



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:12 pm BST

PDB ID : 3MO0
Title : Human G9a-like (GLP, also known as EHMT1) in complex with inhibitor E11
Authors : Chang, Y.; Horton, J.R.; Cheng, X.
Deposited on : 2010-04-22
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

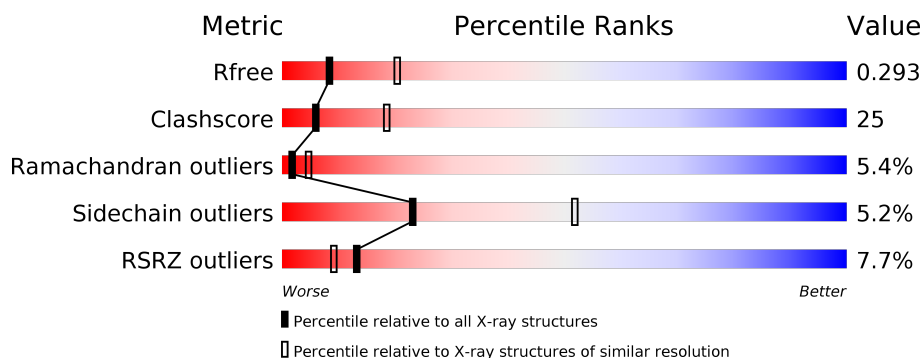
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	285	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>29%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	285	<div> <div>8%</div> <div> <div></div> <div>48%</div> <div>31%</div> <div>6%</div> <div>15%</div> </div> </div>

2 Entry composition [i](#)

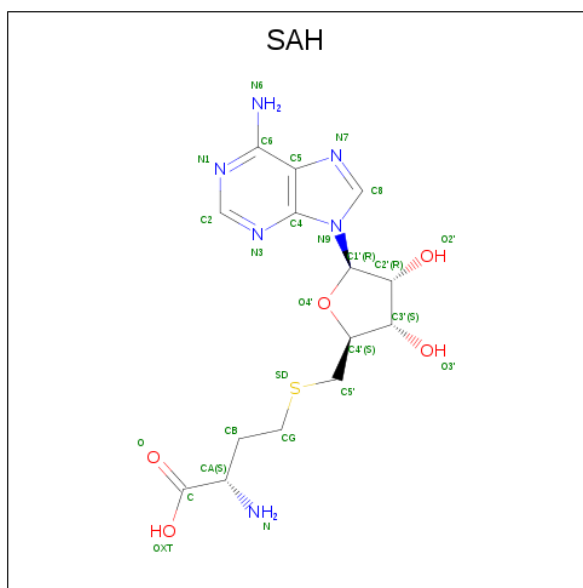
There are 6 unique types of molecules in this entry. The entry contains 4074 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

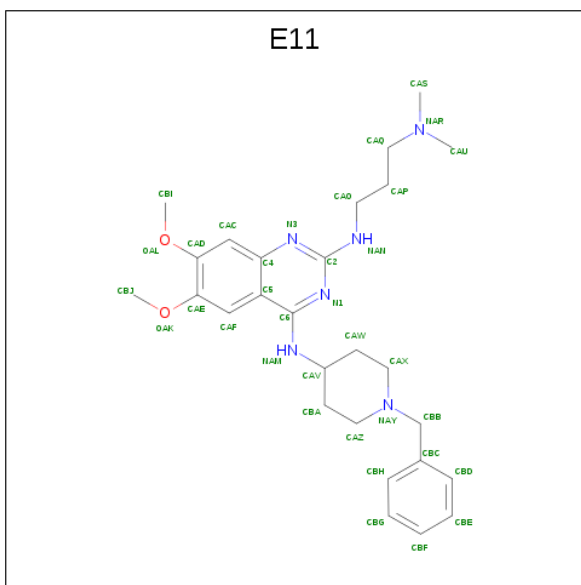
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	2	0
			2005	1250	366	365	24			
1	B	242	Total	C	N	O	S	0	0	0
			1850	1152	334	343	21			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is N 4 -(1-benzylpiperidin-4-yl)-N 2 -[3-(dimethylamino)propyl]-6,7-dimethoxyquinazoline-2,4-diamine (three-letter code: E11) (formula: $C_{27}H_{38}N_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 35	C 27	N 6	O 2	0	1
3	A	1	Total 35	C 27	N 6	O 2	0	1
3	B	1	Total 35	C 27	N 6	O 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	5	Total Zn 5 5	0	0
4	A	5	Total Zn 5 5	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

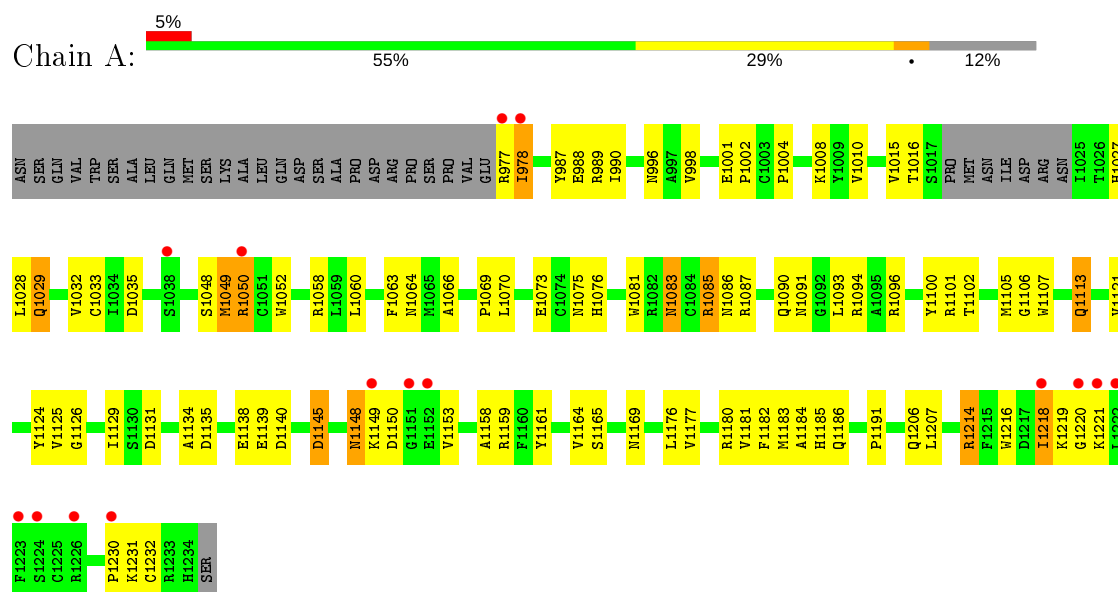
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	22	Total	O	0	0
			22	22		
6	B	22	Total	O	0	0
			22	22		

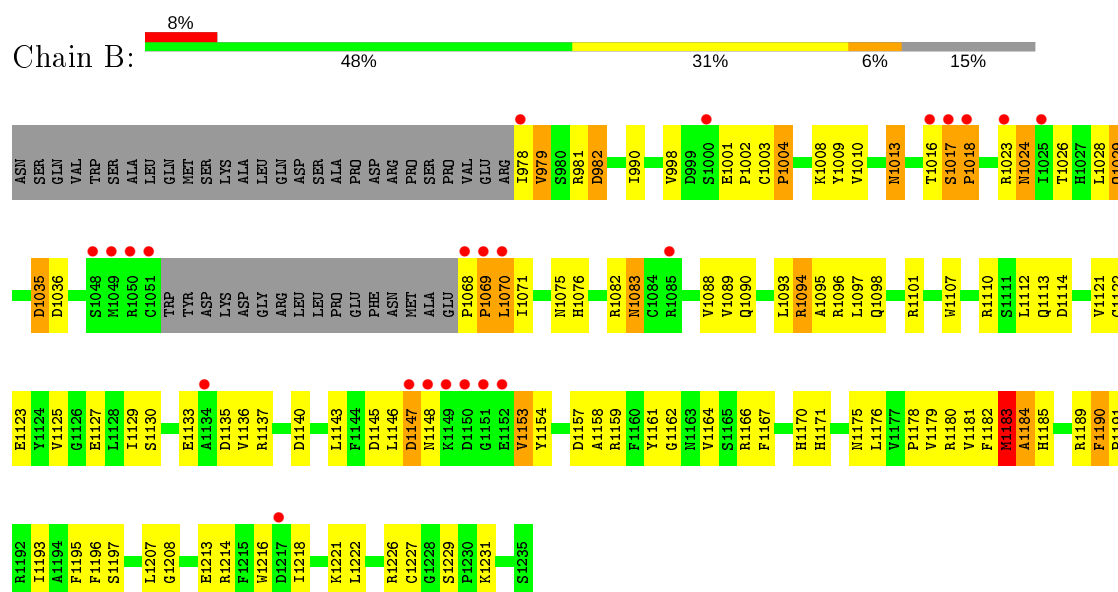
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.30 Å 94.50 Å 138.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 2.78 34.55 – 2.78	Depositor EDS
% Data completeness (in resolution range)	85.5 (34.55-2.78) 85.5 (34.55-2.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.76 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.306 0.220 , 0.293	Depositor DCC
R_{free} test set	739 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4074	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: E11, ZN, SAH, EDO

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	0.41	0/2054	0.61	0/2781
1	B	0.39	0/1893	0.62	0/2570
All	All	0.40	0/3947	0.61	0/5351

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2005	0	1845	91	0
1	B	1850	0	1676	97	0
2	A	26	0	19	0	0
2	B	26	0	19	1	0
3	A	70	0	76	24	0
3	B	35	0	38	13	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	8	0	12	0	0
6	A	22	0	0	0	0
6	B	22	0	0	1	0
All	All	4074	0	3685	192	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 25.

