



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 08:27 am BST

PDB ID : 3MO5  
Title : Human G9a-like (GLP, also known as EHMT1) in complex with inhibitor E72  
Authors : Chang, Y.; Horton, J.R.; Cheng, X.  
Deposited on : 2010-04-22  
Resolution : 2.14 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](mailto: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.

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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

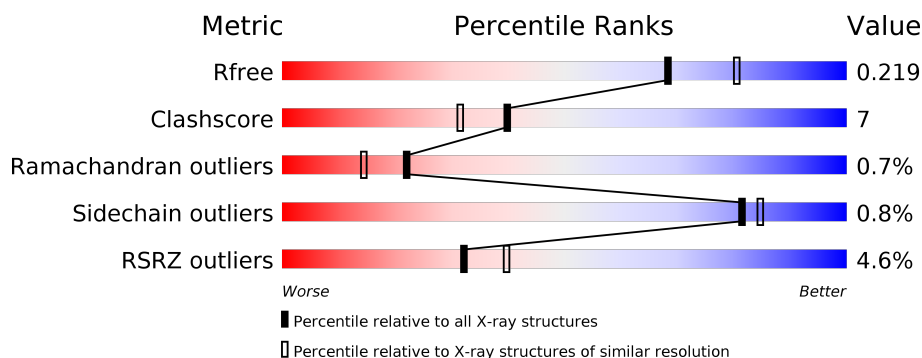
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>3%</div> <div> <div></div> <div>78%</div> <div>11%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	285	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	285	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	285	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9067 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.

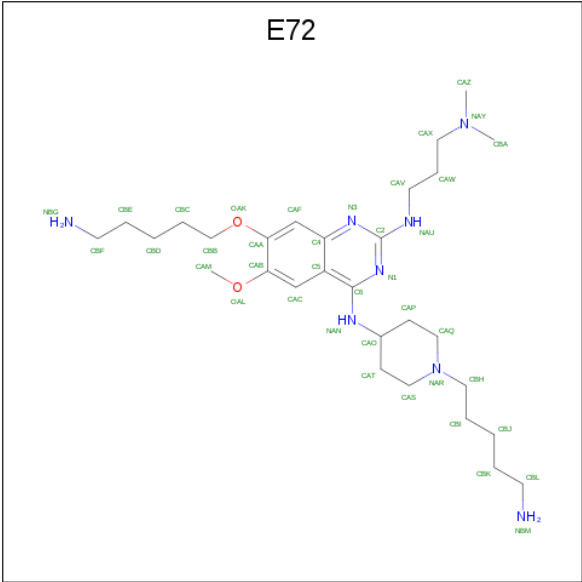
- Molecule 1 is a protein called Histone-lysine N-methyltransferase, H3 lysine-9 specific 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2022	1262	363	373	24			
1	B	258	Total	C	N	O	S	0	0	0
			2050	1282	366	377	25			
1	C	258	Total	C	N	O	S	0	0	0
			2053	1282	368	378	25			
1	D	256	Total	C	N	O	S	0	0	0
			2019	1263	359	372	25			

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

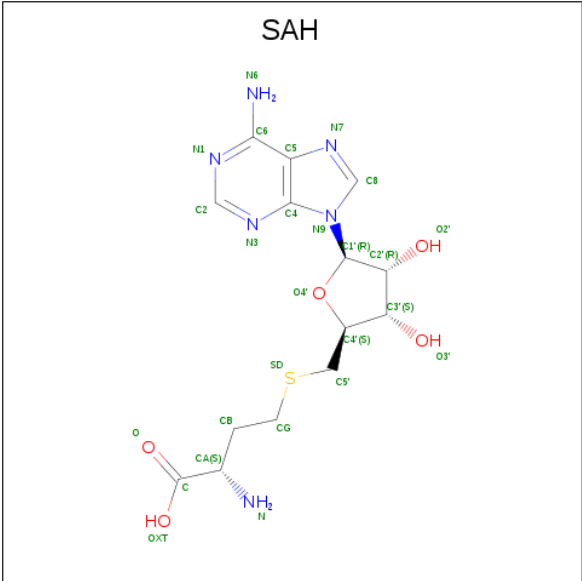
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Zn	0	0
			4	4		
2	A	4	Total	Zn	0	0
			4	4		
2	D	4	Total	Zn	0	0
			4	4		
2	C	4	Total	Zn	0	0
			4	4		

- Molecule 3 is 7-[(5-aminopentyl)oxy]-N 4 -[1-(5-aminopentyl)piperidin-4-yl]-N 2 -[3-(dimethylamino)propyl]-6-methoxyquinazoline-2,4-diamine (three-letter code: E72) (formula: C<sub>29</sub>H<sub>52</sub>N<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			39	29	8	2		
3	B	1	Total	C	N	O	0	0
			39	29	8	2		
3	C	1	Total	C	N	O	0	0
			39	29	8	2		
3	D	1	Total	C	N	O	0	0
			39	29	8	2		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



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

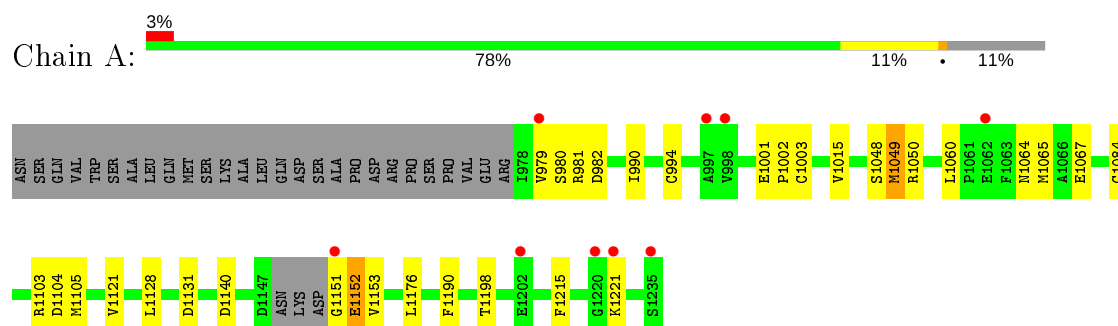
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		
5	B	201	Total	O	0	0
			201	201		
5	C	182	Total	O	0	0
			182	182		
5	D	123	Total	O	0	0
			123	123		

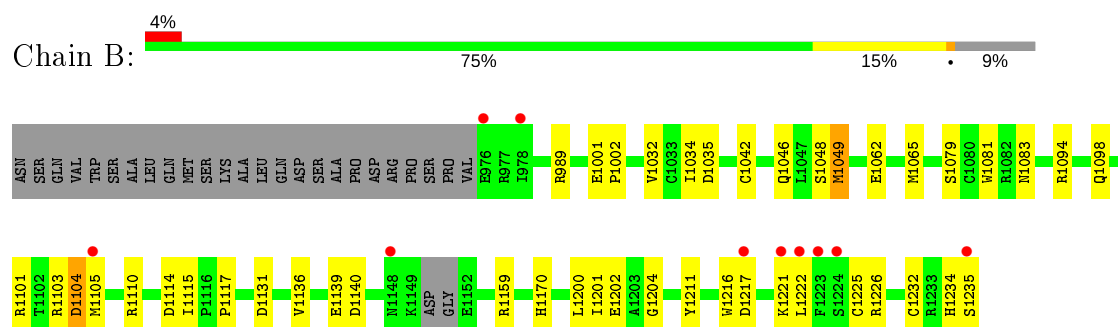
### 3 Residue-property plots [i](#)

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.

