	2.25	0.48
1:G:27:ASN:O	1:G:318:ILE:HG13	2.14	0.48
1:B:109:ASP:OD2	1:B:112:THR:OG1	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PHE:CD1	1:B:150:LEU:HD11	2.49	0.47
1:C:244:LEU:HD13	1:C:347:VAL:HG22	1.94	0.47
1:D:50:PHE:HZ	1:D:84:MET:HG3	1.79	0.47
1:E:109:ASP:OD2	1:E:112:THR:OG1	2.32	0.47
1:A:169:LEU:HD13	1:A:267:ASN:HD22	1.79	0.47
1:H:60:ILE:HD12	1:H:84:MET:HE2	1.96	0.47
1:H:279:LYS:NZ	1:H:283:GLU:OE2	2.40	0.47
1:E:228:ARG:NH2	1:E:277:GLU:OE2	2.47	0.47
1:B:303:MET:HA	1:B:311:ARG:HD3	1.96	0.47
1:A:302:GLN:HA	1:A:303:MET:CB	2.44	0.47
1:C:350:ASP:OD1	1:C:350:ASP:N	2.47	0.47
1:D:336:MET:HE3	1:D:340:TYR:HE2	1.78	0.47
1:H:166:PRO:HB2	1:H:169:LEU:HD23	1.96	0.47
1:H:266:PHE:CD1	1:H:330:GLN:HG3	2.49	0.47
1:D:17:THR:HA	1:D:18:GLY:HA2	1.57	0.47
1:E:169:LEU:HA	1:E:177:LEU:HD12	1.96	0.47
1:A:48:THR:O	1:A:52:LYS:HG2	2.14	0.47
1:C:184:ILE:HD11	1:C:196:TYR:HB2	1.97	0.47
1:D:169:LEU:HD13	1:D:267:ASN:HD22	1.78	0.47
1:F:65:LEU:HA	1:F:66:GLY:HA2	1.71	0.47
1:H:15:MET:HE3	1:H:322:PHE:HB2	1.95	0.47
1:D:65:LEU:HA	1:D:103:ASN:HB3	1.97	0.47
1:F:211:ARG:O	1:F:215:VAL:HG23	2.15	0.47
1:G:92:ASN:HA	1:G:93:CYS:HA	1.49	0.47
1:G:65:LEU:HA	1:G:103:ASN:HB3	1.97	0.47
1:A:77:ILE:HG12	1:A:100:VAL:HG11	1.96	0.46
1:C:242:TRP:HZ3	1:C:323:THR:HG21	1.79	0.46
1:G:221:MET:HB3	1:G:365:LEU:HB2	1.97	0.46
1:C:76:VAL:O	1:C:80:ILE:HG12	2.15	0.46
1:G:109:ASP:OD2	1:G:112:THR:OG1	2.24	0.46
1:B:17:THR:HB	1:B:109:ASP:HB2	1.97	0.46
1:A:9:VAL:HG21	1:A:164:GLN:HA	1.96	0.46
1:D:266:PHE:CD1	1:D:330:GLN:HG3	2.50	0.46
1:F:170:THR:HA	1:F:171:SER:HA	1.72	0.46
1:H:71:PRO:HA	1:H:74:PHE:CD2	2.51	0.46
1:A:24:TYR:HA	1:A:321:ALA:HB1	1.98	0.46
1:E:157:TYR:OH	1:E:360:SER:OG	2.28	0.46
1:C:24:TYR:OH	1:C:31:THR:HG21	2.16	0.46
1:E:320:ARG:HE	1:E:324:GLU:CD	2.23	0.46
1:G:302:GLN:HA	1:G:303:MET:HB2	1.97	0.46
1:D:363:LEU:HD22	1:D:365:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:VAL:HA	1:A:322:PHE:CE2	2.51	0.46
1:C:333:HIS:HA	1:C:336:MET:HG2	1.97	0.46
1:F:345:HIS:O	1:F:349:SER:OG	2.26	0.46
1:H:57:PHE:HA	1:H:58:GLN:HA	1.51	0.46
1:C:302:GLN:HA	1:C:303:MET:CB	2.43	0.46
1:E:25:VAL:HG23	1:E:71:PRO:HD3	1.98	0.46
1:E:170:THR:HA	1:E:171:SER:HA	1.56	0.46
1:E:319:VAL:O	1:E:323:THR:OG1	2.25	0.46
1:B:319:VAL:HA	1:B:322:PHE:CE2	2.51	0.46
1:H:71:PRO:HA	1:H:74:PHE:HD2	1.80	0.46
1:B:43:GLU:HB3	1:B:83:MET:HE3	1.98	0.45
1:B:57:PHE:HA	1:B:58:GLN:HA	1.50	0.45
1:C:141:HIS:ND1	1:C:163:THR:HG23	2.32	0.45
1:F:350:ASP:OD1	1:F:350:ASP:N	2.48	0.45
1:G:303:MET:HE3	1:G:303:MET:HA	1.98	0.45
1:B:139:SER:HA	2:B:501:SAH:N1	2.31	0.45
1:C:296:PHE:CZ	1:C:360:SER:HB2	2.51	0.45
1:D:57:PHE:HA	1:D:58:GLN:HA	1.51	0.45
1:H:307:ASP:O	1:H:311:ARG:HG3	2.17	0.45
1:D:179:LYS:HA	1:D:180:GLY:HA2	1.61	0.45
1:B:50:PHE:HA	1:B:56:LEU:HD11	1.97	0.45
1:C:20:GLY:HA2	1:C:21:GLU:HA	1.70	0.45
1:F:84:MET:HE3	1:F:84:MET:HB2	1.87	0.45
1:A:50:PHE:CZ	1:A:84:MET:HG3	2.48	0.45
1:H:75:ALA:O	1:H:79:THR:HG22	2.17	0.45
1:B:75:ALA:O	1:B:79:THR:HG23	2.17	0.45
1:E:37:MET:HG3	1:E:298:LEU:HD21	1.99	0.45
1:E:249:ILE:HG12	1:E:339:LEU:HD11	1.98	0.45
1:G:189:PRO:HB2	1:G:191:VAL:HG23	1.98	0.45
1:H:81:LYS:O	1:H:85:GLU:N	2.48	0.45
1:E:319:VAL:HA	1:E:322:PHE:CE2	2.51	0.45
1:B:166:PRO:HG2	1:B:196:TYR:CE1	2.51	0.45
1:D:303:MET:H	1:D:311:ARG:HD3	1.82	0.45
1:H:31:THR:OG1	3:H:502:EXU:N9	2.50	0.45
1:H:126:CYS:HA	1:H:127:GLU:HA	1.63	0.45
1:B:189:PRO:HA	1:B:190:PRO:HA	1.84	0.45
1:B:235:ASP:O	1:B:238:SER:OG	2.32	0.45
1:A:202:GLU:HG2	1:A:206:MET:HE3	1.99	0.45
1:A:237:GLN:HE22	1:A:359:THR:HG1	1.59	0.45
1:E:136:VAL:HG21	1:E:145:PHE:HE2	1.82	0.45
1:F:302:GLN:CA	1:F:303:MET:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:O	1:B:26:GLN:NE2	2.50	0.44
1:B:52:LYS:C	1:B:54:PHE:H	2.25	0.44
1:F:77:ILE:HG12	1:F:100:VAL:HG11	1.99	0.44
1:G:75:ALA:O	1:G:79:THR:HG22	2.17	0.44
1:C:57:PHE:HA	1:C:58:GLN:HA	1.53	0.44
1:F:34:VAL:HG11	1:F:157:TYR:CE1	2.52	0.44
1:B:19:GLU:H	1:B:20:GLY:CA	2.29	0.44
1:A:102:MET:HE2	1:A:113:LEU:HD21	2.00	0.44
1:A:285:ASP:OD2	1:A:287:SER:OG	2.33	0.44
1:A:301:LEU:O	1:A:303:MET:HB2	2.17	0.44
1:B:120:LYS:H	1:B:120:LYS:HG2	1.64	0.44
1:A:104:ASP:OD1	1:A:105:LEU:N	2.50	0.44
1:D:169:LEU:HD13	1:D:267:ASN:ND2	2.32	0.44
1:E:245:LEU:O	1:E:249:ILE:HG13	2.17	0.44
1:F:50:PHE:HZ	1:F:84:MET:HG3	1.82	0.44
1:H:302:GLN:CA	1:H:303:MET:HB3	2.37	0.44
1:D:111:ASN:O	1:D:115:LYS:HB2	2.17	0.44
1:G:243:GLU:O	1:G:247:ILE:HG13	2.18	0.44
1:A:221:MET:HE3	1:A:221:MET:HB2	1.72	0.44
1:E:16:ASN:HB3	1:E:23:SER:HA	1.99	0.44
1:B:53:ASP:HA	1:B:56:LEU:HD13	2.00	0.44
1:A:79:THR:HG22	1:A:82:ARG:NH1	2.32	0.44
1:G:50:PHE:HZ	1:G:84:MET:HG3	1.83	0.44
1:G:145:PHE:CD2	1:G:150:LEU:HD11	2.53	0.44
1:B:211:ARG:O	1:B:215:VAL:HG22	2.18	0.44
1:D:315:PHE:O	1:D:318:ILE:HG22	2.18	0.44
1:D:340:TYR:O	1:D:344:THR:OG1	2.29	0.44
1:F:34:VAL:HG11	1:F:157:TYR:HE1	1.82	0.44
1:F:307:ASP:OD1	1:F:308:LYS:N	2.51	0.44
1:H:84:MET:HE1	1:H:98:LEU:HD13	2.00	0.44
1:H:157:TYR:N	1:H:224:ILE:O	2.43	0.44
1:F:176:ALA:HA	1:F:177:LEU:HA	1.86	0.43
1:F:301:LEU:O	1:F:303:MET:HB2	2.18	0.43
1:F:303:MET:H	1:F:311:ARG:HD3	1.82	0.43
1:B:261:ASP:O	1:B:265:THR:OG1	2.30	0.43
1:A:45:ALA:HB1	1:A:220:CYS:SG	2.58	0.43
1:C:77:ILE:HG23	1:C:100:VAL:HG21	1.99	0.43
1:D:99:GLN:NE2	1:D:134:MET:SD	2.91	0.43
1:G:57:PHE:HA	1:G:58:GLN:HA	1.52	0.43
1:H:178:ASN:HB3	1:H:267:ASN:HD21	1.82	0.43
1:C:170:THR:HA	1:C:171:SER:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:GLU:OE1	1:E:334:GLU:N	2.39	0.43
1:F:302:GLN:HA	1:F:303:MET:CB	2.45	0.43
1:G:196:TYR:HB3	1:G:271:TYR:CD1	2.54	0.43
1:C:163:THR:OG1	1:C:203:ASP:OD2	2.37	0.43
1:D:221:MET:HE3	1:D:221:MET:HB2	1.80	0.43
1:C:189:PRO:O	1:C:192:VAL:HG22	2.19	0.43
1:D:296:PHE:HE1	1:D:298:LEU:HD11	1.84	0.43
1:A:52:LYS:O	1:A:54:PHE:N	2.39	0.43
1:A:166:PRO:HG2	1:A:196:TYR:CE1	2.54	0.43
1:E:46:VAL:HG11	1:E:83:MET:HB3	2.00	0.43