All (192) 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:1131:ASP:O	3:A:2001[A]:E11:HAU	1.29	1.29
1:A:1131:ASP:OD2	3:A:2001[A]:E11:CAU	1.96	1.13
1:A:1131:ASP:O	3:A:2001[A]:E11:CAU	1.99	1.11
1:A:1131:ASP:OD2	3:A:2001[A]:E11:HAU	1.50	1.11
1:B:1013:ASN:HD22	1:B:1125:VAL:HG13	1.29	0.97
1:B:1096:ARG:H	1:B:1113:GLN:HE21	1.04	0.96
1:A:1214[A]:ARG:HH21	1:A:1214[A]:ARG:HB3	1.35	0.91
1:B:1146:LEU:HD13	1:B:1190:PHE:HA	1.56	0.85
1:A:1131:ASP:OD2	3:A:2001[A]:E11:HAUB	1.78	0.82
3:B:2003:E11:HAPA	3:B:2003:E11:N1	1.95	0.81
1:B:1096:ARG:H	1:B:1113:GLN:NE2	1.76	0.81
1:B:1029:GLN:HE21	1:B:1075:ASN:ND2	1.80	0.79
1:B:978:ILE:HG22	1:B:979:VAL:HG13	1.64	0.79
1:B:990:ILE:HD12	1:B:990:ILE:O	1.82	0.79
1:A:990:ILE:O	1:A:990:ILE:HD12	1.84	0.77
1:A:1131:ASP:C	3:A:2001[A]:E11:HAU	2.04	0.76
1:A:1048:SER:O	1:A:1049:MET:HB2	1.85	0.76
1:A:1138:GLU:HG2	3:A:2001[A]:E11:HBF	1.69	0.74
1:B:1182:PHE:CZ	1:B:1191:PRO:HB3	2.25	0.72
1:B:1013:ASN:HD21	1:B:1125:VAL:HA	1.55	0.71
1:B:1145:ASP:OD1	3:B:2003:E11:HAC	1.90	0.71
1:B:1017:SER:H	1:B:1018:PRO:CD	2.04	0.70
1:A:1138:GLU:HG2	3:A:2002[B]:E11:HBF	1.72	0.70
1:B:1013:ASN:ND2	1:B:1125:VAL:HG13	2.03	0.69
1:A:1131:ASP:OD2	3:A:2002[B]:E11:HAP	1.94	0.68
1:B:978:ILE:O	1:B:979:VAL:HG22	1.94	0.67
1:A:1073:GLU:HA	1:A:1086:ASN:ND2	2.09	0.67
1:B:1140:ASP:OD2	3:B:2003:E11:HAF	1.93	0.67
1:B:1221:LYS:O	1:B:1222:LEU:HD23	1.94	0.66
1:A:1214[A]:ARG:NH2	1:A:1214[A]:ARG:HB3	2.09	0.66
1:A:998:VAL:HG21	1:A:1101:ARG:O	1.95	0.66
1:A:1214[B]:ARG:HH21	3:A:2002[B]:E11:HBI	1.62	0.65
1:A:1070:LEU:HD22	1:A:1182:PHE:HE2	1.61	0.64
1:A:1214[B]:ARG:HB2	3:A:2002[B]:E11:HBI	1.79	0.64
1:A:1016:THR:HA	1:B:1024:ASN:CB	2.27	0.64
1:B:1140:ASP:HB2	1:B:1143:LEU:HD12	1.79	0.64
1:B:1135:ASP:HA	3:B:2003:E11:HAZ	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:ASP:O	3:A:2002[B]:E11:HBJA	1.98	0.63
1:B:1153:VAL:HG12	1:B:1154:TYR:N	2.15	0.61
1:A:1169:ASN:ND2	1:A:1206:GLN:OE1	2.32	0.61
1:B:1068:PRO:N	1:B:1069:PRO:CD	2.63	0.61
1:A:1033:CYS:HB3	1:A:1035:ASP:OD1	2.01	0.60
1:B:1068:PRO:N	1:B:1069:PRO:HD2	2.15	0.60
1:A:1182:PHE:CZ	1:A:1191:PRO:HB3	2.36	0.60
1:A:1070:LEU:HD23	1:A:1180[A]:ARG:HB2	1.83	0.59
1:B:1029:GLN:HE21	1:B:1075:ASN:HD21	1.47	0.59
1:A:1214[B]:ARG:HH21	3:A:2002[B]:E11:CBI	2.13	0.59
1:A:1218:ILE:HG12	3:A:2001[A]:E11:HBJB	1.84	0.58
1:B:1178:PRO:HB3	1:B:1195:PHE:HE1	1.68	0.58
1:A:1129:ILE:HD11	1:A:1134:ALA:HB2	1.85	0.57
1:B:1029:GLN:NE2	1:B:1075:ASN:ND2	2.52	0.57
1:A:1140:ASP:O	3:A:2001[A]:E11:HBJA	2.04	0.57
1:B:978:ILE:HG12	1:B:1002:PRO:HA	1.87	0.57
1:A:1180[B]:ARG:N	1:A:1180[B]:ARG:HD2	2.20	0.56
1:B:1148:ASN:HB3	1:B:1189:ARG:HA	1.86	0.56
3:B:2003:E11:CAS	3:B:2003:E11:HAW	2.36	0.56
1:B:1146:LEU:HD12	1:B:1154:TYR:CB	2.35	0.55
1:B:1183:MET:HE1	1:B:1184:ALA:HB2	1.89	0.54
1:A:1063:PHE:CZ	1:A:1069:PRO:HD2	2.42	0.54
1:A:1096:ARG:HB2	1:A:1113:GLN:HG2	1.88	0.54
1:B:1123:GLU:HB2	1:B:1193:ILE:O	2.07	0.54
1:B:1158:ALA:HA	1:B:1161:TYR:O	2.09	0.53
1:A:1140:ASP:OD2	3:A:2002[B]:E11:HAF	2.09	0.53
1:B:979:VAL:HG23	1:B:979:VAL:O	2.06	0.53
1:A:1216:TRP:O	1:A:1220:GLY:HA3	2.08	0.53
1:B:1089:VAL:HG21	1:B:1181:VAL:HG21	1.91	0.53
1:A:1073:GLU:OE1	1:A:1090:GLN:HG2	2.09	0.53
1:B:1098:GLN:HB2	1:B:1112:LEU:HD11	1.90	0.52
1:A:1058:ARG:NH1	1:A:1058:ARG:HG3	2.24	0.52
1:A:1070:LEU:HD23	1:A:1180[B]:ARG:HB2	1.91	0.52
1:A:1058:ARG:HH11	1:A:1058:ARG:HG3	1.75	0.52
1:B:1070:LEU:HD23	1:B:1180:ARG:HB2	1.91	0.52
1:B:1133:GLU:O	1:B:1136:VAL:HB	2.11	0.51
3:B:2003:E11:HAW	3:B:2003:E11:HAS	1.93	0.51
1:A:977:ARG:HG3	1:A:978:ILE:N	2.25	0.51
1:B:1166:ARG:NH1	1:B:1167:PHE:CZ	2.79	0.51
1:A:1218:ILE:HG12	3:A:2002[B]:E11:HBJB	1.92	0.51
1:A:1001:GLU:HG3	1:A:1002:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:ASN:OD1	1:A:1066:ALA:HB3	2.11	0.51
3:B:2003:E11:CAP	3:B:2003:E11:N1	2.64	0.51
1:A:1124:TYR:CD1	1:A:1165:SER:HB3	2.46	0.51
1:A:1131:ASP:HB2	1:A:1153:VAL:O	2.11	0.50
1:B:978:ILE:HG12	1:B:1002:PRO:CA	2.41	0.50
1:B:990:ILE:HD12	1:B:990:ILE:C	2.31	0.50
1:A:1010:VAL:HG12	1:B:1076:HIS:HB2	1.94	0.50
1:B:1127:GLU:OE2	1:B:1137:ARG:NH2	2.43	0.50
1:B:1026:THR:OG1	1:B:1185:HIS:HA	2.11	0.50
1:A:1048:SER:O	1:A:1049:MET:CB	2.59	0.50
1:A:1083:ASN:HD22	1:A:1083:ASN:H	1.58	0.50
1:B:1153:VAL:CG1	1:B:1154:TYR:N	2.74	0.50
1:B:1176:LEU:HB2	1:B:1208:GLY:O	2.11	0.50
1:A:1131:ASP:O	3:A:2001[A]:E11:HAUA	2.04	0.50
1:A:1086:ASN:O	1:A:1087:ARG:HG2	2.11	0.49
1:B:1001:GLU:OE2	1:B:1002:PRO:HD2	2.12	0.49
1:B:978:ILE:HG12	1:B:1002:PRO:HB3	1.95	0.49
1:A:1148:ASN:O	1:A:1150:ASP:N	2.43	0.48
1:A:1135:ASP:HB2	3:A:2001[A]:E11:NAR	2.28	0.48
1:B:1178:PRO:HB3	1:B:1195:PHE:CE1	2.46	0.48
3:B:2003:E11:HAV	3:B:2003:E11:HASB	1.95	0.48
1:A:1081:TRP:CH2	1:B:981:ARG:NH2	2.80	0.48
1:A:1145:ASP:OD2	3:A:2002[B]:E11:HBIB	2.13	0.48
1:A:1085:ARG:NH1	1:A:1085:ARG:HG2	2.29	0.48