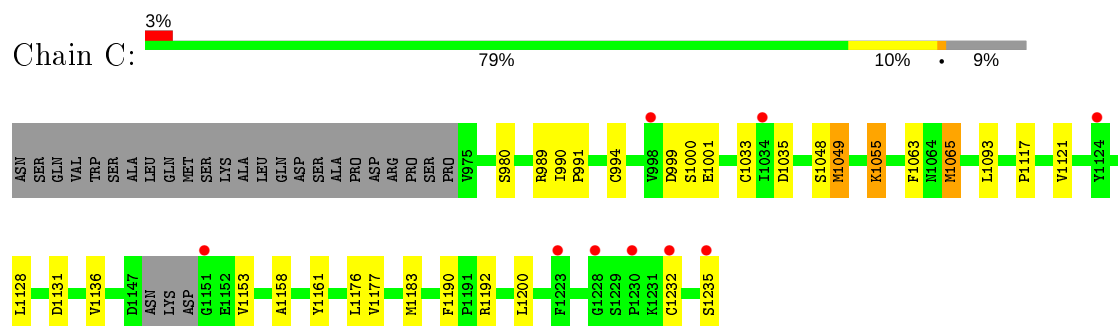
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5



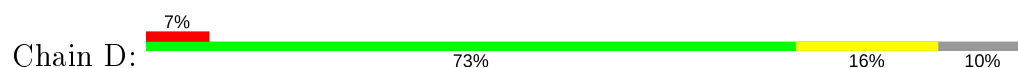
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5

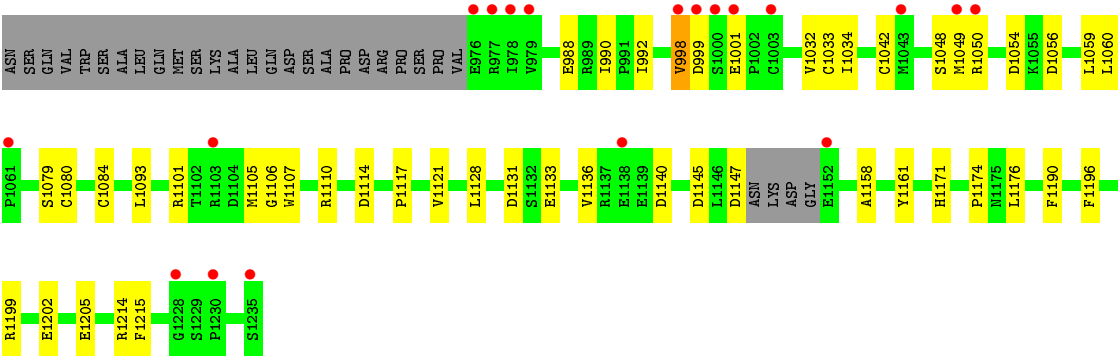


- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 5



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.90 Å 162.90 Å 69.10 Å 90.00° 99.00° 90.00°	Depositor
Resolution (Å)	34.14 – 2.14 34.12 – 2.13	Depositor EDS
% Data completeness (in resolution range)	93.3 (34.14-2.14) 92.2 (34.12-2.13)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.12 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.196 , 0.233 0.185 , 0.219	Depositor DCC
$R_{free}$ test set	3646 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: E72, ZN, SAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.33	0/2072	0.57	0/2807
1	B	0.33	0/2100	0.57	0/2844
1	C	0.33	0/2103	0.57	0/2848
1	D	0.31	0/2069	0.54	0/2807
All	All	0.33	0/8344	0.57	0/11306

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	2022	0	1879	30	0
1	B	2050	0	1916	31	0
1	C	2053	0	1916	24	0
1	D	2019	0	1868	35	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	39	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	39	0	52	4	0
3	C	39	0	52	1	0
3	D	39	0	52	3	0
4	C	26	0	18	0	0
4	D	26	0	20	2	0
5	A	193	0	0	0	0
5	B	201	0	0	0	0
5	C	182	0	0	1	0
5	D	123	0	0	1	0
All	All	9067	0	7825	118	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 7.

