Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 07:15 AM EDT

PDB ID	:	3MO2
Title	:	human G9a-like (GLP, also known as EHMT1) in complex with inhibitor E67
Authors	:	Chang, Y.; Horton, J.R.; Cheng, X.
Deposited on	:	2010-04-22
Resolution	:	2.49 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 (i) 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 (i)) were used in the production of this report:

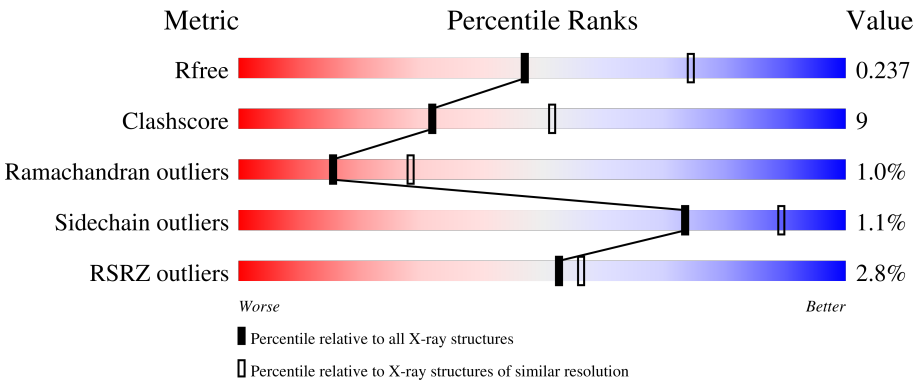
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	285	5% 67% 22% • 11%
1	B	285	2% 77% 12% • 9%
1	C	285	2% 75% 15% 9%
1	D	285	2% 69% 20% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8719 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.

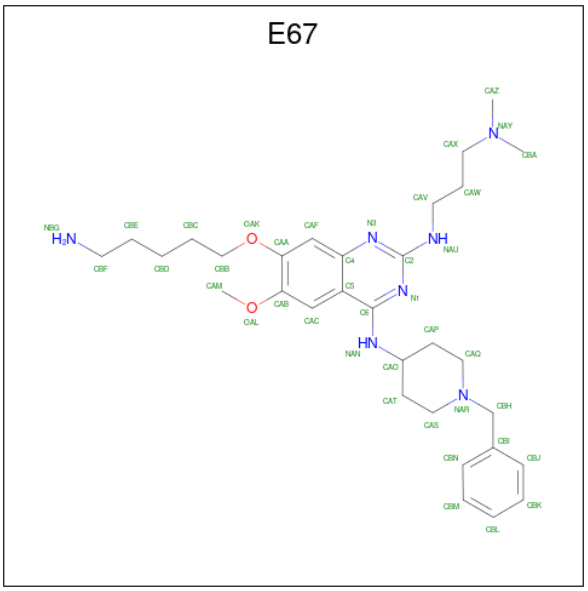
- Molecule 1 is a protein called Histone-lysine N-methyltransferase, H3 lysine-9 specific 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2016	1259	363	370	24	0	0	0
1	B	258	2046	1279	367	375	25	0	0	0
1	C	258	2040	1274	365	376	25	0	0	0
1	D	256	1992	1249	353	365	25	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

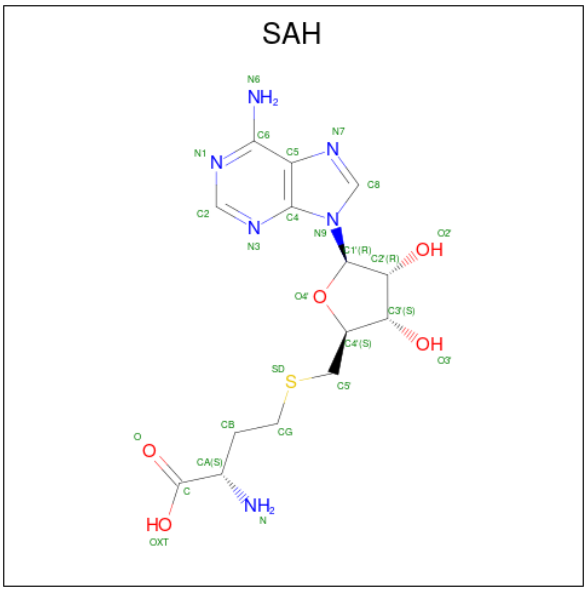
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	4	4	4	0	0
2	B	4	4	4	0	0
2	C	4	4	4	0	0
2	D	4	4	4	0	0

- Molecule 3 is 7-[(5-aminopentyl)oxy]-N 4 -(1-benzylpiperidin-4-yl)-N 2 -[3-(dimethylamino) propyl]-6-methoxyquinazoline-2,4-diamine (three-letter code: E67) (formula: $C_{31}H_{47}N_7O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	40	31	7	2	0	0
			Total	C	N	O		
3	B	1	40	31	7	2	0	0
			Total	C	N	O		
3	C	1	40	31	7	2	0	0
			Total	C	N	O		
3	D	1	40	31	7	2	0	0

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 5 is water.

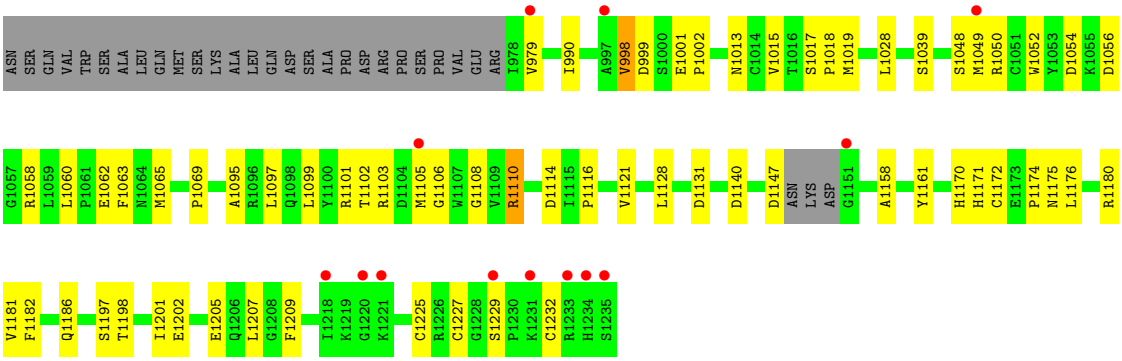
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	110	110	110	0	0
			Total	O		
5	B	107	107	107	0	0
			Total	O		
5	C	114	114	114	0	0
			Total	O		
5	D	66	66	66	0	0

3 Residue-property plots (i)

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

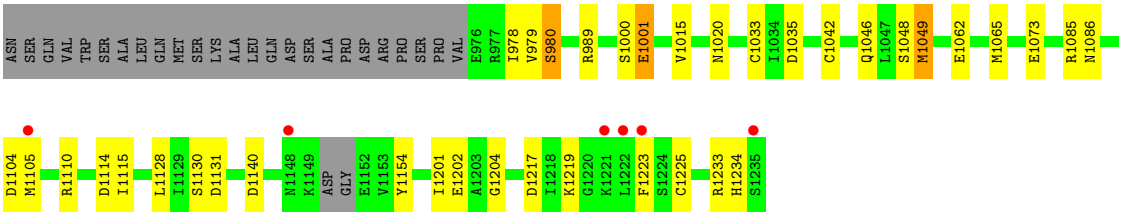
• Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain A:



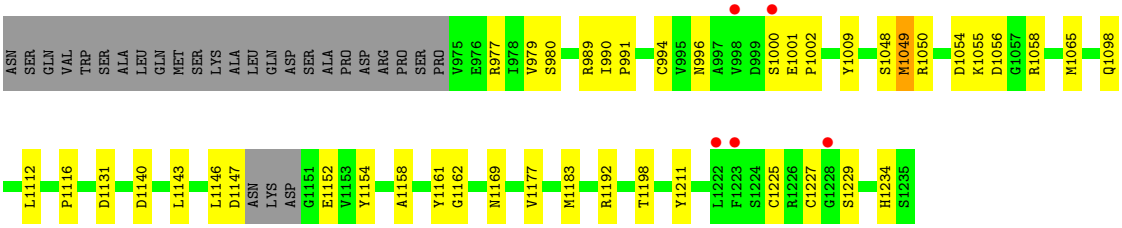
• Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain B:



• Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

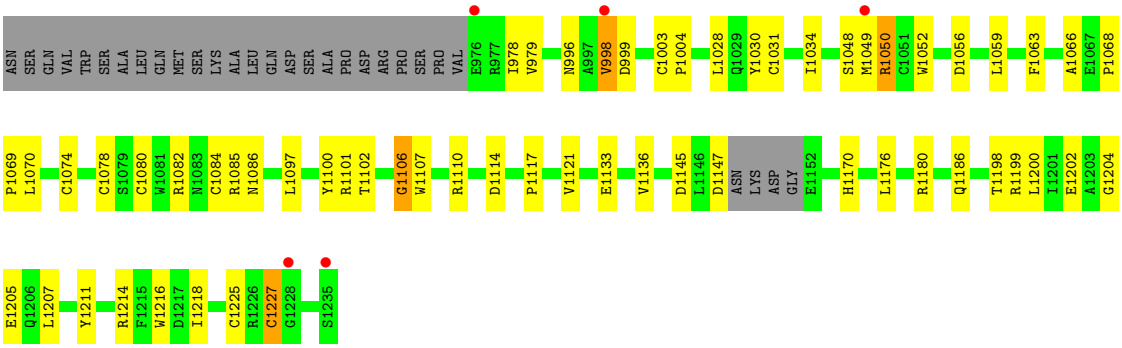
Chain C:



• Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

Chain D:

2%
69%
20%
10%


ASN SER GLN VAL TRP SER ALA LEU GLN MET SER LYS ALA LEU GLN ASP SER ALA PRO ASP ARG PRO SER PRO VAL E976 R977 I978 V979 N996 A997 V998 D999 C1003 P1004 L1028 Q1029 Y1030 C1031 I1034 S1048 M1049 R1050 C1051 W1052 D1056 L1059 F1063 A1066 E1067 P1068
P1069 L1070 C1074 C1078 S1079 C1080 W1081 R1082 N1083 C1084 R1085 N1086 L1097 Y1100 R1101 T1102 G1106 W1107 R1110 D1114 P1117 V1121 E1133 V1136 D1145 L1146 D1147 ASN LYS ASP GLY E1152 H1170 L1176 R1180 Q1186 T1198 R1199 L1200 I1201 E1202 A1203 G1204
E1205 Q1206 L1207 Y1211 R1214 F1215 W1216 D1217 I1218 C1225 R1226 C1227 G1228 S1235

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.70Å 163.00Å 69.30Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	31.83 – 2.49 31.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	91.5 (31.83-2.49) 91.3 (31.82-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.192 , 0.248 0.181 , 0.237	Depositor DCC
R_{free} test set	2165 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8719	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: E67, SAH, ZN

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	0.35	0/2066	0.58	0/2800
1	B	0.36	0/2096	0.58	0/2839
1	C	0.36	0/2090	0.58	0/2832
1	D	0.34	0/2042	0.56	0/2774
All	All	0.35	0/8294	0.57	0/11245

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2016	0	1871	50	0
1	B	2046	0	1906	25	0
1	C	2040	0	1892	29	0
1	D	1992	0	1824	39	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	40	0	47	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	40	0	47	2	0
3	C	40	0	47	3	0
3	D	40	0	47	0	0
4	C	26	0	19	0	0
4	D	26	0	20	0	0
5	A	110	0	0	2	0
5	B	107	0	0	0	0
5	C	114	0	0	1	0
5	D	66	0	0	2	0
All	All	8719	0	7720	142	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 9.