1:A:977:ARG:O	1:A:978:ILE:HB	2.14	0.48
1:A:1158:ALA:HA	1:A:1161:TYR:O	2.14	0.47
1:B:1148:ASN:CB	1:B:1189:ARG:HA	2.44	0.47
1:B:1071:ILE:HD12	1:B:1179:VAL:HG11	1.96	0.47
1:A:988:GLU:OE2	1:A:988:GLU:HA	2.15	0.47
1:B:1096:ARG:N	1:B:1113:GLN:HE21	1.89	0.47
1:B:1140:ASP:OD2	3:B:2003:E11:HBJB	2.15	0.47
1:B:1017:SER:H	1:B:1018:PRO:HD3	1.76	0.47
1:B:1157:ASP:OD1	1:B:1159:ARG:HB3	2.15	0.47
1:A:1148:ASN:C	1:A:1150:ASP:H	2.18	0.46
1:B:981:ARG:O	1:B:982:ASP:HB2	2.14	0.46
1:A:1093:LEU:HD12	1:A:1121:VAL:O	2.15	0.46
1:A:996:ASN:ND2	1:A:1001:GLU:O	2.48	0.46
1:A:1004:PRO:HD3	1:A:1107:TRP:CZ2	2.51	0.46
1:A:1176:LEU:HD11	1:A:1207:LEU:HB3	1.98	0.46
1:B:1129:ILE:HG13	1:B:1130:SER:N	2.31	0.46
1:A:1008:LYS:HB3	1:A:1161:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:VAL:HG12	1:A:1183:MET:HE2	1.98	0.46
1:A:1214[B]:ARG:NH2	3:A:2002[B]:E11:HBI	2.29	0.45
1:A:1076:HIS:H	1:A:1076:HIS:HD1	1.63	0.45
1:A:1214[A]:ARG:HB2	3:A:2001[A]:E11:HBIA	1.97	0.45
1:B:1182:PHE:CE1	1:B:1191:PRO:HB3	2.50	0.45
1:A:1073:GLU:HA	1:A:1086:ASN:HD21	1.80	0.45
1:A:989:ARG:NH2	1:A:1094:ARG:HE	2.15	0.45
1:B:1171:HIS:CE1	1:B:1229:SER:HB2	2.52	0.45
1:B:1176:LEU:HA	1:B:1196:PHE:O	2.17	0.45
1:B:1026:THR:C	1:B:1028:LEU:H	2.18	0.45
1:B:1159:ARG:HH11	1:B:1159:ARG:HG3	1.82	0.45
1:B:1218:ILE:HG22	1:B:1218:ILE:O	2.16	0.45
1:A:1015:VAL:HG23	1:A:1015:VAL:O	2.17	0.45
1:B:1133:GLU:HA	1:B:1136:VAL:CG2	2.46	0.45
1:A:1129:ILE:CD1	1:A:1134:ALA:HB2	2.47	0.44
1:B:1147:ASP:HB2	1:B:1180:ARG:HH22	1.82	0.44
1:A:989:ARG:CZ	1:A:1094:ARG:HE	2.31	0.44
1:B:1094:ARG:HG3	6:B:39:HOH:O	2.16	0.44
3:B:2003:E11:CAV	3:B:2003:E11:HASB	2.48	0.44
1:A:1085:ARG:HH11	1:A:1085:ARG:HG2	1.81	0.44
1:B:1148:ASN:OD1	1:B:1153:VAL:N	2.50	0.44
1:B:990:ILE:HD11	1:B:1093:LEU:HD21	1.99	0.44
1:B:1213:GLU:O	1:B:1214:ARG:C	2.54	0.44
1:B:1029:GLN:HG3	1:B:1029:GLN:O	2.18	0.44
1:B:1170:HIS:CG	1:B:1171:HIS:N	2.86	0.43
1:A:1052:TRP:O	1:A:1060:LEU:HG	2.18	0.43
3:B:2003:E11:CBH	3:B:2003:E11:HAXA	2.48	0.43
1:A:1184:ALA:O	1:A:1185:HIS:HB2	2.19	0.43
1:B:1009:TYR:HA	1:B:1162:GLY:O	2.18	0.43
1:B:1035:ASP:HB2	1:B:1036:ASP:H	1.65	0.43
1:B:1013:ASN:ND2	1:B:1125:VAL:HA	2.29	0.43
1:A:989:ARG:NH2	1:A:1091:ASN:O	2.32	0.43
1:B:1002:PRO:O	1:B:1003:CYS:C	2.57	0.43
1:B:1082:ARG:HG3	1:B:1082:ARG:O	2.18	0.43
1:B:1090:GLN:OE1	1:B:1183:MET:CE	2.67	0.43
1:B:1164:VAL:O	1:B:1164:VAL:HG22	2.19	0.43
1:B:1133:GLU:HA	1:B:1136:VAL:HG23	2.01	0.43
1:B:1146:LEU:O	1:B:1180:ARG:NH2	2.52	0.43
1:B:1159:ARG:NH1	1:B:1159:ARG:HG3	2.34	0.43
1:B:1175:ASN:O	1:B:1197:SER:HA	2.19	0.42
1:B:1101:ARG:HB2	1:B:1107:TRP:CZ3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:VAL:HG11	1:B:1076:HIS:HD2	1.83	0.42
1:A:1145:ASP:OD2	3:A:2001[A]:E11:HBIB	2.19	0.42
1:A:1131:ASP:OD2	3:A:2001[A]:E11:CAS	2.68	0.42
1:A:1177:VAL:HG13	1:A:1177:VAL:O	2.20	0.42
1:B:1029:GLN:HE21	1:B:1075:ASN:HD22	1.65	0.42
1:B:1094:ARG:HD3	1:B:1095:ALA:N	2.34	0.42
3:B:2003:E11:HAPA	3:B:2003:E11:HASB	1.60	0.42
1:B:1183:MET:HE1	1:B:1184:ALA:N	2.34	0.42
1:A:1139:GLU:HG2	1:A:1159:ARG:HD3	2.01	0.42
1:B:1229:SER:C	1:B:1231:LYS:H	2.22	0.42
1:B:1226:ARG:H	2:B:102:SAH:HN62	1.68	0.42
1:A:1048:SER:C	1:A:1050:ARG:H	2.24	0.41
1:B:979:VAL:O	1:B:979:VAL:CG2	2.68	0.41
1:A:1028:LEU:O	1:A:1029:GLN:CB	2.67	0.41
3:B:2003:E11:HASB	3:B:2003:E11:HAW	2.02	0.41
1:A:1139:GLU:OE1	1:A:1139:GLU:HA	2.20	0.41
1:A:1125:VAL:HG12	1:A:1126:GLY:N	2.36	0.41
1:B:1017:SER:H	1:B:1018:PRO:HD2	1.83	0.41
1:A:1100:TYR:OH	1:A:1206:GLN:HG3	2.20	0.41
1:A:1102:THR:OG1	1:A:1106:GLY:N	2.54	0.41
1:B:1097:LEU:HD22	1:B:1207:LEU:HD11	2.03	0.41
1:B:1123:GLU:HG3	1:B:1125:VAL:HG23	2.03	0.41
1:A:1075:ASN:CB	1:A:1184:ALA:HB2	2.51	0.41
1:B:1216:TRP:C	1:B:1218:ILE:N	2.72	0.40
1:A:1094:ARG:HD3	1:A:1094:ARG:HA	1.81	0.40
1:A:1105:MET:CE	1:A:1206:GLN:HE22	2.34	0.40
1:B:1004:PRO:HD3	1:B:1107:TRP:CE2	2.56	0.40
1:A:1219:LYS:C	1:A:1221:LYS:H	2.24	0.40
1:B:1083:ASN:HD22	1:B:1083:ASN:H	1.70	0.40
1:B:1121:VAL:O	1:B:1122:CYS:HB3	2.22	0.40
1:B:1146:LEU:O	1:B:1147:ASP:CB	2.70	0.40
1:A:987:TYR:CD1	1:B:1082:ARG:HB2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/285 (87%)	205 (82%)	36 (14%)	8 (3%)	4	12
1	B	238/285 (84%)	188 (79%)	32 (13%)	18 (8%)	1	2
All	All	487/570 (85%)	393 (81%)	68 (14%)	26 (5%)	2	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1029	GLN
1	A	1231	LYS
1	B	1017	SER
1	B	1023	ARG
1	B	1069	PRO
1	B	1070	LEU
1	B	1153	VAL
1	B	1184	ALA
1	A	1149	LYS
1	B	982	ASP
1	B	998	VAL
1	B	1024	ASN
1	B	1147	ASP
1	B	1183	MET
1	A	978	ILE
1	A	1049	MET
1	A	1232	CYS
1	B	1016	THR
1	B	979	VAL
1	B	1004	PRO
1	B	1013	ASN
1	B	1018	PRO
1	A	1164	VAL
1	B	1088	VAL
1	B	1190	PHE
1	A	1230	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	214/257 (83%)	202 (94%)	12 (6%)	21	48
1	B	194/257 (76%)	184 (95%)	10 (5%)	23	52
All	All	408/514 (79%)	386 (95%)	22 (5%)	23	50