All (118) 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:D:1050:ARG:HH22	1:D:1060:LEU:HD12	1.30	0.95
1:B:989:ARG:NH1	1:B:1094:ARG:HE	1.71	0.87
1:D:1101:ARG:NH1	1:D:1106:GLY:HA2	1.93	0.83
1:A:1131:ASP:HB2	1:A:1153:VAL:HG23	1.62	0.82
1:D:1080:CYS:SG	5:D:548:HOH:O	2.40	0.78
1:A:1151:GLY:O	1:A:1152:GLU:HG2	1.85	0.76
1:A:1050:ARG:HH12	1:A:1060:LEU:HD12	1.50	0.74
1:D:1050:ARG:NH2	1:D:1060:LEU:HD12	2.05	0.70
1:B:1083:ASN:O	1:C:1055:LYS:HE3	1.94	0.68
1:A:990:ILE:O	1:A:990:ILE:HD12	1.94	0.67
1:A:1050:ARG:NH1	1:A:1060:LEU:HD12	2.09	0.66
1:D:1117:PRO:HB3	1:D:1199:ARG:HA	1.78	0.65
1:B:1034:ILE:HD12	1:B:1035:ASP:N	2.12	0.65
1:D:1101:ARG:HH12	1:D:1106:GLY:HA2	1.62	0.65
1:D:1131:ASP:OD1	3:D:4:E72:HAZA	1.96	0.64
1:D:1048:SER:O	1:D:1049:MET:HB2	1.98	0.63
1:B:1048:SER:O	1:B:1049:MET:HB2	2.00	0.60
1:B:1062:GLU:OE1	1:B:1062:GLU:N	2.31	0.60
1:A:1048:SER:O	1:A:1049:MET:HB2	2.02	0.59
1:C:1065:MET:CE	1:C:1177:VAL:HG11	2.33	0.58
1:B:1139:GLU:HG2	1:B:1159:ARG:HD3	1.84	0.58
1:B:1001:GLU:HG3	1:B:1101:ARG:NH2	2.20	0.57
1:A:1221:LYS:NZ	1:A:1221:LYS:HB2	2.19	0.57
1:D:1133:GLU:O	1:D:1136:VAL:HG22	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1128:LEU:HD21	1:C:1190:PHE:CD1	2.41	0.56
1:B:1131:ASP:OD2	3:B:2:E72:HAZA	2.05	0.56
1:C:1121:VAL:HG21	1:C:1176:LEU:HD21	1.88	0.55
1:C:1232:CYS:SG	1:C:1235:SER:HB3	2.47	0.54
1:D:1101:ARG:HH11	1:D:1106:GLY:HA2	1.73	0.54
1:D:1110:ARG:HB2	1:D:1205:GLU:O	2.07	0.54
1:A:1152:GLU:HG3	1:A:1152:GLU:O	2.08	0.54
1:D:990:ILE:HD11	1:D:1093:LEU:HD13	1.90	0.54
1:B:1140:ASP:O	3:B:2:E72:HAMA	2.07	0.54
1:D:988:GLU:HB3	1:D:1093:LEU:HD12	1.90	0.53
1:B:1232:CYS:SG	1:B:1235:SER:HB3	2.49	0.53
1:B:1042:CYS:O	1:B:1046:GLN:HG3	2.09	0.53
1:C:1048:SER:O	1:C:1049:MET:HB2	2.08	0.53
1:C:989:ARG:HD3	1:C:1093:LEU:O	2.08	0.52
1:B:1217:ASP:O	1:B:1221:LYS:HE2	2.08	0.52
1:D:990:ILE:O	1:D:990:ILE:HD12	2.10	0.52
1:A:979:VAL:HG23	1:A:1003:CYS:HB2	1.91	0.52
1:D:1215:PHE:HB2	3:D:4:E72:HBC	1.92	0.52
1:B:1103:ARG:C	1:B:1105:MET:H	2.13	0.51
1:C:1065:MET:HE2	1:C:1177:VAL:HG11	1.91	0.51
1:D:992:ILE:HD11	1:D:1093:LEU:HD11	1.92	0.51
1:A:1140:ASP:OD2	3:A:1236:E72:HAC	2.11	0.51
1:B:1104:ASP:OD2	1:B:1226:ARG:NE	2.41	0.51
1:C:1131:ASP:HB2	1:C:1153:VAL:HG23	1.92	0.51
1:C:980:SER:HB3	1:C:994:CYS:HB3	1.93	0.51
1:B:989:ARG:HH12	1:B:1094:ARG:HH21	1.57	0.50
1:A:1048:SER:O	1:A:1049:MET:CB	2.60	0.49
1:C:1033:CYS:HB3	1:C:1035:ASP:OD1	2.12	0.49
1:D:1121:VAL:HG21	1:D:1176:LEU:HD21	1.94	0.49
1:D:999:ASP:OD1	1:D:1001:GLU:HB2	2.12	0.49
1:A:1065:MET:CE	1:A:1198:THR:HA	2.43	0.49
1:A:1221:LYS:HB2	1:A:1221:LYS:HZ2	1.77	0.49
1:A:1103:ARG:C	1:A:1105:MET:H	2.16	0.49
1:C:1065:MET:HE2	1:C:1177:VAL:CG1	2.42	0.49
1:C:990:ILE:HG23	1:C:991:PRO:HD2	1.93	0.49
1:B:1221:LYS:C	1:B:1222:LEU:HD12	2.33	0.49
1:A:1152:GLU:CG	1:A:1152:GLU:O	2.60	0.48
1:B:1131:ASP:OD2	3:B:2:E72:HAVA	2.14	0.48
1:D:1033:CYS:SG	1:D:1042:CYS:HA	2.53	0.48
1:D:1128:LEU:HD21	1:D:1190:PHE:CD1	2.48	0.48
1:B:1170:HIS:CE1	1:B:1216:TRP:HE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1171:HIS:O	1:D:1174:PRO:HD3	2.14	0.47
1:D:1048:SER:C	1:D:1050:ARG:H	2.18	0.47
1:B:1032:VAL:HA	1:B:1079:SER:OG	2.15	0.47
1:B:1225:CYS:HB2	1:B:1234:HIS:HB2	1.97	0.46
1:D:1054:ASP:OD1	1:D:1056:ASP:N	2.49	0.46
1:A:990:ILE:C	1:A:990:ILE:HD12	2.34	0.46
1:C:1063:PHE:CD2	1:C:1065:MET:HE1	2.50	0.46
1:A:982:ASP:HB3	1:B:1081:TRP:CH2	2.52	0.45
1:B:1110:ARG:HD3	1:B:1204:GLY:HA2	1.99	0.45
1:A:1140:ASP:O	3:A:1236:E72:HAMA	2.17	0.44
1:A:981:ARG:HD2	1:C:1117:PRO:HG2	2.00	0.43
1:B:1114:ASP:OD1	1:B:1202:GLU:HA	2.18	0.43
1:A:1064:ASN:ND2	1:A:1067:GLU:HB3	2.32	0.43
1:D:1117:PRO:HB3	1:D:1199:ARG:CA	2.46	0.43
1:B:1034:ILE:C	1:B:1034:ILE:HD12	2.39	0.43
1:D:1158:ALA:HA	1:D:1161:TYR:O	2.19	0.43
1:C:1048:SER:O	1:C:1049:MET:CB	2.66	0.43
1:D:1114:ASP:OD1	1:D:1202:GLU:HA	2.18	0.43
1:C:1065:MET:HG3	1:C:1177:VAL:HG11	2.01	0.43
1:A:1001:GLU:HA	1:A:1002:PRO:HD3	1.91	0.43
1:B:1170:HIS:HB2	1:B:1211:TYR:CG	2.54	0.42
1:D:1001:GLU:HG3	1:D:1101:ARG:HH21	1.83	0.42
1:D:1140:ASP:O	3:D:4:E72:HAMA	2.19	0.42
1:A:1064:ASN:HD21	1:A:1067:GLU:HB3	1.84	0.42
1:A:1221:LYS:CB	1:A:1221:LYS:NZ	2.83	0.42
1:A:1128:LEU:HD21	1:A:1190:PHE:CD1	2.55	0.42
1:C:999:ASP:HB2	1:C:1000:SER:H	1.71	0.42
1:C:1001:GLU:OE1	1:C:1001:GLU:HA	2.20	0.42
1:D:1034:ILE:HD12	1:D:1034:ILE:C	2.40	0.42
1:C:1183:MET:HE3	1:C:1192:ARG:HD3	2.02	0.42
1:B:1115:ILE:HB	1:B:1201:ILE:HB	2.02	0.42
1:D:1049:MET:O	1:D:1050:ARG:HB2	2.20	0.41
1:C:1093:LEU:HD12	5:C:33:HOH:O	2.20	0.41
1:D:998:VAL:HG12	1:D:999:ASP:N	2.35	0.41
4:D:104:SAH:O4'	4:D:104:SAH:HG2	2.21	0.41
1:D:1145:ASP:OD2	1:D:1214:ARG:HD2	2.20	0.41
1:B:1117:PRO:HG3	1:B:1200:LEU:N	2.34	0.41
1:D:1032:VAL:HA	1:D:1079:SER:OG	2.20	0.41
1:A:980:SER:HB3	1:A:994:CYS:HB3	2.02	0.41
1:A:979:VAL:CG2	1:A:1003:CYS:HB2	2.49	0.41
1:A:1015:VAL:HG12	1:A:1128:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:VAL:HG21	1:A:1176:LEU:HD21	2.03	0.41
1:C:1136:VAL:HA	3:C:1236:E72:HBJ	2.03	0.41
1:C:1158:ALA:HA	1:C:1161:TYR:O	2.20	0.41
1:C:1117:PRO:HG3	1:C:1200:LEU:N	2.36	0.41
1:B:1048:SER:O	1:B:1049:MET:CB	2.65	0.41
1:D:1107:TRP:O	4:D:104:SAH:N	2.54	0.41
1:D:1059:LEU:HD11	1:D:1196:PHE:CG	2.55	0.41
1:B:1001:GLU:HA	1:B:1002:PRO:HD3	1.80	0.40
1:B:1136:VAL:HA	3:B:2:E72:HBJ	2.03	0.40
1:A:1065:MET:HE3	1:A:1198:THR:HA	2.03	0.40
1:A:1215:PHE:HB2	3:A:1236:E72:HBC	2.04	0.40
1:B:1098:GLN:OE1	1:B:1110:ARG:NH1	2.52	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	251/285 (88%)	235 (94%)	13 (5%)	3 (1%)	13	6
1	B	254/285 (89%)	239 (94%)	14 (6%)	1 (0%)	34	29
1	C	254/285 (89%)	237 (93%)	16 (6%)	1 (0%)	34	29
1	D	252/285 (88%)	231 (92%)	19 (8%)	2 (1%)	19	11
All	All	1011/1140 (89%)	942 (93%)	62 (6%)	7 (1%)	22	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1105	MET
1	A	1049	MET
1	C	1049	MET

