



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:13 AM UTC

PDB ID : 5HFJ / pdb_00005hfj
Title : crystal structure of M1.HpyAVI-SAM complex
Authors : Ma, B.; Liu, W.; Zhang, H.
Deposited on : 2016-01-07
Resolution : 3.10 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

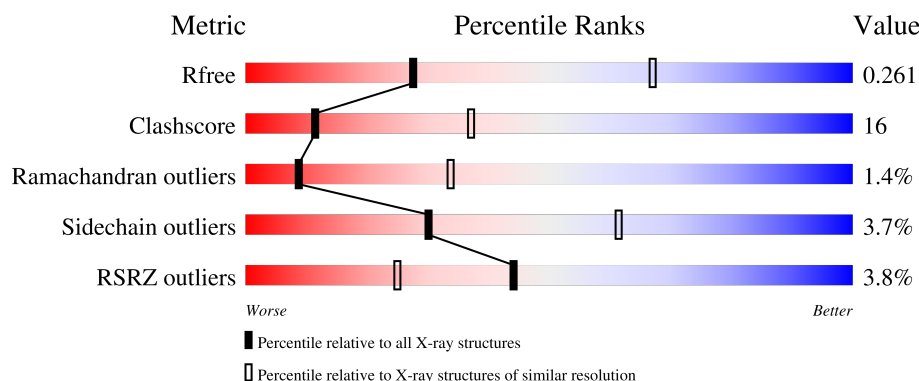
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	232	3% 58% 24% 13%
1	B	232	3% 60% 19% 16%
1	C	232	3% 57% 28% 12%
1	D	232	3% 50% 26% 19%
1	E	232	5% 50% 27% 6% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	232	
1	G	232	
1	H	232	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAM	E	301	-	-	X	-

2 Entry composition

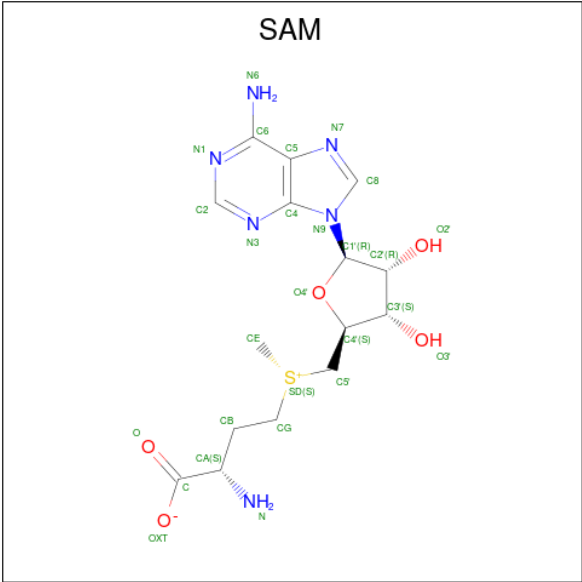
There are 2 unique types of molecules in this entry. The entry contains 13194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenine specific DNA methyltransferase (DpnA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1661	1087	278	288	8			
1	B	194	Total	C	N	O	S	0	0	0
			1611	1054	272	277	8			
1	C	204	Total	C	N	O	S	0	0	0
			1684	1098	284	294	8			
1	D	188	Total	C	N	O	S	0	0	0
			1558	1021	260	269	8			
1	E	193	Total	C	N	O	S	0	0	0
			1600	1045	270	277	8			
1	F	194	Total	C	N	O	S	0	0	0
			1605	1050	269	278	8			
1	G	200	Total	C	N	O	S	0	0	0
			1662	1086	279	289	8			
1	H	193	Total	C	N	O	S	0	0	0
			1597	1044	268	277	8			

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).

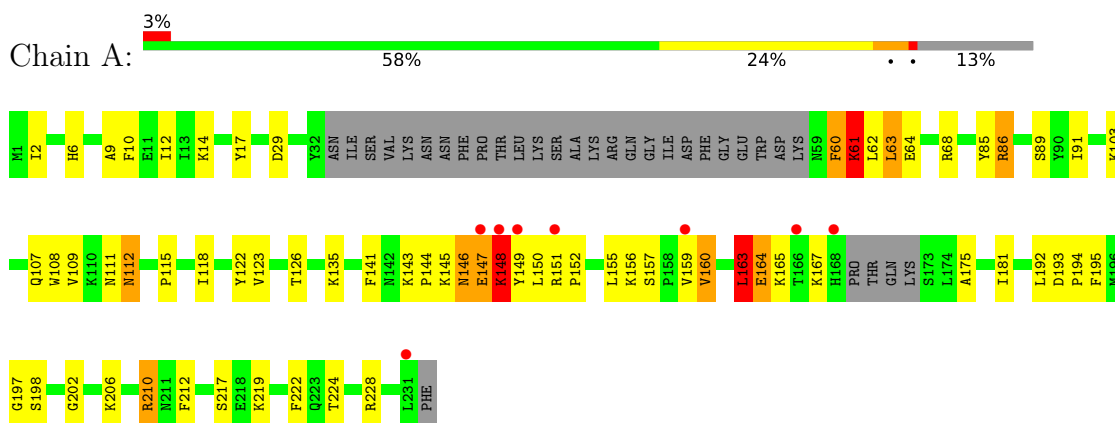


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

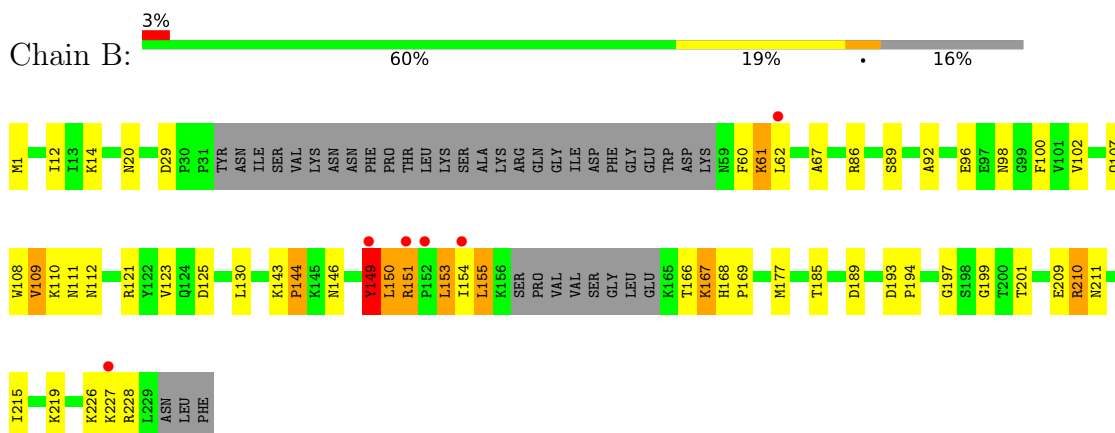
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

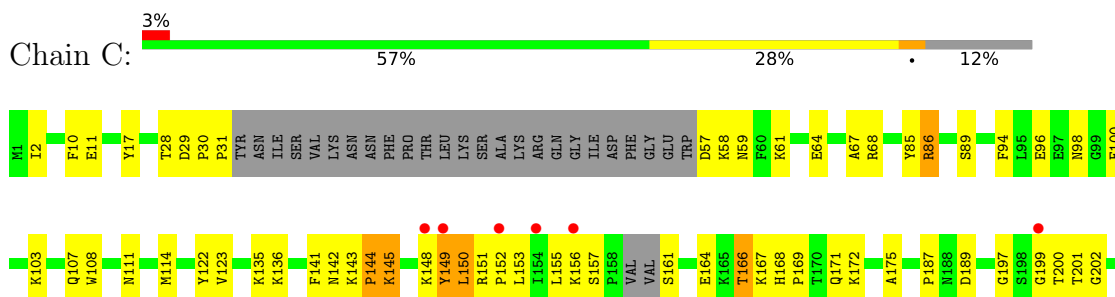
• Molecule 1: Adenine specific DNA methyltransferase (DpnA)



• Molecule 1: Adenine specific DNA methyltransferase (DpnA)

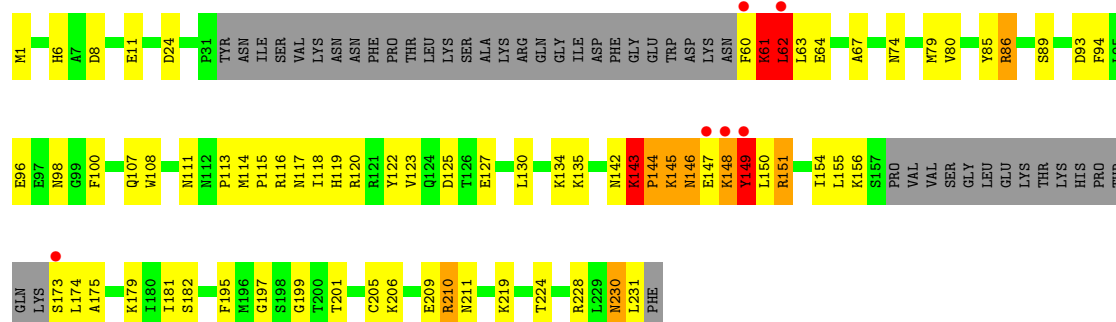


• Molecule 1: Adenine specific DNA methyltransferase (DpnA)

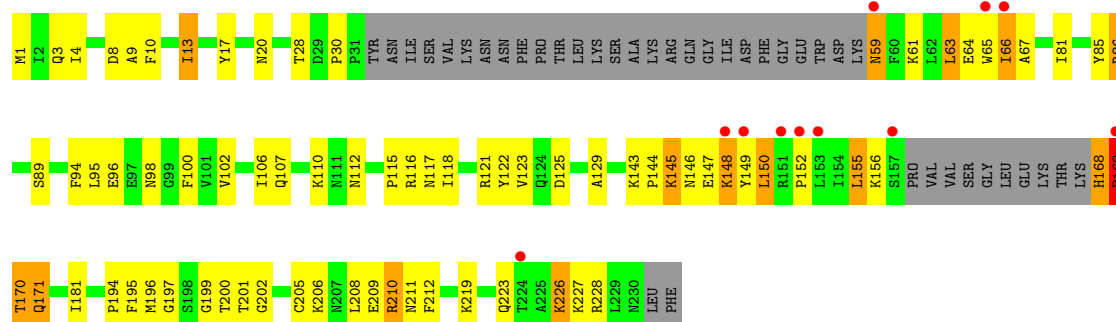




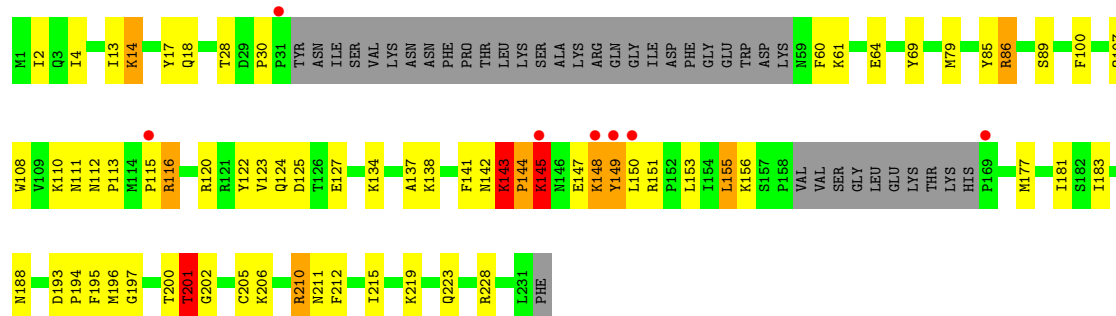
- Molecule 1: Adenine specific DNA methyltransferase (DpnA)



- Molecule 1: Adenine specific DNA methyltransferase (DpnA)