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1027	HIS
1	A	1032	VAL
1	A	1050	ARG
1	A	1083	ASN
1	A	1085	ARG
1	A	1113	GLN
1	A	1145	ASP
1	A	1148	ASN
1	A	1186	GLN
1	A	1214[A]	ARG
1	A	1214[B]	ARG
1	A	1218	ILE
1	B	1008	LYS
1	B	1010	VAL
1	B	1029	GLN
1	B	1035	ASP
1	B	1083	ASN
1	B	1094	ARG
1	B	1110	ARG
1	B	1114	ASP
1	B	1183	MET
1	B	1227	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1027	HIS
1	A	1083	ASN
1	B	1013	ASN
1	B	1029	GLN

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Mol	Chain	Res	Type
1	B	1083	ASN
1	B	1113	GLN
1	B	1186	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAH	A	101	-	21,28,28	1.83	4 (19%)	20,40,40	2.22	7 (35%)
5	EDO	B	1	-	3,3,3	0.52	0	2,2,2	0.26	0
3	E11	B	2003	-	37,38,38	1.09	1 (2%)	51,51,51	1.81	14 (27%)
5	EDO	B	2	-	3,3,3	0.57	0	2,2,2	0.17	0
3	E11	A	2002[B]	-	37,38,38	1.10	1 (2%)	51,51,51	1.80	13 (25%)
2	SAH	B	102	-	21,28,28	1.87	4 (19%)	20,40,40	2.20	8 (40%)
3	E11	A	2001[A]	-	37,38,38	1.07	1 (2%)	51,51,51	1.76	12 (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
2	SAH	A	101	-	-	3/7/31/31	0/3/3/3
5	EDO	B	1	-	-	0/1/1/1	-
3	E11	B	2003	-	-	10/19/29/29	0/4/4/4
5	EDO	B	2	-	-	1/1/1/1	-
3	E11	A	2002[B]	-	-	4/19/29/29	0/4/4/4
2	SAH	B	102	-	-	3/7/31/31	0/3/3/3
3	E11	A	2001[A]	-	-	8/19/29/29	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	102	SAH	O4'-C1'	5.35	1.48	1.41
3	A	2002[B]	E11	C6-C5	-4.54	1.39	1.44
3	B	2003	E11	C6-C5	-4.41	1.39	1.44
2	A	101	SAH	O4'-C1'	4.36	1.47	1.41
3	A	2001[A]	E11	C6-C5	-4.25	1.39	1.44
2	A	101	SAH	C2-N3	3.87	1.38	1.32
2	B	102	SAH	C2-N3	3.67	1.38	1.32
2	A	101	SAH	CA-N	2.81	1.53	1.47
2	B	102	SAH	C8-N7	-2.65	1.30	1.34
2	A	101	SAH	C8-N7	-2.62	1.30	1.34
2	B	102	SAH	CA-N	2.60	1.52	1.47

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	102	SAH	O4'-C1'-C2'	-5.12	99.44	106.93
2	A	101	SAH	C3'-C2'-C1'	4.54	107.81	100.98
3	B	2003	E11	C6-C5-C4	4.33	118.61	115.88
3	A	2001[A]	E11	C6-C5-C4	4.25	118.56	115.88
2	B	102	SAH	N3-C2-N1	-4.18	122.15	128.68
3	A	2002[B]	E11	CAF-C5-C6	-4.16	121.13	124.88
3	A	2002[B]	E11	C6-C5-C4	4.13	118.48	115.88
3	B	2003	E11	CAF-C5-C6	-4.11	121.17	124.88
2	A	101	SAH	O4'-C1'-C2'	-4.11	100.93	106.93
2	A	101	SAH	N3-C2-N1	-4.08	122.30	128.68
3	A	2001[A]	E11	CAF-C5-C6	-4.06	121.22	124.88
2	A	101	SAH	CB-CG-SD	-4.03	104.28	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002[B]	E11	CBJ-OAK-CAE	-3.88	111.68	117.53
3	A	2002[B]	E11	CBI-OAL-CAD	-3.87	111.68	117.53
3	A	2001[A]	E11	CBJ-OAK-CAE	-3.81	111.77	117.53
3	B	2003	E11	CBI-OAL-CAD	-3.70	111.94	117.53
2	B	102	SAH	CB-CG-SD	-3.64	105.15	113.31
3	B	2003	E11	CBJ-OAK-CAE	-3.61	112.08	117.53
3	B	2003	E11	N3-C2-N1	-3.58	120.57	126.23
3	A	2001[A]	E11	N3-C2-N1	-3.50	120.69	126.23
3	A	2001[A]	E11	CBI-OAL-CAD	-3.49	112.26	117.53
3	B	2003	E11	OAL-CAD-CAC	-3.45	120.77	125.24
3	B	2003	E11	OAK-CAE-CAF	-3.43	120.80	125.24
3	A	2002[B]	E11	N3-C2-N1	-3.42	120.82	126.23
3	A	2002[B]	E11	OAK-CAE-CAF	-3.27	121.01	125.24
3	A	2001[A]	E11	OAK-CAE-CAF	-3.24	121.05	125.24
3	A	2001[A]	E11	C2-N3-C4	3.22	120.85	115.60
3	B	2003	E11	C2-N3-C4	3.22	120.84	115.60
3	A	2001[A]	E11	OAL-CAD-CAC	-3.21	121.08	125.24
3	A	2002[B]	E11	C2-N3-C4	3.21	120.83	115.60
3	A	2002[B]	E11	OAL-CAD-CAC	-3.14	121.17	125.24
3	A	2002[B]	E11	C5-C4-N3	-3.09	119.53	122.81
3	B	2003	E11	C5-C4-N3	-3.08	119.54	122.81
3	A	2001[A]	E11	C5-C4-N3	-3.07	119.55	122.81
2	B	102	SAH	C3'-C2'-C1'	3.02	105.53	100.98
3	B	2003	E11	OAL-CAD-CAE	2.84	119.36	115.41
2	B	102	SAH	C2-N1-C6	2.83	123.60	118.75
3	A	2002[B]	E11	OAK-CAE-CAD	2.71	119.18	115.41
3	B	2003	E11	OAK-CAE-CAD	2.59	119.02	115.41
2	A	101	SAH	C2-N1-C6	2.57	123.15	118.75
2	B	102	SAH	C1'-N9-C4	-2.53	122.20	126.64
3	A	2001[A]	E11	OAK-CAE-CAD	2.53	118.93	115.41
2	A	101	SAH	C1'-N9-C4	-2.50	122.25	126.64
3	A	2001[A]	E11	OAL-CAD-CAE	2.46	118.84	115.41
3	B	2003	E11	C6-NAM-CAV	-2.33	119.73	124.16
3	A	2002[B]	E11	CAO-NAN-C2	-2.29	119.78	123.75
3	A	2002[B]	E11	OAL-CAD-CAE	2.23	118.52	115.41
3	B	2003	E11	CAO-NAN-C2	-2.20	119.94	123.75
3	A	2002[B]	E11	C6-NAM-CAV	-2.17	120.03	124.16
2	A	101	SAH	C5-C6-N6	2.17	123.64	120.35
2	B	102	SAH	C5-C6-N6	2.08	123.52	120.35
3	B	2003	E11	C2-N1-C6	2.05	121.08	116.39
3	A	2001[A]	E11	C2-N1-C6	2.01	120.99	116.39
2	B	102	SAH	C5-C6-N1	-2.01	115.81	120.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2003	E11	CAP-CAO-NAN-C2
2	B	102	SAH	CA-CB-CG-SD
2	A	101	SAH	CA-CB-CG-SD
3	B	2003	E11	CAP-CAQ-NAR-CAS
3	B	2003	E11	CAP-CAQ-NAR-CAU
3	A	2001[A]	E11	CAP-CAQ-NAR-CAS
3	A	2001[A]	E11	CAP-CAQ-NAR-CAU
3	B	2003	E11	N3-C2-NAN-CAO
3	A	2001[A]	E11	CAO-CAP-CAQ-NAR
3	B	2003	E11	CAE-CAD-OAL-CBI
3	B	2003	E11	N1-C2-NAN-CAO
3	A	2001[A]	E11	CAD-CAE-OAK-CBJ
3	A	2002[B]	E11	CAF-CAE-OAK-CBJ
3	A	2001[A]	E11	CAF-CAE-OAK-CBJ
3	B	2003	E11	CAF-CAE-OAK-CBJ
3	A	2002[B]	E11	CAD-CAE-OAK-CBJ
2	A	101	SAH	C3'-C4'-C5'-SD
2	B	102	SAH	CB-CG-SD-C5'
3	B	2003	E11	CAC-CAD-OAL-CBI
3	B	2003	E11	CAD-CAE-OAK-CBJ
3	A	2001[A]	E11	CAE-CAD-OAL-CBI
5	B	2	EDO	O1-C1-C2-O2
3	A	2001[A]	E11	CAP-CAO-NAN-C2
3	A	2002[B]	E11	CAE-CAD-OAL-CBI
3	B	2003	E11	CAO-CAP-CAQ-NAR
3	A	2002[B]	E11	CAC-CAD-OAL-CBI
3	A	2001[A]	E11	CAC-CAD-OAL-CBI
2	A	101	SAH	CB-CG-SD-C5'
2	B	102	SAH	C3'-C4'-C5'-SD