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Mol	Chain	Res	Type
1	A	1104	ASP
1	A	1152	GLU
1	B	1049	MET
1	D	998	VAL

### 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	221/257 (86%)	220 (100%)	1 (0%)	88	91
1	B	225/257 (88%)	223 (99%)	2 (1%)	78	81
1	C	225/257 (88%)	223 (99%)	2 (1%)	78	81
1	D	220/257 (86%)	218 (99%)	2 (1%)	78	81
All	All	891/1028 (87%)	884 (99%)	7 (1%)	81	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1084	CYS
1	B	1065	MET
1	B	1104	ASP
1	C	1055	LYS
1	C	1065	MET
1	D	1084	CYS
1	D	1147	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1046	GLN
1	A	1064	ASN
1	A	1086	ASN

### 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 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	E72	C	1236	-	40,41,41	1.19	4 (10%)	52,52,52	1.70	10 (19%)
3	E72	A	1236	-	40,41,41	1.23	4 (10%)	52,52,52	1.65	10 (19%)
3	E72	B	2	-	40,41,41	1.24	4 (10%)	52,52,52	1.61	11 (21%)
4	SAH	C	103	-	21,28,28	4.01	18 (85%)	20,40,40	2.67	11 (55%)
3	E72	D	4	-	40,41,41	1.26	4 (10%)	52,52,52	1.69	13 (25%)
4	SAH	D	104	-	21,28,28	0.91	1 (4%)	20,40,40	1.33	1 (5%)

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	E72	C	1236	-	-	8/26/36/36	0/3/3/3
3	E72	A	1236	-	-	9/26/36/36	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	E72	B	2	-	-	13/26/36/36	0/3/3/3
4	SAH	C	103	-	-	3/7/31/31	0/3/3/3
3	E72	D	4	-	-	11/26/36/36	0/3/3/3
4	SAH	D	104	-	-	3/7/31/31	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	103	SAH	O3'-C3'	-7.06	1.26	1.43
4	C	103	SAH	O4'-C1'	-6.62	1.31	1.41
4	C	103	SAH	C8-N7	-6.35	1.23	1.34
4	C	103	SAH	C4-N3	-5.32	1.28	1.35
4	C	103	SAH	C3'-C4'	-5.13	1.39	1.53
4	C	103	SAH	C2'-C3'	-5.09	1.39	1.53
4	C	103	SAH	CG-SD	-4.75	1.63	1.81
3	B	2	E72	CAF-CAA	3.97	1.43	1.36
4	C	103	SAH	C2-N1	-3.84	1.26	1.33
3	C	1236	E72	CAF-CAA	3.80	1.43	1.36
3	A	1236	E72	CAF-CAA	3.75	1.43	1.36
3	D	4	E72	CAC-CAB	3.72	1.43	1.36
4	C	103	SAH	C2'-C1'	-3.66	1.48	1.53
4	C	103	SAH	O4'-C4'	-3.58	1.37	1.45
3	D	4	E72	CAF-CAA	3.54	1.42	1.36
3	B	2	E72	CAC-CAB	3.53	1.42	1.36
3	A	1236	E72	CAC-CAB	3.43	1.42	1.36
3	B	2	E72	C6-N1	3.27	1.37	1.32
3	A	1236	E72	C6-N1	3.26	1.37	1.32
3	D	4	E72	C6-N1	3.23	1.37	1.32
4	C	103	SAH	C5-N7	-3.21	1.28	1.39
3	C	1236	E72	C6-C5	-3.11	1.40	1.44
3	C	1236	E72	CAC-CAB	3.11	1.42	1.36
3	A	1236	E72	C6-C5	-3.03	1.41	1.44
4	C	103	SAH	C5'-SD	-3.00	1.68	1.80
4	C	103	SAH	C5-C4	-2.90	1.33	1.40
3	B	2	E72	C6-C5	-2.82	1.41	1.44
4	C	103	SAH	C2-N3	-2.82	1.27	1.32
3	C	1236	E72	C6-N1	2.77	1.36	1.32
3	D	4	E72	C6-C5	-2.77	1.41	1.44
4	C	103	SAH	C5'-C4'	2.43	1.62	1.52
4	D	104	SAH	O4'-C1'	2.27	1.44	1.41
4	C	103	SAH	C6-N6	-2.25	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	103	SAH	O2'-C2'	-2.18	1.37	1.43
4	C	103	SAH	C6-N1	-2.01	1.28	1.37

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	103	SAH	C5-C6-N6	4.89	127.78	120.35
4	D	104	SAH	N3-C2-N1	-4.60	121.48	128.68
4	C	103	SAH	C4-C5-N7	-4.38	104.84	109.40
4	C	103	SAH	O3'-C3'-C2'	-4.25	98.06	111.82
4	C	103	SAH	N3-C2-N1	-4.16	122.18	128.68
3	C	1236	E72	OAL-CAB-CAC	-3.98	120.09	125.24
3	B	2	E72	N3-C2-N1	-3.96	119.96	126.23
3	D	4	E72	N3-C2-N1	-3.92	120.03	126.23
4	C	103	SAH	CB-CG-SD	3.90	122.05	113.31
3	C	1236	E72	CAC-C5-C6	-3.88	121.38	124.88
3	A	1236	E72	N3-C2-N1	-3.85	120.13	126.23
3	C	1236	E72	N3-C2-N1	-3.83	120.18	126.23
3	A	1236	E72	CAC-C5-C6	-3.72	121.52	124.88
3	C	1236	E72	C6-C5-C4	3.70	118.21	115.88
3	D	4	E72	CAC-C5-C6	-3.64	121.59	124.88
3	B	2	E72	CAC-C5-C6	-3.62	121.62	124.88
3	D	4	E72	C6-C5-C4	3.60	118.14	115.88
3	A	1236	E72	CAM-OAL-CAB	-3.56	112.16	117.53
3	A	1236	E72	OAL-CAB-CAC	-3.54	120.66	125.24
4	C	103	SAH	N6-C6-N1	-3.50	111.30	118.57
3	D	4	E72	OAL-CAB-CAC	-3.50	120.71	125.24
3	D	4	E72	C2-N3-C4	3.49	121.29	115.60
3	A	1236	E72	C6-C5-C4	3.49	118.08	115.88
3	B	2	E72	C2-N3-C4	3.49	121.28	115.60
3	B	2	E72	C6-C5-C4	3.46	118.06	115.88
3	A	1236	E72	C2-N3-C4	3.38	121.10	115.60
3	D	4	E72	OAK-CAA-CAF	-3.35	119.52	125.19
3	C	1236	E72	C2-N3-C4	3.26	120.92	115.60
3	C	1236	E72	CAM-OAL-CAB	-3.24	112.64	117.53
3	C	1236	E72	OAL-CAB-CAA	3.23	119.90	115.41
3	B	2	E72	CAM-OAL-CAB	-3.22	112.66	117.53
3	D	4	E72	OAL-CAB-CAA	3.16	119.82	115.41
3	C	1236	E72	C5-C4-N3	-3.08	119.55	122.81
3	B	2	E72	OAL-CAB-CAC	-3.01	121.34	125.24
3	C	1236	E72	OAK-CAA-CAF	-3.00	120.11	125.19
3	B	2	E72	C5-C4-N3	-2.99	119.64	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	E72	CAM-OAL-CAB	-2.96	113.06	117.53
3	A	1236	E72	OAL-CAB-CAA	2.86	119.39	115.41
4	C	103	SAH	O3'-C3'-C4'	-2.85	102.82	111.05
3	D	4	E72	C5-C4-N3	-2.82	119.82	122.81
3	A	1236	E72	OAK-CAA-CAF	-2.81	120.43	125.19
3	A	1236	E72	C5-C4-N3	-2.79	119.85	122.81
4	C	103	SAH	C5'-C4'-C3'	-2.71	108.28	115.06
3	B	2	E72	OAL-CAB-CAA	2.48	118.87	115.41
3	D	4	E72	CBB-OAK-CAA	-2.43	111.73	117.69
4	C	103	SAH	C4'-C5'-SD	2.37	122.29	113.78
4	C	103	SAH	O4'-C4'-C5'	2.33	114.84	108.83
3	A	1236	E72	C2-N1-C6	2.32	121.69	116.39
4	C	103	SAH	O2'-C2'-C3'	-2.31	104.36	111.82
3	D	4	E72	NAU-C2-N1	2.29	121.15	117.19
3	C	1236	E72	C2-N1-C6	2.26	121.57	116.39
3	B	2	E72	NAU-C2-N1	2.25	121.09	117.19
3	D	4	E72	OAK-CAA-CAB	2.21	120.30	115.73
3	D	4	E72	C2-N1-C6	2.21	121.45	116.39
3	B	2	E72	C2-N1-C6	2.19	121.39	116.39
3	B	2	E72	OAK-CAA-CAF	-2.15	121.55	125.19