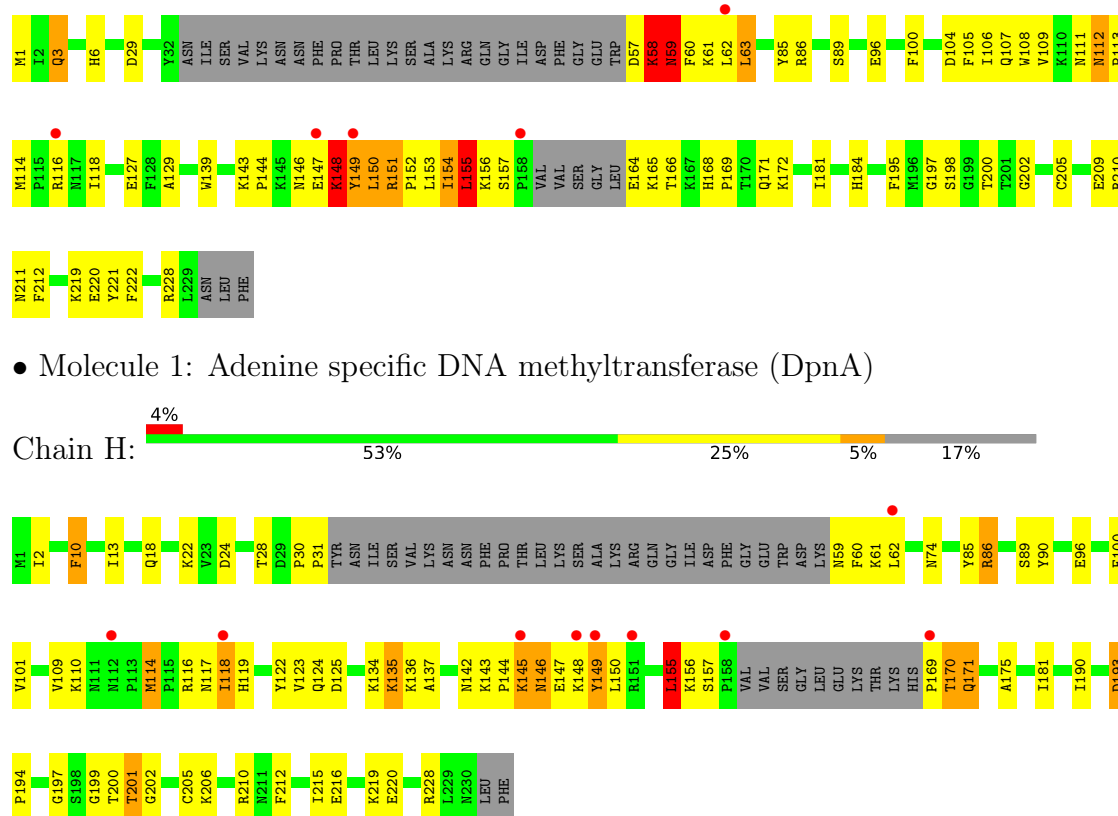


- Molecule 1: Adenine specific DNA methyltransferase (DpnA)



- Molecule 1: Adenine specific DNA methyltransferase (DpnA)





- Molecule 1: Adenine specific DNA methyltransferase (DpnA)

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	135.60Å 135.60Å 265.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.91 – 3.10 48.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.91-3.10) 99.9 (48.91-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.221 , 0.276 (Not available) , 0.261	Depositor DCC
R_{free} test set	1997 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.129 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13194	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.48	0/1703	1.12	14/2300 (0.6%)
1	B	0.43	0/1652	1.07	9/2229 (0.4%)
1	C	0.42	0/1726	1.15	14/2329 (0.6%)
1	D	0.43	0/1597	1.15	19/2156 (0.9%)
1	E	0.50	0/1641	1.10	11/2216 (0.5%)
1	F	0.46	1/1646 (0.1%)	1.04	6/2223 (0.3%)
1	G	0.46	0/1705	1.24	21/2301 (0.9%)
1	H	0.46	0/1638	1.07	13/2212 (0.6%)
All	All	0.46	1/13308 (0.0%)	1.12	107/17966 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	1
1	D	0	3
1	F	0	2
1	H	0	2
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	143	LYS	CA-C	5.36	1.58	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	TYR	CA-C-N	12.63	144.44	121.70
1	A	149	TYR	C-N-CA	12.63	144.44	121.70
1	G	149	TYR	N-CA-C	12.51	125.49	108.23
1	C	143	LYS	CA-C-N	11.40	134.09	119.84
1	C	143	LYS	C-N-CA	11.40	134.09	119.84
1	G	112	ASN	CA-C-N	11.32	133.99	119.84
1	G	112	ASN	C-N-CA	11.32	133.99	119.84
1	E	168	HIS	C-N-CD	-8.39	102.15	120.60
1	E	168	HIS	CA-C-N	8.36	147.07	127.00
1	E	168	HIS	C-N-CA	8.36	147.07	127.00
1	E	169	PRO	CA-C-N	8.33	136.69	121.70
1	E	169	PRO	C-N-CA	8.33	136.69	121.70
1	C	210	ARG	N-CA-C	8.28	123.11	112.92
1	A	148	LYS	N-CA-C	8.28	128.44	110.80
1	C	149	TYR	N-CA-C	8.04	119.16	108.07
1	F	145	LYS	N-CA-C	-7.98	99.77	110.55
1	D	143	LYS	CA-C-N	7.95	127.84	120.21
1	D	143	LYS	C-N-CA	7.95	127.84	120.21
1	A	146	ASN	N-CA-C	7.87	122.46	113.02
1	G	147	GLU	N-CA-C	7.70	121.95	109.40
1	H	143	LYS	CA-C-N	7.69	129.45	119.84
1	H	143	LYS	C-N-CA	7.69	129.45	119.84
1	C	59	ASN	N-CA-C	-7.61	103.59	113.17
1	B	155	LEU	N-CA-C	7.58	120.09	110.24
1	G	59	ASN	N-CA-C	7.52	120.82	107.80
1	A	210	ARG	N-CA-C	7.38	121.99	112.92
1	H	135	LYS	N-CA-C	7.31	118.93	110.97
1	B	153	LEU	N-CA-C	7.26	120.38	108.99
1	G	63	LEU	N-CA-C	-7.20	104.06	112.92
1	C	166	THR	N-CA-C	7.09	121.51	112.86
1	D	62	LEU	CA-CB-CG	7.06	141.02	116.30
1	E	148	LYS	CB-CA-C	-7.05	107.40	115.79
1	H	146	ASN	CB-CA-C	-7.05	108.43	116.54
1	G	151	ARG	CA-C-N	6.99	127.29	119.32
1	G	151	ARG	C-N-CA	6.99	127.29	119.32
1	D	151	ARG	CA-C-N	6.90	126.42	119.24
1	D	151	ARG	C-N-CA	6.90	126.42	119.24
1	G	154	ILE	N-CA-C	-6.87	106.03	112.83
1	D	146	ASN	N-CA-C	6.74	120.47	111.30
1	G	58	LYS	CA-C-N	-6.68	112.76	122.44
1	G	58	LYS	C-N-CA	-6.68	112.76	122.44
1	A	147	GLU	N-CA-C	6.56	124.78	110.80
1	H	171	GLN	N-CA-C	6.55	124.74	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	148	LYS	CB-CA-C	-6.38	108.19	115.79
1	F	148	LYS	CB-CA-C	-6.36	107.49	115.89
1	G	114	MET	CA-C-N	6.35	142.25	127.00
1	G	114	MET	C-N-CA	6.35	142.25	127.00
1	A	112	ASN	CA-C-N	-6.27	114.19	120.21
1	A	112	ASN	C-N-CA	-6.27	114.19	120.21
1	A	135	LYS	N-CA-C	6.22	117.75	110.97
1	H	60	PHE	N-CA-C	-6.22	105.73	113.38
1	B	228	ARG	N-CA-C	-6.22	105.18	112.89
1	B	226	LYS	N-CA-C	6.20	117.70	111.07
1	C	57	ASP	CA-C-N	-6.13	113.27	123.33
1	C	57	ASP	C-N-CA	-6.13	113.27	123.33
1	B	61	LYS	CA-C-N	6.03	132.55	121.70
1	B	61	LYS	C-N-CA	6.03	132.55	121.70
1	F	142	ASN	N-CA-C	6.03	123.64	110.80
1	H	10	PHE	N-CA-C	6.01	118.80	111.82
1	G	114	MET	C-N-CD	-6.00	107.41	120.60
1	B	219	LYS	N-CA-C	5.97	117.87	111.36
1	G	146	ASN	N-CA-C	-5.92	98.20	110.80
1	D	143	LYS	CB-CA-C	5.79	115.90	110.17
1	D	116	ARG	N-CA-C	5.75	117.97	109.69
1	G	3	GLN	N-CA-C	5.75	118.48	108.76
1	A	147	GLU	CA-C-N	5.67	132.36	121.54
1	A	147	GLU	C-N-CA	5.67	132.36	121.54
1	E	143	LYS	CA-C-N	5.64	126.89	119.84
1	E	143	LYS	C-N-CA	5.64	126.89	119.84
1	G	148	LYS	N-CA-C	5.62	119.66	109.32
1	E	210	ARG	N-CA-C	5.46	119.64	112.92
1	C	135	LYS	N-CA-C	5.45	116.91	110.97
1	H	155	LEU	N-CA-C	5.40	115.37	108.24
1	D	149	TYR	N-CA-C	5.37	122.24	110.80
1	H	201	THR	N-CA-C	-5.36	105.10	111.69
1	E	155	LEU	N-CA-C	5.34	115.29	108.24
1	H	114	MET	CA-C-N	5.30	139.72	127.00
1	H	114	MET	C-N-CA	5.30	139.72	127.00
1	C	230	ASN	N-CA-C	5.29	122.06	110.80
1	D	154	ILE	CA-C-N	-5.29	111.45	121.54
1	D	154	ILE	C-N-CA	-5.29	111.45	121.54
1	H	193	ASP	CA-C-N	5.28	125.09	119.28
1	H	193	ASP	C-N-CA	5.28	125.09	119.28
1	F	201	THR	N-CA-C	-5.24	105.24	111.69
1	A	149	TYR	O-C-N	-5.24	115.62	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	LYS	CA-C-N	5.23	129.84	122.46
1	D	145	LYS	C-N-CA	5.23	129.84	122.46
1	E	66	ILE	CB-CA-C	-5.20	105.32	111.97
1	G	155	LEU	CA-CB-CG	5.17	134.38	116.30
1	D	117	ASN	N-CA-C	-5.16	106.28	112.58
1	D	210	ARG	N-CA-C	5.15	119.25	112.92
1	B	144	PRO	CA-C-O	-5.14	115.50	122.08
1	D	144	PRO	CA-C-O	-5.14	115.06	122.31
1	D	148	LYS	CA-C-N	5.13	131.35	121.54
1	D	148	LYS	C-N-CA	5.13	131.35	121.54
1	G	150	LEU	CA-C-N	-5.11	116.14	122.42
1	G	150	LEU	C-N-CA	-5.11	116.14	122.42
1	D	143	LYS	CA-CB-CG	5.09	124.28	114.10
1	C	151	ARG	CA-C-N	5.08	125.12	119.32
1	C	151	ARG	C-N-CA	5.08	125.12	119.32
1	B	210	ARG	N-CA-C	5.07	119.15	112.92
1	C	114	MET	CA-C-N	5.07	139.17	127.00
1	C	114	MET	C-N-CA	5.07	139.17	127.00
1	A	193	ASP	CA-C-N	5.07	124.85	119.28
1	A	193	ASP	C-N-CA	5.07	124.85	119.28
1	F	210	ARG	N-CA-C	5.06	119.15	112.92
1	F	144	PRO	CA-N-CD	-5.05	104.94	112.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	LYS	Peptide
1	A	163	LEU	Peptide
1	A	60	PHE	Peptide
1	A	61	LYS	Peptide
1	C	167	LYS	Peptide
1	D	114	MET	Peptide
1	D	230	ASN	Peptide
1	D	61	LYS	Peptide
1	F	143	LYS	Peptide
1	F	145	LYS	Peptide
1	H	155	LEU	Peptide
1	H	170	THR	Peptide

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	1661	0	1687	65	0
1	B	1611	0	1641	41	1
1	C	1684	0	1712	53	0
1	D	1558	0	1582	55	0
1	E	1600	0	1619	73	1
1	F	1605	0	1631	62	0
1	G	1662	0	1685	60	0
1	H	1597	0	1620	61	0
2	A	27	0	22	7	0
2	B	27	0	22	2	0
2	C	27	0	22	6	0
2	D	27	0	22	2	0
2	E	27	0	22	9	0
2	F	27	0	22	4	0
2	G	27	0	22	6	0
2	H	27	0	22	6	0
All	All	13194	0	13353	428	1

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 16.