1:E:189:PRO:HA	1:E:190:PRO:HD3	1.88	0.43
1:E:302:GLN:HA	1:E:303:MET:CB	2.48	0.43
1:F:60:ILE:HG23	1:F:98:LEU:HD13	1.99	0.43
1:H:199:GLN:HG3	1:H:203:ASP:OD1	2.19	0.43
1:H:200:PHE:CE2	1:H:273:PRO:HG3	2.53	0.43
1:F:45:ALA:O	1:F:48:THR:OG1	2.36	0.43
1:A:189:PRO:HA	1:A:190:PRO:HD3	1.85	0.43
1:F:64:ASP:OD2	1:F:73:THR:OG1	2.32	0.43
1:G:346:ILE:O	1:G:350:ASP:HB2	2.19	0.43
1:E:99:GLN:HE21	1:E:134:MET:HE1	1.83	0.43
1:E:363:LEU:HD22	1:E:365:LEU:HD21	2.01	0.43
1:G:171:SER:N	1:G:172:ARG:HA	2.20	0.43
1:G:291:ASP:OD2	1:G:366:SER:OG	2.25	0.43
1:B:164:GLN:HG3	1:B:199:GLN:NE2	2.34	0.42
1:B:211:ARG:O	1:B:214:GLU:N	2.51	0.42
1:A:228:ARG:HG3	1:A:230:SER:O	2.19	0.42
1:D:324:GLU:O	1:D:328:SER:HB2	2.19	0.42
1:E:17:THR:OG1	1:E:18:GLY:N	2.52	0.42
1:E:196:TYR:HB3	1:E:271:TYR:CD1	2.54	0.42
1:G:188:SER:HA	1:G:189:PRO:HD2	1.87	0.42
1:H:233:PRO:O	1:H:238:SER:OG	2.29	0.42
1:G:170:THR:HA	1:G:171:SER:HA	1.64	0.42
1:G:252:LEU:HD11	1:G:339:LEU:HA	2.01	0.42
1:B:114:PHE:O	1:B:118:SER:N	2.52	0.42
1:B:241:ILE:HD11	1:B:315:PHE:HZ	1.84	0.42
1:C:27:ASN:HD22	1:C:321:ALA:HB2	1.85	0.42
1:D:178:ASN:CB	1:D:267:ASN:HD21	2.33	0.42
1:E:191:VAL:HA	1:E:194:GLU:HB2	2.00	0.42
1:H:245:LEU:HD23	1:H:245:LEU:HA	1.91	0.42
1:A:15:MET:HG2	2:A:501:SAH:O3'	2.20	0.42
1:D:143:ARG:HH22	1:D:147:ARG:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:253:VAL:CG1	1:G:260:GLU:HB3	2.46	0.42
1:C:235:ASP:O	1:C:238:SER:OG	2.36	0.42
1:C:299:ASP:OD1	1:C:299:ASP:N	2.51	0.42
1:G:79:THR:HB	1:G:82:ARG:HH11	1.84	0.42
1:G:228:ARG:NH2	1:G:277:GLU:OE2	2.53	0.42
1:H:179:LYS:HA	1:H:180:GLY:HA2	1.78	0.42
1:B:315:PHE:HA	1:B:318:ILE:HG22	2.01	0.42
1:A:179:LYS:HA	1:A:180:GLY:HA2	1.57	0.42
1:C:171:SER:H	1:C:172:ARG:HA	1.85	0.42
1:F:179:LYS:HA	1:F:180:GLY:HA2	1.55	0.42
1:G:180:GLY:HA2	1:G:263:LEU:HD13	2.02	0.42
1:A:76:VAL:HG11	1:A:154:HIS:CE1	2.55	0.42
1:E:84:MET:HB2	1:E:84:MET:HE3	1.75	0.42
1:F:316:ALA:HB2	1:F:344:THR:HG23	2.02	0.42
1:B:302:GLN:HA	1:B:303:MET:HB3	2.00	0.42
1:A:184:ILE:HD11	1:A:196:TYR:HB2	2.01	0.42
1:C:45:ALA:HB1	1:C:220:CYS:SG	2.60	0.42
1:D:184:ILE:HG12	1:D:192:VAL:HG12	2.02	0.42
1:E:171:SER:HA	1:E:175:LEU:N	2.35	0.42
1:F:236:MET:O	1:F:240:PHE:N	2.53	0.42
1:B:302:GLN:HA	1:B:303:MET:HB2	2.02	0.42
1:D:300:SER:OG	1:D:356:PRO:O	2.34	0.42
1:G:84:MET:HG2	1:G:129:VAL:HG11	2.02	0.42
1:A:170:THR:HA	1:A:171:SER:HA	1.54	0.41
1:G:315:PHE:HA	1:G:318:ILE:HG22	2.02	0.41
1:H:50:PHE:HZ	1:H:84:MET:HG3	1.85	0.41
1:H:324:GLU:HB3	1:H:325:PRO:HD3	2.02	0.41
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.91	0.41
1:A:220:CYS:SG	1:A:221:MET:N	2.94	0.41
1:D:16:ASN:HB3	1:D:23:SER:HA	2.03	0.41
1:B:237:GLN:HA	1:B:356:PRO:HB2	2.01	0.41
1:C:44:ASN:O	1:C:48:THR:HG23	2.21	0.41
1:G:268:ILE:HD11	1:G:327:ILE:HD11	2.01	0.41
1:A:57:PHE:HA	1:A:58:GLN:HA	1.51	0.41
1:C:50:PHE:CE2	1:C:84:MET:HG2	2.55	0.41
1:D:153:VAL:HB	1:D:221:MET:HG3	2.03	0.41
1:E:182:ILE:HB	1:E:268:ILE:HG12	2.01	0.41
1:F:296:PHE:CE2	1:F:298:LEU:HD11	2.55	0.41
1:F:336:MET:HE3	1:F:340:TYR:HE2	1.85	0.41
1:B:27:ASN:O	1:B:318:ILE:HG13	2.21	0.41
1:F:211:ARG:O	1:F:214:GLU:N	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ARG:HH11	1:G:353:ALA:HB3	1.84	0.41
1:H:216:VAL:HG22	1:H:217:PRO:HD2	2.01	0.41
1:C:226:ARG:HH12	1:C:241:ILE:HG13	1.84	0.41
1:D:45:ALA:O	1:D:48:THR:OG1	2.37	0.41
1:D:109:ASP:OD2	1:D:112:THR:OG1	2.27	0.41
1:G:266:PHE:CD1	1:G:330:GLN:HG3	2.55	0.41
1:H:306:ASN:OD1	1:H:306:ASN:N	2.52	0.41
1:B:207:PHE:O	1:B:211:ARG:HG2	2.21	0.41
1:A:176:ALA:HA	1:A:177:LEU:HA	1.84	0.41
1:A:342:LYS:O	1:A:346:ILE:HG13	2.21	0.41
1:F:143:ARG:NH2	1:F:145:PHE:O	2.53	0.41
1:B:9:VAL:HG11	1:B:164:GLN:HA	2.03	0.41
1:A:53:ASP:O	1:A:56:LEU:HB2	2.21	0.41
1:C:80:ILE:HG22	1:C:84:MET:HE3	2.01	0.41
1:C:205:THR:O	1:C:209:ASN:N	2.35	0.41
1:E:186:LYS:HD2	1:E:234:SER:HB2	2.02	0.41
1:E:223:LEU:HB2	1:E:363:LEU:HB2	2.03	0.41
1:F:39:MET:N	1:F:40:PRO:HD2	2.36	0.41
1:F:190:PRO:HA	1:F:192:VAL:N	2.36	0.41
1:G:48:THR:O	1:G:52:LYS:N	2.42	0.41
1:H:52:LYS:C	1:H:54:PHE:H	2.28	0.41
1:H:278:VAL:HA	1:H:281:ILE:HD12	2.03	0.41
1:H:319:VAL:HA	1:H:322:PHE:CE2	2.56	0.41
1:B:156:SER:O	2:B:501:SAH:HB2	2.21	0.40
1:A:333:HIS:HA	1:A:336:MET:HG2	2.02	0.40
1:D:196:TYR:HB3	1:D:271:TYR:CD1	2.56	0.40
1:H:16:ASN:HB2	1:H:321:ALA:O	2.21	0.40
1:H:196:TYR:HB3	1:H:271:TYR:CD1	2.57	0.40
1:H:333:HIS:HA	1:H:336:MET:HG2	2.03	0.40
1:A:18:GLY:HA2	1:A:19:GLU:HA	1.93	0.40
1:C:52:LYS:O	1:C:54:PHE:N	2.48	0.40
1:C:207:PHE:O	1:C:211:ARG:HB2	2.21	0.40
1:D:84:MET:O	1:D:88:CYS:HB2	2.21	0.40
1:E:84:MET:O	1:E:88:CYS:N	2.53	0.40
1:E:302:GLN:HA	1:E:303:MET:HB3	2.03	0.40
1:F:147:ARG:HA	1:F:213:GLN:O	2.22	0.40
1:H:218:ASN:O	1:H:218:ASN:ND2	2.41	0.40
1:B:84:MET:HB2	1:B:84:MET:HE3	1.81	0.40
1:A:75:ALA:O	1:A:79:THR:HG23	2.21	0.40
1:A:84:MET:HE3	1:A:84:MET:HB2	1.82	0.40
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:ILE:HG23	1:F:100:VAL:HG21	2.02	0.40
1:G:324:GLU:HB3	1:G:325:PRO:HD3	2.02	0.40
1:B:243:GLU:O	1:B:247:ILE:HG13	2.22	0.40
1:B:320:ARG:O	1:B:324:GLU:HB2	2.22	0.40
1:F:27:ASN:O	1:F:318:ILE:HG13	2.22	0.40
1:B:228:ARG:HD3	1:B:233:PRO:HA	2.04	0.40
1:D:145:PHE:CD2	1:D:150:LEU:HD11	2.56	0.40
1:F:227:GLY:HA2	1:F:272:PHE:HB3	2.04	0.40
1:G:202:GLU:HG2	1:G:206:MET:HE2	2.04	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	352/363 (97%)	330 (94%)	21 (6%)	1 (0%)	36	64
1	B	344/363 (95%)	324 (94%)	18 (5%)	2 (1%)	21	52
1	C	339/363 (93%)	322 (95%)	17 (5%)	0	100	100
1	D	352/363 (97%)	329 (94%)	22 (6%)	1 (0%)	36	64
1	E	352/363 (97%)	329 (94%)	21 (6%)	2 (1%)	21	52
1	F	341/363 (94%)	319 (94%)	20 (6%)	2 (1%)	21	52
1	G	351/363 (97%)	330 (94%)	19 (5%)	2 (1%)	21	52
1	H	349/363 (96%)	327 (94%)	20 (6%)	2 (1%)	21	52
All	All	2780/2904 (96%)	2610 (94%)	158 (6%)	12 (0%)	30	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	127	GLU