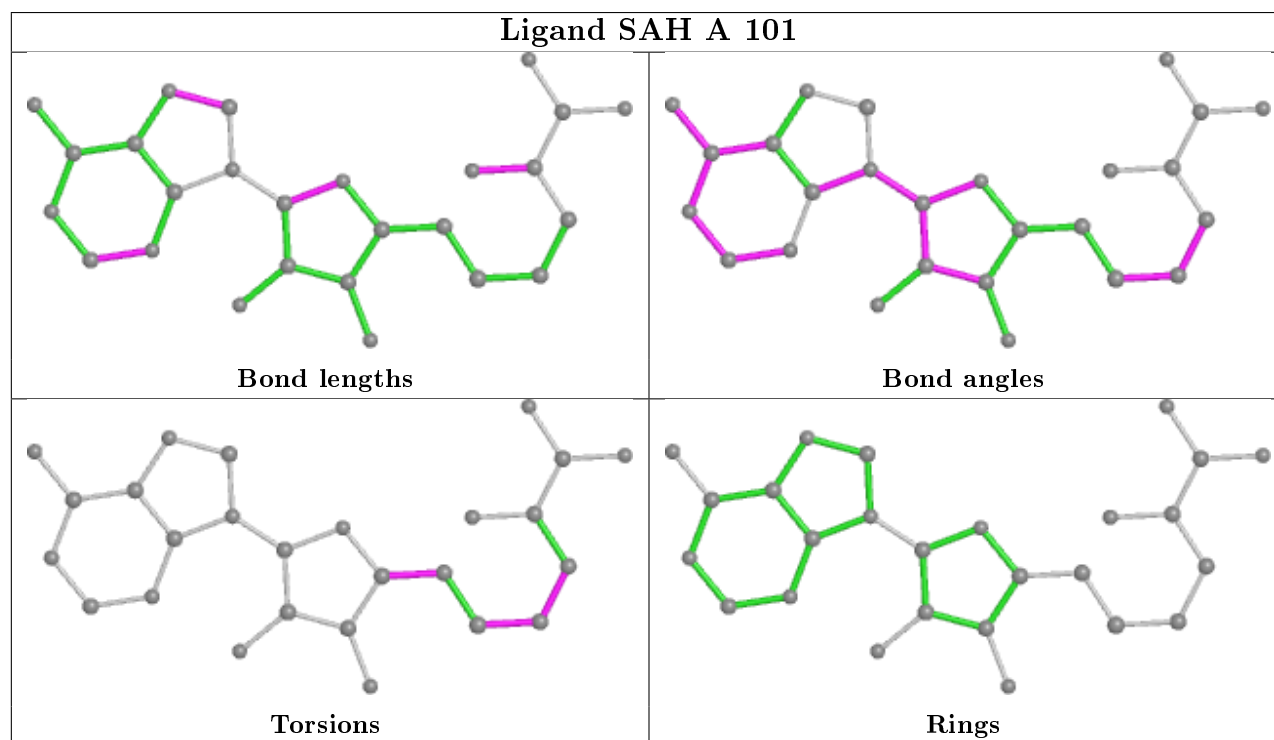
There are no ring outliers.

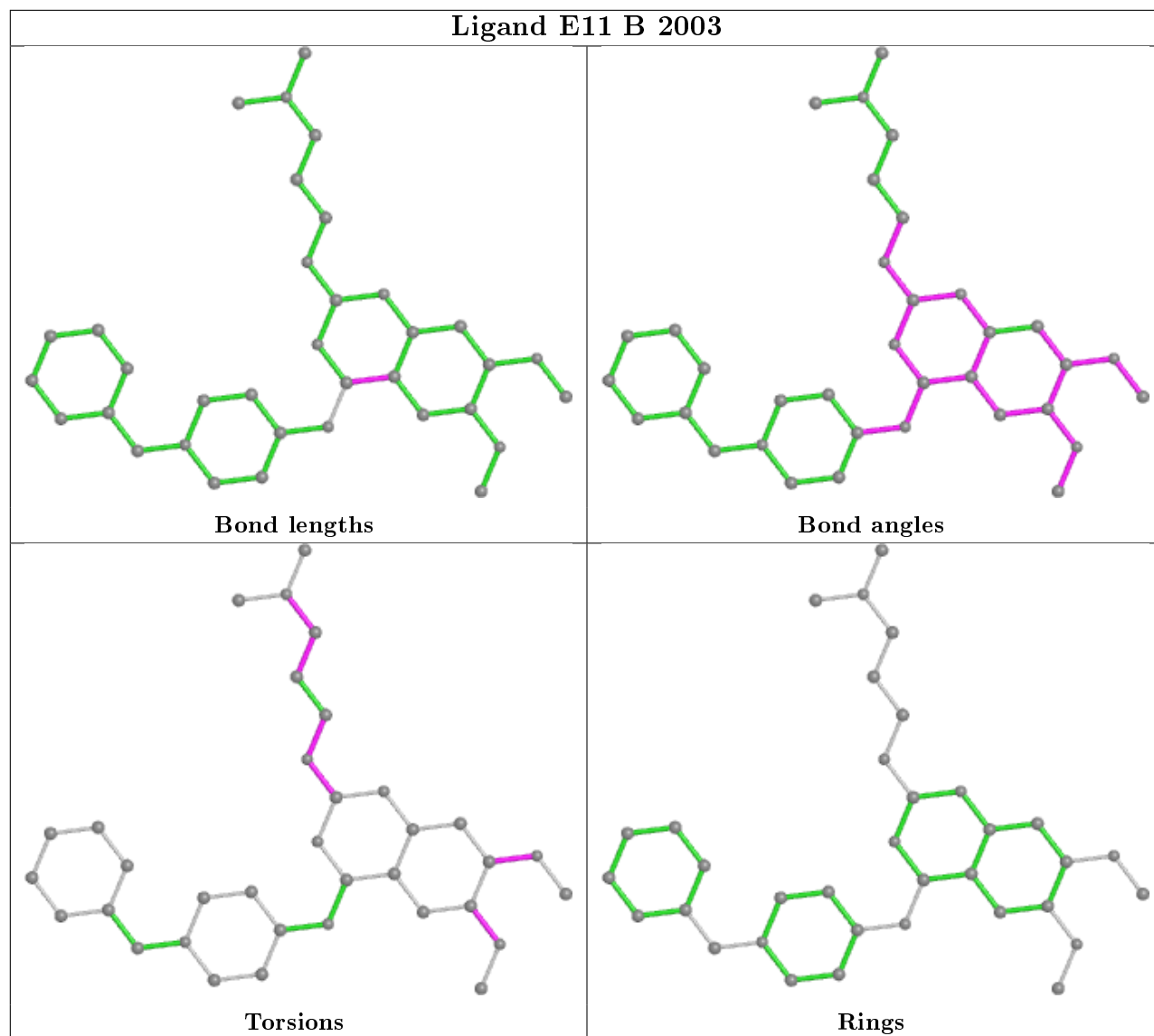
4 monomers are involved in 38 short contacts:

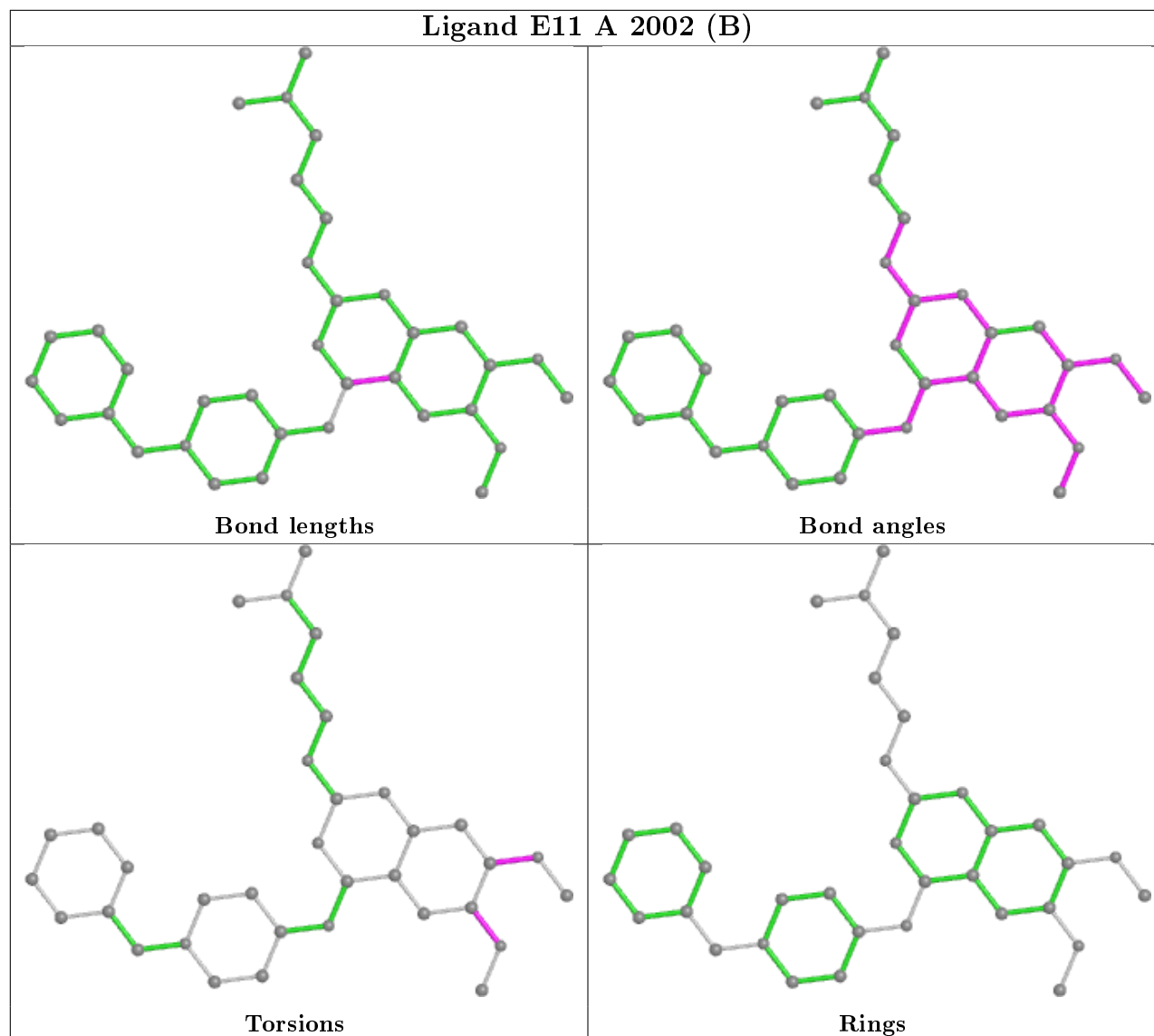
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2003	E11	13	0
3	A	2002[B]	E11	10	0
2	B	102	SAH	1	0
3	A	2001[A]	E11	14	0

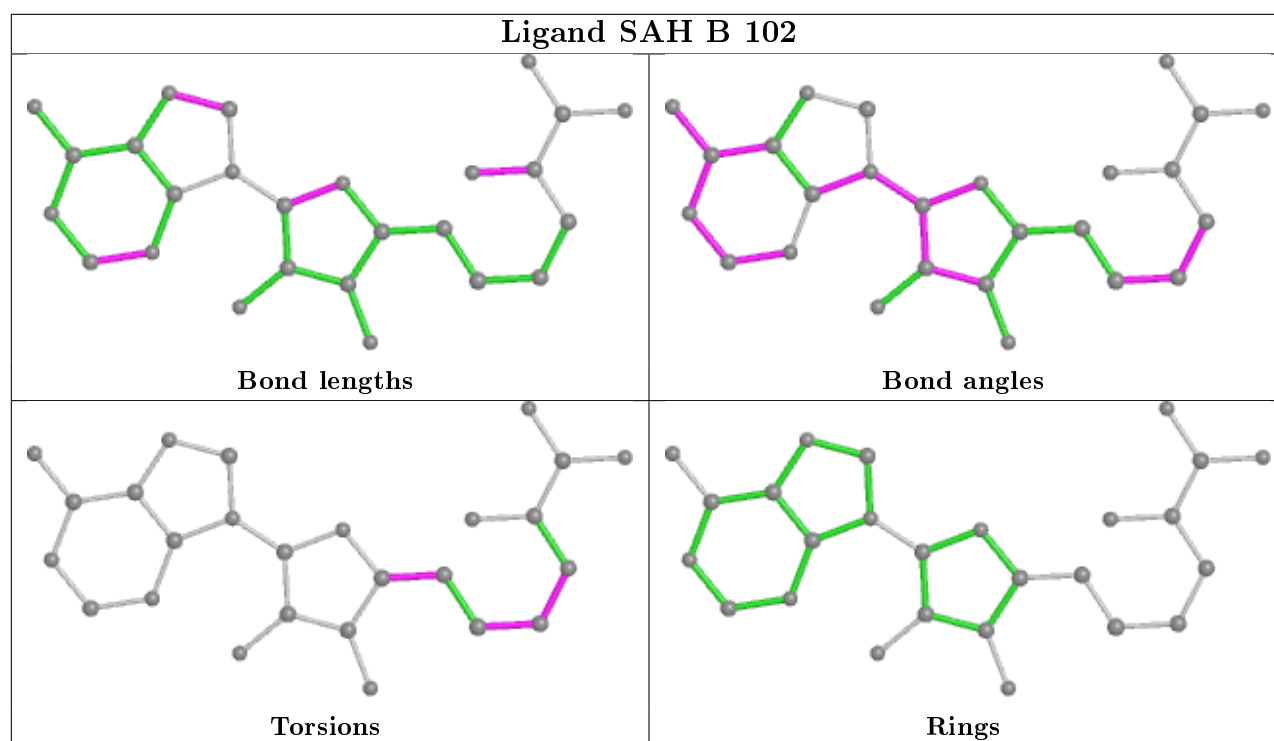
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