All (428) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD23	1:A:157:SER:H	1.25	1.02
1:G:151:ARG:HH22	1:G:154:ILE:HG22	1.34	0.91
1:G:153:LEU:HG	1:G:155:LEU:H	1.38	0.88
1:F:13:ILE:HG13	1:F:17:TYR:HE2	1.42	0.84
1:B:108:TRP:HE1	1:B:155:LEU:HB3	1.43	0.82
1:H:101:VAL:HG23	1:H:135:LYS:HD2	1.60	0.82
1:A:163:LEU:HD13	1:A:224:THR:HG21	1.64	0.80
1:C:111:ASN:HB2	1:C:156:LYS:HA	1.65	0.79
1:E:226:LYS:HG2	1:E:227:LYS:N	1.99	0.77
1:D:89:SER:HB2	1:H:89:SER:HB2	1.68	0.75
1:F:122:TYR:HD1	1:G:149:TYR:HB3	1.51	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:B:123:VAL:O	1.87	0.75
1:B:185:THR:OG1	1:B:210:ARG:NH1	2.20	0.74
1:H:197:GLY:HA3	2:H:301:SAM:HB1	1.67	0.74
1:E:59:ASN:OD1	1:E:59:ASN:N	2.18	0.73
1:A:89:SER:HB2	1:B:89:SER:HB2	1.71	0.73
1:G:60:PHE:HB3	1:G:62:LEU:HG	1.69	0.72
1:B:153:LEU:HG	1:B:155:LEU:H	1.54	0.72
1:C:103:LYS:O	1:E:121:ARG:NH2	2.23	0.72
1:F:89:SER:HB2	1:G:89:SER:HB2	1.72	0.71
1:F:147:GLU:HB2	1:G:118:ILE:HD11	1.70	0.71
1:C:149:TYR:HB3	1:E:122:TYR:HD1	1.55	0.71
1:E:1:MET:SD	1:E:3:GLN:NE2	2.64	0.71
1:C:153:LEU:HG	1:C:155:LEU:H	1.55	0.71
1:B:197:GLY:HA3	2:B:301:SAM:HB1	1.71	0.71
1:F:123:VAL:O	1:G:150:LEU:HD12	1.90	0.70
1:A:108:TRP:HE1	1:A:155:LEU:HB3	1.56	0.70
1:F:143:LYS:CG	1:F:144:PRO:HD3	2.22	0.70
1:F:188:ASN:OD1	1:F:211:ASN:ND2	2.24	0.70
1:A:163:LEU:O	1:A:165:LYS:N	2.25	0.70
1:F:122:TYR:HH	1:G:184:HIS:HE2	1.39	0.70
1:B:1:MET:N	1:B:211:ASN:OD1	2.25	0.70
1:E:147:GLU:HG3	1:E:148:LYS:HG3	1.74	0.69
1:F:111:ASN:HD22	1:F:156:LYS:HD3	1.57	0.69
1:G:168:HIS:HD2	1:G:169:PRO:HD2	1.58	0.68
1:A:197:GLY:HA3	2:A:301:SAM:HB1	1.75	0.68
1:G:168:HIS:CD2	1:G:169:PRO:HD2	2.29	0.67
1:F:134:LYS:HB3	1:F:137:ALA:HB2	1.76	0.67
1:E:66:ILE:HD12	1:E:94:PHE:CD2	2.29	0.67
1:B:60:PHE:HB2	1:B:62:LEU:HD12	1.77	0.67
1:H:117:ASN:O	1:H:119:HIS:N	2.20	0.67
1:A:165:LYS:HE3	1:A:167:LYS:HB2	1.76	0.66
1:H:59:ASN:OD1	1:H:61:LYS:NZ	2.27	0.66
1:C:200:THR:OG1	1:C:228:ARG:NH1	2.18	0.66
1:C:89:SER:HB2	1:E:89:SER:HB2	1.77	0.66
1:A:155:LEU:HD12	1:A:175:ALA:HB3	1.78	0.66
1:F:143:LYS:HG3	1:F:144:PRO:HD3	1.76	0.66
1:A:115:PRO:HB2	1:A:118:ILE:HD11	1.77	0.65
1:C:122:TYR:HD1	1:E:149:TYR:HB3	1.60	0.65
1:H:200:THR:OG1	1:H:228:ARG:NH1	2.29	0.65
1:F:112:ASN:HB2	1:H:145:LYS:HD2	1.78	0.65
1:F:14:LYS:HA	1:F:17:TYR:CD2	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LYS:HE3	1:D:231:LEU:HD21	1.78	0.64
1:A:122:TYR:HD1	1:B:149:TYR:HB3	1.62	0.64
1:F:143:LYS:HG3	1:F:144:PRO:CD	2.28	0.64
1:A:6:HIS:NE2	1:A:217:SER:O	2.30	0.64
1:G:1:MET:N	1:G:211:ASN:OD1	2.29	0.64
1:A:107:GLN:HE21	1:A:126:THR:HG21	1.61	0.63
1:E:223:GLN:O	1:E:226:LYS:HD3	1.99	0.63
1:G:168:HIS:CE1	2:G:301:SAM:HN2	2.16	0.63
1:E:66:ILE:HD12	1:E:94:PHE:HD2	1.62	0.62
1:A:109:VAL:HG23	1:A:151:ARG:HH11	1.65	0.62
1:F:153:LEU:HD23	1:F:155:LEU:HD12	1.81	0.62
1:F:113:PRO:HD2	1:G:148:LYS:NZ	2.15	0.61
1:H:170:THR:OG1	2:H:301:SAM:HG1	2.00	0.61
1:C:216:GLU:OE2	2:C:301:SAM:O2'	2.14	0.61
1:C:85:TYR:CE1	1:C:86:ARG:HD3	2.36	0.61
1:F:85:TYR:CE1	1:F:86:ARG:HD3	2.35	0.60
1:D:63:LEU:HD23	1:D:94:PHE:CD1	2.36	0.60
1:A:150:LEU:HD13	1:B:125:ASP:OD1	2.01	0.60
1:F:200:THR:OG1	1:F:228:ARG:NH1	2.33	0.60
1:E:195:PHE:HD1	2:E:301:SAM:C8	2.14	0.59
1:A:163:LEU:HD11	1:A:198:SER:HB2	1.85	0.59
1:C:157:SER:HG	1:C:161:SER:N	2.00	0.59
1:A:109:VAL:HG23	1:A:151:ARG:NH1	2.18	0.59
1:E:170:THR:HG22	1:E:171:GLN:H	1.66	0.59
1:G:151:ARG:NH2	1:G:154:ILE:HG22	2.12	0.59
1:H:155:LEU:HD21	1:H:175:ALA:HB3	1.84	0.59
1:D:155:LEU:O	1:D:156:LYS:HD3	2.02	0.58
1:D:155:LEU:HG	1:D:156:LYS:N	2.19	0.58
1:E:1:MET:N	1:E:211:ASN:OD1	2.36	0.58
1:A:85:TYR:CE1	1:A:86:ARG:HD3	2.38	0.58
1:A:159:VAL:HG23	1:A:160:VAL:H	1.68	0.58
1:D:1:MET:N	1:D:211:ASN:OD1	2.37	0.58
1:E:169:PRO:HG2	2:E:301:SAM:N	2.18	0.58
1:F:177:MET:HE2	1:F:201:THR:HG22	1.85	0.58
1:D:63:LEU:HD23	1:D:94:PHE:CG	2.38	0.57
1:D:175:ALA:O	1:D:179:LYS:HD3	2.05	0.57
1:D:60:PHE:HB3	1:D:62:LEU:HG	1.87	0.57
1:E:169:PRO:HG2	2:E:301:SAM:HN2	1.69	0.57
1:H:2:ILE:HD11	1:H:206:LYS:HB2	1.85	0.57
1:A:2:ILE:HD11	1:A:206:LYS:HB2	1.87	0.57
1:A:60:PHE:HA	1:A:61:LYS:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:ILE:HG13	1:F:17:TYR:CE2	2.32	0.57
1:F:111:ASN:ND2	1:F:155:LEU:O	2.38	0.57
1:G:198:SER:H	2:G:301:SAM:HN1	1.53	0.56
1:E:219:LYS:O	1:E:223:GLN:N	2.36	0.56
1:A:112:ASN:ND2	1:A:156:LYS:O	2.38	0.56
1:F:143:LYS:HG2	1:F:149:TYR:OH	2.06	0.56
1:A:144:PRO:C	1:A:146:ASN:H	2.14	0.56
1:D:85:TYR:CE1	1:D:86:ARG:HD3	2.41	0.56
1:H:144:PRO:HD2	1:H:149:TYR:OH	2.05	0.56
1:D:62:LEU:HD13	1:D:63:LEU:HB2	1.87	0.56
1:B:29:ASP:HB3	2:B:301:SAM:HN2	1.70	0.55
1:C:2:ILE:HD11	1:C:206:LYS:HB2	1.88	0.55
1:D:147:GLU:HG2	1:D:149:TYR:HD2	1.72	0.55
1:D:63:LEU:HB3	1:D:94:PHE:CD2	2.41	0.55
1:C:122:TYR:CD1	1:E:149:TYR:HB3	2.40	0.55
1:H:145:LYS:CG	1:H:146:ASN:H	2.20	0.55
1:D:111:ASN:HB2	1:D:155:LEU:O	2.06	0.55
1:G:57:ASP:OD1	1:G:58:LYS:N	2.37	0.55
1:B:143:LYS:HG2	1:B:144:PRO:O	2.07	0.54
1:C:164:GLU:O	1:C:166:THR:HG23	2.07	0.54
1:D:181:ILE:HG21	1:D:210:ARG:HG3	1.90	0.54
1:F:113:PRO:O	1:H:145:LYS:HD3	2.07	0.54
1:H:110:LYS:HA	1:H:155:LEU:O	2.08	0.54
1:A:165:LYS:NZ	2:A:301:SAM:O3'	2.24	0.54
1:A:163:LEU:HD21	1:A:228:ARG:HD2	1.89	0.54
1:F:2:ILE:HD11	1:F:206:LYS:HB2	1.88	0.54
1:D:118:ILE:HG13	1:D:119:HIS:H	1.73	0.54
1:A:165:LYS:HE2	2:A:301:SAM:HB1	1.89	0.54
1:H:114:MET:HG3	1:H:116:ARG:NH1	2.21	0.54
1:D:173:SER:OG	1:D:174:LEU:N	2.40	0.54
1:E:8:ASP:OD1	2:E:301:SAM:N6	2.39	0.54
1:A:60:PHE:HA	1:A:61:LYS:CB	2.38	0.53
1:B:167:LYS:O	1:B:167:LYS:HG3	2.08	0.53
1:G:197:GLY:HA3	2:G:301:SAM:N	2.23	0.53
1:A:151:ARG:HD2	1:B:151:ARG:HH22	1.72	0.53
1:C:31:PRO:HG3	2:C:301:SAM:C8	2.38	0.53
1:E:96:GLU:HA	1:E:100:PHE:O	2.08	0.53
1:A:63:LEU:HD11	1:A:91:ILE:HG12	1.90	0.53
1:E:30:PRO:HA	1:E:195:PHE:CD2	2.44	0.53
1:G:200:THR:OG1	1:G:228:ARG:NH1	2.40	0.53
1:A:156:LYS:O	1:A:157:SER:OG	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:PHE:HE2	1:G:107:GLN:HE21	1.57	0.53
1:A:6:HIS:CE1	1:A:219:LYS:HD3	2.43	0.53
1:G:153:LEU:HG	1:G:155:LEU:N	2.15	0.53
1:D:197:GLY:HA3	2:D:301:SAM:HB1	1.91	0.53
1:E:208:LEU:O	1:E:210:ARG:NH1	2.41	0.53
1:D:123:VAL:HG12	1:H:149:TYR:O	2.10	0.52
1:E:168:HIS:CD2	1:E:168:HIS:O	2.62	0.52
1:C:10:PHE:CZ	1:C:61:LYS:HG2	2.44	0.52
1:G:111:ASN:ND2	1:G:156:LYS:HD3	2.24	0.52
1:E:66:ILE:CD1	1:E:94:PHE:HD2	2.23	0.52
1:E:219:LYS:O	1:E:223:GLN:HG2	2.08	0.52
1:H:134:LYS:HB3	1:H:137:ALA:HB2	1.91	0.52
1:E:112:ASN:HB3	1:E:156:LYS:HD2	1.91	0.52
1:H:219:LYS:HG3	1:H:220:GLU:N	2.24	0.52
1:E:9:ALA:H	2:E:301:SAM:HN61	1.57	0.52
1:E:168:HIS:O	1:E:168:HIS:HD2	1.93	0.52
1:A:163:LEU:HB2	1:A:164:GLU:HG3	1.91	0.51
1:E:181:ILE:CG2	1:E:210:ARG:HG3	2.41	0.51
1:A:167:LYS:HD3	2:A:301:SAM:HE1	1.92	0.51
1:H:202:GLY:HA2	1:H:212:PHE:CG	2.46	0.51
1:F:13:ILE:HD13	1:F:69:TYR:CZ	2.45	0.51
1:D:146:ASN:OD1	1:D:148:LYS:NZ	2.44	0.51
1:C:226:LYS:HE2	1:C:231:LEU:HB3	1.93	0.51
1:F:14:LYS:HA	1:F:17:TYR:HD2	1.75	0.51
1:G:85:TYR:CE1	1:G:86:ARG:HD3	2.46	0.50
1:D:146:ASN:HA	1:D:148:LYS:NZ	2.27	0.50
1:D:181:ILE:CG2	1:D:210:ARG:HG3	2.42	0.50
1:F:120:ARG:NH2	1:G:139:TRP:O	2.43	0.50
1:F:219:LYS:HD3	1:F:219:LYS:N	2.27	0.50
1:D:205:CYS:HA	1:D:210:ARG:HB2	1.94	0.50
1:F:113:PRO:HD2	1:G:148:LYS:HZ1	1.77	0.50
1:C:168:HIS:HD2	1:C:221:TYR:CE1	2.30	0.50
1:F:155:LEU:CD2	1:F:156:LYS:H	2.25	0.50
1:H:96:GLU:HA	1:H:100:PHE:O	2.11	0.50
1:B:111:ASN:OD1	1:B:154:ILE:O	2.29	0.49
1:F:144:PRO:HB2	1:F:145:LYS:O	2.12	0.49
1:A:155:LEU:CD1	1:A:175:ALA:HB3	2.41	0.49
1:G:166:THR:OG1	1:G:171:GLN:OE1	2.21	0.49
1:A:195:PHE:HB3	2:A:301:SAM:O4'	2.12	0.49
1:C:150:LEU:HD22	1:E:123:VAL:O	2.11	0.49
1:E:155:LEU:HD12	1:E:156:LYS:H	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:LYS:HG2	1:G:220:GLU:N	2.27	0.49
1:E:205:CYS:HA	1:E:210:ARG:HB2	1.94	0.49
1:H:156:LYS:O	1:H:157:SER:OG	2.22	0.49
1:D:61:LYS:NZ	1:D:64:GLU:OE1	2.37	0.49
1:F:205:CYS:HA	1:F:210:ARG:HB2	1.95	0.49
1:B:12:ILE:HG21	1:B:215:ILE:HD13	1.94	0.49
1:C:149:TYR:HB3	1:E:122:TYR:CD1	2.41	0.49
1:G:143:LYS:HA	1:G:149:TYR:OH	2.13	0.49
1:D:118:ILE:HG22	1:H:148:LYS:HA	1.94	0.49
1:G:172:LYS:O	1:G:200:THR:HG21	2.13	0.49
1:H:197:GLY:HA3	2:H:301:SAM:CB	2.40	0.49
1:A:143:LYS:HG2	1:A:144:PRO:O	2.12	0.49
1:C:96:GLU:HA	1:C:100:PHE:O	2.13	0.49
1:D:8:ASP:HB3	1:D:11:GLU:HG2	1.95	0.49
1:F:108:TRP:HE3	1:F:127:GLU:HB2	1.77	0.49
1:B:166:THR:OG1	1:B:167:LYS:N	2.45	0.49
1:D:150:LEU:HD12	1:H:123:VAL:O	2.13	0.49
1:E:117:ASN:HB3	1:E:121:ARG:HG2	1.95	0.48
1:F:202:GLY:HA2	1:F:212:PHE:CG	2.48	0.48
1:H:145:LYS:HG2	1:H:146:ASN:H	1.78	0.48
1:E:85:TYR:CE1	1:E:86:ARG:HD3	2.48	0.48
1:G:219:LYS:HG2	1:G:220:GLU:H	1.78	0.48
1:H:85:TYR:CE1	1:H:86:ARG:HD3	2.48	0.48
1:H:181:ILE:CG2	1:H:210:ARG:HG3	2.43	0.48
1:C:28:THR:HG23	1:C:30:PRO:HD3	1.94	0.48
1:D:230:ASN:N	1:D:231:LEU:HB2	2.29	0.48
1:F:124:GLN:NE2	1:G:104:ASP:OD2	2.40	0.48
1:A:107:GLN:HE21	1:A:126:THR:CG2	2.27	0.48
1:B:67:ALA:HA	1:B:98:ASN:ND2	2.28	0.48
1:H:59:ASN:HB3	1:H:62:LEU:CD1	2.43	0.48
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.56	0.48
1:G:205:CYS:HA	1:G:210:ARG:HB2	1.94	0.48
1:A:123:VAL:O	1:B:150:LEU:HD22	2.14	0.48
1:B:227:LYS:HA	1:B:227:LYS:HD3	1.70	0.48
1:F:143:LYS:HG2	1:F:144:PRO:HD3	1.95	0.48
1:E:197:GLY:HA3	2:E:301:SAM:N	2.29	0.48
1:C:166:THR:OG1	1:C:171:GLN:OE1	2.30	0.47
1:H:199:GLY:C	1:H:201:THR:H	2.22	0.47
1:A:62:LEU:HD12	1:A:62:LEU:O	2.13	0.47