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Mol	Chain	Res	Type
1	E	127	GLU
1	E	125	LYS
1	G	303	MET
1	F	53	ASP
1	F	54	PHE
1	G	92	ASN
1	A	126	CYS
1	B	190	PRO
1	H	184	ILE
1	B	189	PRO
1	H	189	PRO

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	268/323 (83%)	250 (93%)	18 (7%)	15	42
1	B	241/323 (75%)	218 (90%)	23 (10%)	8	29
1	C	231/323 (72%)	208 (90%)	23 (10%)	7	27
1	D	274/323 (85%)	249 (91%)	25 (9%)	9	30
1	E	268/323 (83%)	245 (91%)	23 (9%)	10	32
1	F	206/323 (64%)	181 (88%)	25 (12%)	5	20
1	G	272/323 (84%)	240 (88%)	32 (12%)	5	20
1	H	222/323 (69%)	194 (87%)	28 (13%)	4	18
All	All	1982/2584 (77%)	1785 (90%)	197 (10%)	7	27

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	25	VAL
1	B	47	GLU
1	B	74	PHE

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Mol	Chain	Res	Type
1	B	120	LYS
1	B	140	PHE
1	B	186	LYS
1	B	187	THR
1	B	192	VAL
1	B	202	GLU
1	B	224	ILE
1	B	226	ARG
1	B	228	ARG
1	B	232	ASP
1	B	245	LEU
1	B	265	THR
1	B	275	LEU
1	B	288	PHE
1	B	301	LEU
1	B	333	HIS
1	B	336	MET
1	B	339	LEU
1	B	366	SER
1	A	25	VAL
1	A	31	THR
1	A	42	LEU
1	A	76	VAL
1	A	96	LEU
1	A	130	SER
1	A	134	MET
1	A	158	SER
1	A	177	LEU
1	A	191	VAL
1	A	224	ILE
1	A	263	LEU
1	A	278	VAL
1	A	297	GLU
1	A	301	LEU
1	A	303	MET
1	A	314	LYS
1	A	345	HIS
1	C	25	VAL
1	C	32	GLU
1	C	76	VAL
1	C	79	THR
1	C	102	MET

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Mol	Chain	Res	Type
1	C	163	THR
1	C	211	ARG
1	C	214	GLU
1	C	226	ARG
1	C	243	GLU
1	C	251	GLU
1	C	275	LEU
1	C	287	SER
1	C	297	GLU
1	C	299	ASP
1	C	301	LEU
1	C	303	MET
1	C	323	THR
1	C	330	GLN
1	C	344	THR
1	C	350	ASP
1	C	360	SER
1	C	363	LEU
1	D	31	THR
1	D	60	ILE
1	D	76	VAL
1	D	83	MET
1	D	88	CYS
1	D	95	THR
1	D	120	LYS
1	D	158	SER
1	D	191	VAL
1	D	205	THR
1	D	211	ARG
1	D	263	LEU
1	D	265	THR
1	D	275	LEU
1	D	297	GLU
1	D	298	LEU
1	D	301	LEU
1	D	306	ASN
1	D	314	LYS
1	D	318	ILE
1	D	328	SER
1	D	339	LEU
1	D	342	LYS
1	D	354	LYS

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Mol	Chain	Res	Type
1	D	367	LYS
1	E	25	VAL
1	E	28	SER
1	E	31	THR
1	E	32	GLU
1	E	42	LEU
1	E	76	VAL
1	E	133	VAL
1	E	134	MET
1	E	158	SER
1	E	186	LYS
1	E	194	GLU
1	E	211	ARG
1	E	226	ARG
1	E	247	ILE
1	E	263	LEU
1	E	301	LEU
1	E	303	MET
1	E	309	TRP
1	E	326	ILE
1	E	329	ASN
1	E	344	THR
1	E	347	VAL
1	E	369	VAL
1	F	17	THR
1	F	25	VAL
1	F	26	GLN
1	F	31	THR
1	F	65	LEU
1	F	76	VAL
1	F	84	MET
1	F	111	ASN
1	F	131	CYS
1	F	140	PHE
1	F	152	LEU
1	F	158	SER
1	F	177	LEU
1	F	215	VAL
1	F	234	SER
1	F	237	GLN
1	F	243	GLU
1	F	245	LEU

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Mol	Chain	Res	Type
1	F	247	ILE
1	F	253	VAL
1	F	303	MET
1	F	317	LYS
1	F	324	GLU
1	F	328	SER
1	F	344	THR
1	G	15	MET
1	G	31	THR
1	G	51	SER
1	G	76	VAL
1	G	79	THR
1	G	129	VAL
1	G	130	SER
1	G	158	SER
1	G	159	VAL
1	G	177	LEU
1	G	187	THR
1	G	191	VAL
1	G	193	ARG
1	G	211	ARG
1	G	225	LEU
1	G	263	LEU
1	G	268	ILE
1	G	287	SER
1	G	294	GLU
1	G	297	GLU
1	G	299	ASP
1	G	301	LEU
1	G	306	ASN
1	G	314	LYS
1	G	329	ASN
1	G	330	GLN
1	G	336	MET
1	G	341	ASP
1	G	345	HIS
1	G	349	SER
1	G	363	LEU
1	G	369	VAL
1	H	12	VAL
1	H	15	MET
1	H	17	THR

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Mol	Chain	Res	Type
1	H	48	THR
1	H	76	VAL
1	H	79	THR
1	H	140	PHE
1	H	159	VAL
1	H	169	LEU
1	H	186	LYS
1	H	187	THR
1	H	194	GLU
1	H	197	LEU
1	H	201	HIS
1	H	204	PHE
1	H	215	VAL
1	H	216	VAL
1	H	218	ASN
1	H	223	LEU
1	H	241	ILE
1	H	268	ILE
1	H	283	GLU
1	H	297	GLU
1	H	299	ASP
1	H	306	ASN
1	H	344	THR
1	H	363	LEU
1	H	366	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	26	GLN
1	B	55	HIS
1	B	103	ASN
1	B	237	GLN
1	A	108	ASN
1	A	199	GLN
1	A	201	HIS
1	A	213	GLN
1	A	237	GLN
1	A	267	ASN
1	A	330	GLN
1	C	27	ASN
1	C	72	ASN