All (142) 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:1001:GLU:HB3	1:A:1101:ARG:HH12	1.42	0.83
1:C:980:SER:HB3	1:C:994:CYS:HB3	1.66	0.77
1:B:1062:GLU:OE1	1:B:1062:GLU:N	2.20	0.74
1:D:1170:HIS:CD2	1:D:1216:TRP:HE1	2.06	0.73
1:D:1031:CYS:SG	5:D:295:HOH:O	2.46	0.72
1:B:978:ILE:HD12	1:B:978:ILE:H	1.53	0.71
1:A:1001:GLU:HB3	1:A:1101:ARG:NH1	2.05	0.70
1:D:1114:ASP:OD1	1:D:1202:GLU:HA	1.93	0.68
1:C:1131:ASP:OD1	3:C:1236:E67:HAWA	1.93	0.67
1:A:1140:ASP:O	3:A:1:E67:HAMA	1.94	0.67
1:D:1170:HIS:CD2	1:D:1211:TYR:H	2.13	0.66
1:B:1048:SER:O	1:B:1049:MET:HB2	1.94	0.66
1:A:998:VAL:HG21	1:A:1102:THR:O	1.97	0.65
1:B:989:ARG:HH11	1:B:989:ARG:HG2	1.62	0.65
1:A:1001:GLU:CB	1:A:1101:ARG:HH12	2.09	0.65
1:A:1048:SER:O	1:A:1049:MET:HB2	1.97	0.64
1:C:1065:MET:HE3	1:C:1198:THR:HA	1.79	0.64
1:A:1114:ASP:OD1	1:A:1202:GLU:HA	1.98	0.64
1:D:1133:GLU:O	1:D:1136:VAL:HG12	1.99	0.62
1:A:1052:TRP:O	1:A:1060:LEU:HD13	2.00	0.61
1:B:1131:ASP:OD2	3:B:2:E67:HAWA	2.01	0.61
1:D:1100:TYR:CE1	1:D:1102:THR:HG22	2.36	0.60
1:D:1225:CYS:SG	1:D:1227:CYS:HB3	2.43	0.59
1:D:1048:SER:O	1:D:1049:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:MET:CE	1:C:1198:THR:HA	2.34	0.57
1:B:1015:VAL:HG12	1:B:1128:LEU:HB3	1.86	0.57
1:D:1117:PRO:HG3	1:D:1200:LEU:N	2.20	0.57
1:A:1121:VAL:HG21	1:A:1176:LEU:HD21	1.88	0.56
1:A:1225:CYS:SG	1:A:1227:CYS:HB3	2.45	0.56
1:D:1170:HIS:HD2	1:D:1211:TYR:H	1.54	0.55
1:B:1219:LYS:HB3	1:B:1223:PHE:CZ	2.42	0.55
1:D:998:VAL:HG12	1:D:999:ASP:N	2.22	0.54
1:D:1145:ASP:OD2	1:D:1214:ARG:HD2	2.08	0.54
1:A:1101:ARG:HD2	1:A:1106:GLY:O	2.08	0.54
1:A:1028:LEU:HD23	1:A:1186:GLN:HG3	1.90	0.54
1:A:1054:ASP:OD1	1:A:1056:ASP:N	2.41	0.54
1:D:1034:ILE:HD12	1:D:1034:ILE:C	2.29	0.53
1:B:978:ILE:HD12	1:B:978:ILE:N	2.21	0.53
1:B:1114:ASP:OD1	1:B:1202:GLU:HA	2.09	0.53
1:C:979:VAL:HG21	1:C:1002:PRO:HA	1.90	0.53
1:B:1085:ARG:HA	1:C:1055:LYS:HD2	1.92	0.52
1:C:1048:SER:O	1:C:1049:MET:HB2	2.09	0.52
1:D:1110:ARG:HD2	1:D:1204:GLY:HA2	1.91	0.52
1:A:1065:MET:CE	1:A:1198:THR:HA	2.40	0.52
1:B:989:ARG:HG2	1:B:989:ARG:NH1	2.24	0.52
1:A:1097:LEU:HD22	1:A:1207:LEU:HD11	1.92	0.51
1:C:979:VAL:HG22	1:C:979:VAL:O	2.11	0.51
1:A:998:VAL:HG12	1:A:999:ASP:N	2.24	0.50
1:D:996:ASN:ND2	1:D:999:ASP:O	2.45	0.50
1:B:1110:ARG:HD3	1:B:1204:GLY:HA2	1.92	0.50
1:D:1101:ARG:NH1	1:D:1106:GLY:HA2	2.27	0.50
1:B:1225:CYS:HB2	1:B:1234:HIS:HB2	1.94	0.49
1:D:1202:GLU:O	1:D:1205:GLU:HB2	2.11	0.49
1:A:1174:PRO:HB3	1:A:1209:PHE:HA	1.93	0.49
1:A:1101:ARG:HE	1:A:1105:MET:C	2.14	0.49
1:A:1172:CYS:SG	1:A:1232:CYS:HA	2.53	0.49
1:C:979:VAL:HG12	1:C:994:CYS:O	2.12	0.48
1:B:978:ILE:H	1:B:978:ILE:CD1	2.25	0.48
1:C:1065:MET:SD	1:C:1177:VAL:HG11	2.54	0.48
1:A:979:VAL:HG12	1:A:979:VAL:O	2.12	0.48
1:A:1181:VAL:HG12	1:A:1182:PHE:N	2.29	0.48
1:A:1015:VAL:HG12	1:A:1128:LEU:HB3	1.96	0.48
1:A:1028:LEU:CD2	1:A:1186:GLN:HG3	2.44	0.48
1:B:1115:ILE:HB	1:B:1201:ILE:HB	1.97	0.47
1:C:1000:SER:O	1:C:1001:GLU:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:VAL:HG11	1:A:1002:PRO:HA	1.94	0.47
1:A:1060:LEU:HB3	1:A:1062:GLU:OE1	2.13	0.47
1:A:1175:ASN:O	1:A:1197:SER:HA	2.14	0.47
1:C:1098:GLN:NE2	1:C:1112:LEU:HD21	2.28	0.47
1:C:990:ILE:HG23	1:C:991:PRO:HD2	1.95	0.47
1:C:1140:ASP:HB3	3:C:1236:E67:HATA	1.96	0.47
1:A:1174:PRO:CB	1:A:1209:PHE:HA	2.45	0.47
1:B:1073:GLU:HA	1:B:1086:ASN:ND2	2.29	0.47
1:C:1169:ASN:HA	1:C:1211:TYR:OH	2.15	0.47
1:D:1121:VAL:HG21	1:D:1176:LEU:HD21	1.96	0.47
1:A:1158:ALA:HA	1:A:1161:TYR:O	2.15	0.46
1:A:990:ILE:HD11	1:A:1095:ALA:O	2.15	0.46
1:D:1063:PHE:CZ	1:D:1069:PRO:HD2	2.51	0.46
1:C:989:ARG:HH11	1:C:989:ARG:HG2	1.81	0.46
1:D:1048:SER:C	1:D:1050:ARG:H	2.18	0.46
1:B:1000:SER:O	1:B:1001:GLU:C	2.54	0.46
1:A:1058:ARG:NE	1:A:1116:PRO:HB2	2.31	0.46
1:A:1131:ASP:OD1	3:A:1:E67:HAWA	2.15	0.46
1:A:1017:SER:HB2	1:A:1018:PRO:CD	2.46	0.45
1:A:1110:ARG:HB2	1:A:1205:GLU:O	2.16	0.45
1:A:1013:ASN:HB2	5:A:228:HOH:O	2.15	0.45
1:D:1004:PRO:HD3	1:D:1107:TRP:CZ2	2.52	0.45
1:A:999:ASP:OD1	1:A:1101:ARG:NH1	2.50	0.45
1:D:1066:ALA:O	1:D:1068:PRO:HD3	2.16	0.45
1:D:1214:ARG:O	1:D:1218:ILE:HG13	2.17	0.45
1:B:1033:CYS:HB3	1:B:1035:ASP:OD1	2.17	0.44
1:C:1050:ARG:NH1	5:C:292:HOH:O	2.49	0.44
1:C:977:ARG:HG2	1:C:996:ASN:O	2.17	0.44
1:B:979:VAL:O	1:B:980:SER:HB2	2.17	0.44
1:C:1058:ARG:HE	1:C:1116:PRO:HB2	1.83	0.44
1:D:1097:LEU:HD22	1:D:1207:LEU:HD11	1.99	0.44
1:D:1117:PRO:HG3	1:D:1199:ARG:C	2.37	0.44
1:D:1028:LEU:HD23	1:D:1186:GLN:HG3	2.00	0.44
1:D:1176:LEU:HD11	1:D:1207:LEU:HB3	2.00	0.44
1:C:1183:MET:HE3	1:C:1192:ARG:HD3	1.99	0.43
1:A:1065:MET:HE1	1:A:1198:THR:HA	2.01	0.43
1:A:1114:ASP:HA	1:A:1201:ILE:O	2.18	0.43
1:A:1019:MET:HA	5:A:269:HOH:O	2.18	0.43
1:C:1048:SER:O	1:C:1049:MET:CB	2.66	0.43
1:C:1227:CYS:SG	1:C:1229:SER:HB3	2.58	0.43
1:D:1117:PRO:HG3	1:D:1199:ARG:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:LEU:HD12	1:A:1108:GLY:O	2.18	0.43
1:A:1103:ARG:C	1:A:1105:MET:H	2.21	0.43
1:A:1180:ARG:HH11	1:A:1180:ARG:HG3	1.84	0.43
1:C:1158:ALA:HA	1:C:1161:TYR:O	2.19	0.43
1:A:1065:MET:HE3	1:A:1198:THR:HA	2.01	0.42
1:B:1062:GLU:H	1:B:1062:GLU:CD	2.17	0.42
1:D:1110:ARG:HB2	1:D:1205:GLU:O	2.19	0.42
1:D:1170:HIS:HD2	1:D:1211:TYR:HB2	1.84	0.42
1:D:1080:CYS:HA	5:D:263:HOH:O	2.18	0.42
1:A:1227:CYS:SG	1:A:1229:SER:HB3	2.59	0.42
1:B:1233:ARG:HB2	1:B:1233:ARG:NH1	2.34	0.42
1:B:1104:ASP:O	1:B:1105:MET:HB2	2.19	0.42
1:A:1058:ARG:HH21	1:A:1116:PRO:HD2	1.83	0.42
1:A:1048:SER:C	1:A:1050:ARG:H	2.23	0.42
1:C:1146:LEU:O	1:C:1147:ASP:C	2.56	0.42
1:A:1058:ARG:HE	1:A:1116:PRO:HB2	1.84	0.42
1:D:1070:LEU:HD21	1:D:1180:ARG:CZ	2.50	0.41
1:B:1042:CYS:O	1:B:1046:GLN:HG3	2.21	0.41
1:C:1054:ASP:OD1	1:C:1056:ASP:N	2.54	0.41
1:D:979:VAL:CB	1:D:1003:CYS:HB2	2.50	0.41
1:A:1170:HIS:CG	1:A:1171:HIS:N	2.88	0.41
1:B:1140:ASP:OD2	3:B:2:E67:HAC	2.21	0.41
1:D:1052:TRP:O	1:D:1059:LEU:HA	2.20	0.41
1:A:1054:ASP:OD1	1:A:1054:ASP:C	2.60	0.41
1:C:1143:LEU:O	3:C:1236:E67:HBE	2.21	0.40
1:D:1074:CYS:SG	1:D:1086:ASN:HB3	2.61	0.40
1:B:1130:SER:HA	1:B:1154:TYR:CD1	2.56	0.40
1:C:1225:CYS:HB2	1:C:1234:HIS:HB2	2.03	0.40
1:A:1140:ASP:OD2	3:A:1:E67:HAC	2.21	0.40
1:D:1170:HIS:HB2	1:D:1211:TYR:CD1	2.56	0.40
1:D:1198:THR:O	1:D:1199:ARG:HB3	2.21	0.40
1:A:1063:PHE:CZ	1:A:1069:PRO:HD2	2.56	0.40
1:C:1009:TYR:HA	1:C:1162:GLY:O	2.21	0.40
1:D:1030:TYR:HB2	1:D:1078:CYS:HA	2.04	0.40
1:D:1082:ARG:HG3	1:D:1082:ARG:O	2.22	0.40
1:C:1152:GLU:HG2	1:C:1154:TYR:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	251/285 (88%)	226 (90%)	24 (10%)	1 (0%)	34 54
1	B	254/285 (89%)	233 (92%)	17 (7%)	4 (2%)	9 17
1	C	254/285 (89%)	229 (90%)	24 (9%)	1 (0%)	34 54
1	D	252/285 (88%)	221 (88%)	27 (11%)	4 (2%)	9 17
All	All	1011/1140 (89%)	909 (90%)	92 (9%)	10 (1%)	15 28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	998	VAL
1	B	980	SER
1	B	1020	ASN
1	C	1049	MET
1	D	1106	GLY
1	D	1050	ARG
1	B	1001	GLU
1	B	1049	MET
1	D	978	ILE
1	A	998	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	219/257 (85%)	216 (99%)	3 (1%)	67 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	223/257 (87%)	221 (99%)	2 (1%)	78 92
1	C	222/257 (86%)	222 (100%)	0	100 100
1	D	213/257 (83%)	208 (98%)	5 (2%)	50 76
All	All	877/1028 (85%)	867 (99%)	10 (1%)	73 89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1039	SER
1	A	1110	ARG
1	A	1147	ASP
1	B	1065	MET
1	B	1217	ASP
1	D	1056	ASP
1	D	1084	CYS
1	D	1085	ARG
1	D	1147	ASP
1	D	1227	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1064	ASN
1	A	1234	HIS
1	D	1041	ASN
1	D	1170	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 16 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	E67	D	4	-	42,43,43	1.99	11 (26%)	56,56,56	1.69	11 (19%)
3	E67	B	2	-	42,43,43	2.00	11 (26%)	56,56,56	1.81	12 (21%)
4	SAH	D	104	-	24,28,28	1.27	2 (8%)	25,40,40	2.95	4 (16%)
4	SAH	C	103	-	24,28,28	0.90	1 (4%)	25,40,40	3.68	4 (16%)
3	E67	C	1236	-	42,43,43	2.02	11 (26%)	56,56,56	1.81	13 (23%)
3	E67	A	1	-	42,43,43	1.99	11 (26%)	56,56,56	1.79	13 (23%)

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	E67	D	4	-	-	3/24/34/34	0/4/4/4
3	E67	B	2	-	-	3/24/34/34	0/4/4/4
4	SAH	D	104	-	-	3/11/31/31	0/3/3/3
4	SAH	C	103	-	-	3/11/31/31	0/3/3/3
3	E67	C	1236	-	-	6/24/34/34	0/4/4/4
3	E67	A	1	-	-	5/24/34/34	0/4/4/4