1:C:202:GLY:HA2	1:C:212:PHE:CG	2.49	0.47
1:E:63:LEU:HD21	1:E:94:PHE:CD1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:LEU:HG	1:F:155:LEU:H	1.79	0.47
1:G:96:GLU:HA	1:G:100:PHE:O	2.14	0.47
1:A:150:LEU:O	1:A:150:LEU:HD23	2.15	0.47
1:G:108:TRP:CZ2	1:G:155:LEU:HD22	2.50	0.47
1:A:10:PHE:HE2	1:A:64:GLU:HG3	1.80	0.47
1:A:163:LEU:HD11	1:A:198:SER:CB	2.45	0.47
1:C:144:PRO:HB2	1:C:145:LYS:HG3	1.96	0.47
1:C:187:PRO:HA	1:C:210:ARG:NH1	2.30	0.47
1:G:107:GLN:O	1:G:152:PRO:HD2	2.13	0.47
1:A:29:ASP:O	2:A:301:SAM:HE3	2.15	0.47
1:E:115:PRO:HA	1:E:123:VAL:HG23	1.97	0.47
1:G:1:MET:HE2	1:G:3:GLN:NE2	2.29	0.47
1:G:6:HIS:HB2	1:G:222:PHE:CD2	2.49	0.47
1:A:29:ASP:HB3	2:A:301:SAM:HN2	1.79	0.47
1:B:96:GLU:HA	1:B:100:PHE:O	2.15	0.47
1:C:205:CYS:HA	1:C:210:ARG:HB2	1.96	0.47
1:H:101:VAL:HG23	1:H:135:LYS:CD	2.39	0.47
1:H:117:ASN:C	1:H:119:HIS:H	2.16	0.47
1:C:123:VAL:O	1:E:150:LEU:HD22	2.15	0.47
1:E:169:PRO:HB2	1:E:170:THR:HB	1.97	0.47
1:F:85:TYR:HE1	1:F:86:ARG:HD3	1.79	0.47
1:C:197:GLY:HA3	2:C:301:SAM:HB2	1.96	0.46
1:G:111:ASN:HD21	1:G:156:LYS:HD3	1.78	0.46
1:G:111:ASN:HD22	1:G:156:LYS:HA	1.80	0.46
1:C:17:TYR:OH	1:C:68:ARG:O	2.32	0.46
1:D:224:THR:O	1:D:228:ARG:HG3	2.16	0.46
1:H:145:LYS:HG2	1:H:146:ASN:N	2.30	0.46
1:D:143:LYS:HZ1	1:D:146:ASN:HA	1.81	0.46
1:E:61:LYS:O	1:E:64:GLU:N	2.44	0.46
1:G:106:ILE:CG1	1:G:129:ALA:HB3	2.46	0.46
1:D:24:ASP:OD1	1:D:74:ASN:ND2	2.43	0.46
1:D:122:TYR:HB3	1:H:150:LEU:HD13	1.97	0.46
1:G:109:VAL:HB	1:G:151:ARG:NH2	2.30	0.46
1:H:149:TYR:O	1:H:150:LEU:HB2	2.16	0.46
1:F:149:TYR:C	1:F:150:LEU:HD23	2.41	0.46
1:E:181:ILE:HG21	1:E:210:ARG:HG3	1.98	0.46
1:G:195:PHE:HB3	2:G:301:SAM:O4'	2.15	0.46
1:B:112:ASN:N	1:B:112:ASN:OD1	2.47	0.46
1:C:148:LYS:O	1:C:149:TYR:HD1	1.99	0.46
1:E:168:HIS:HB3	1:E:170:THR:O	2.16	0.46
1:A:122:TYR:CD1	1:B:149:TYR:HB3	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LYS:HA	1:A:222:PHE:HB3	1.98	0.46
1:D:96:GLU:HA	1:D:100:PHE:O	2.15	0.46
1:F:13:ILE:O	1:F:17:TYR:HD2	1.99	0.46
1:H:145:LYS:HB3	1:H:145:LYS:HE3	1.45	0.46
1:C:168:HIS:CE1	2:C:301:SAM:HG1	2.52	0.45
1:A:144:PRO:C	1:A:146:ASN:N	2.75	0.45
1:D:6:HIS:NE2	1:D:219:LYS:HG2	2.30	0.45
1:G:155:LEU:O	1:G:156:LYS:HD3	2.16	0.45
1:H:24:ASP:HB2	1:H:190:ILE:H	1.81	0.45
1:E:81:ILE:HD12	1:E:95:LEU:HD11	1.99	0.45
1:C:187:PRO:O	1:C:210:ARG:HD3	2.16	0.45
1:E:96:GLU:HG3	1:E:102:VAL:HG23	1.97	0.45
1:E:200:THR:OG1	1:E:228:ARG:NH1	2.49	0.45
1:D:205:CYS:O	1:D:209:GLU:N	2.50	0.45
1:F:197:GLY:HA3	2:F:301:SAM:HB2	1.98	0.45
1:C:155:LEU:HD22	1:C:175:ALA:HB3	1.99	0.45
1:H:31:PRO:HG3	2:H:301:SAM:C8	2.47	0.45
1:E:155:LEU:CG	1:E:156:LYS:H	2.30	0.45
1:G:168:HIS:HE1	2:G:301:SAM:HN2	1.61	0.45
1:F:115:PRO:O	1:F:116:ARG:HG2	2.17	0.45
1:C:168:HIS:HB3	1:C:169:PRO:C	2.42	0.44
1:F:13:ILE:HD13	1:F:69:TYR:CE2	2.52	0.44
1:H:194:PRO:O	1:H:215:ILE:HB	2.16	0.44
1:E:28:THR:HG23	1:E:30:PRO:HD3	1.99	0.44
1:F:195:PHE:HB3	2:F:301:SAM:O4'	2.17	0.44
2:C:301:SAM:H4'	2:C:301:SAM:HE3	1.62	0.44
1:D:199:GLY:C	1:D:201:THR:H	2.25	0.44
1:C:108:TRP:HE1	1:C:155:LEU:HB3	1.83	0.44
1:D:67:ALA:HA	1:D:98:ASN:ND2	2.32	0.44
1:D:108:TRP:CD1	1:D:127:GLU:HB2	2.53	0.44
1:A:163:LEU:O	1:A:163:LEU:HD12	2.18	0.44
1:D:143:LYS:HG2	1:H:118:ILE:O	2.18	0.44
1:C:61:LYS:HG3	1:C:64:GLU:OE1	2.18	0.44
1:D:148:LYS:C	1:D:149:TYR:CG	2.96	0.44
1:H:216:GLU:OE2	2:H:301:SAM:O2'	2.22	0.44
1:F:219:LYS:O	1:F:223:GLN:HG2	2.18	0.44
1:H:10:PHE:O	1:H:13:ILE:HG22	2.18	0.44
1:D:111:ASN:HB2	1:D:156:LYS:HD3	2.00	0.44
1:D:143:LYS:HA	1:D:144:PRO:HD2	1.80	0.44
1:E:4:ILE:HB	1:E:196:MET:HE1	1.99	0.44
1:E:205:CYS:O	1:E:209:GLU:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ILE:CG2	1:F:210:ARG:HG3	2.48	0.44
1:B:189:ASP:O	1:B:211:ASN:HB2	2.18	0.43
1:B:199:GLY:C	1:B:201:THR:H	2.26	0.43
1:G:108:TRP:CZ2	1:G:155:LEU:HD13	2.53	0.43
1:H:109:VAL:HA	1:H:125:ASP:O	2.17	0.43
1:E:107:GLN:O	1:E:152:PRO:HD2	2.17	0.43
1:F:61:LYS:HA	1:F:64:GLU:HB3	1.99	0.43
1:A:103:LYS:O	1:B:121:ARG:NH2	2.42	0.43
1:B:194:PRO:O	1:B:215:ILE:HB	2.18	0.43
1:G:143:LYS:HG2	1:G:144:PRO:O	2.18	0.43
1:C:67:ALA:HA	1:C:98:ASN:OD1	2.18	0.43
1:C:150:LEU:HD13	1:E:122:TYR:HB3	1.99	0.43
1:E:195:PHE:HB3	2:E:301:SAM:O4'	2.19	0.43
1:G:108:TRP:HE3	1:G:127:GLU:HB2	1.84	0.43
1:D:125:ASP:OD1	1:H:150:LEU:HD23	2.19	0.43
1:D:209:GLU:OE2	1:E:206:LYS:HE2	2.19	0.43
2:H:301:SAM:HE3	2:H:301:SAM:H4'	1.68	0.43
1:F:28:THR:HG23	1:F:30:PRO:HD3	2.00	0.43
1:F:110:LYS:HG3	1:F:125:ASP:O	2.18	0.43
1:F:196:MET:O	2:F:301:SAM:HA	2.18	0.43
1:G:106:ILE:HG12	1:G:129:ALA:HB3	2.01	0.43
1:G:59:ASN:OD1	1:G:61:LYS:HG3	2.19	0.43
1:B:143:LYS:NZ	1:B:146:ASN:O	2.46	0.43
1:G:164:GLU:HG2	1:G:165:LYS:H	1.82	0.43
1:D:80:VAL:HA	1:D:130:LEU:O	2.19	0.42
1:D:195:PHE:HB3	2:D:301:SAM:O4'	2.19	0.42
1:E:195:PHE:HD1	2:E:301:SAM:N7	2.17	0.42
1:E:66:ILE:HD13	1:E:66:ILE:HG21	1.84	0.42
1:H:59:ASN:HB3	1:H:62:LEU:HD11	2.01	0.42
1:A:151:ARG:HH21	1:B:151:ARG:HH22	1.66	0.42
1:C:85:TYR:HE1	1:C:86:ARG:HD3	1.82	0.42
1:E:65:TRP:CH2	1:E:81:ILE:HD13	2.53	0.42
1:A:10:PHE:CE2	1:A:64:GLU:HG3	2.55	0.42
1:C:150:LEU:HD23	1:E:125:ASP:OD1	2.19	0.42
1:D:143:LYS:NZ	1:D:146:ASN:HA	2.33	0.42
1:E:145:LYS:HE3	1:E:145:LYS:HB2	1.81	0.42
1:H:150:LEU:HD12	1:H:150:LEU:HA	1.84	0.42
1:A:9:ALA:HA	1:A:12:ILE:HG22	2.00	0.42
1:A:115:PRO:CB	1:A:118:ILE:HD11	2.47	0.42
1:B:153:LEU:HG	1:B:155:LEU:N	2.30	0.42
1:D:93:ASP:OD2	1:H:90:TYR:OH	2.24	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:TRP:HE1	1:E:194:PRO:HG3	1.85	0.42
1:H:142:ASN:O	1:H:144:PRO:HD3	2.20	0.42
1:C:67:ALA:HB2	1:C:94:PHE:CE2	2.54	0.42
1:C:122:TYR:HB3	1:E:150:LEU:HD13	2.01	0.42
1:C:189:ASP:O	1:C:211:ASN:HB2	2.19	0.42
1:F:107:GLN:O	1:F:151:ARG:HG3	2.19	0.42
1:G:108:TRP:HZ2	1:G:155:LEU:HD22	1.85	0.42
1:C:172:LYS:O	1:C:200:THR:HG21	2.19	0.42
1:E:10:PHE:HA	1:E:13:ILE:HD11	2.02	0.42
1:F:60:PHE:O	1:F:64:GLU:N	2.53	0.42
1:G:29:ASP:O	2:G:301:SAM:HE3	2.20	0.42
1:H:145:LYS:CG	1:H:146:ASN:N	2.83	0.42
1:F:153:LEU:HG	1:F:155:LEU:N	2.34	0.42
1:C:141:PHE:O	1:C:142:ASN:HB2	2.19	0.42
1:D:107:GLN:O	1:D:151:ARG:HG3	2.20	0.42
1:D:155:LEU:HG	1:D:156:LYS:H	1.84	0.42
1:E:67:ALA:HA	1:E:98:ASN:OD1	2.19	0.42
1:H:205:CYS:HA	1:H:210:ARG:HB2	2.01	0.42
1:A:111:ASN:HB2	1:A:156:LYS:HA	2.02	0.42
1:C:148:LYS:HE2	1:C:148:LYS:HB2	1.93	0.42
1:E:144:PRO:HG2	1:E:146:ASN:HB3	2.01	0.42
1:A:6:HIS:NE2	1:A:219:LYS:HD3	2.35	0.41
1:A:108:TRP:NE1	1:A:155:LEU:HB3	2.29	0.41
1:B:166:THR:HG23	1:B:168:HIS:H	1.85	0.41
1:C:205:CYS:CA	1:C:210:ARG:HB2	2.50	0.41
1:C:199:GLY:C	1:C:201:THR:H	2.27	0.41
1:H:148:LYS:HE3	1:H:148:LYS:HB2	1.91	0.41
1:B:177:MET:HE2	1:B:201:THR:HG23	2.02	0.41
1:C:107:GLN:O	1:C:152:PRO:HD2	2.20	0.41
1:D:113:PRO:HG2	1:H:148:LYS:HD2	2.02	0.41
1:A:17:TYR:OH	1:A:68:ARG:O	2.26	0.41
1:B:14:LYS:HB3	1:B:14:LYS:HE3	1.80	0.41
1:B:96:GLU:HG3	1:B:102:VAL:HG23	2.01	0.41
1:F:4:ILE:HB	1:F:196:MET:HE1	2.02	0.41
1:G:111:ASN:ND2	1:G:156:LYS:HA	2.35	0.41
1:G:181:ILE:HG21	1:G:210:ARG:HG3	2.01	0.41
1:H:22:LYS:HB3	1:H:74:ASN:OD1	2.20	0.41
1:A:62:LEU:H	1:A:62:LEU:HG	1.84	0.41
1:B:193:ASP:HA	1:B:194:PRO:HD2	1.91	0.41
1:F:108:TRP:HE1	1:F:155:LEU:HB3	1.84	0.41
1:F:148:LYS:HB3	1:F:149:TYR:H	1.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:GLY:HA3	2:F:301:SAM:CB	2.50	0.41
1:G:150:LEU:HD23	1:G:150:LEU:O	2.20	0.41
1:A:107:GLN:NE2	1:B:107:GLN:HE22	2.18	0.41
1:C:172:LYS:HD3	1:C:172:LYS:HA	1.90	0.41
2:E:301:SAM:HE2	2:E:301:SAM:HB1	1.84	0.41
1:G:168:HIS:CD2	1:G:221:TYR:CZ	3.09	0.41
1:A:181:ILE:HG21	1:A:210:ARG:HG3	2.01	0.41
1:A:192:LEU:HG	1:A:194:PRO:HD3	2.02	0.41
1:D:79:MET:HG3	1:D:100:PHE:CE2	2.56	0.41
1:E:202:GLY:HA2	1:E:212:PHE:CG	2.55	0.41
1:F:79:MET:HG3	1:F:100:PHE:CE2	2.56	0.41
1:H:144:PRO:HD2	1:H:149:TYR:CE2	2.56	0.41
1:H:146:ASN:CB	1:H:149:TYR:HE1	2.34	0.41
1:A:181:ILE:CG2	1:A:210:ARG:HG3	2.49	0.41
1:A:202:GLY:HA2	1:A:212:PHE:CG	2.56	0.41
1:B:168:HIS:CG	1:B:169:PRO:HD2	2.56	0.41
1:E:110:LYS:HG3	1:E:125:ASP:O	2.20	0.41
1:A:107:GLN:HE22	1:B:107:GLN:HE22	1.67	0.41
1:A:107:GLN:O	1:A:152:PRO:HD2	2.20	0.41
1:B:109:VAL:HA	1:B:125:ASP:O	2.21	0.41
1:C:29:ASP:CG	1:C:172:LYS:HZ2	2.27	0.41
1:E:106:ILE:CG1	1:E:129:ALA:HB3	2.51	0.41
1:E:155:LEU:HG	1:E:156:LYS:N	2.35	0.41
1:E:169:PRO:HB2	1:E:170:THR:CB	2.51	0.41
1:F:193:ASP:HA	1:F:194:PRO:HD2	1.93	0.41
1:H:155:LEU:HD21	1:H:175:ALA:CB	2.49	0.41
1:C:136:LYS:HD3	1:C:136:LYS:HA	1.77	0.41
1:F:141:PHE:O	1:F:183:ILE:O	2.39	0.41
1:G:181:ILE:CG2	1:G:210:ARG:HG3	2.51	0.41
1:H:61:LYS:HB2	1:H:61:LYS:HE2	1.51	0.41
1:H:193:ASP:HA	1:H:194:PRO:HD2	1.90	0.41
1:D:62:LEU:HD13	1:D:63:LEU:HD22	2.03	0.40
1:D:142:ASN:HB2	1:D:182:SER:O	2.21	0.40
1:D:150:LEU:HA	1:H:122:TYR:CD1	2.57	0.40
1:E:65:TRP:HE1	1:E:194:PRO:CG	2.34	0.40
1:E:199:GLY:C	1:E:201:THR:H	2.29	0.40
1:F:113:PRO:HD2	1:G:148:LYS:HZ2	1.84	0.40
1:F:194:PRO:O	1:F:215:ILE:HB	2.20	0.40
1:B:61:LYS:HA	1:B:62:LEU:HB2	2.02	0.40
1:C:172:LYS:HG2	2:C:301:SAM:HN1	1.85	0.40
1:G:205:CYS:O	1:G:209:GLU:N	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ILE:O	1:E:17:TYR:N	2.48	0.40
1:E:28:THR:HG21	1:E:65:TRP:CZ2	2.56	0.40
1:H:169:PRO:HB2	1:H:170:THR:H	1.69	0.40
1:B:92:ALA:HB2	1:B:130:LEU:HD11	2.04	0.40
1:G:202:GLY:HA2	1:G:212:PHE:CG	2.56	0.40
1:H:28:THR:HG23	1:H:30:PRO:HD3	2.02	0.40
1:H:59:ASN:CG	1:H:61:LYS:HZ1	2.28	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ASN:OD1	1:E:20:ASN:ND2[6_564]	2.16	0.04