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Mol	Chain	Res	Type
1	C	103	ASN
1	C	154	HIS
1	C	267	ASN
1	D	99	GLN
1	D	199	GLN
1	D	229	GLN
1	D	237	GLN
1	D	267	ASN
1	E	27	ASN
1	E	72	ASN
1	E	237	GLN
1	E	267	ASN
1	F	26	GLN
1	F	108	ASN
1	F	199	GLN
1	F	213	GLN
1	G	72	ASN
1	G	201	HIS
1	G	267	ASN
1	H	26	GLN
1	H	199	GLN
1	H	267	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
3	EXU	A	502	-	16,16,16	1.11	3 (18%)	24,25,25	1.60	5 (20%)
3	EXU	E	502	-	16,16,16	1.13	3 (18%)	24,25,25	1.58	4 (16%)
2	SAH	D	501	-	27,28,28	1.09	4 (14%)	36,40,40	2.08	10 (27%)
2	SAH	H	501	-	27,28,28	1.09	3 (11%)	36,40,40	2.05	10 (27%)
3	EXU	F	502	-	16,16,16	1.11	3 (18%)	24,25,25	1.56	4 (16%)
3	EXU	H	502	-	16,16,16	1.12	3 (18%)	24,25,25	1.57	4 (16%)
2	SAH	G	501	-	27,28,28	1.09	4 (14%)	36,40,40	2.01	9 (25%)
3	EXU	B	502	-	16,16,16	1.14	3 (18%)	24,25,25	1.60	5 (20%)
2	SAH	A	501	-	27,28,28	1.09	3 (11%)	36,40,40	2.11	10 (27%)
2	SAH	F	501	-	21,21,28	1.13	2 (9%)	30,31,40	2.09	8 (26%)
2	SAH	B	501	-	27,28,28	1.10	4 (14%)	36,40,40	2.07	10 (27%)
3	EXU	G	502	-	16,16,16	1.12	3 (18%)	24,25,25	1.63	5 (20%)
3	EXU	C	502	-	16,16,16	1.11	3 (18%)	24,25,25	1.57	4 (16%)
2	SAH	C	501	-	21,21,28	1.15	3 (14%)	30,31,40	2.10	8 (26%)
3	EXU	D	502	-	16,16,16	1.10	3 (18%)	24,25,25	1.59	4 (16%)
2	SAH	E	501	-	27,28,28	1.11	4 (14%)	36,40,40	2.16	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EXU	A	502	-	-	-	0/2/2/2
3	EXU	E	502	-	-	-	0/2/2/2
2	SAH	D	501	-	-	6/15/31/31	0/3/3/3
2	SAH	H	501	-	-	4/15/31/31	0/3/3/3
3	EXU	F	502	-	-	-	0/2/2/2
3	EXU	H	502	-	-	-	0/2/2/2
2	SAH	G	501	-	-	4/15/31/31	0/3/3/3
3	EXU	B	502	-	-	-	0/2/2/2
2	SAH	A	501	-	-	8/15/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	F	501	-	-	0/6/22/31	0/3/3/3
2	SAH	B	501	-	-	2/15/31/31	0/3/3/3
3	EXU	G	502	-	-	-	0/2/2/2
3	EXU	C	502	-	-	-	0/2/2/2
2	SAH	C	501	-	-	0/6/22/31	0/3/3/3
3	EXU	D	502	-	-	-	0/2/2/2
2	SAH	E	501	-	-	4/15/31/31	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAH	C2-N3	2.62	1.38	1.33
2	C	501	SAH	C2-N1	2.59	1.38	1.33
2	D	501	SAH	C2-N3	2.59	1.38	1.33
2	H	501	SAH	C2-N3	2.59	1.38	1.33
2	F	501	SAH	C2-N3	2.58	1.38	1.33
2	B	501	SAH	C2-N1	2.57	1.38	1.33
2	E	501	SAH	C2-N1	2.54	1.38	1.33
2	C	501	SAH	C2-N3	2.53	1.38	1.33
2	G	501	SAH	C2-N1	2.53	1.38	1.33
2	H	501	SAH	C2-N1	2.53	1.38	1.33
2	G	501	SAH	C2-N3	2.52	1.38	1.33
2	B	501	SAH	C2-N3	2.52	1.38	1.33
2	E	501	SAH	C2-N3	2.51	1.38	1.33
2	F	501	SAH	C2-N1	2.51	1.38	1.33
2	D	501	SAH	C2-N1	2.46	1.38	1.33
3	A	502	EXU	CAK-N3	-2.44	1.42	1.47
2	A	501	SAH	C2-N1	2.42	1.38	1.33
3	E	502	EXU	CAJ-N1	-2.39	1.42	1.47
3	B	502	EXU	CAK-N3	-2.39	1.42	1.47
3	G	502	EXU	CAK-N3	-2.39	1.42	1.47
3	H	502	EXU	CAK-N3	-2.38	1.42	1.47
2	E	501	SAH	OXT-C	-2.38	1.23	1.30
3	D	502	EXU	CAK-N3	-2.36	1.42	1.47
3	E	502	EXU	CAK-N3	-2.36	1.42	1.47
3	C	502	EXU	CAK-N3	-2.36	1.42	1.47
3	D	502	EXU	CAJ-N1	-2.35	1.42	1.47
3	B	502	EXU	CAJ-N1	-2.34	1.42	1.47
3	F	502	EXU	CAK-N3	-2.33	1.42	1.47
3	H	502	EXU	CAJ-N1	-2.32	1.42	1.47
3	G	502	EXU	CAJ-N1	-2.32	1.42	1.47
3	F	502	EXU	CAJ-N1	-2.32	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	EXU	CAJ-N1	-2.28	1.43	1.47
3	C	502	EXU	CAJ-N1	-2.28	1.43	1.47
2	G	501	SAH	OXT-C	-2.27	1.23	1.30
2	H	501	SAH	OXT-C	-2.27	1.23	1.30
2	B	501	SAH	OXT-C	-2.25	1.23	1.30
2	D	501	SAH	OXT-C	-2.25	1.23	1.30
2	A	501	SAH	OXT-C	-2.24	1.23	1.30
3	E	502	EXU	CAL-N7	-2.20	1.43	1.47
3	B	502	EXU	CAL-N7	-2.20	1.43	1.47
2	C	501	SAH	C8-N7	2.16	1.35	1.31
3	C	502	EXU	CAL-N7	-2.16	1.43	1.47
3	G	502	EXU	CAL-N7	-2.14	1.43	1.47
2	B	501	SAH	C5-N7	-2.12	1.35	1.39
3	F	502	EXU	CAL-N7	-2.10	1.43	1.47
3	H	502	EXU	CAL-N7	-2.10	1.43	1.47
3	A	502	EXU	CAL-N7	-2.08	1.43	1.47
3	D	502	EXU	CAL-N7	-2.05	1.43	1.47
2	D	501	SAH	C5-N7	-2.02	1.35	1.39
2	G	501	SAH	C5-N7	-2.02	1.35	1.39
2	E	501	SAH	C5-N7	-2.02	1.35	1.39

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SAH	N3-C2-N1	-5.67	120.00	128.58
2	D	501	SAH	N3-C2-N1	-5.66	120.01	128.58
2	E	501	SAH	N3-C2-N1	-5.62	120.07	128.58
2	F	501	SAH	N3-C2-N1	-5.60	120.11	128.58
2	G	501	SAH	N3-C2-N1	-5.56	120.17	128.58
2	A	501	SAH	N3-C2-N1	-5.53	120.22	128.58
2	C	501	SAH	N3-C2-N1	-5.50	120.26	128.58
2	H	501	SAH	N3-C2-N1	-5.43	120.36	128.58
2	E	501	SAH	C5'-SD-CG	-5.35	86.39	102.26
3	C	502	EXU	C5-C6-N1	4.58	120.46	112.06
3	B	502	EXU	C5-C6-N1	4.55	120.39	112.06
3	F	502	EXU	C5-C6-N1	4.52	120.34	112.06
3	G	502	EXU	C5-C6-N1	4.51	120.33	112.06
3	E	502	EXU	C5-C6-N1	4.48	120.26	112.06
3	D	502	EXU	C5-C6-N1	4.46	120.24	112.06
3	A	502	EXU	C5-C6-N1	4.45	120.21	112.06
2	A	501	SAH	C5'-SD-CG	-4.45	89.07	102.26
2	C	501	SAH	C5-C4-N3	-4.44	120.60	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SAH	C5-C4-N3	-4.40	120.66	126.72
2	H	501	SAH	C5-C4-N3	-4.37	120.71	126.72
2	D	501	SAH	C5-C4-N3	-4.26	120.84	126.72
2	F	501	SAH	C5-C4-N3	-4.26	120.85	126.72
2	B	501	SAH	C5-C4-N3	-4.11	121.06	126.72
2	E	501	SAH	N9-C8-N7	-4.10	108.11	113.94
2	E	501	SAH	C5-C4-N3	-4.08	121.09	126.72
2	G	501	SAH	C5-C4-N3	-4.08	121.10	126.72
2	C	501	SAH	N9-C8-N7	-4.02	108.23	113.94
2	F	501	SAH	N9-C8-N7	-4.00	108.26	113.94
2	D	501	SAH	C5'-SD-CG	-3.98	90.45	102.26
2	A	501	SAH	N9-C8-N7	-3.98	108.29	113.94
2	G	501	SAH	N9-C8-N7	-3.91	108.38	113.94
2	B	501	SAH	N9-C8-N7	-3.83	108.50	113.94
3	H	502	EXU	C5-C6-N1	3.81	119.04	112.06
2	D	501	SAH	N9-C8-N7	-3.76	108.59	113.94
2	B	501	SAH	C5'-SD-CG	-3.76	91.11	102.26
2	H	501	SAH	N9-C8-N7	-3.71	108.68	113.94
2	E	501	SAH	C5-N7-C8	3.64	109.17	103.45
2	H	501	SAH	C5'-SD-CG	-3.63	91.49	102.26
2	A	501	SAH	C5-N7-C8	3.63	109.15	103.45
2	D	501	SAH	C5-N7-C8	3.58	109.07	103.45
2	F	501	SAH	C5-N7-C8	3.56	109.05	103.45
2	H	501	SAH	C5-N7-C8	3.50	108.95	103.45
2	C	501	SAH	C5-N7-C8	3.50	108.94	103.45
2	G	501	SAH	C5-N7-C8	3.47	108.91	103.45
2	G	501	SAH	C5'-SD-CG	-3.47	91.97	102.26
2	B	501	SAH	C5-N7-C8	3.39	108.78	103.45
2	C	501	SAH	C2-N3-C4	3.38	120.09	111.83
2	D	501	SAH	C2-N3-C4	3.37	120.06	111.83
2	A	501	SAH	C2-N3-C4	3.37	120.05	111.83
3	H	502	EXU	C6-N1-C2	-3.35	120.22	125.66
2	F	501	SAH	C2-N3-C4	3.34	120.00	111.83
2	E	501	SAH	C2-N3-C4	3.29	119.88	111.83
2	H	501	SAH	C2-N3-C4	3.29	119.86	111.83
2	G	501	SAH	C2-N3-C4	3.20	119.66	111.83
2	B	501	SAH	C2-N3-C4	3.20	119.64	111.83
2	B	501	SAH	OXT-C-O	-3.18	116.87	124.08
2	H	501	SAH	OXT-C-O	-3.16	116.90	124.08
3	B	502	EXU	C6-N1-C2	-3.12	120.58	125.66
3	A	502	EXU	O6-C6-C5	-3.10	120.02	126.38
3	A	502	EXU	C6-N1-C2	-3.08	120.65	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	EXU	C6-N1-C2	-3.07	120.67	125.66
3	H	502	EXU	O6-C6-C5	-3.06	120.10	126.38
3	G	502	EXU	C6-C5-N7	3.03	134.80	131.26
3	C	502	EXU	C6-N1-C2	-2.99	120.79	125.66
3	D	502	EXU	C6-N1-C2	-2.99	120.80	125.66
3	G	502	EXU	C6-N1-C2	-2.95	120.87	125.66
2	A	501	SAH	N3-C4-N9	2.91	132.12	127.17
2	C	501	SAH	N3-C4-N9	2.91	132.12	127.17
3	B	502	EXU	C6-C5-N7	2.88	134.63	131.26
3	H	502	EXU	C6-C5-N7	2.87	134.61	131.26
2	D	501	SAH	O4'-C1'-N9	2.84	113.55	108.09
3	G	502	EXU	O6-C6-C5	-2.82	120.61	126.38
2	D	501	SAH	OXT-C-O	-2.82	117.68	124.08
2	D	501	SAH	C4-C5-N7	-2.79	107.39	110.58
2	G	501	SAH	OXT-C-O	-2.79	117.75	124.08
3	D	502	EXU	O6-C6-C5	-2.77	120.71	126.38
2	B	501	SAH	N3-C4-N9	2.77	131.88	127.17
2	E	501	SAH	N3-C4-N9	2.76	131.87	127.17
2	F	501	SAH	N3-C4-N9	2.76	131.85	127.17
2	A	501	SAH	OXT-C-O	-2.73	117.89	124.08
3	C	502	EXU	O6-C6-C5	-2.73	120.79	126.38
2	E	501	SAH	OXT-C-O	-2.72	117.90	124.08
3	E	502	EXU	C6-N1-C2	-2.71	121.26	125.66
3	E	502	EXU	O6-C6-C5	-2.71	120.84	126.38
2	H	501	SAH	C4-C5-N7	-2.70	107.49	110.58
2	H	501	SAH	N3-C4-N9	2.70	131.75	127.17
2	G	501	SAH	N3-C4-N9	2.69	131.75	127.17
3	F	502	EXU	O6-C6-C5	-2.68	120.90	126.38
3	B	502	EXU	O6-C6-C5	-2.62	121.00	126.38
3	E	502	EXU	C6-C5-N7	2.62	134.32	131.26
2	A	501	SAH	C4-C5-N7	-2.62	107.59	110.58
2	B	501	SAH	O4'-C1'-N9	2.61	113.11	108.09
3	C	502	EXU	C6-C5-N7	2.60	134.30	131.26
2	F	501	SAH	C4-C5-N7	-2.60	107.61	110.58
2	D	501	SAH	N3-C4-N9	2.57	131.54	127.17
2	H	501	SAH	O4'-C1'-N9	2.56	113.00	108.09
2	E	501	SAH	C4-C5-N7	-2.55	107.67	110.58
2	C	501	SAH	O4'-C1'-N9	2.49	112.87	108.09
2	F	501	SAH	O4'-C1'-N9	2.45	112.80	108.09
2	G	501	SAH	C4-C5-N7	-2.45	107.78	110.58
3	D	502	EXU	C6-C5-N7	2.43	134.10	131.26
3	A	502	EXU	C6-C5-N7	2.43	134.10	131.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	EXU	C6-C5-N7	2.42	134.09	131.26
2	C	501	SAH	C4-C5-N7	-2.41	107.83	110.58
2	B	501	SAH	C4-C5-N7	-2.33	107.92	110.58
2	A	501	SAH	O4'-C1'-N9	2.29	112.48	108.09
3	A	502	EXU	CAK-N3-C4	-2.27	117.86	120.98
3	G	502	EXU	CAK-N3-C4	-2.21	117.94	120.98
2	E	501	SAH	C4-N9-C8	2.16	108.00	105.74
3	B	502	EXU	CAK-N3-C4	-2.05	118.16	120.98