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1236	E72	CAA-CAB-OAL-CAM
3	B	2	E72	CAW-CAX-NAY-CAZ
3	A	1236	E72	CAC-CAB-OAL-CAM
3	B	2	E72	CAA-CAB-OAL-CAM
3	C	1236	E72	CAC-CAB-OAL-CAM
3	C	1236	E72	CAA-CAB-OAL-CAM
3	B	2	E72	CAC-CAB-OAL-CAM
3	D	4	E72	CAC-CAB-OAL-CAM
3	D	4	E72	CAA-CAB-OAL-CAM
3	B	2	E72	CAW-CAX-NAY-CBA
3	C	1236	E72	NAR-CBH-CBI-CBJ
3	B	2	E72	CBC-CBD-CBE-CBF
3	D	4	E72	CAV-CAW-CAX-NAY
3	B	2	E72	CBB-CBC-CBD-CBE
3	D	4	E72	CAW-CAX-NAY-CAZ
3	D	4	E72	CAB-CAA-OAK-CBB
3	B	2	E72	NAR-CBH-CBI-CBJ

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Mol	Chain	Res	Type	Atoms
3	D	4	E72	CBI-CBJ-CBK-CBL
3	B	2	E72	CAV-CAW-CAX-NAY
3	A	1236	E72	CAB-CAA-OAK-CBB
3	C	1236	E72	CAB-CAA-OAK-CBB
3	D	4	E72	CAF-CAA-OAK-CBB
3	B	2	E72	CAB-CAA-OAK-CBB
3	C	1236	E72	CAV-CAW-CAX-NAY
3	B	2	E72	CBI-CBH-NAR-CAQ
4	C	103	SAH	CA-CB-CG-SD
4	D	104	SAH	CA-CB-CG-SD
3	A	1236	E72	CAF-CAA-OAK-CBB
3	C	1236	E72	CAF-CAA-OAK-CBB
3	A	1236	E72	CBI-CBH-NAR-CAQ
3	B	2	E72	CAF-CAA-OAK-CBB
3	A	1236	E72	OAK-CBB-CBC-CBD
3	C	1236	E72	OAK-CBB-CBC-CBD
4	C	103	SAH	CB-CG-SD-C5'
3	B	2	E72	CBI-CBH-NAR-CAS
3	A	1236	E72	CAV-CAW-CAX-NAY
3	C	1236	E72	CBI-CBH-NAR-CAQ
3	A	1236	E72	CBI-CBH-NAR-CAS
3	D	4	E72	CBB-CBC-CBD-CBE
3	D	4	E72	CBJ-CBK-CBL-NBM
4	C	103	SAH	C-CA-CB-CG
4	D	104	SAH	C-CA-CB-CG
4	D	104	SAH	CB-CG-SD-C5'
3	A	1236	E72	NAU-CAV-CAW-CAX
3	B	2	E72	CBC-CBB-OAK-CAA
3	D	4	E72	CAW-CAX-NAY-CBA
3	D	4	E72	CBI-CBH-NAR-CAQ

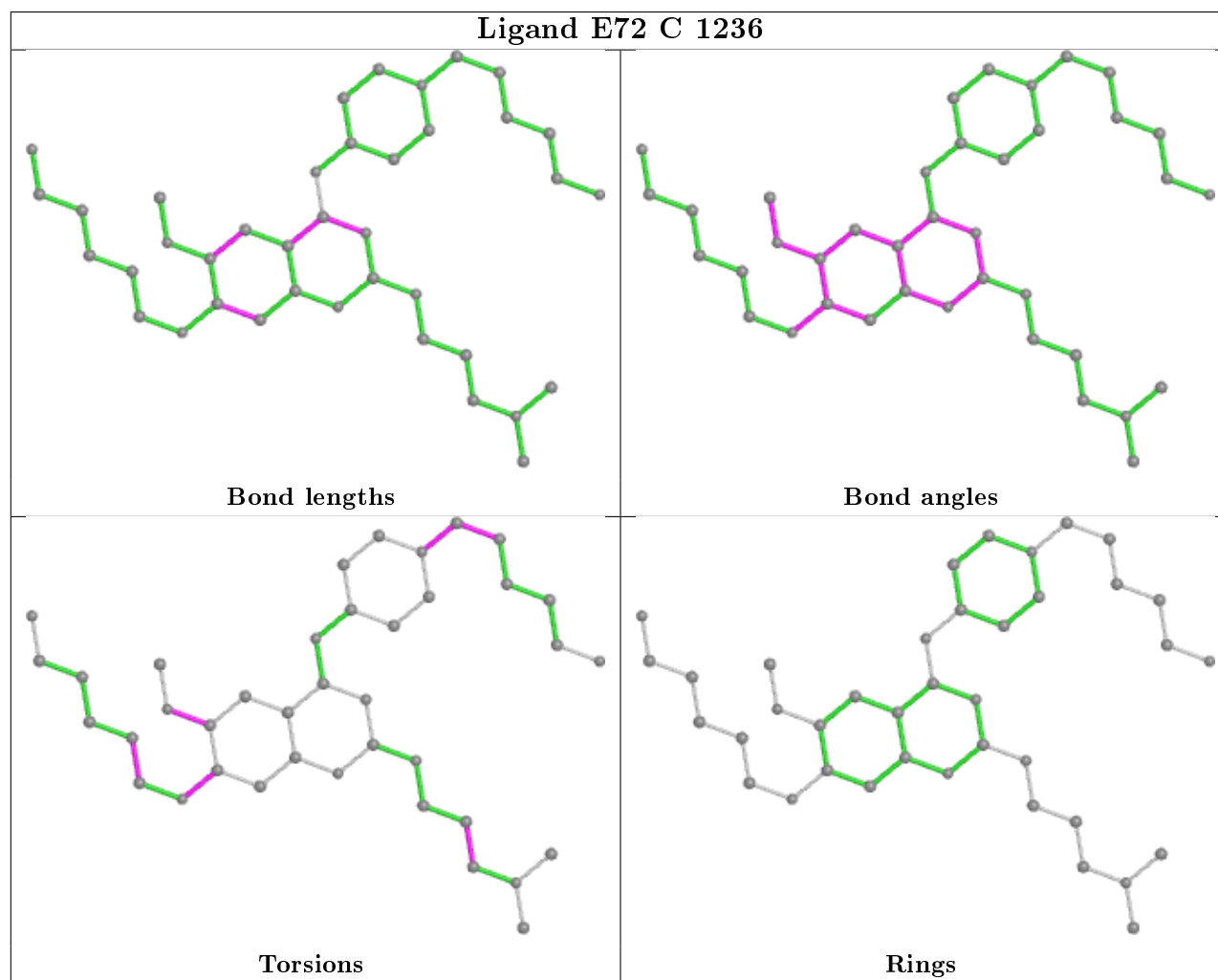
There are no ring outliers.