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	195/232 (84%)	178 (91%)	12 (6%)	5 (3%)	4	21
1	B	188/232 (81%)	176 (94%)	10 (5%)	2 (1%)	11	39
1	C	198/232 (85%)	181 (91%)	15 (8%)	2 (1%)	12	41
1	D	182/232 (78%)	168 (92%)	12 (7%)	2 (1%)	11	39
1	E	187/232 (81%)	171 (91%)	12 (6%)	4 (2%)	5	25
1	F	188/232 (81%)	171 (91%)	16 (8%)	1 (0%)	24	57
1	G	194/232 (84%)	175 (90%)	16 (8%)	3 (2%)	8	32
1	H	187/232 (81%)	169 (90%)	15 (8%)	3 (2%)	7	30
All	All	1519/1856 (82%)	1389 (91%)	108 (7%)	22 (1%)	9	34

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	118	ILE
1	E	171	GLN
1	G	155	LEU
1	A	148	LYS
1	C	150	LEU
1	E	150	LEU
1	F	149	TYR
1	A	141	PHE
1	A	145	LYS
1	A	147	GLU
1	A	164	GLU
1	B	150	LEU
1	H	149	TYR
1	H	171	GLN
1	B	149	TYR
1	C	144	PRO
1	D	149	TYR
1	G	148	LYS
1	D	115	PRO
1	G	157	SER
1	E	118	ILE
1	E	169	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	182/210 (87%)	175 (96%)	7 (4%)	29	60
1	B	176/210 (84%)	169 (96%)	7 (4%)	28	60
1	C	185/210 (88%)	181 (98%)	4 (2%)	45	71
1	D	170/210 (81%)	162 (95%)	8 (5%)	23	55
1	E	175/210 (83%)	167 (95%)	8 (5%)	24	55
1	F	176/210 (84%)	169 (96%)	7 (4%)	28	60
1	G	182/210 (87%)	177 (97%)	5 (3%)	39	67
1	H	175/210 (83%)	169 (97%)	6 (3%)	32	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1421/1680 (85%)	1369 (96%)	52 (4%)	30 61

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	61	LYS
1	A	63	LEU
1	A	86	ARG
1	A	148	LYS
1	A	160	VAL
1	A	163	LEU
1	B	86	ARG
1	B	109	VAL
1	B	110	LYS
1	B	149	TYR
1	B	151	ARG
1	B	167	LYS
1	B	209	GLU
1	C	11	GLU
1	C	58	LYS
1	C	86	ARG
1	C	145	LYS
1	D	61	LYS
1	D	62	LEU
1	D	86	ARG
1	D	120	ARG
1	D	134	LYS
1	D	135	LYS
1	D	143	LYS
1	D	145	LYS
1	E	13	ILE
1	E	59	ASN
1	E	63	LEU
1	E	86	ARG
1	E	116	ARG
1	E	145	LYS
1	E	170	THR
1	E	226	LYS
1	F	14	LYS
1	F	18	GLN
1	F	86	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	116	ARG
1	F	138	LYS
1	F	155	LEU
1	F	201	THR
1	G	58	LYS
1	G	59	ASN
1	G	63	LEU
1	G	116	ARG
1	G	155	LEU
1	H	18	GLN
1	H	86	ARG
1	H	124	GLN
1	H	136	LYS
1	H	145	LYS
1	H	147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	119	HIS
1	B	111	ASN
1	C	119	HIS
1	E	59	ASN
1	E	168	HIS
1	F	107	GLN
1	F	111	ASN
1	G	107	GLN
1	G	168	HIS
1	H	18	GLN
1	H	146	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](#)

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	SAM	D	301	-	27,29,29	1.10	4 (14%)	34,42,42	2.01	9 (26%)
2	SAM	G	301	-	27,29,29	1.11	4 (14%)	34,42,42	2.01	9 (26%)
2	SAM	A	301	-	27,29,29	1.10	4 (14%)	34,42,42	1.98	9 (26%)
2	SAM	C	301	-	27,29,29	1.12	4 (14%)	34,42,42	2.24	11 (32%)
2	SAM	F	301	-	27,29,29	1.13	4 (14%)	34,42,42	1.99	9 (26%)
2	SAM	B	301	-	27,29,29	1.09	4 (14%)	34,42,42	1.99	8 (23%)
2	SAM	E	301	-	27,29,29	1.12	4 (14%)	34,42,42	2.14	10 (29%)
2	SAM	H	301	-	27,29,29	1.11	4 (14%)	34,42,42	2.17	9 (26%)