There are no chirality outliers.

All (28) torsion outliers are listed below:

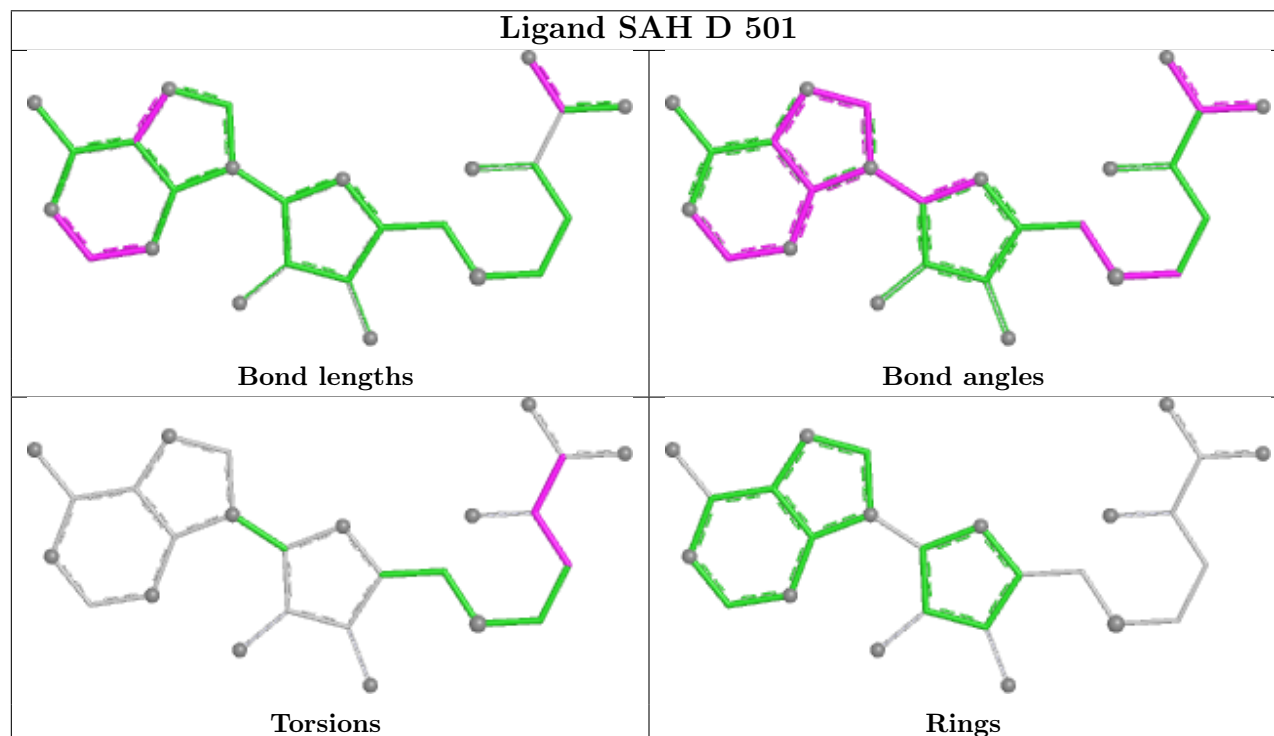
Mol	Chain	Res	Type	Atoms
2	B	501	SAH	C-CA-CB-CG
2	E	501	SAH	C3'-C4'-C5'-SD
2	A	501	SAH	CA-CB-CG-SD
2	H	501	SAH	OXT-C-CA-N
2	B	501	SAH	CA-CB-CG-SD
2	A	501	SAH	C-CA-CB-CG
2	A	501	SAH	OXT-C-CA-N
2	D	501	SAH	C-CA-CB-CG
2	G	501	SAH	C-CA-CB-CG
2	D	501	SAH	N-CA-CB-CG
2	E	501	SAH	OXT-C-CA-CB
2	A	501	SAH	O4'-C4'-C5'-SD
2	E	501	SAH	O4'-C4'-C5'-SD
2	E	501	SAH	O-C-CA-CB
2	G	501	SAH	OXT-C-CA-CB
2	G	501	SAH	CB-CG-SD-C5'
2	G	501	SAH	O-C-CA-CB
2	H	501	SAH	C-CA-CB-CG
2	H	501	SAH	CB-CG-SD-C5'
2	A	501	SAH	O-C-CA-CB
2	D	501	SAH	O-C-CA-CB
2	D	501	SAH	OXT-C-CA-CB
2	A	501	SAH	OXT-C-CA-CB
2	A	501	SAH	N-CA-CB-CG
2	A	501	SAH	C3'-C4'-C5'-SD
2	D	501	SAH	OXT-C-CA-N
2	D	501	SAH	O-C-CA-N
2	H	501	SAH	O-C-CA-N

There are no ring outliers.

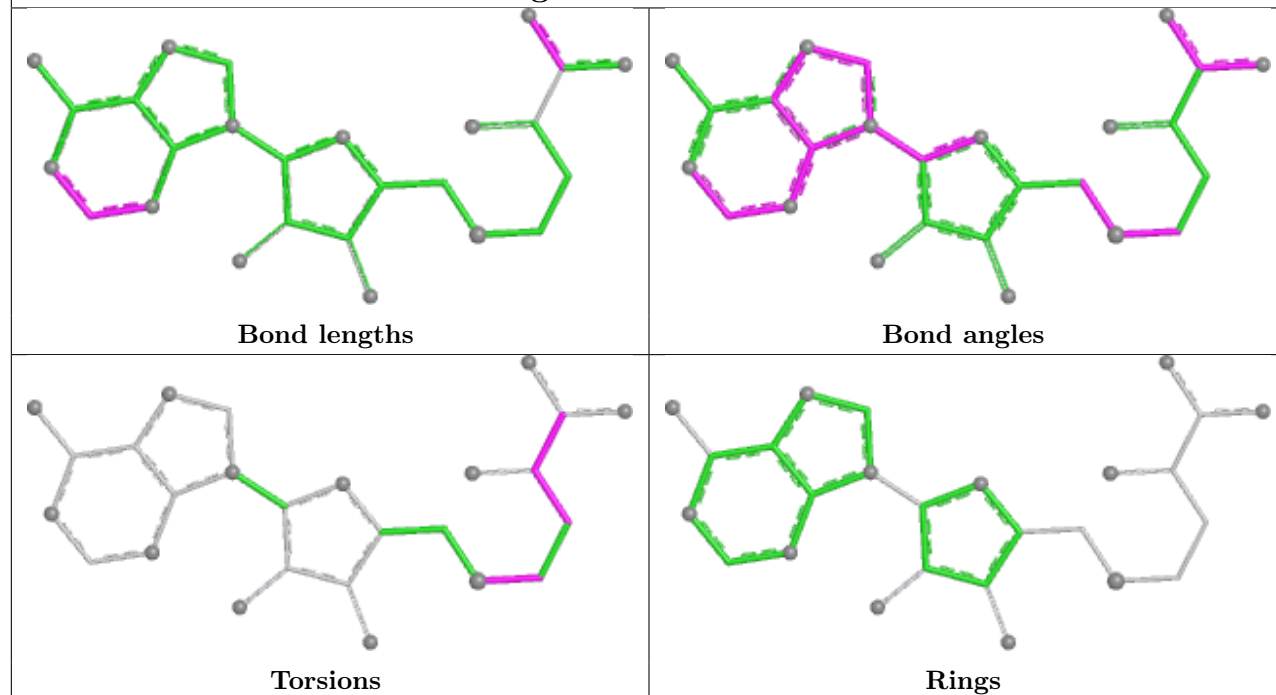
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	SAH	1	0
2	H	501	SAH	1	0
3	H	502	EXU	1	0
2	A	501	SAH	2	0
2	F	501	SAH	1	0
2	B	501	SAH	4	0
2	C	501	SAH	1	0
2	E	501	SAH	4	0