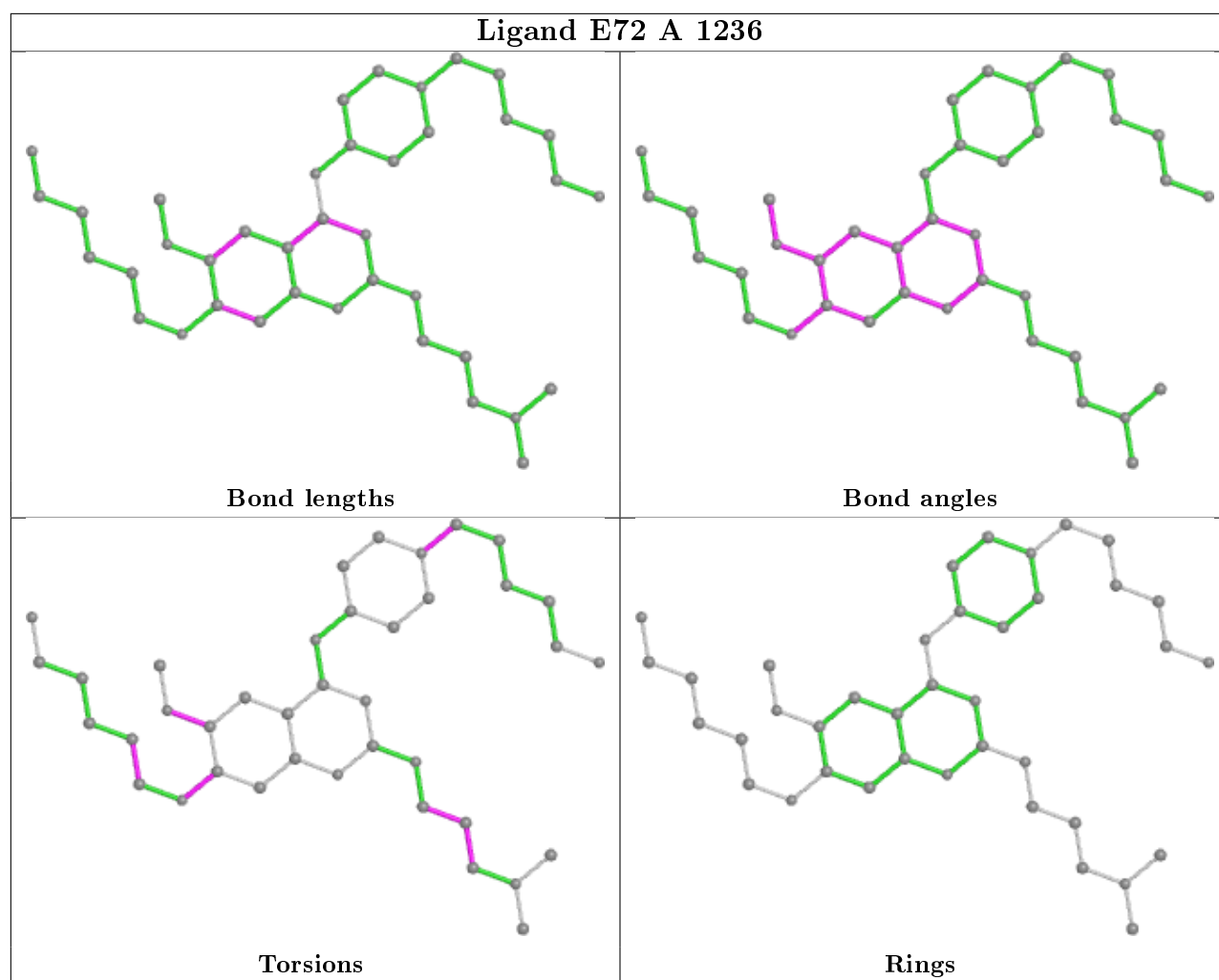
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1236	E72	1	0
3	A	1236	E72	3	0
3	B	2	E72	4	0
3	D	4	E72	3	0
4	D	104	SAH	2	0