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	SAM	D	301	-	-	9/17/33/33	0/3/3/3
2	SAM	G	301	-	-	9/17/33/33	0/3/3/3
2	SAM	A	301	-	-	5/17/33/33	0/3/3/3
2	SAM	C	301	-	-	9/17/33/33	0/3/3/3
2	SAM	F	301	-	-	6/17/33/33	0/3/3/3
2	SAM	B	301	-	-	7/17/33/33	0/3/3/3
2	SAM	E	301	-	-	11/17/33/33	0/3/3/3
2	SAM	H	301	-	-	10/17/33/33	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SAM	C2-N3	2.70	1.38	1.33
2	C	301	SAM	C2-N1	2.65	1.38	1.33
2	F	301	SAM	C2-N1	2.63	1.38	1.33
2	H	301	SAM	C2-N3	2.63	1.38	1.33
2	D	301	SAM	C2-N3	2.59	1.38	1.33
2	E	301	SAM	C2-N3	2.58	1.38	1.33
2	D	301	SAM	C2-N1	2.57	1.38	1.33
2	F	301	SAM	C2-N3	2.57	1.38	1.33
2	G	301	SAM	C2-N3	2.56	1.38	1.33
2	B	301	SAM	C2-N1	2.56	1.38	1.33
2	H	301	SAM	C2-N1	2.55	1.38	1.33
2	G	301	SAM	C2-N1	2.53	1.38	1.33
2	E	301	SAM	C2-N1	2.53	1.38	1.33
2	A	301	SAM	C2-N1	2.50	1.38	1.33
2	B	301	SAM	C2-N3	2.47	1.38	1.33
2	A	301	SAM	C2-N3	2.30	1.38	1.33
2	A	301	SAM	C8-N7	2.26	1.36	1.31
2	A	301	SAM	OXT-C	-2.25	1.23	1.30
2	C	301	SAM	OXT-C	-2.25	1.23	1.30
2	H	301	SAM	OXT-C	-2.24	1.23	1.30
2	B	301	SAM	OXT-C	-2.22	1.23	1.30
2	D	301	SAM	OXT-C	-2.21	1.23	1.30
2	E	301	SAM	OXT-C	-2.21	1.23	1.30
2	F	301	SAM	OXT-C	-2.19	1.23	1.30
2	G	301	SAM	C8-N7	2.18	1.35	1.31
2	B	301	SAM	C8-N7	2.18	1.35	1.31
2	G	301	SAM	OXT-C	-2.18	1.23	1.30
2	F	301	SAM	C8-N7	2.16	1.35	1.31
2	D	301	SAM	C8-N7	2.14	1.35	1.31
2	H	301	SAM	C8-N7	2.13	1.35	1.31
2	E	301	SAM	C5-N7	-2.11	1.35	1.39
2	C	301	SAM	C8-N7	2.11	1.35	1.31

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	SAM	N3-C2-N1	-5.92	119.62	128.58
2	F	301	SAM	N3-C2-N1	-5.72	119.93	128.58
2	B	301	SAM	N3-C2-N1	-5.67	120.00	128.58
2	G	301	SAM	N3-C2-N1	-5.63	120.06	128.58
2	C	301	SAM	N3-C2-N1	-5.57	120.16	128.58
2	D	301	SAM	N3-C2-N1	-5.56	120.16	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	SAM	N3-C2-N1	-5.55	120.18	128.58
2	E	301	SAM	N3-C2-N1	-5.48	120.28	128.58
2	E	301	SAM	C5-C4-N3	-5.46	119.19	126.72
2	C	301	SAM	O4'-C1'-N9	4.86	117.42	108.09
2	C	301	SAM	C5-C4-N3	-4.86	120.03	126.72
2	H	301	SAM	C5-C4-N3	-4.71	120.23	126.72
2	D	301	SAM	C5-C4-N3	-4.67	120.28	126.72
2	G	301	SAM	C5-C4-N3	-4.51	120.50	126.72
2	B	301	SAM	C5-C4-N3	-4.43	120.62	126.72
2	H	301	SAM	O4'-C1'-N9	4.39	116.53	108.09
2	F	301	SAM	C5-C4-N3	-4.37	120.70	126.72
2	A	301	SAM	N9-C8-N7	-4.17	108.02	113.94
2	F	301	SAM	N9-C8-N7	-4.07	108.17	113.94
2	G	301	SAM	N9-C8-N7	-3.89	108.42	113.94
2	B	301	SAM	N9-C8-N7	-3.89	108.42	113.94
2	E	301	SAM	N3-C4-N9	3.89	133.78	127.17
2	A	301	SAM	C5-C4-N3	-3.88	121.37	126.72
2	H	301	SAM	N9-C8-N7	-3.86	108.46	113.94
2	D	301	SAM	N9-C8-N7	-3.79	108.56	113.94
2	E	301	SAM	C2-N3-C4	3.74	120.98	111.83
2	C	301	SAM	N9-C8-N7	-3.63	108.79	113.94
2	C	301	SAM	C2-N3-C4	3.54	120.49	111.83
2	H	301	SAM	C2-N3-C4	3.50	120.38	111.83
2	D	301	SAM	C2-N3-C4	3.49	120.35	111.83
2	H	301	SAM	C5-N7-C8	3.46	108.89	103.45
2	G	301	SAM	C2-N3-C4	3.46	120.27	111.83
2	F	301	SAM	C2-N3-C4	3.45	120.27	111.83
2	F	301	SAM	C5-N7-C8	3.43	108.84	103.45
2	A	301	SAM	C5-N7-C8	3.42	108.82	103.45
2	C	301	SAM	C5-N7-C8	3.41	108.81	103.45
2	B	301	SAM	C2-N3-C4	3.41	120.16	111.83
2	G	301	SAM	C5-N7-C8	3.38	108.76	103.45
2	D	301	SAM	C5-N7-C8	3.36	108.73	103.45
2	A	301	SAM	C2-N3-C4	3.36	120.03	111.83
2	B	301	SAM	C5-N7-C8	3.34	108.70	103.45
2	E	301	SAM	N9-C8-N7	-3.26	109.31	113.94
2	E	301	SAM	C5-N7-C8	3.20	108.47	103.45
2	C	301	SAM	N3-C4-N9	3.19	132.59	127.17
2	H	301	SAM	N3-C4-N9	3.14	132.51	127.17
2	D	301	SAM	N3-C4-N9	3.09	132.42	127.17
2	G	301	SAM	N3-C4-N9	2.93	132.15	127.17
2	F	301	SAM	N3-C4-N9	2.90	132.10	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	SAM	N3-C4-N9	2.89	132.09	127.17
2	C	301	SAM	O4'-C4'-C5'	2.78	115.91	108.88
2	F	301	SAM	OXT-C-O	-2.78	117.78	124.08
2	D	301	SAM	OXT-C-O	-2.76	117.82	124.08
2	H	301	SAM	OXT-C-O	-2.71	117.92	124.08
2	B	301	SAM	OXT-C-O	-2.70	117.95	124.08
2	E	301	SAM	O4'-C1'-N9	2.67	113.21	108.09
2	A	301	SAM	OXT-C-O	-2.65	118.06	124.08
2	C	301	SAM	OXT-C-O	-2.63	118.11	124.08
2	G	301	SAM	OXT-C-O	-2.62	118.13	124.08
2	G	301	SAM	O4'-C1'-N9	2.62	113.11	108.09
2	E	301	SAM	OXT-C-O	-2.61	118.17	124.08
2	A	301	SAM	C4-C5-N7	-2.50	107.73	110.58
2	D	301	SAM	O4'-C1'-N9	2.46	112.81	108.09
2	H	301	SAM	C4-C5-N7	-2.45	107.78	110.58
2	C	301	SAM	C4-C5-N7	-2.43	107.81	110.58
2	A	301	SAM	N3-C4-N9	2.38	131.22	127.17
2	F	301	SAM	C4-C5-N7	-2.38	107.86	110.58
2	B	301	SAM	C4-C5-N7	-2.36	107.88	110.58
2	G	301	SAM	C4-C5-N7	-2.35	107.89	110.58
2	D	301	SAM	C4-C5-N7	-2.31	107.94	110.58
2	E	301	SAM	C6-C5-C4	2.30	120.32	117.18
2	A	301	SAM	C4-N9-C8	2.16	108.01	105.74
2	E	301	SAM	C4-C5-N7	-2.10	108.18	110.58
2	F	301	SAM	C4-N9-C8	2.10	107.94	105.74
2	C	301	SAM	C6-C5-C4	2.05	119.98	117.18

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	SAM	CB-CG-SD-CE
2	B	301	SAM	N-CA-CB-CG
2	B	301	SAM	CB-CG-SD-C5'
2	C	301	SAM	N-CA-CB-CG
2	C	301	SAM	C-CA-CB-CG
2	C	301	SAM	CB-CG-SD-CE
2	C	301	SAM	C4'-C5'-SD-CE
2	D	301	SAM	N-CA-CB-CG
2	D	301	SAM	CB-CG-SD-C5'
2	E	301	SAM	N-CA-CB-CG
2	E	301	SAM	C-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	301	SAM	O4'-C4'-C5'-SD
2	E	301	SAM	C3'-C4'-C5'-SD
2	F	301	SAM	C-CA-CB-CG
2	G	301	SAM	N-CA-CB-CG
2	H	301	SAM	N-CA-CB-CG
2	H	301	SAM	CA-CB-CG-SD
2	H	301	SAM	CB-CG-SD-CE
2	H	301	SAM	C4'-C5'-SD-CE
2	H	301	SAM	OXT-C-CA-CB
2	E	301	SAM	C2'-C1'-N9-C8
2	E	301	SAM	C2'-C1'-N9-C4
2	H	301	SAM	O-C-CA-CB
2	G	301	SAM	C-CA-CB-CG
2	H	301	SAM	C-CA-CB-CG
2	H	301	SAM	OXT-C-CA-N
2	B	301	SAM	CB-CG-SD-CE
2	D	301	SAM	CB-CG-SD-CE
2	H	301	SAM	O-C-CA-N
2	A	301	SAM	C2'-C1'-N9-C8
2	B	301	SAM	C2'-C1'-N9-C8
2	D	301	SAM	C2'-C1'-N9-C8
2	F	301	SAM	C2'-C1'-N9-C8
2	F	301	SAM	N-CA-CB-CG
2	C	301	SAM	CA-CB-CG-SD
2	E	301	SAM	CA-CB-CG-SD
2	G	301	SAM	CA-CB-CG-SD
2	C	301	SAM	OXT-C-CA-CB
2	A	301	SAM	CB-CG-SD-C5'
2	C	301	SAM	CB-CG-SD-C5'
2	C	301	SAM	O-C-CA-CB
2	E	301	SAM	OXT-C-CA-CB
2	D	301	SAM	OXT-C-CA-CB
2	F	301	SAM	O-C-CA-CB
2	A	301	SAM	C2'-C1'-N9-C4
2	D	301	SAM	C-CA-CB-CG
2	D	301	SAM	O-C-CA-CB
2	E	301	SAM	O-C-CA-CB
2	F	301	SAM	OXT-C-CA-CB
2	G	301	SAM	O-C-CA-N
2	B	301	SAM	OXT-C-CA-CB
2	G	301	SAM	OXT-C-CA-N
2	B	301	SAM	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

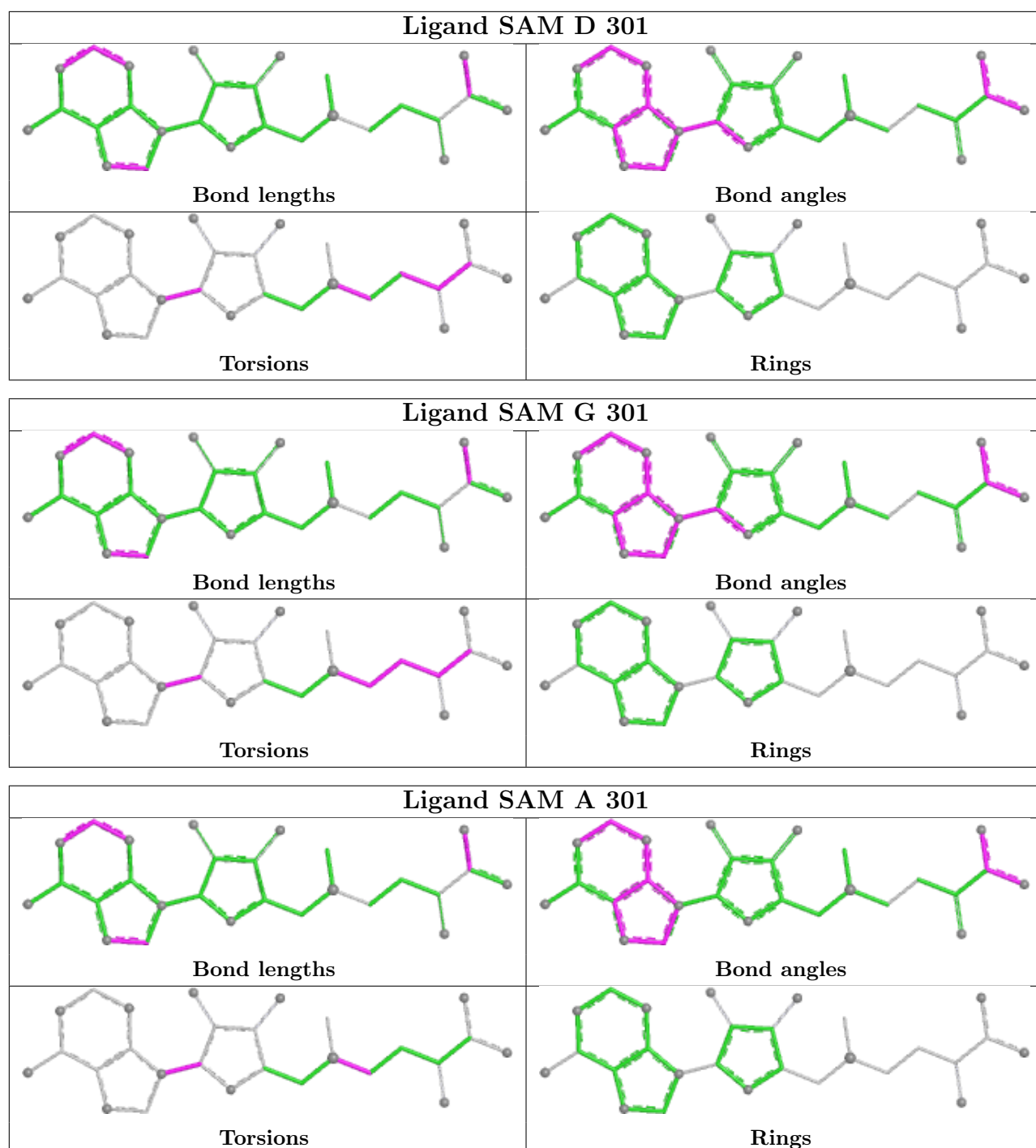
Mol	Chain	Res	Type	Atoms
2	F	301	SAM	O4'-C1'-N9-C8
2	A	301	SAM	O4'-C1'-N9-C8
2	B	301	SAM	O-C-CA-CB
2	G	301	SAM	O-C-CA-CB
2	G	301	SAM	OXT-C-CA-CB
2	G	301	SAM	C2'-C1'-N9-C8
2	D	301	SAM	O4'-C1'-N9-C8
2	C	301	SAM	O4'-C4'-C5'-SD
2	E	301	SAM	CB-CG-SD-C5'
2	G	301	SAM	CB-CG-SD-C5'
2	H	301	SAM	CB-CG-SD-C5'
2	E	301	SAM	O-C-CA-N
2	D	301	SAM	OXT-C-CA-N