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	E67	CBM-CBL	5.76	1.53	1.38
3	D	4	E67	CBM-CBL	5.71	1.53	1.38
3	C	1236	E67	CBM-CBL	5.64	1.53	1.38
3	A	1	E67	CBM-CBL	5.59	1.52	1.38
3	C	1236	E67	CBL-CBK	4.94	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	E67	CBL-CBK	4.85	1.50	1.38
3	B	2	E67	CBL-CBK	4.84	1.50	1.38
4	D	104	SAH	OXT-C	4.78	1.46	1.30
3	D	4	E67	CBL-CBK	4.67	1.50	1.38
3	D	4	E67	CAC-CAB	4.45	1.44	1.36
3	B	2	E67	CAF-CAA	4.28	1.44	1.36
3	D	4	E67	CAF-CAA	4.07	1.43	1.36
3	A	1	E67	CAF-CAA	4.05	1.43	1.36
3	C	1236	E67	CAF-CAA	4.02	1.43	1.36
3	C	1236	E67	CAC-CAB	4.01	1.43	1.36
3	B	2	E67	CAC-CAB	3.94	1.43	1.36
3	A	1	E67	CAC-CAB	3.83	1.43	1.36
3	A	1	E67	CBH-CBI	3.04	1.56	1.51
3	C	1236	E67	CBH-CBI	2.91	1.56	1.51
3	B	2	E67	CBJ-CBI	2.90	1.45	1.38
3	C	1236	E67	CBJ-CBI	2.86	1.45	1.38
3	D	4	E67	CBH-CBI	2.80	1.56	1.51
3	A	1	E67	CBJ-CBI	2.80	1.44	1.38
3	C	1236	E67	CAP-CAQ	2.79	1.60	1.52
3	A	1	E67	C6-C5	-2.77	1.41	1.44
4	C	103	SAH	O4'-C1'	2.73	1.44	1.41
3	B	2	E67	C6-C5	-2.72	1.41	1.44
3	B	2	E67	CBH-CBI	2.70	1.56	1.51
3	C	1236	E67	C6-C5	-2.67	1.41	1.44
3	B	2	E67	CAP-CAQ	2.66	1.59	1.52
3	D	4	E67	CBJ-CBI	2.66	1.44	1.38
3	D	4	E67	C6-N1	2.60	1.36	1.32
3	C	1236	E67	CBN-CBI	2.59	1.44	1.38
3	A	1	E67	C6-N1	2.49	1.36	1.32
3	A	1	E67	CBN-CBI	2.48	1.44	1.38
3	A	1	E67	CAP-CAQ	2.47	1.59	1.52
3	D	4	E67	CAP-CAQ	2.44	1.59	1.52
3	B	2	E67	CBN-CBI	2.37	1.43	1.38
3	D	4	E67	CBN-CBI	2.36	1.43	1.38
4	D	104	SAH	O4'-C1'	2.28	1.44	1.41
3	D	4	E67	C6-C5	-2.26	1.41	1.44
3	C	1236	E67	OAL-CAB	2.17	1.40	1.37
3	D	4	E67	OAL-CAB	2.17	1.40	1.37
3	B	2	E67	CAW-CAX	-2.12	1.43	1.51
3	B	2	E67	OAL-CAB	2.11	1.40	1.37
3	A	1	E67	CBH-NAR	2.08	1.51	1.47
3	C	1236	E67	CBK-CBJ	2.02	1.43	1.38

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	103	SAH	OXT-C-O	-13.55	93.32	124.09
4	D	104	SAH	OXT-C-O	-10.78	99.62	124.09
4	C	103	SAH	OXT-C-CA	10.50	149.16	113.38
4	D	104	SAH	OXT-C-CA	7.29	138.23	113.38
3	B	2	E67	CAV-NAU-C2	-6.43	112.63	123.75
3	C	1236	E67	CAV-NAU-C2	-6.20	113.03	123.75
3	A	1	E67	CAV-NAU-C2	-5.95	113.47	123.75
3	D	4	E67	CAV-NAU-C2	-5.39	114.43	123.75
3	A	1	E67	C6-C5-C4	4.58	118.76	115.88
4	C	103	SAH	N3-C2-N1	-4.53	121.61	128.68
4	D	104	SAH	N3-C2-N1	-4.48	121.68	128.68
3	B	2	E67	C6-C5-C4	4.47	118.69	115.88
3	C	1236	E67	C6-C5-C4	4.25	118.56	115.88
3	B	2	E67	CAC-C5-C6	-4.21	121.08	124.88
3	A	1	E67	CAC-C5-C6	-4.19	121.11	124.88
3	C	1236	E67	CAC-C5-C6	-4.15	121.13	124.88
3	D	4	E67	C6-C5-C4	4.05	118.43	115.88
3	B	2	E67	CAW-CAX-NAY	-3.97	103.04	113.79
3	C	1236	E67	CAW-CAX-NAY	-3.87	103.31	113.79
3	D	4	E67	CAC-C5-C6	-3.72	121.53	124.88
3	C	1236	E67	NAU-C2-N3	3.45	123.16	117.19
3	A	1	E67	N3-C2-N1	-3.44	120.78	126.23
3	A	1	E67	CAW-CAX-NAY	-3.41	104.57	113.79
3	B	2	E67	NAU-C2-N3	3.38	123.04	117.19
3	D	4	E67	CAW-CAX-NAY	-3.38	104.64	113.79
3	D	4	E67	N3-C2-N1	-3.34	120.94	126.23
3	C	1236	E67	N3-C2-N1	-3.22	121.14	126.23
4	D	104	SAH	C5'-C4'-C3'	-3.21	107.03	115.06
4	C	103	SAH	C5'-C4'-C3'	-3.17	107.12	115.06
3	B	2	E67	N3-C2-N1	-3.17	121.21	126.23
3	B	2	E67	C2-N1-C6	3.09	123.46	116.39
3	C	1236	E67	C2-N1-C6	3.05	123.38	116.39
3	A	1	E67	NAU-C2-N3	3.05	122.46	117.19
3	D	4	E67	NAU-C2-N3	2.91	122.22	117.19
3	D	4	E67	C2-N1-C6	2.88	122.98	116.39
3	B	2	E67	C5-C6-N1	-2.78	117.41	121.98
3	A	1	E67	C2-N1-C6	2.76	122.70	116.39
3	D	4	E67	C5-C6-N1	-2.68	117.59	121.98
3	C	1236	E67	C5-C6-N1	-2.59	117.72	121.98
3	A	1	E67	C5-C6-N1	-2.58	117.74	121.98
3	C	1236	E67	C5-C4-N3	-2.46	120.20	122.81
3	A	1	E67	CBI-CBH-NAR	2.41	117.81	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	E67	C2-N3-C4	2.39	119.49	115.60
3	A	1	E67	C2-N3-C4	2.36	119.45	115.60
3	C	1236	E67	OAL-CAB-CAA	2.34	118.67	115.41
3	B	2	E67	C5-C4-N3	-2.34	120.33	122.81
3	D	4	E67	CBI-CBH-NAR	2.28	117.55	113.12
3	C	1236	E67	OAL-CAB-CAC	-2.24	122.34	125.24
3	B	2	E67	OAL-CAB-CAC	-2.19	122.41	125.24
3	B	2	E67	OAL-CAB-CAA	2.19	118.45	115.41
3	A	1	E67	C5-C4-N3	-2.12	120.56	122.81
3	D	4	E67	C5-C4-N3	-2.11	120.57	122.81
3	C	1236	E67	OAK-CAA-CAF	-2.09	121.65	125.19
3	C	1236	E67	C2-N3-C4	2.08	119.00	115.60
3	A	1	E67	OAL-CAB-CAC	-2.06	122.58	125.24
3	A	1	E67	CBH-NAR-CAQ	-2.02	106.56	111.06
3	B	2	E67	C2-N3-C4	2.02	118.89	115.60

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	E67	CAW-CAX-NAY-CAZ
3	B	2	E67	CAW-CAX-NAY-CAZ
3	B	2	E67	CAW-CAX-NAY-CBA
3	C	1236	E67	CAW-CAX-NAY-CBA
3	D	4	E67	CAW-CAX-NAY-CAZ
3	D	4	E67	CAW-CAX-NAY-CBA
3	C	1236	E67	CBB-CBC-CBD-CBE
3	A	1	E67	CAW-CAX-NAY-CBA
3	C	1236	E67	CAW-CAX-NAY-CAZ
3	C	1236	E67	OAK-CBB-CBC-CBD
3	A	1	E67	CAA-CAB-OAL-CAM
3	C	1236	E67	CAB-CAA-OAK-CBB
3	A	1	E67	CBB-CBC-CBD-CBE
4	D	104	SAH	CA-CB-CG-SD
3	A	1	E67	CAC-CAB-OAL-CAM
3	C	1236	E67	CAF-CAA-OAK-CBB
4	C	103	SAH	C3'-C4'-C5'-SD
4	D	104	SAH	C3'-C4'-C5'-SD
3	D	4	E67	OAK-CBB-CBC-CBD
4	C	103	SAH	O4'-C4'-C5'-SD
4	C	103	SAH	CB-CG-SD-C5'
4	D	104	SAH	CB-CG-SD-C5'