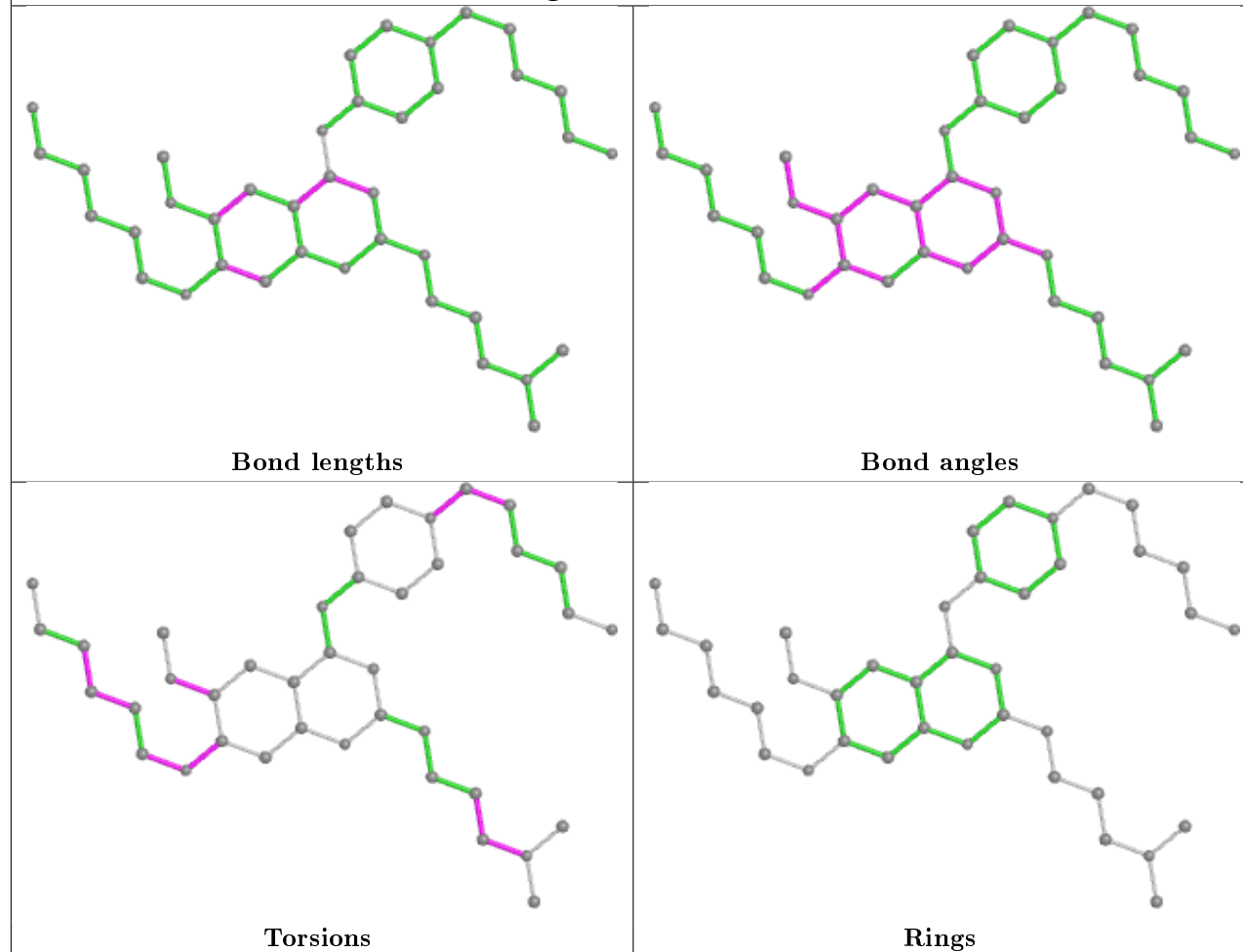
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