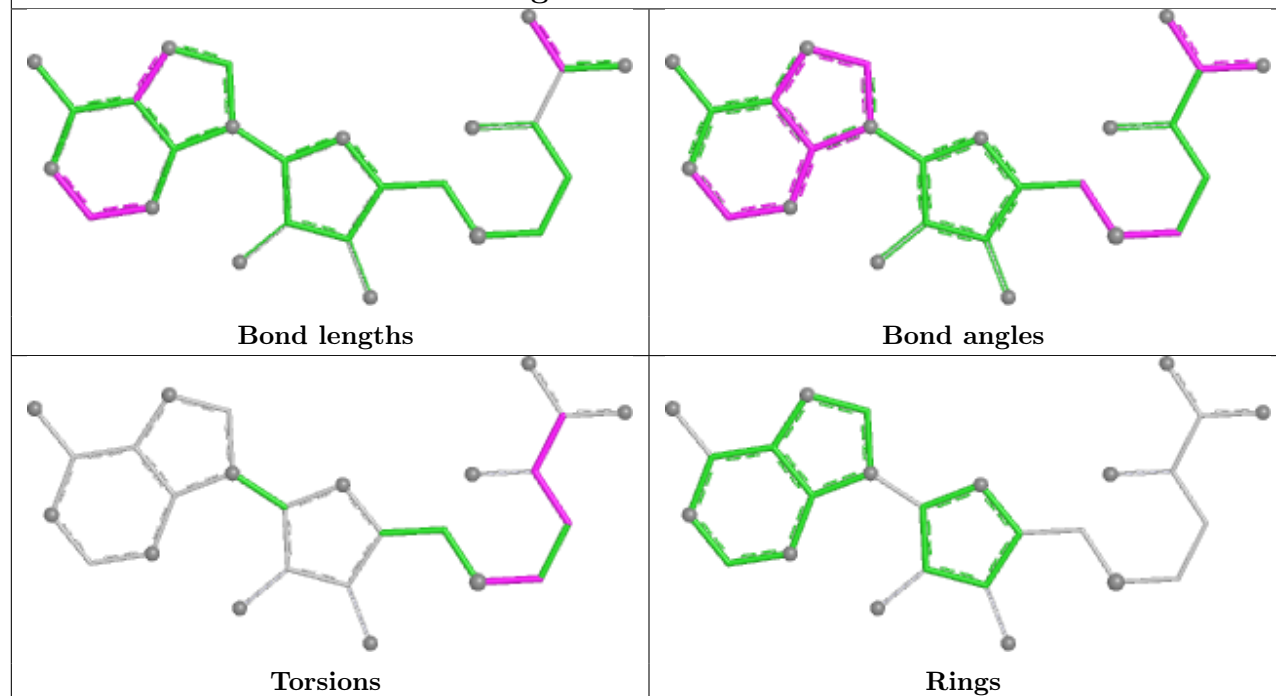
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