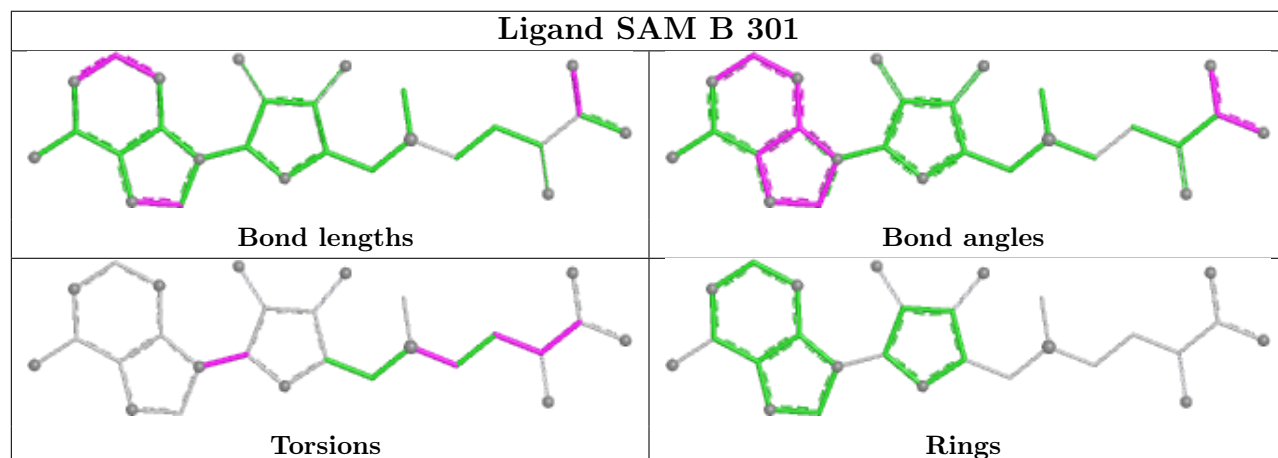
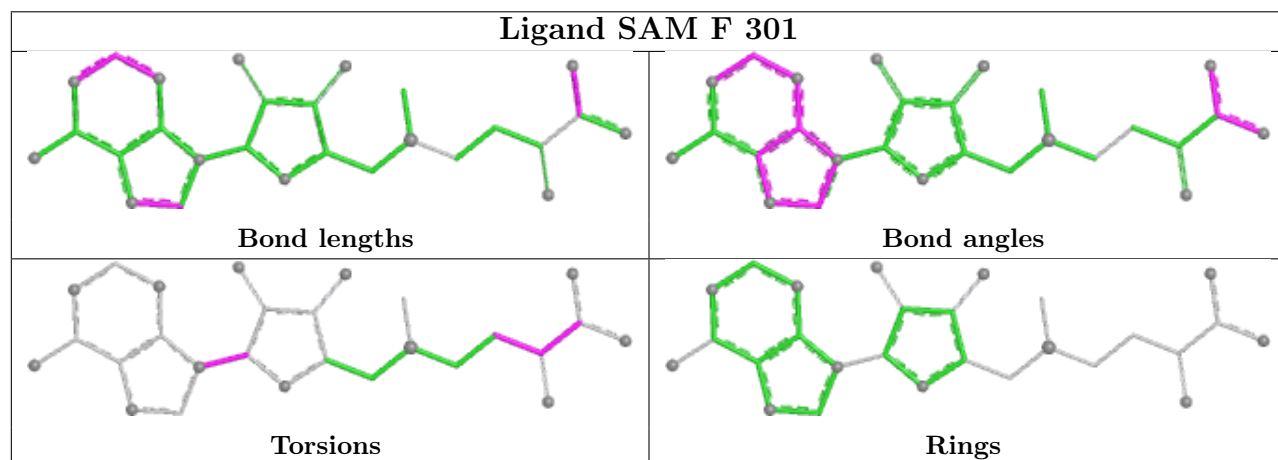
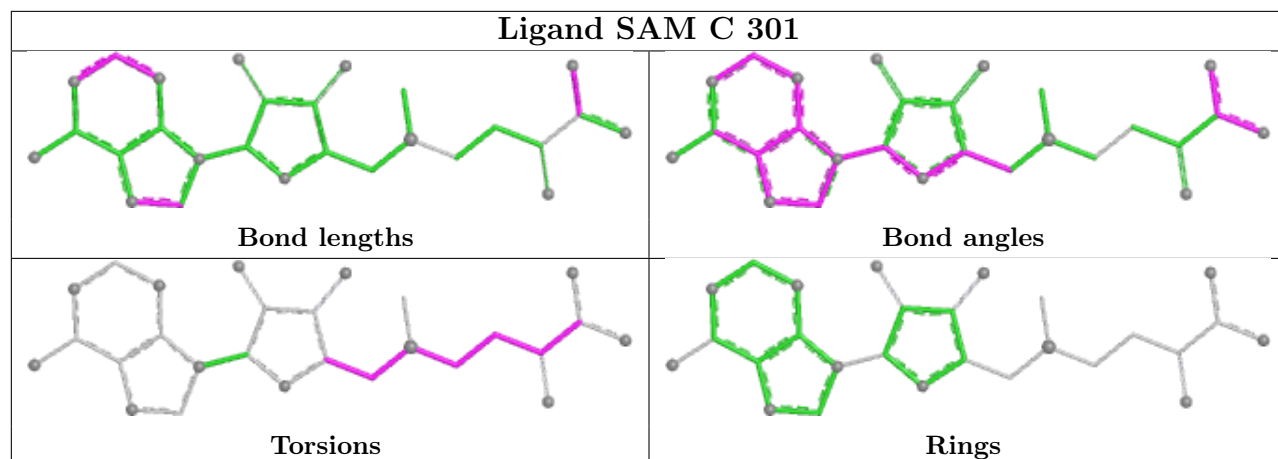
There are no ring outliers.

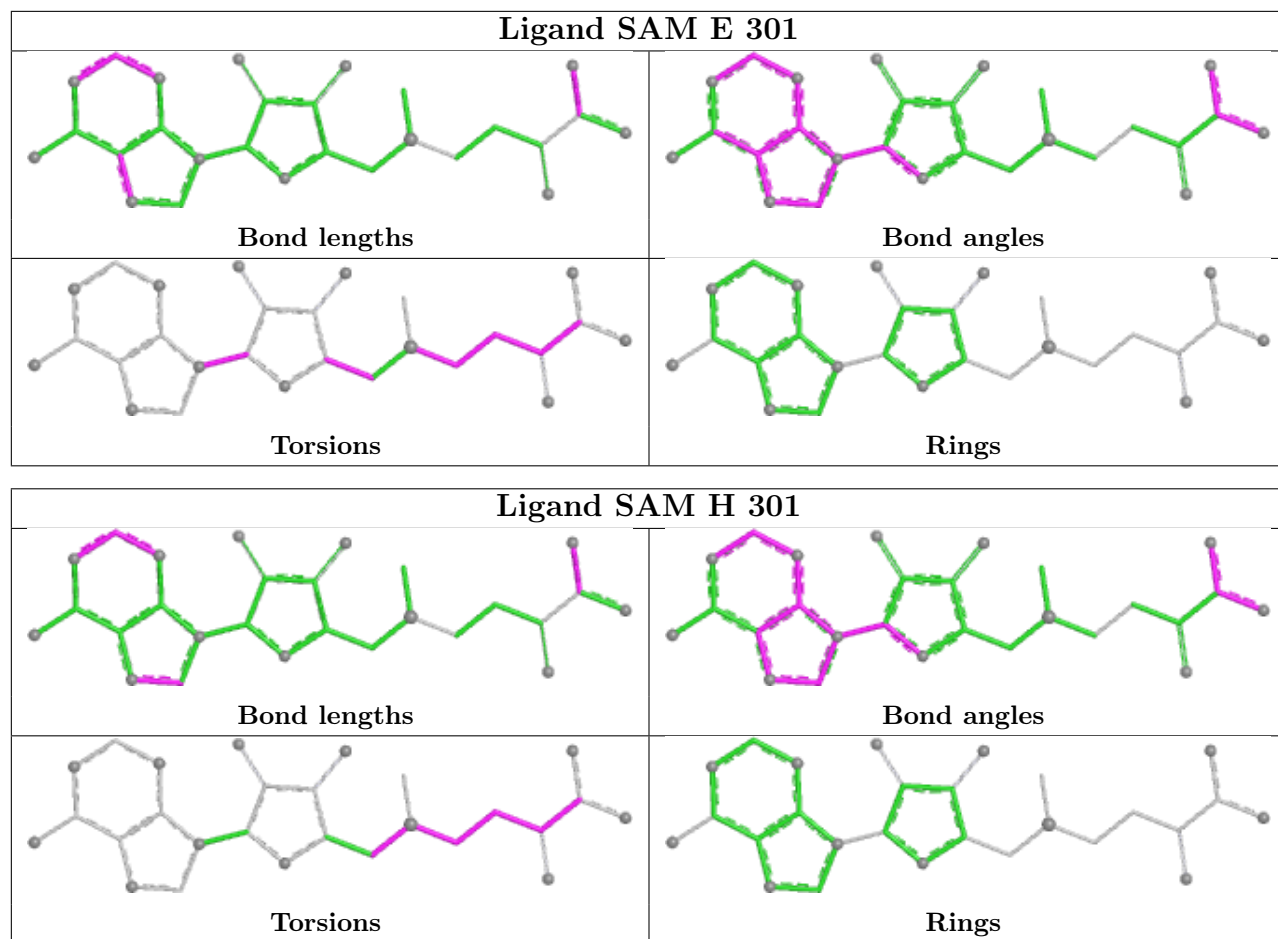
8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	SAM	2	0
2	G	301	SAM	6	0
2	A	301	SAM	7	0
2	C	301	SAM	6	0
2	F	301	SAM	4	0
2	B	301	SAM	2	0
2	E	301	SAM	9	0
2	H	301	SAM	6	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.