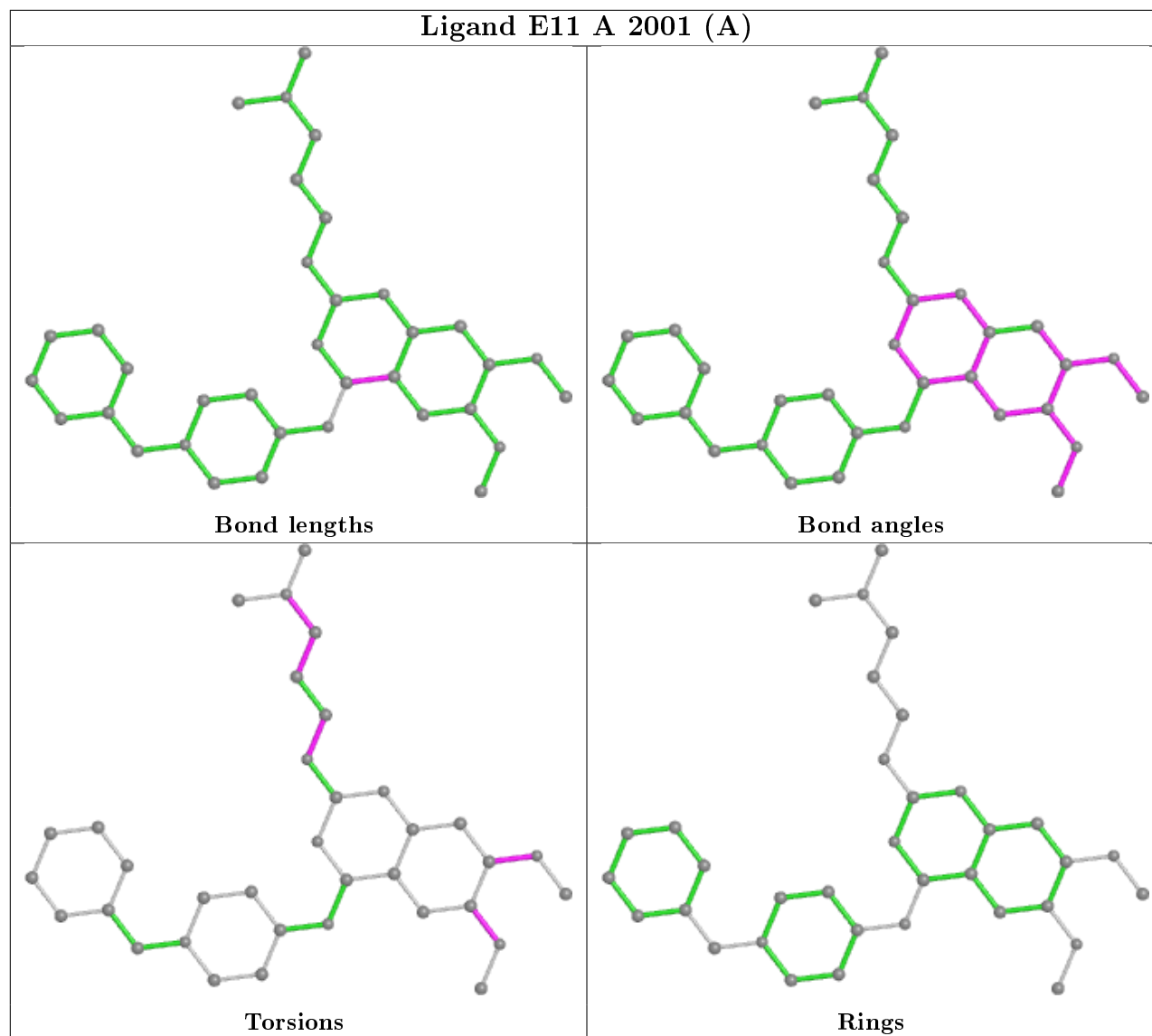
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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	251/285 (88%)	0.33	15 (5%) 21 16	23, 46, 88, 96	0
1	B	242/285 (84%)	0.33	23 (9%) 8 5	28, 53, 105, 113	0
All	All	493/570 (86%)	0.33	38 (7%) 13 9	23, 50, 95, 113	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1051	CYS	7.9
1	B	1017	SER	4.8
1	B	978	ILE	4.7
1	B	1152	GLU	4.2
1	A	1151	GLY	3.8
1	A	978	ILE	3.8
1	B	1068	PRO	3.6
1	B	1050	ARG	3.5
1	A	1226	ARG	3.5
1	B	1151	GLY	3.4
1	B	1018	PRO	3.4
1	B	1069	PRO	3.3
1	A	1223	PHE	3.3
1	B	1025	ILE	3.3
1	A	1230	PRO	3.2
1	B	1016	THR	3.1
1	B	1000	SER	3.1
1	B	1070	LEU	3.0
1	A	1224	SER	2.9
1	A	1149	LYS	2.7
1	B	1085	ARG	2.6
1	B	1150	ASP	2.6
1	B	1048	SER	2.6
1	A	1218	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1134	ALA	2.5
1	A	1222	LEU	2.5
1	B	1149	LYS	2.4
1	A	977	ARG	2.4
1	A	1221	LYS	2.3
1	B	1049	MET	2.3
1	B	1147	ASP	2.2
1	A	1050	ARG	2.2
1	B	1148	ASN	2.2
1	A	1152	GLU	2.2
1	B	1217	ASP	2.1
1	B	1023	ARG	2.1
1	A	1038	SER	2.1
1	A	1220	GLY	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 carbohydrates 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.

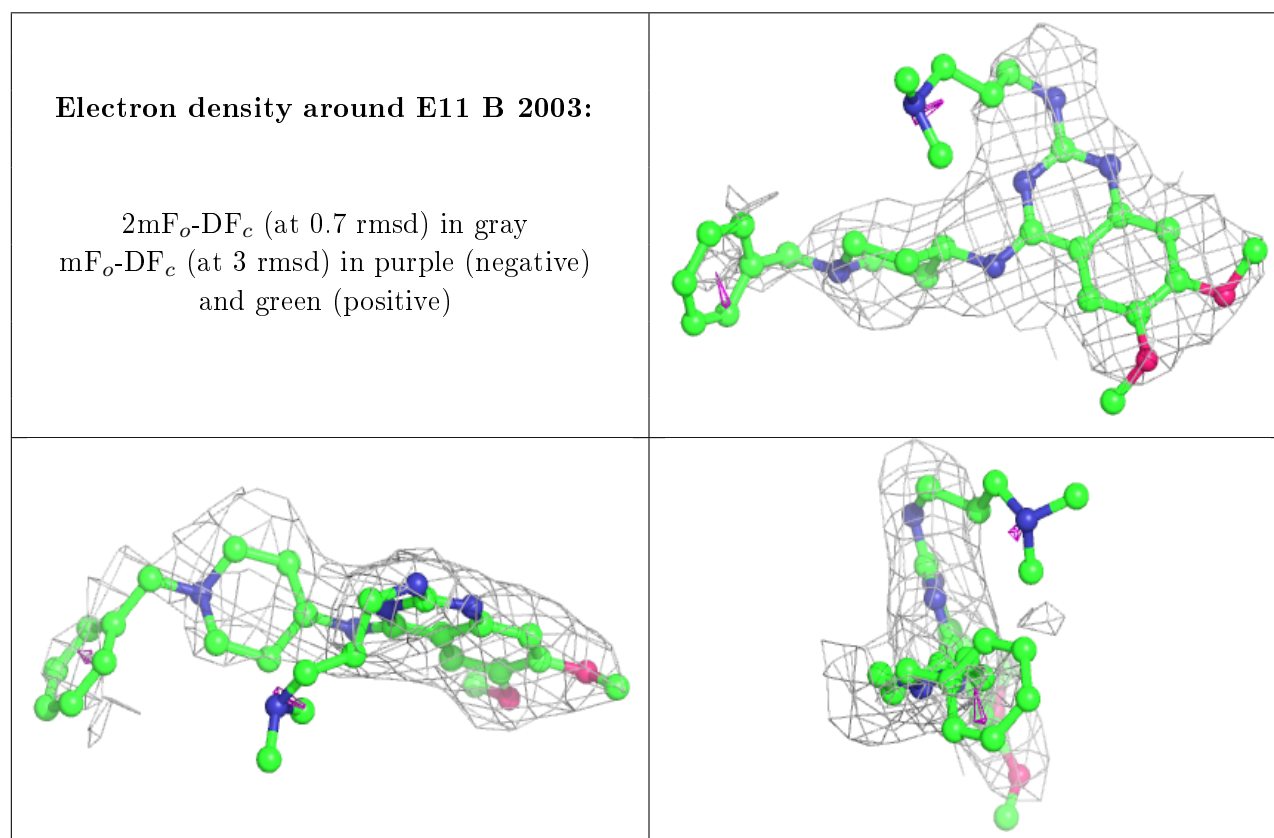
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	E11	B	2003	35/35	0.77	0.36	83,91,101,101	0
3	E11	A	2001[A]	35/35	0.84	0.23	62,66,72,72	35
3	E11	A	2002[B]	35/35	0.85	0.21	59,64,71,71	35
2	SAH	A	101	26/26	0.85	0.23	72,78,79,79	0
5	EDO	B	1	4/4	0.87	0.27	55,59,60,61	0
5	EDO	B	2	4/4	0.90	0.23	60,61,61,63	0
2	SAH	B	102	26/26	0.93	0.18	57,64,65,68	0
4	ZN	A	10	1/1	0.93	0.14	91,91,91,91	0
4	ZN	A	4	1/1	0.98	0.07	70,70,70,70	0