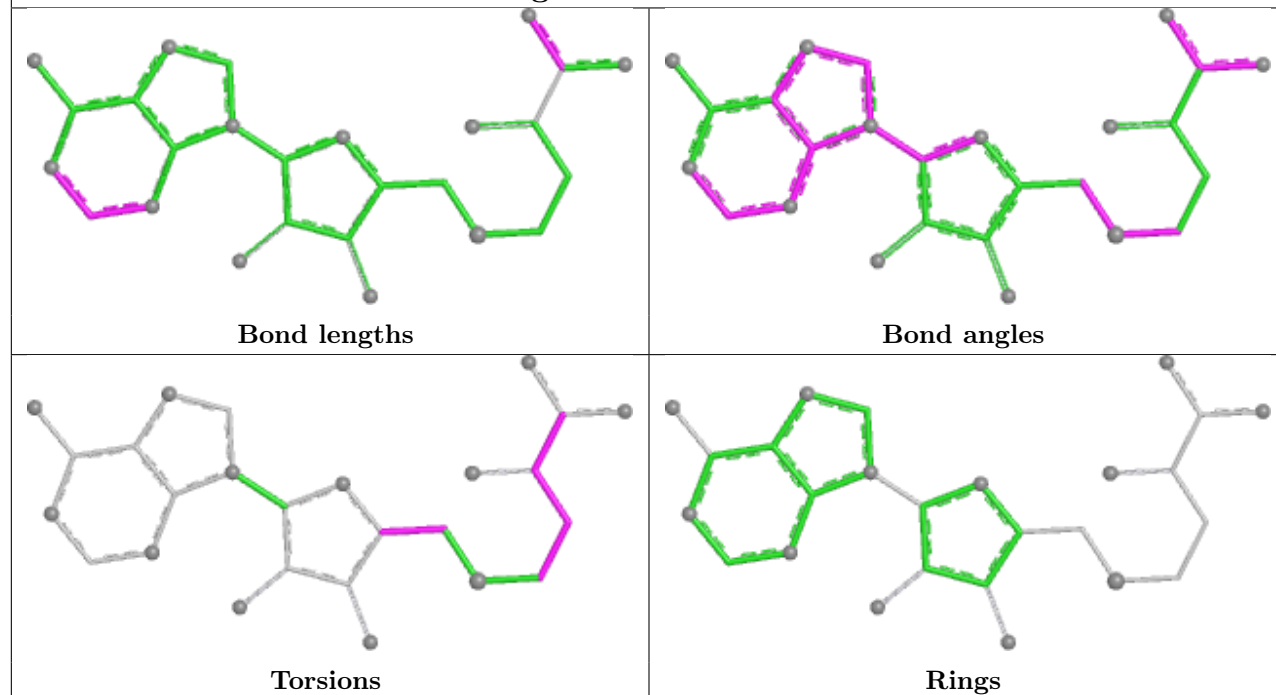
Ligand SAH H 501



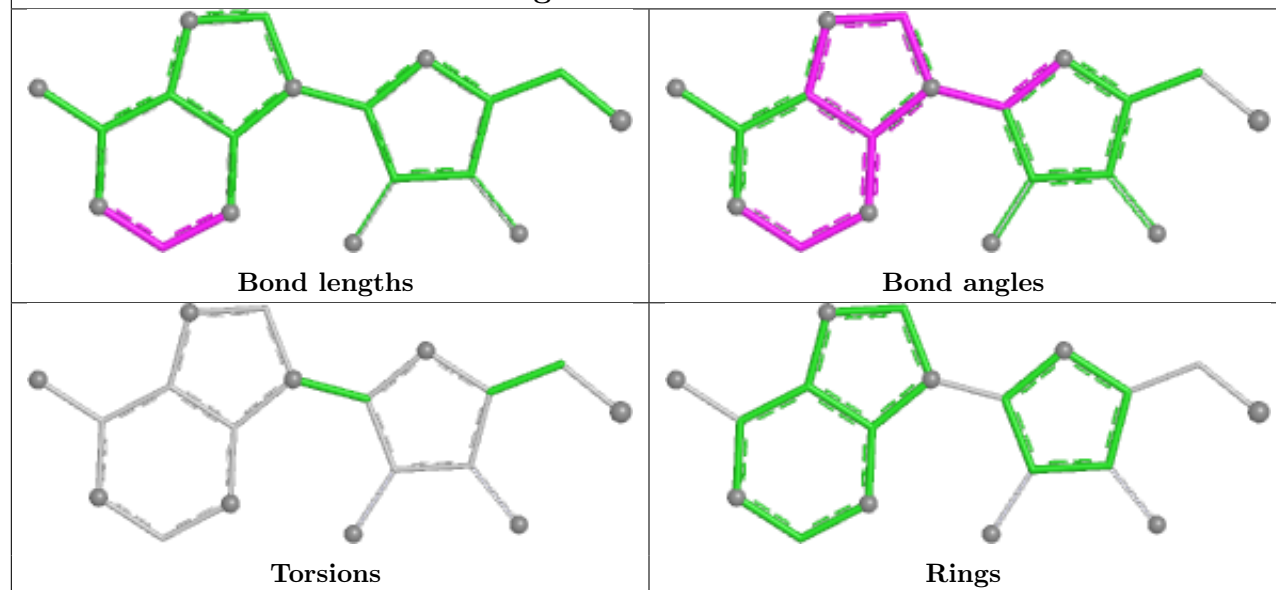
Ligand SAH G 501



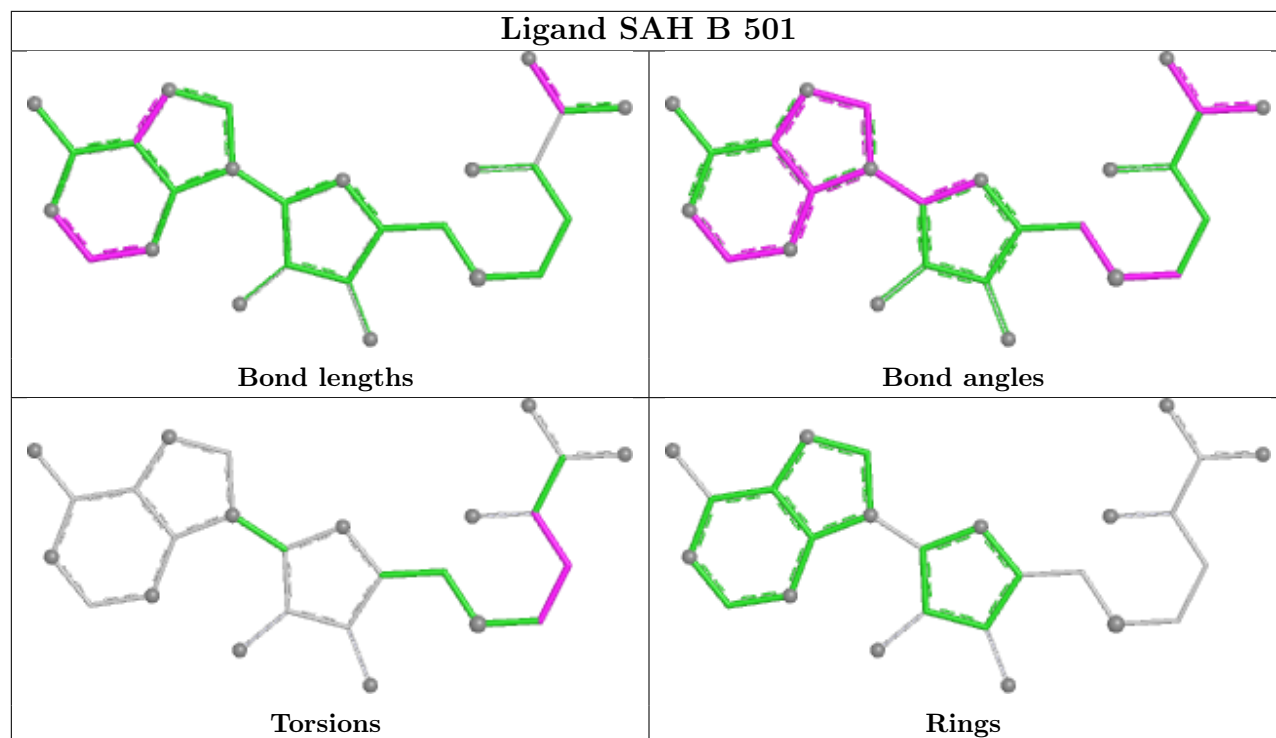
Ligand SAH A 501



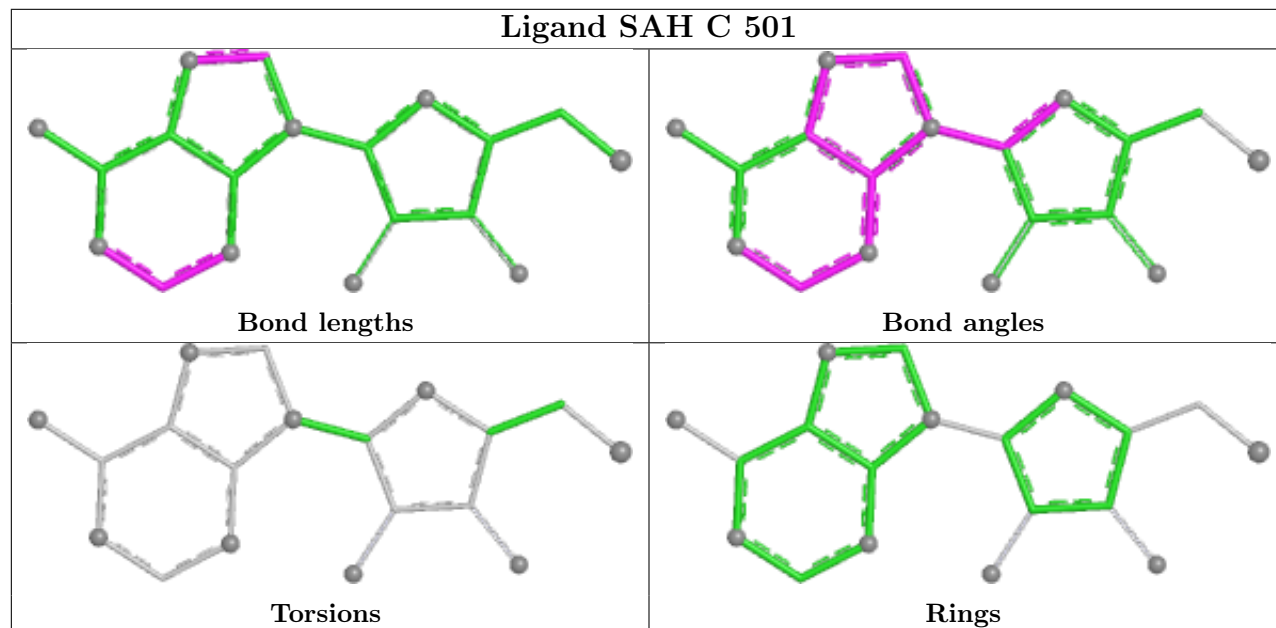
Ligand SAH F 501

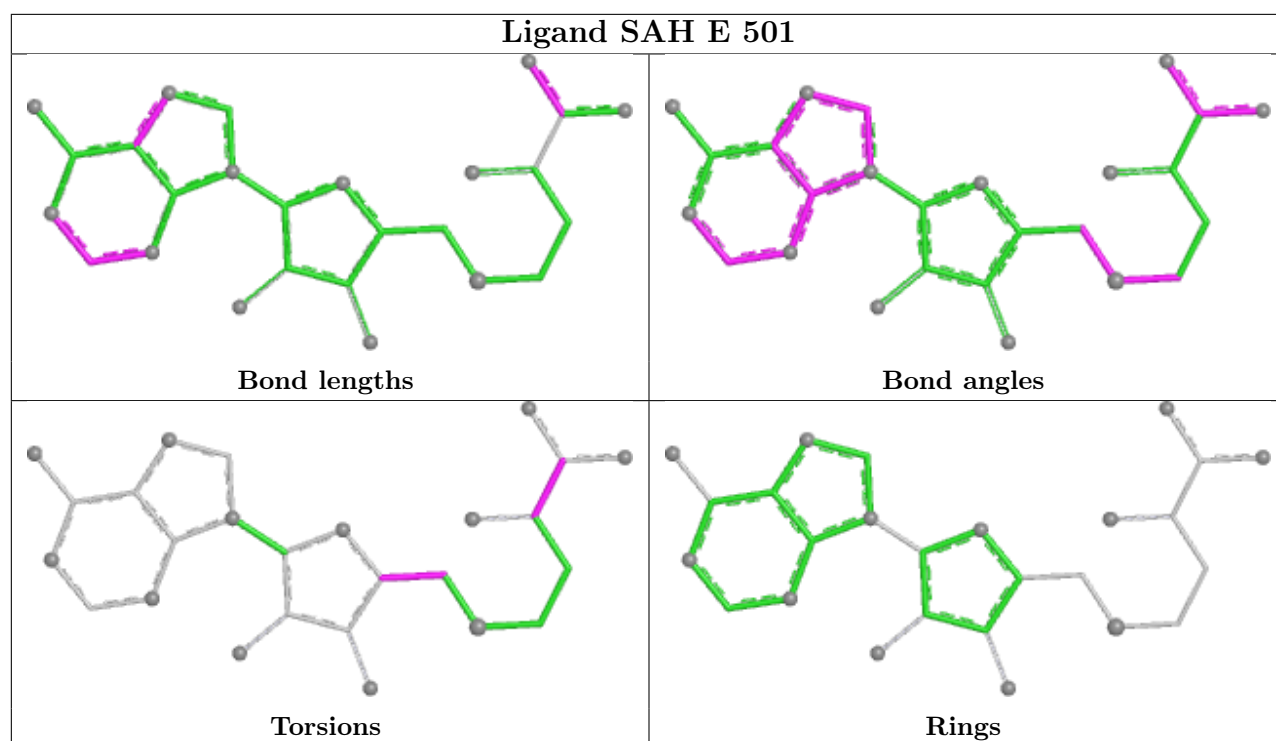


Ligand SAH B 501



Ligand SAH C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	358/363 (98%)	-1.11	0	100	100	15, 46, 98, 149	0
1	B	350/363 (96%)	-0.82	0	100	100	49, 92, 142, 197	0
1	C	347/363 (95%)	-0.86	0	100	100	26, 88, 135, 231	0
1	D	358/363 (98%)	-1.08	0	100	100	21, 51, 107, 161	0
1	E	358/363 (98%)	-1.05	0	100	100	24, 52, 108, 156	0
1	F	351/363 (96%)	-0.73	0	100	100	26, 96, 143, 201	0
1	G	357/363 (98%)	-1.05	0	100	100	19, 48, 100, 176	0
1	H	355/363 (97%)	-0.82	1 (0%)	90	81	26, 88, 138, 175	0
All	All	2834/2904 (97%)	-0.94	1 (0%)	100	100	15, 77, 131, 231	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	168	GLY	4.8

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,

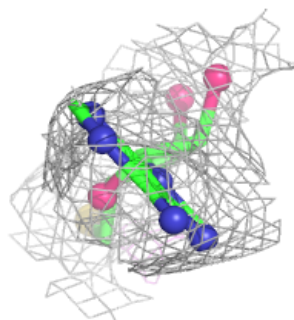
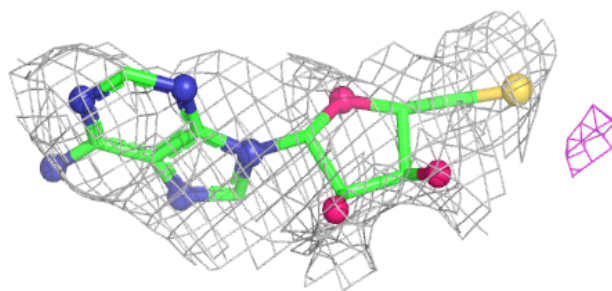
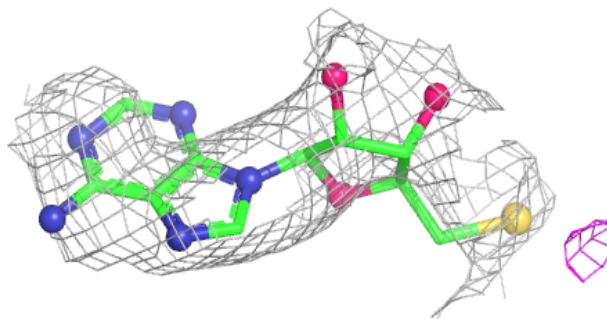
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SAH	F	501	19/26	0.98	0.05	54,72,98,144	0
2	SAH	A	501	26/26	0.99	0.06	12,31,77,128	0
2	SAH	C	501	19/26	0.99	0.04	13,47,88,148	0
2	SAH	D	501	26/26	0.99	0.06	0,28,53,148	0
2	SAH	E	501	26/26	0.99	0.06	21,37,106,142	0
2	SAH	B	501	26/26	0.99	0.06	50,82,97,128	0
2	SAH	G	501	26/26	0.99	0.05	0,29,67,128	0
2	SAH	H	501	26/26	0.99	0.06	31,70,86,157	0
3	EXU	B	502	15/15	0.99	0.07	74,82,89,91	0
3	EXU	A	502	15/15	0.99	0.05	25,40,55,57	0
3	EXU	C	502	15/15	0.99	0.05	47,55,71,87	0
3	EXU	D	502	15/15	0.99	0.07	26,63,78,79	0
3	EXU	E	502	15/15	0.99	0.07	42,56,68,82	0
3	EXU	F	502	15/15	0.99	0.08	89,93,103,110	0
3	EXU	G	502	15/15	0.99	0.05	6,34,50,51	0
3	EXU	H	502	15/15	0.99	0.05	52,64,95,96	0