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Mol	Chain	Res	Type	Atoms
3	B	2	E67	OAK-CBB-CBC-CBD

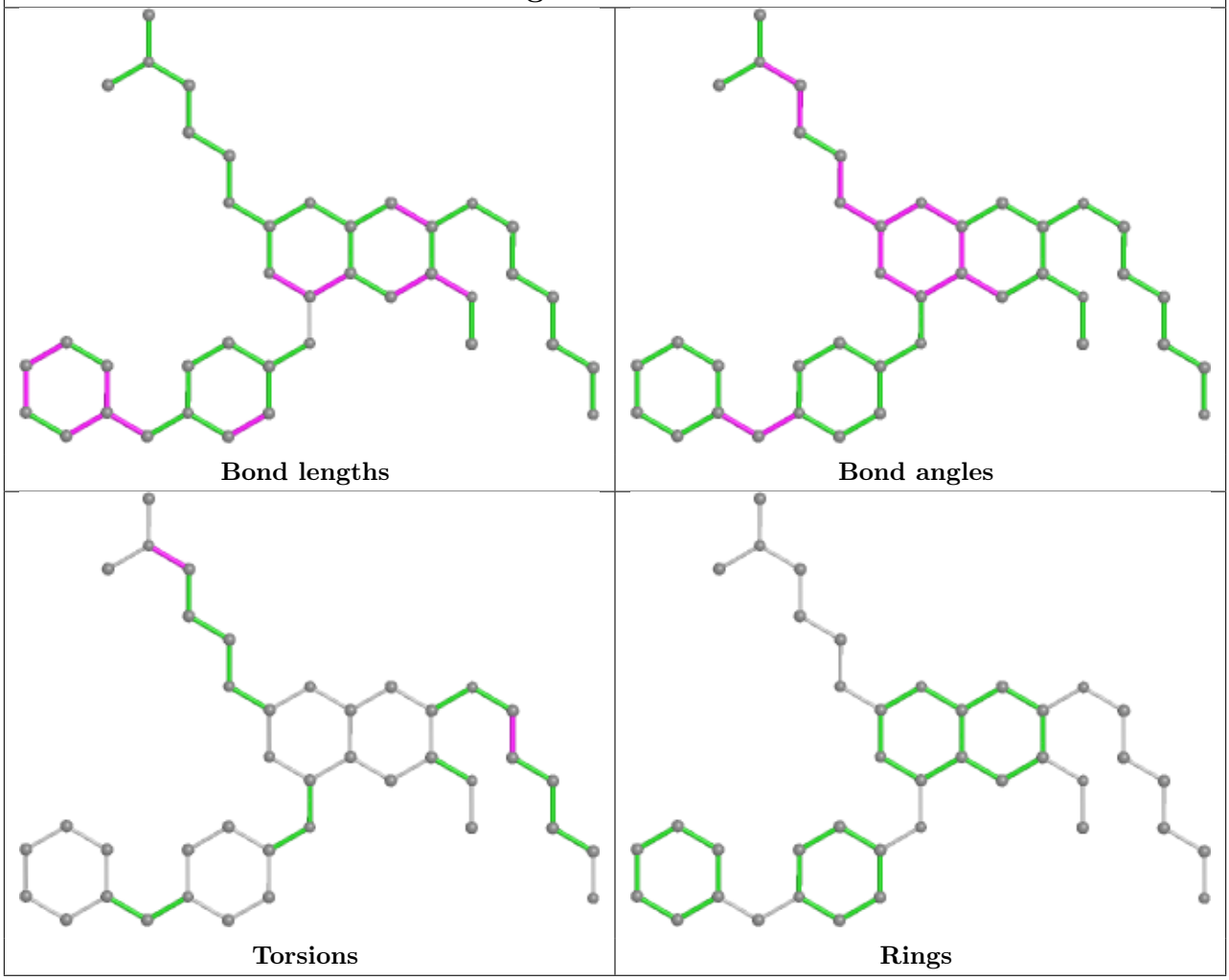
There are no ring outliers.

3 monomers are involved in 8 short contacts:

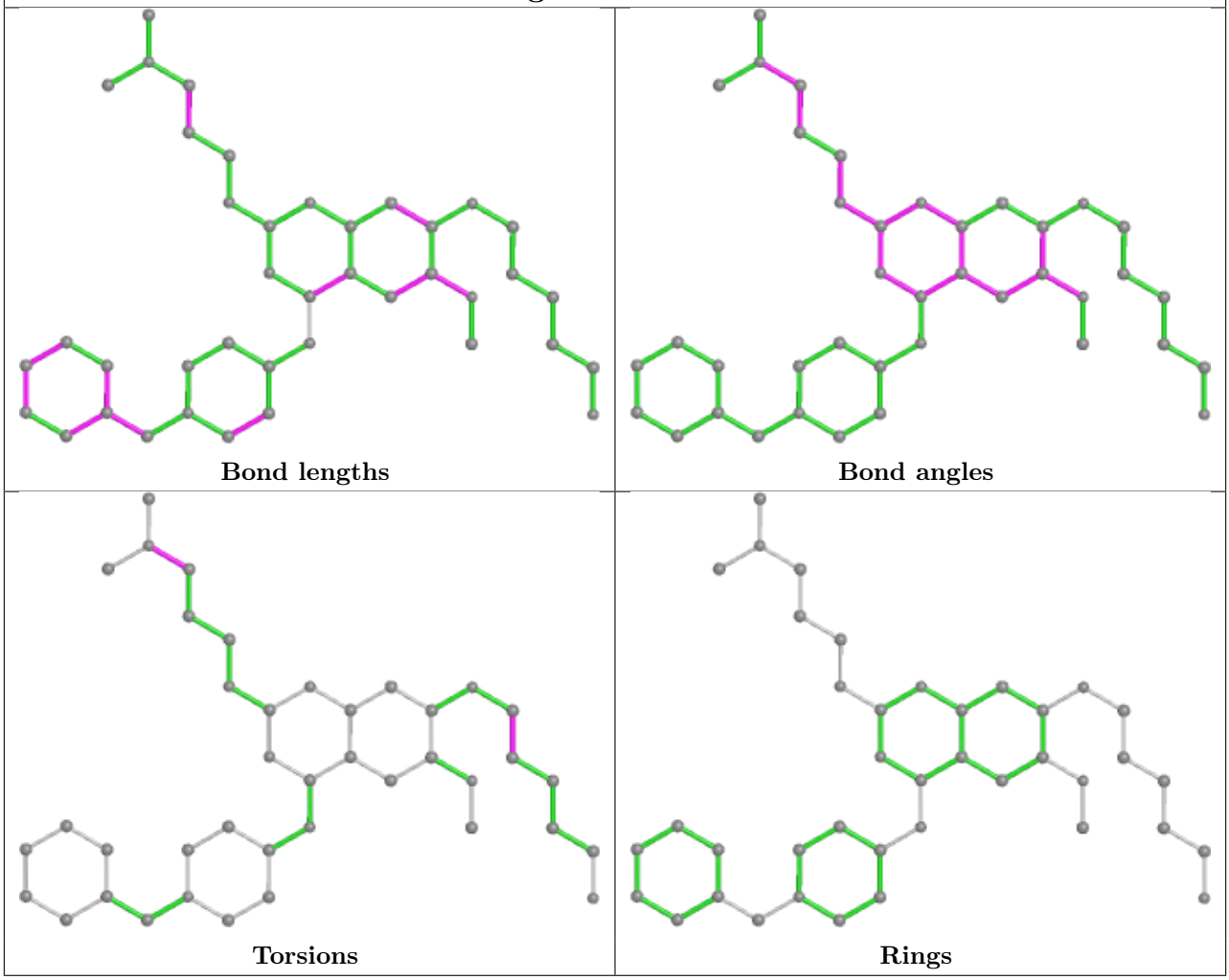
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	E67	2	0
3	C	1236	E67	3	0
3	A	1	E67	3	0