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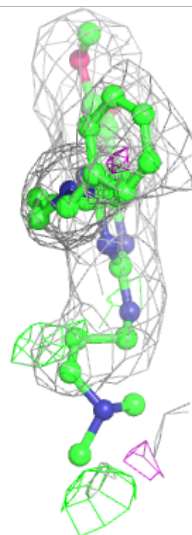
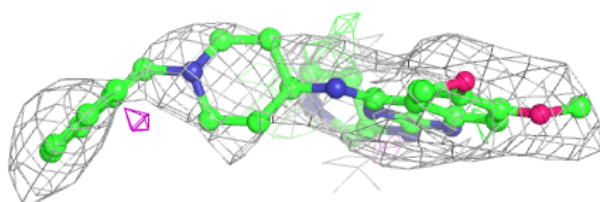
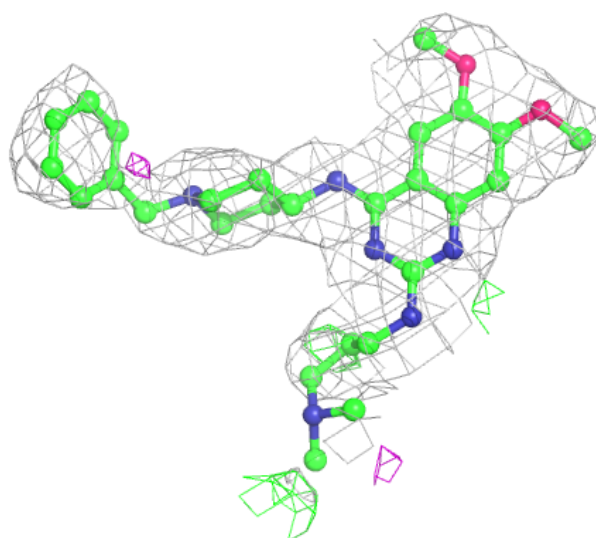
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ZN	A	2	1/1	0.99	0.15	35,35,35,35	0
4	ZN	B	6	1/1	0.99	0.09	37,37,37,37	0
4	ZN	B	5	1/1	0.99	0.11	40,40,40,40	0
4	ZN	A	3	1/1	0.99	0.13	36,36,36,36	0
4	ZN	B	9	1/1	0.99	0.13	53,53,53,53	0
4	ZN	B	7	1/1	0.99	0.10	35,35,35,35	0
4	ZN	B	8	1/1	0.99	0.11	51,51,51,51	0
4	ZN	A	1236	1/1	1.00	0.13	35,35,35,35	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.



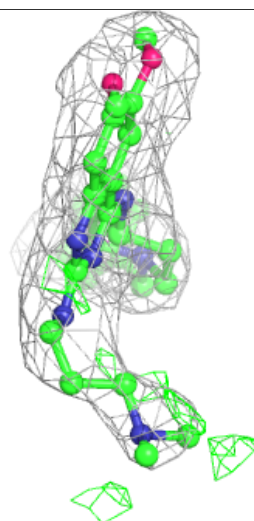
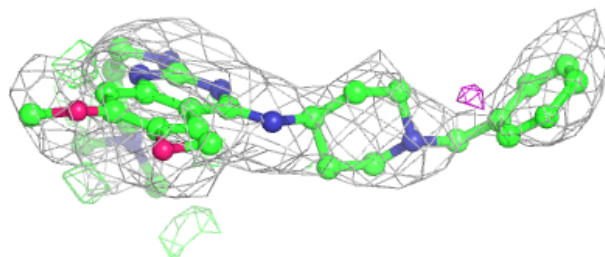
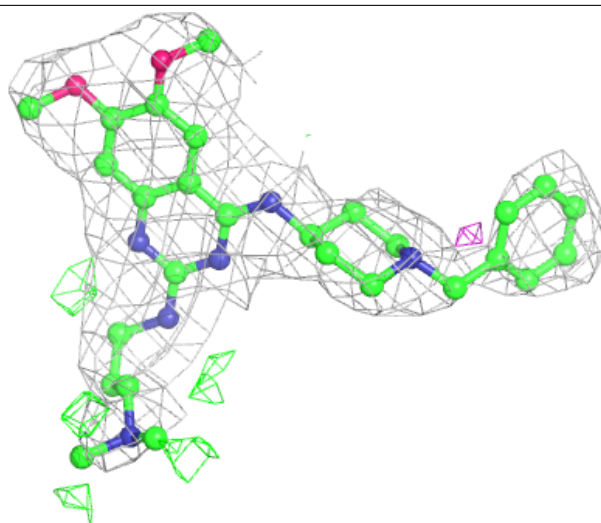
Electron density around E11 A 2001 (A):

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



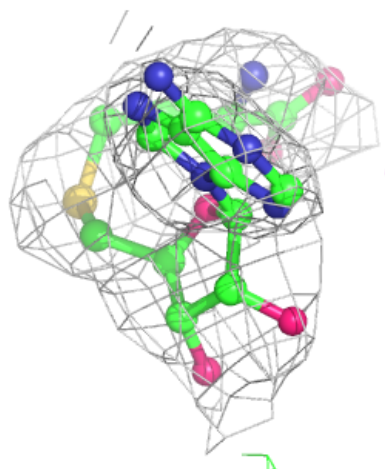
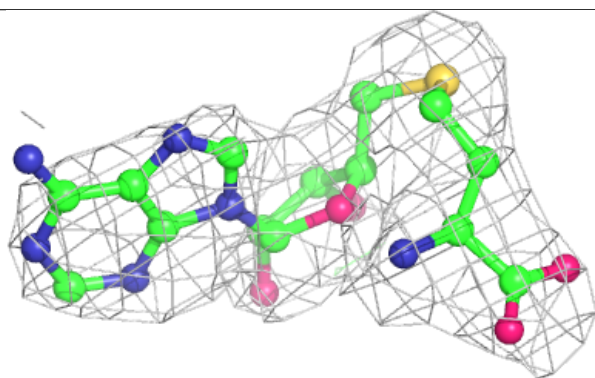
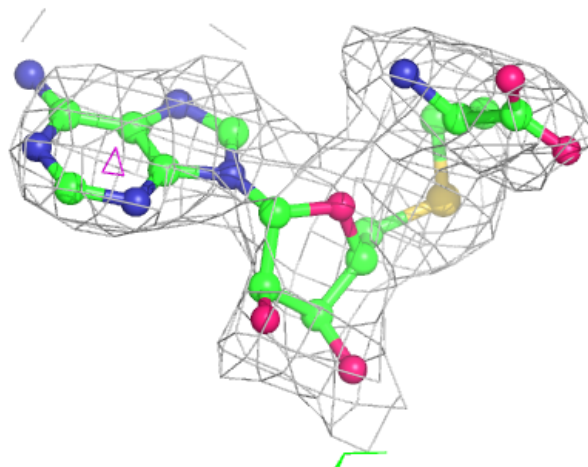
Electron density around E11 A 2002 (B):

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



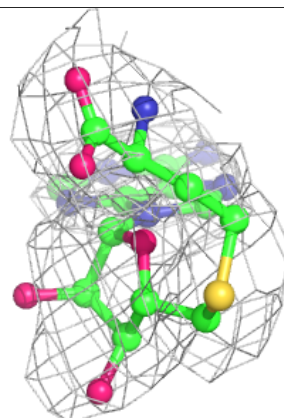
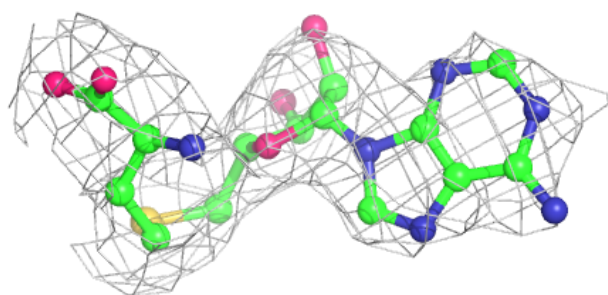
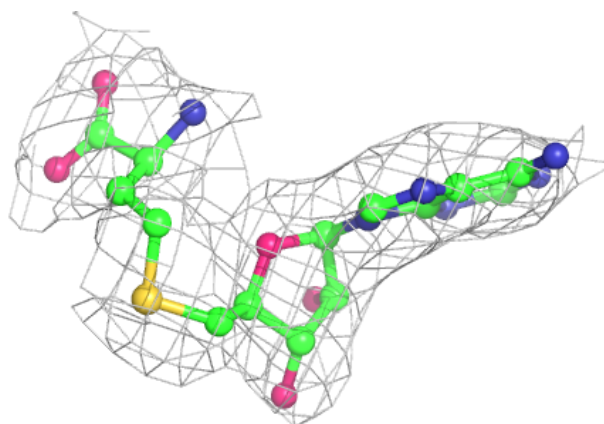
Electron density around SAH A 101:

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



Electron density around SAH B 102:

$2mF_o-DF_c$ (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.