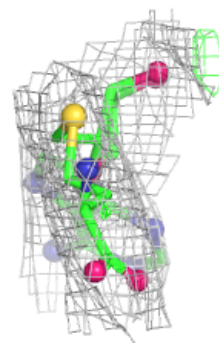
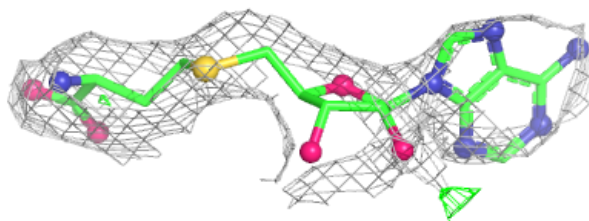
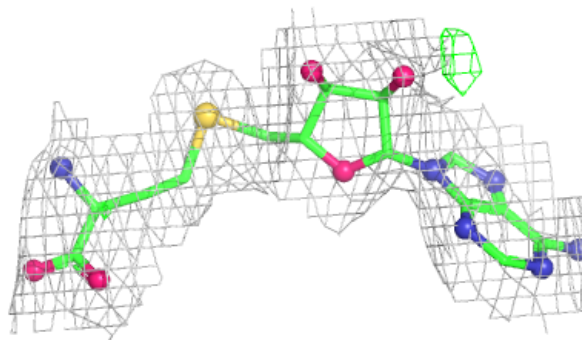
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH F 501:

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

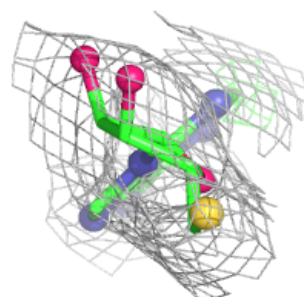
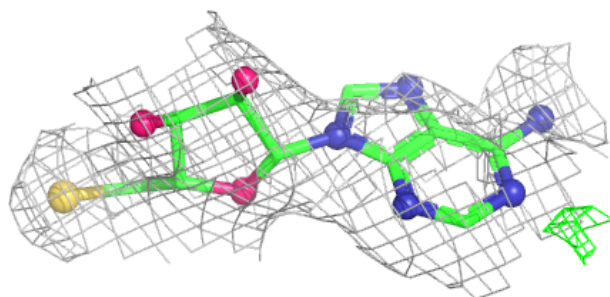
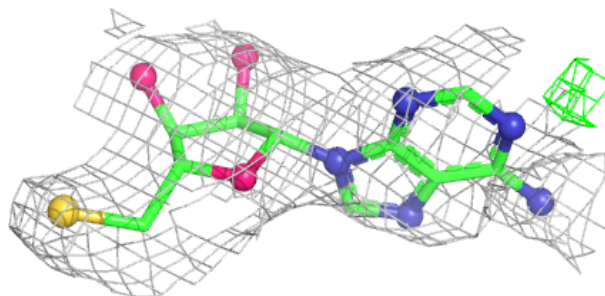
**Electron density around SAH A 501:**

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

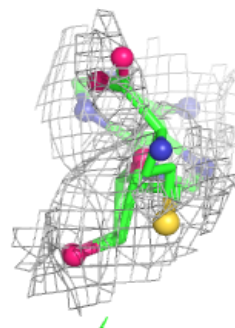
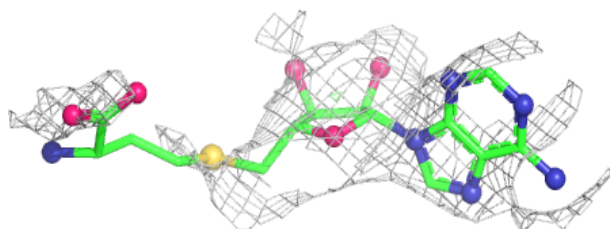
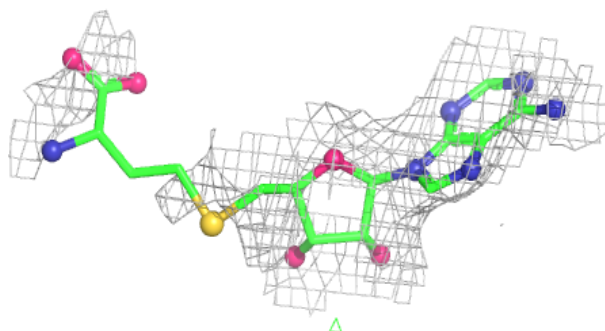


Electron density around SAH C 501:

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

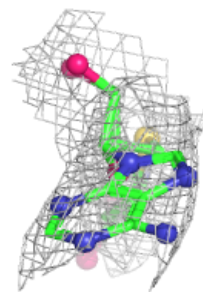
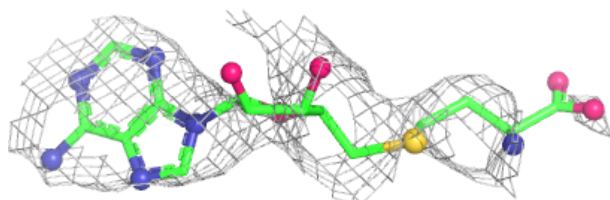
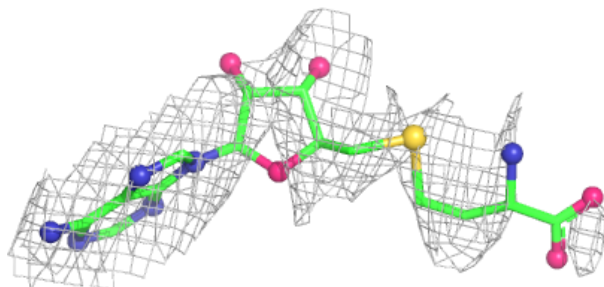
**Electron density around SAH D 501:**

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

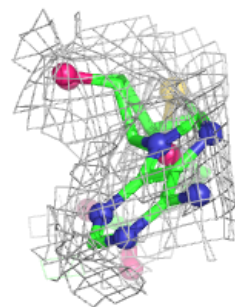
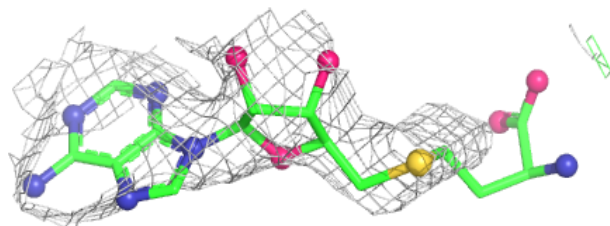
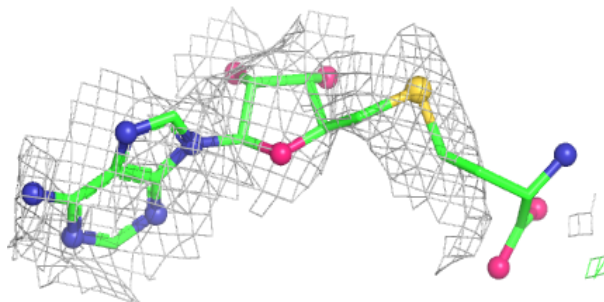


Electron density around SAH E 501:

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

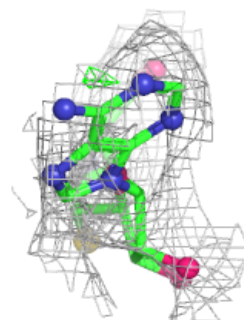
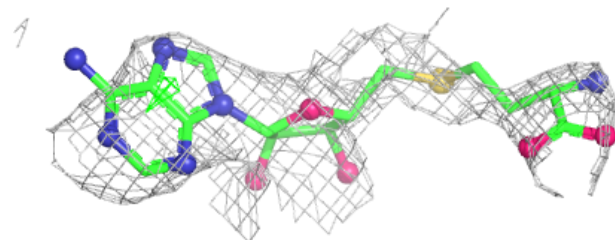
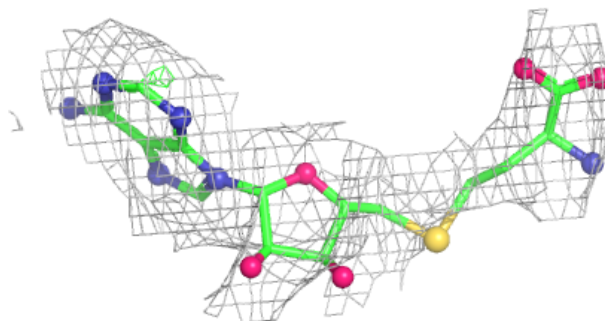
**Electron density around SAH B 501:**

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

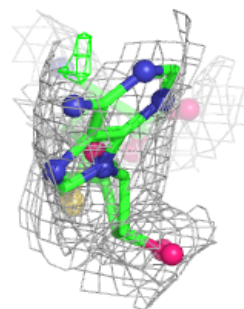
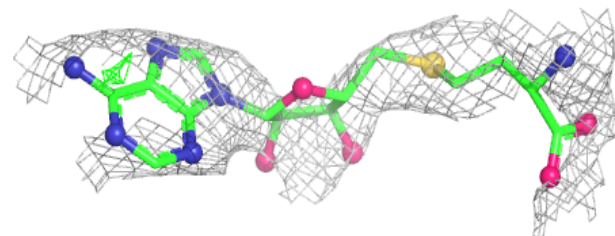
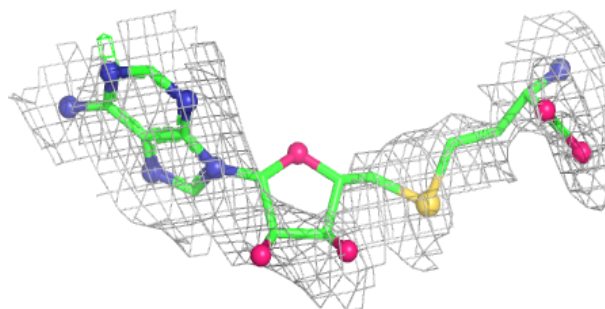


Electron density around SAH G 501:

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

**Electron density around SAH H 501:**

$2mF_o-DF_c$ (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.