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

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	201/232 (86%)	0.15	8 (3%)	42	23	43, 66, 95, 104	0
1	B	194/232 (83%)	0.14	6 (3%)	51	30	42, 70, 101, 113	0
1	C	204/232 (87%)	0.22	7 (3%)	48	28	47, 70, 92, 108	0
1	D	188/232 (81%)	0.15	6 (3%)	50	30	49, 72, 103, 123	0
1	E	193/232 (83%)	0.25	11 (5%)	29	16	47, 70, 108, 123	0
1	F	194/232 (83%)	0.29	7 (3%)	46	26	43, 72, 102, 121	0
1	G	200/232 (86%)	0.18	5 (2%)	58	37	46, 72, 109, 131	0
1	H	193/232 (83%)	0.24	9 (4%)	36	19	49, 74, 107, 133	0
All	All	1567/1856 (84%)	0.20	59 (3%)	44	25	42, 71, 104, 133	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	169	PRO	4.6
1	B	149	TYR	4.5
1	D	149	TYR	4.2
1	H	149	TYR	4.2
1	G	149	TYR	4.1
1	A	149	TYR	3.7
1	B	151	ARG	3.5
1	H	112	ASN	3.3
1	D	62	LEU	3.2
1	E	157	SER	3.2
1	C	231	LEU	3.1
1	F	31	PRO	3.0
1	E	149	TYR	3.0
1	A	231	LEU	2.9
1	A	166	THR	2.8
1	E	224	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	2.8
1	D	60	PHE	2.7
1	H	118	ILE	2.6
1	A	159	VAL	2.6
1	F	150	LEU	2.6
1	F	115	PRO	2.6
1	E	152	PRO	2.6
1	A	168	HIS	2.6
1	D	173	SER	2.6
1	G	158	PRO	2.6
1	B	227	LYS	2.6
1	E	151	ARG	2.6
1	G	116	ARG	2.6
1	B	62	LEU	2.5
1	G	62	LEU	2.5
1	C	154	ILE	2.5
1	E	59	ASN	2.5
1	E	153	LEU	2.5
1	D	147	GLU	2.4
1	A	151	ARG	2.4
1	H	62	LEU	2.4
1	F	145	LYS	2.4
1	H	158	PRO	2.4
1	G	147	GLU	2.4
1	F	169	PRO	2.4
1	E	148	LYS	2.3
1	E	66	ILE	2.3
1	C	156	LYS	2.3
1	C	152	PRO	2.3
1	H	151	ARG	2.2
1	B	154	ILE	2.2
1	H	145	LYS	2.2
1	F	149	TYR	2.1
1	A	147	GLU	2.1
1	B	152	PRO	2.1
1	C	199	GLY	2.1
1	E	169	PRO	2.1
1	F	148	LYS	2.1
1	C	148	LYS	2.0
1	E	65	TRP	2.0
1	C	149	TYR	2.0
1	D	148	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	148	LYS	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](#)

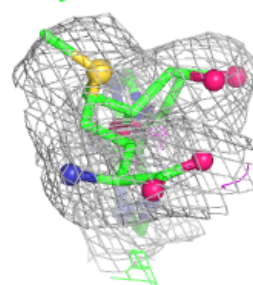
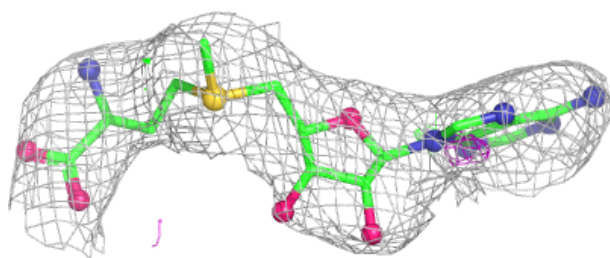
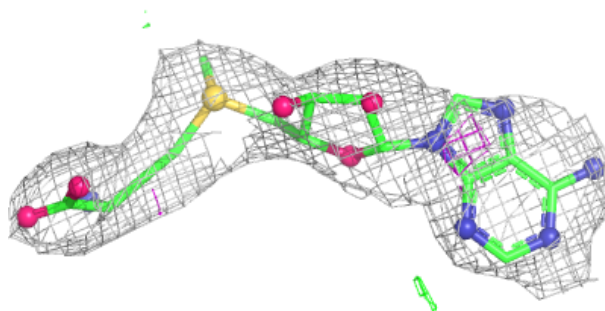
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SAM	D	301	27/27	0.84	0.14	73,90,99,122	0
2	SAM	E	301	27/27	0.85	0.16	62,74,100,101	0
2	SAM	H	301	27/27	0.90	0.11	67,74,88,141	0
2	SAM	G	301	27/27	0.92	0.11	57,63,70,70	0
2	SAM	C	301	27/27	0.92	0.10	49,63,80,132	0
2	SAM	B	301	27/27	0.93	0.10	52,70,74,79	0
2	SAM	A	301	27/27	0.94	0.09	53,66,80,86	0
2	SAM	F	301	27/27	0.94	0.09	37,68,74,114	0

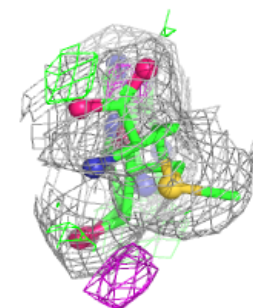
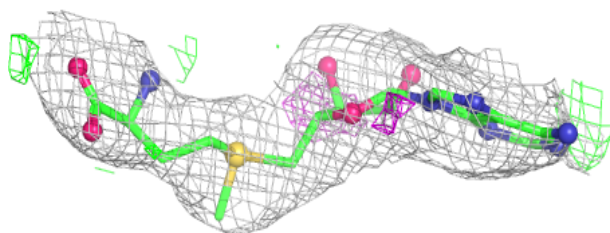
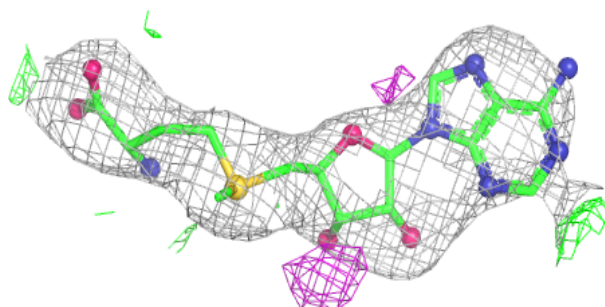
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM 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)

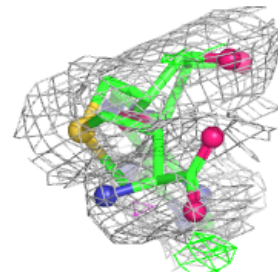
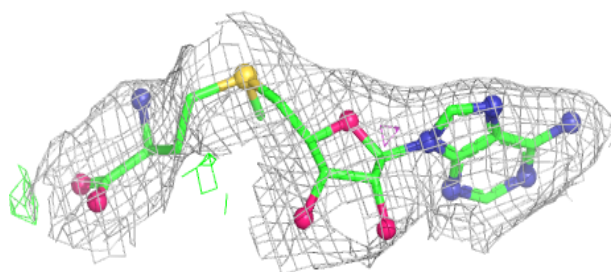
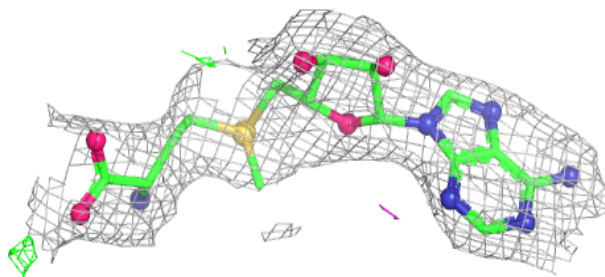
**Electron density around SAM E 301:**

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

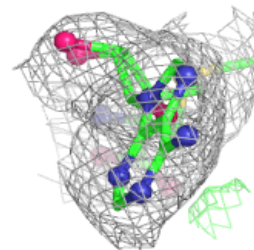
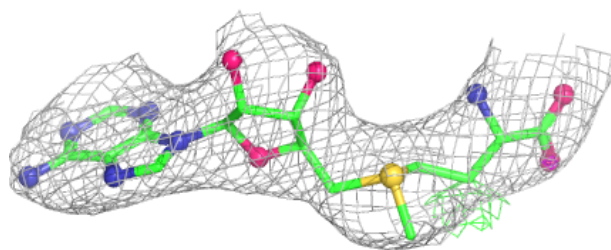
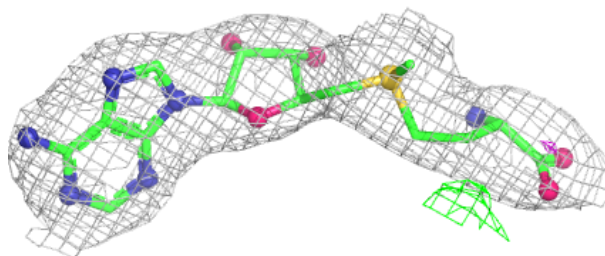


Electron density around SAM H 301:

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

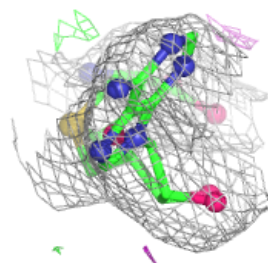
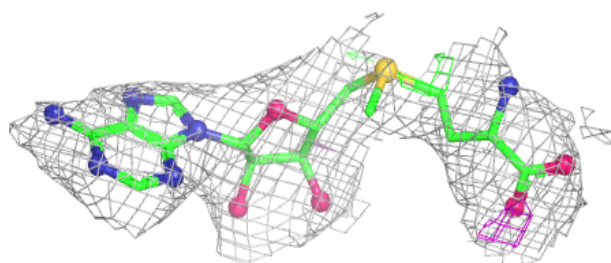
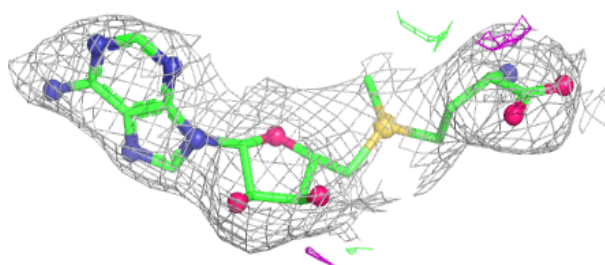
**Electron density around SAM G 301:**

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

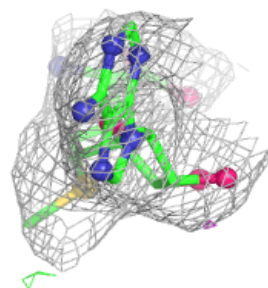
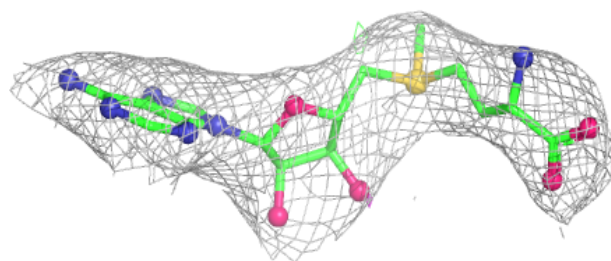
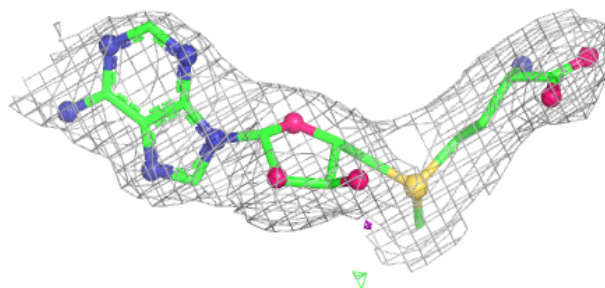


Electron density around SAM C 301:

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

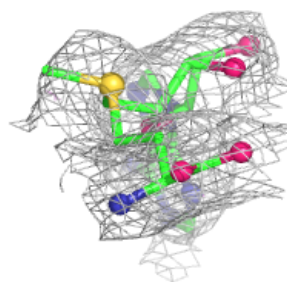
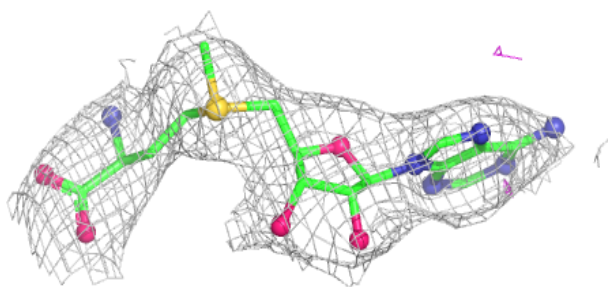
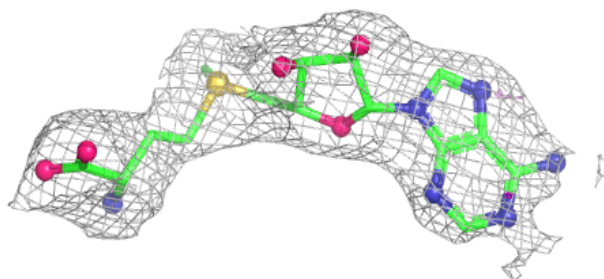
**Electron density around SAM B 301:**

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

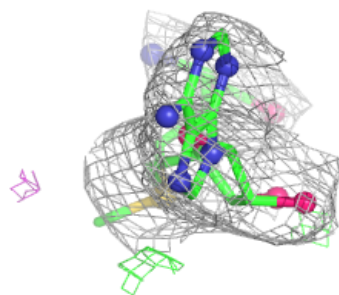
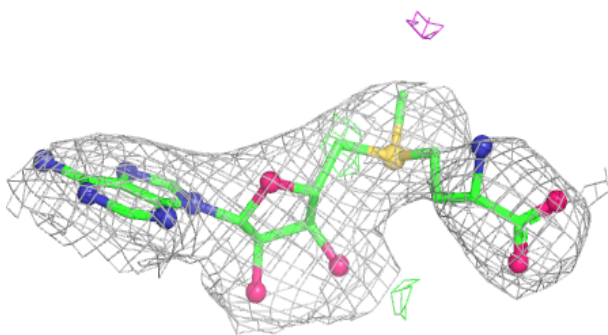
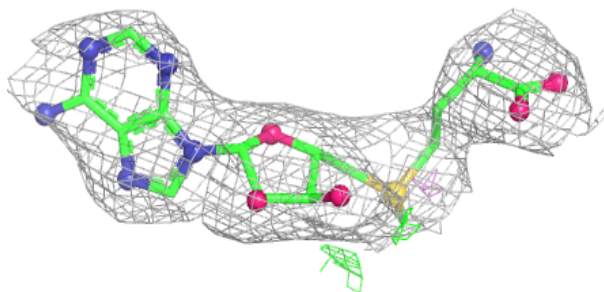


Electron density around SAM A 301:

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

**Electron density around SAM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.