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

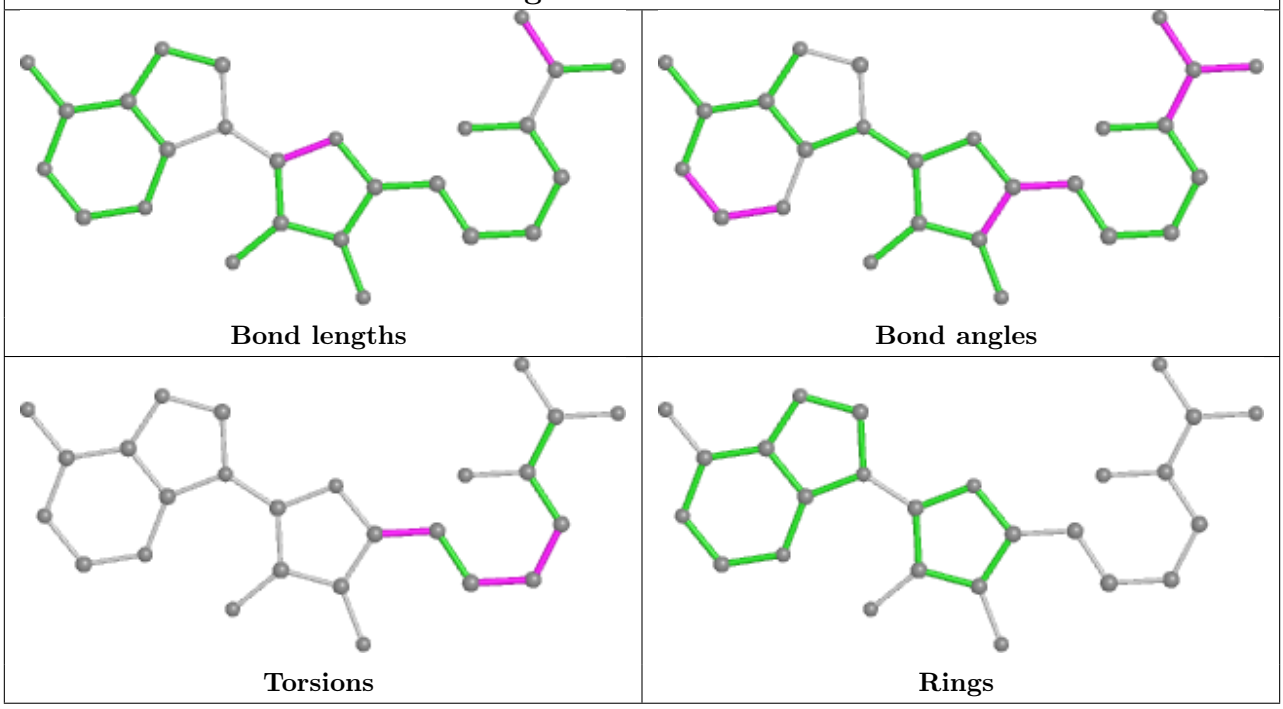
Ligand E67 D 4



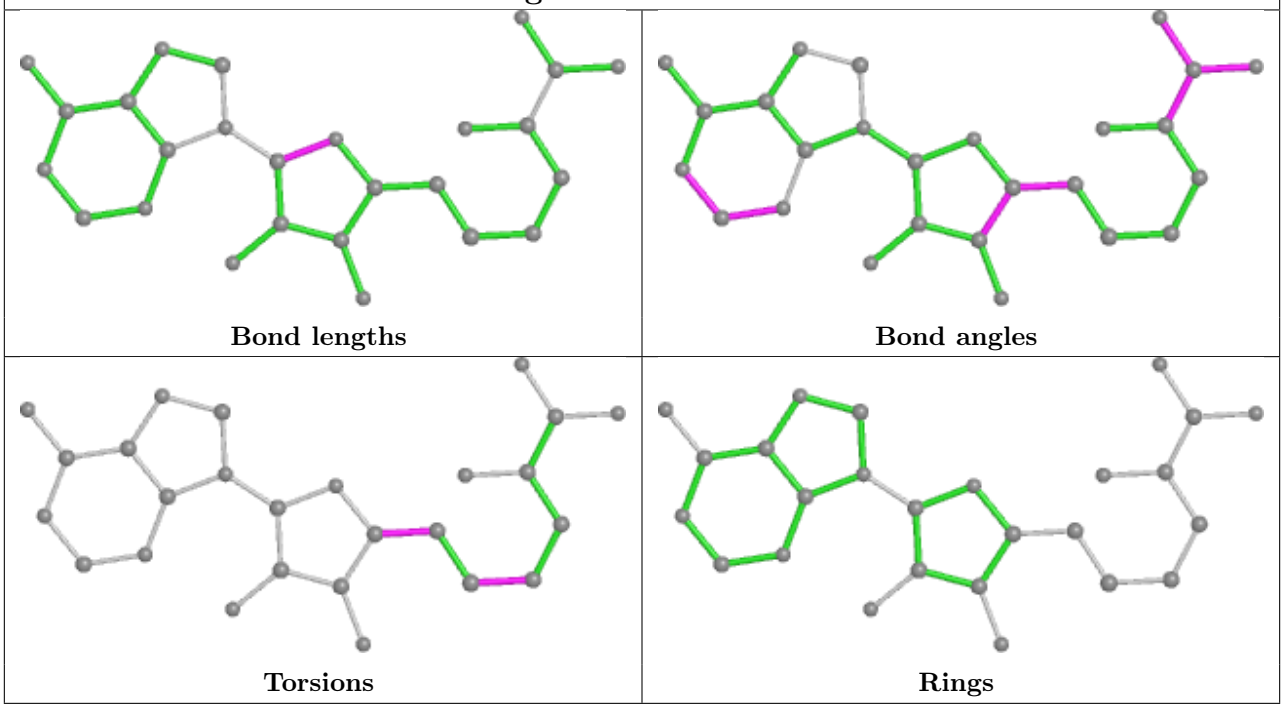
Ligand E67 B 2



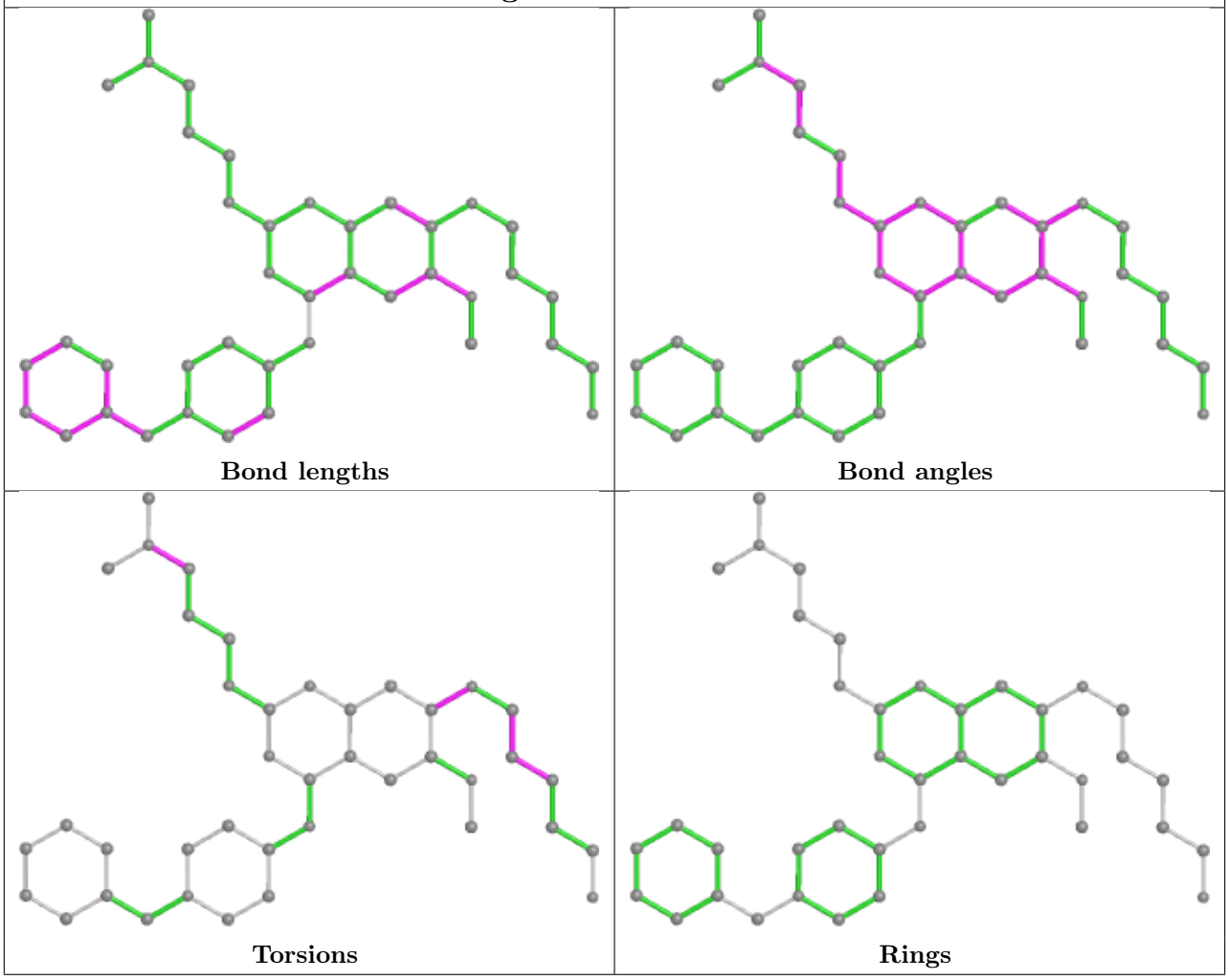
Ligand SAH D 104



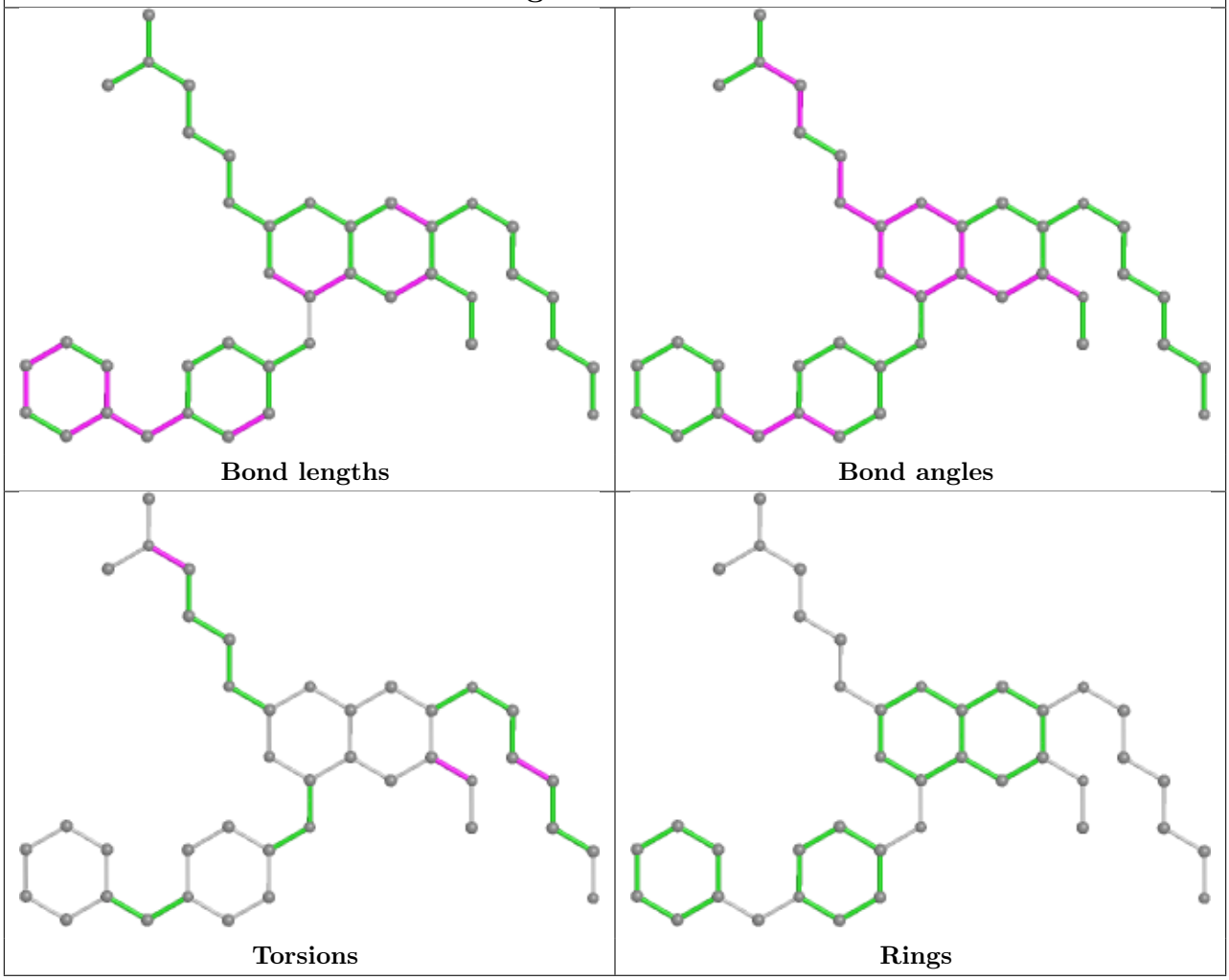
Ligand SAH C 103



Ligand E67 C 1236



Ligand E67 A 1



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(Å^2)	Q<0.9
1	A	255/285 (89%)	-0.00	13 (5%)	28	29	15, 35, 62, 71	0
1	B	258/285 (90%)	-0.20	6 (2%)	60	63	18, 33, 58, 70	0
1	C	258/285 (90%)	-0.16	5 (1%)	66	69	15, 33, 56, 66	0
1	D	256/285 (89%)	0.03	5 (1%)	65	68	23, 44, 64, 75	0
All	All	1027/1140 (90%)	-0.09	29 (2%)	53	56	15, 36, 61, 75	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1235	SER	4.9
1	B	1105	MET	4.7
1	A	1220	GLY	4.2
1	D	976	GLU	3.9
1	D	998	VAL	3.8
1	A	1151	GLY	3.4
1	C	998	VAL	3.4
1	A	1105	MET	3.1
1	A	979	VAL	2.9
1	D	1228	GLY	2.8
1	C	1222	LEU	2.8
1	A	1218	ILE	2.6
1	A	1221	LYS	2.6
1	A	1229	SER	2.5
1	B	1235	SER	2.5
1	C	1228	GLY	2.4
1	B	1222	LEU	2.3
1	A	997	ALA	2.3
1	D	1235	SER	2.3
1	B	1221	LYS	2.2
1	B	1148	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1234	HIS	2.1
1	A	1233	ARG	2.1
1	A	1049	MET	2.0
1	C	1000	SER	2.0
1	C	1223	PHE	2.0
1	D	1049	MET	2.0
1	A	1231	LYS	2.0
1	B	1223	PHE	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 monosaccharides 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
3	E67	A	1	40/40	0.77	0.26	42,49,65,66	0
3	E67	D	4	40/40	0.84	0.23	40,49,63,64	0
4	SAH	D	104	26/26	0.85	0.21	66,67,68,69	0
3	E67	C	1236	40/40	0.88	0.19	37,43,60,61	0
4	SAH	C	103	26/26	0.91	0.15	51,57,59,60	0
3	E67	B	2	40/40	0.92	0.17	37,41,53,54	0
2	ZN	B	8	1/1	0.97	0.06	41,41,41,41	0
2	ZN	D	8	1/1	0.98	0.05	55,55,55,55	0
2	ZN	D	7	1/1	0.99	0.08	37,37,37,37	0
2	ZN	A	341	1/1	0.99	0.10	18,18,18,18	0
2	ZN	A	343	1/1	0.99	0.05	51,51,51,51	0
2	ZN	B	7	1/1	0.99	0.07	31,31,31,31	0
2	ZN	A	340	1/1	0.99	0.10	22,22,22,22	0
2	ZN	C	3	1/1	0.99	0.09	25,25,25,25	0
2	ZN	C	4	1/1	0.99	0.05	46,46,46,46	0

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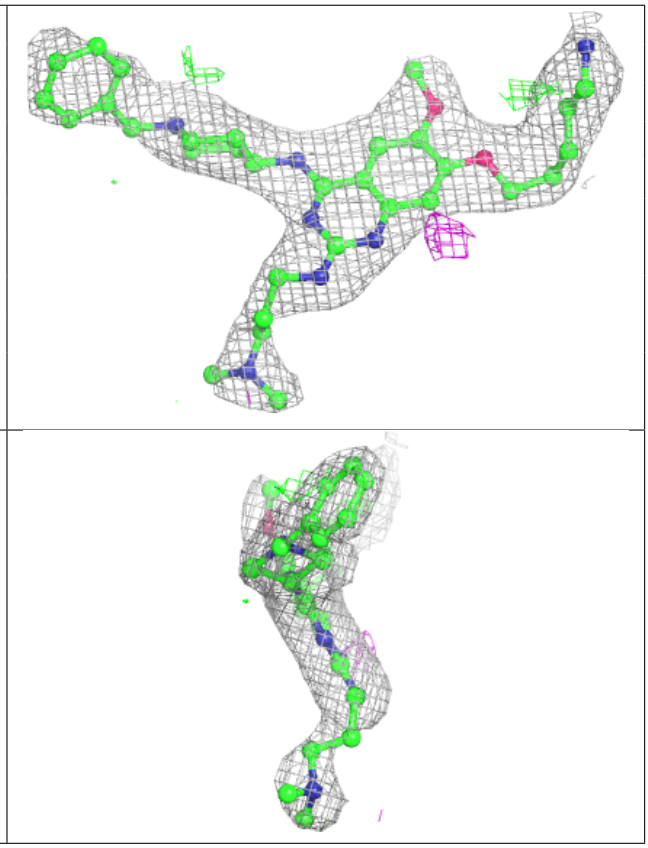
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	6	1/1	0.99	0.08	32,32,32,32	0
2	ZN	B	6	1/1	1.00	0.10	24,24,24,24	0
2	ZN	A	342	1/1	1.00	0.09	19,19,19,19	0
2	ZN	D	5	1/1	1.00	0.07	37,37,37,37	0
2	ZN	B	5	1/1	1.00	0.07	25,25,25,25	0
2	ZN	C	1	1/1	1.00	0.08	26,26,26,26	0
2	ZN	C	2	1/1	1.00	0.08	24,24,24,24	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.

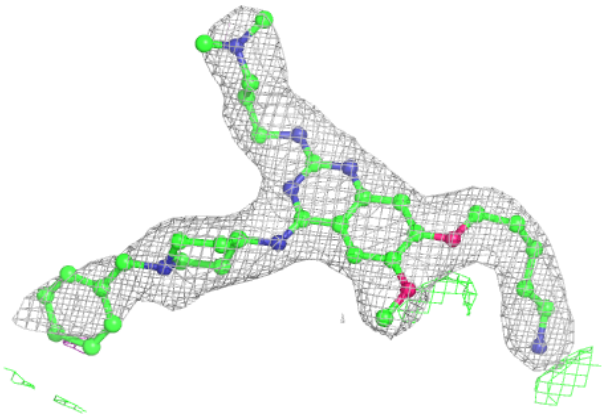
Electron density around E67 A 1:

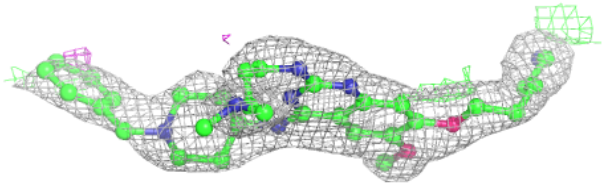
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

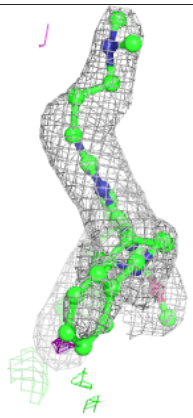


Electron density around E67 D 4:

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

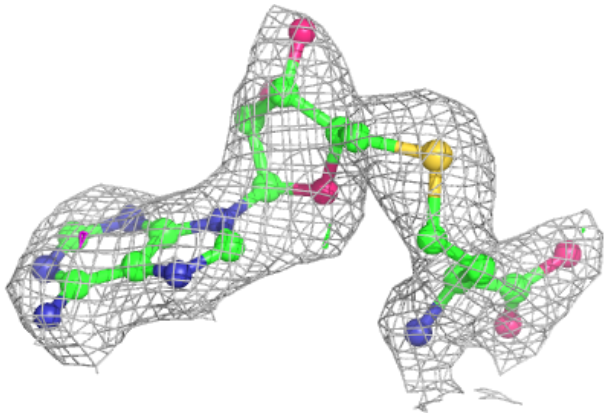


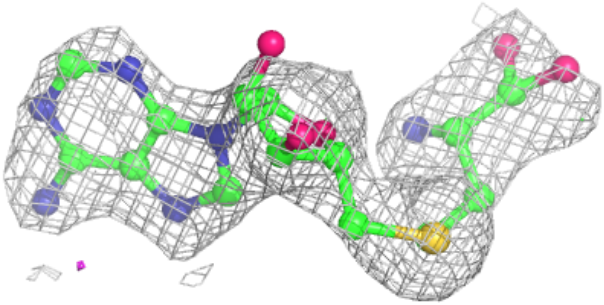


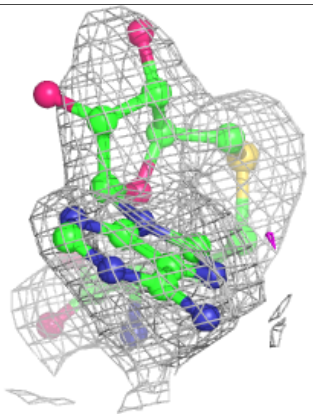


Electron density around SAH D 104:

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

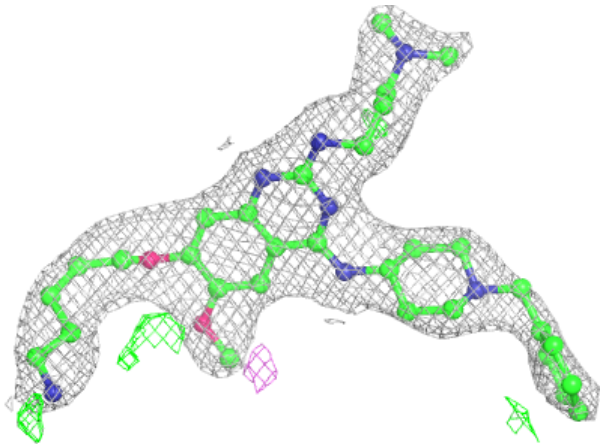


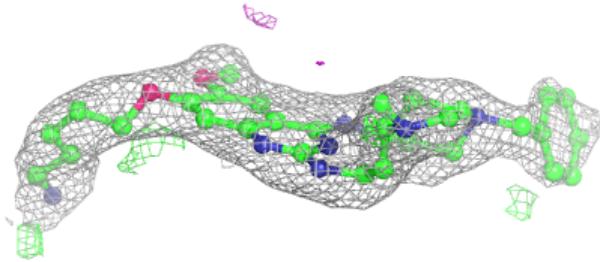


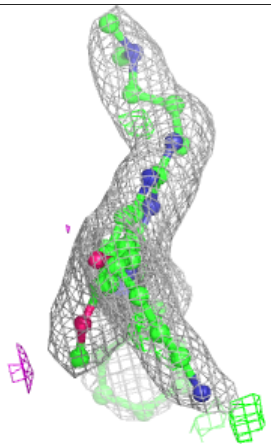


Electron density around E67 C 1236:

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

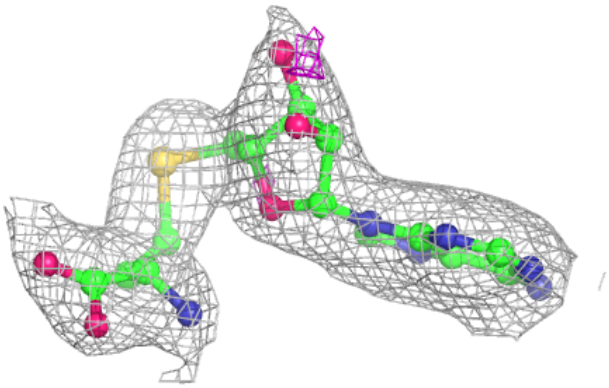


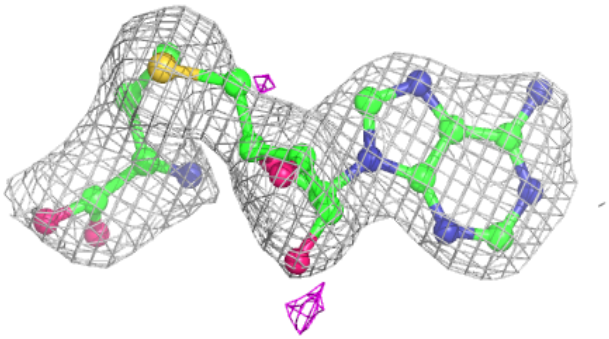


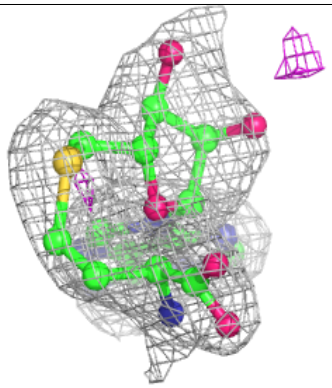


Electron density around SAH C 103:

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

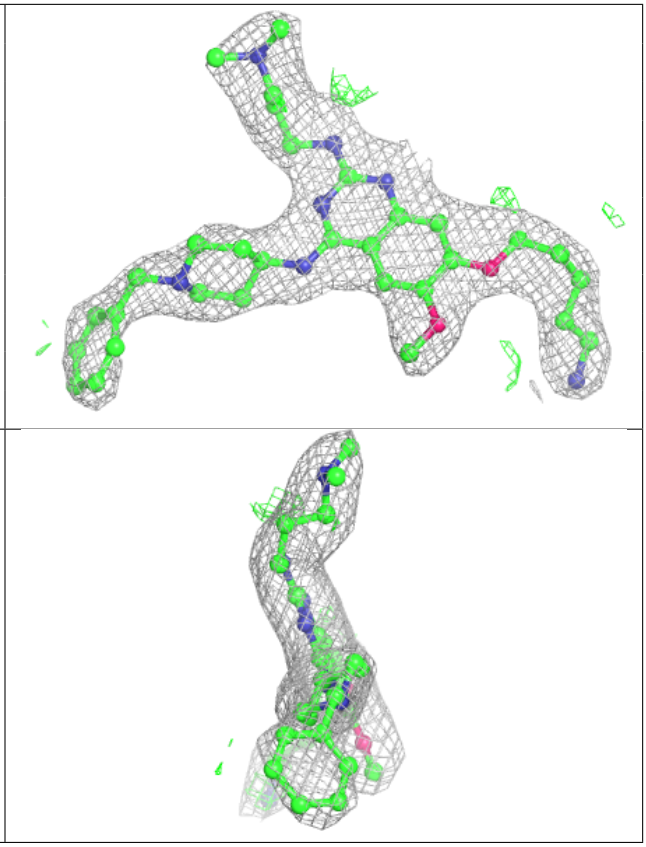






Electron density around E67 B 2:

$2mF_o$-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.