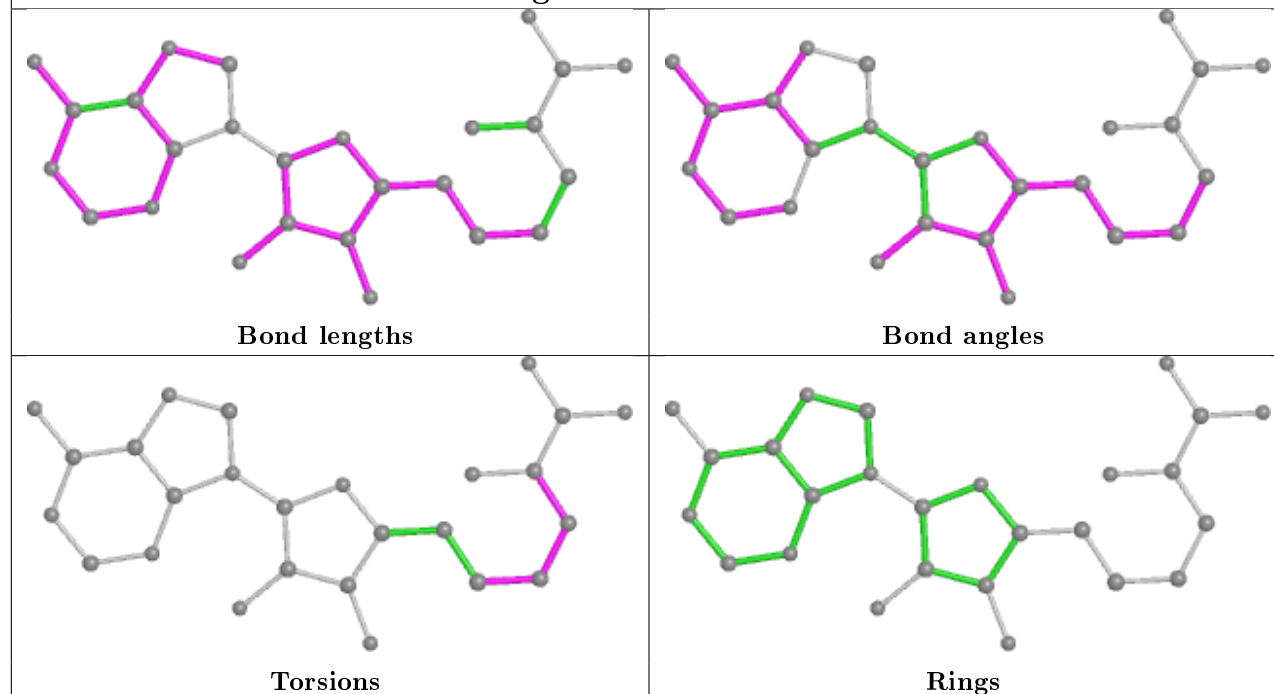


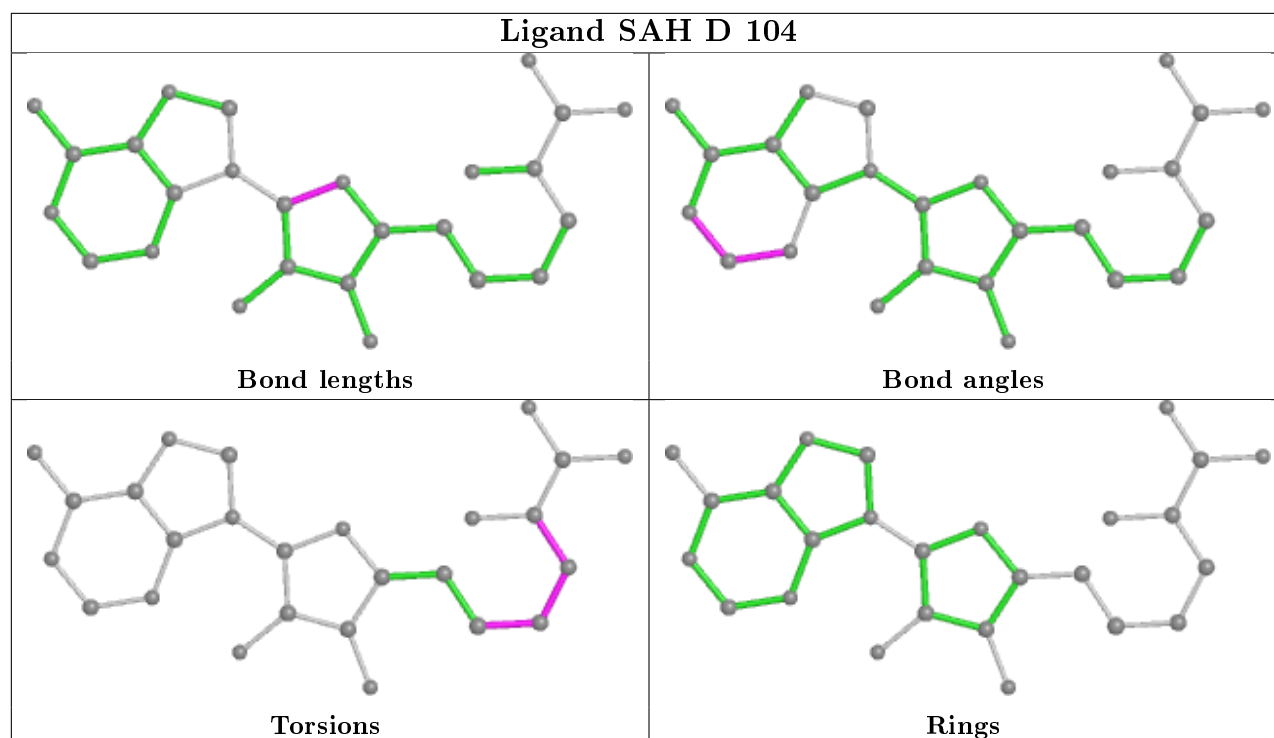
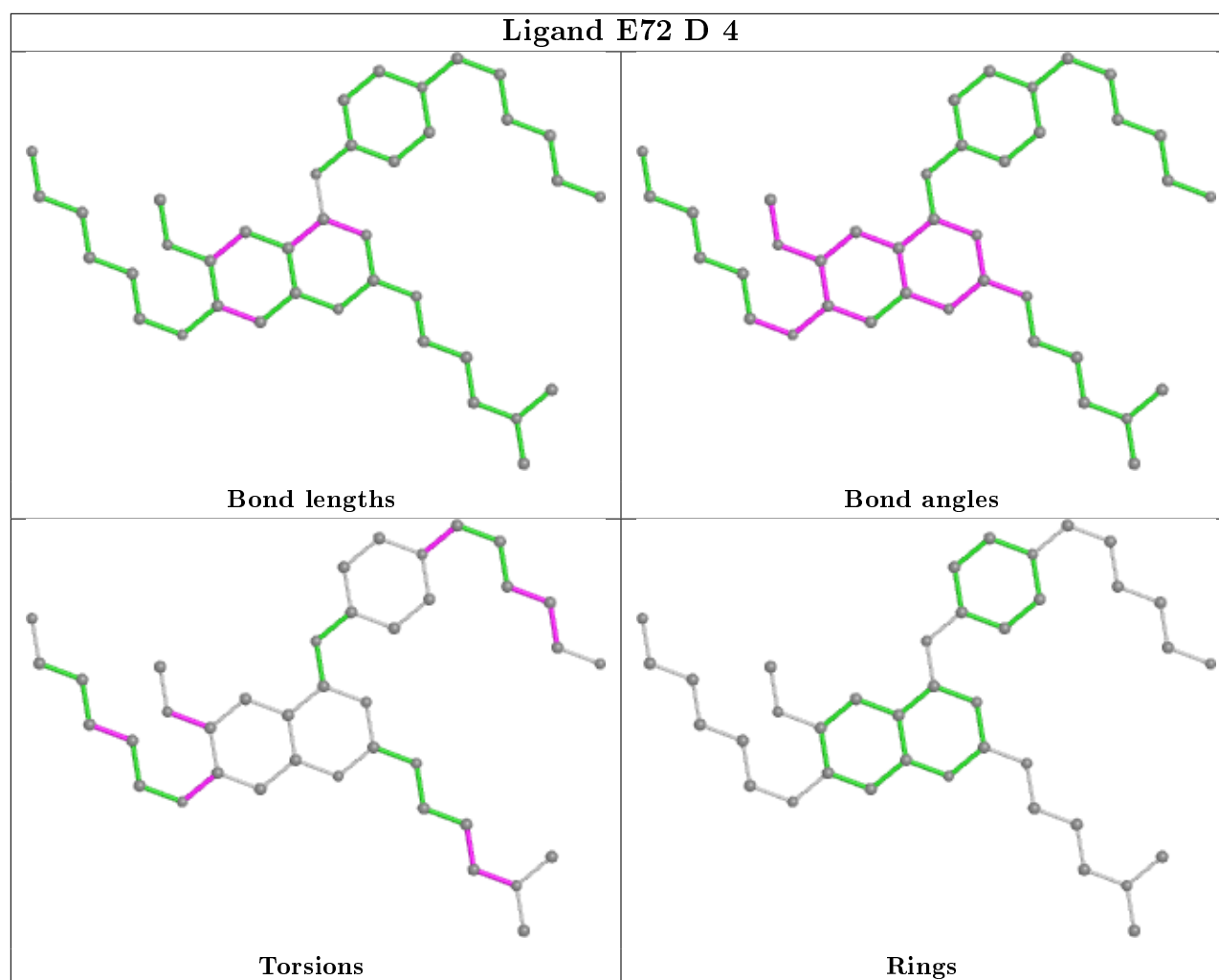


## Ligand E72 B 2



## Ligand SAH C 103





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	255/285 (89%)	0.16	9 (3%) 44 51	17, 32, 54, 59	0
1	B	258/285 (90%)	0.15	10 (3%) 39 47	18, 31, 53, 69	0
1	C	258/285 (90%)	0.09	9 (3%) 44 51	21, 32, 53, 58	0
1	D	256/285 (89%)	0.51	19 (7%) 14 18	26, 41, 61, 71	0
All	All	1027/1140 (90%)	0.23	47 (4%) 32 40	17, 34, 56, 71	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	979	VAL	5.7
1	D	1235	SER	5.2
1	B	1222	LEU	4.9
1	A	979	VAL	4.8
1	D	1228	GLY	4.6
1	A	1235	SER	4.6
1	D	1000	SER	4.2
1	B	1235	SER	3.9
1	D	978	ILE	3.5
1	B	976	GLU	3.5
1	D	976	GLU	3.4
1	B	1105	MET	3.4
1	D	1049	MET	3.4
1	A	997	ALA	3.3
1	B	1148	ASN	3.2
1	D	998	VAL	3.0
1	A	1221	LYS	3.0
1	C	998	VAL	2.9
1	D	1043	MET	2.9
1	C	1151	GLY	2.9
1	A	1202	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	1230	PRO	2.9
1	C	1034	ILE	2.8
1	A	998	VAL	2.7
1	D	977	ARG	2.7
1	C	1228	GLY	2.6
1	C	1230	PRO	2.6
1	C	1232	CYS	2.6
1	D	1050	ARG	2.5
1	C	1223	PHE	2.5
1	B	1217	ASP	2.5
1	A	1151	GLY	2.5
1	D	999	ASP	2.4
1	B	1221	LYS	2.4
1	D	1152	GLU	2.3
1	D	1061	PRO	2.3
1	C	1235	SER	2.3
1	B	1224	SER	2.3
1	D	1103	ARG	2.2
1	B	1223	PHE	2.2
1	D	1138	GLU	2.1
1	B	978	ILE	2.1
1	D	1001	GLU	2.1
1	D	1003	CYS	2.1
1	A	1220	GLY	2.0
1	A	1062	GLU	2.0
1	C	1124	TYR	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](#)

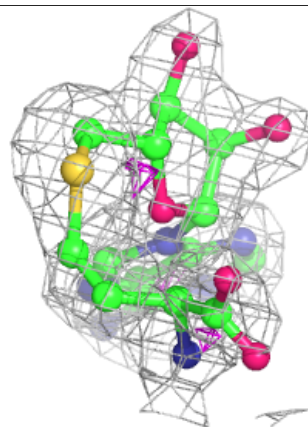
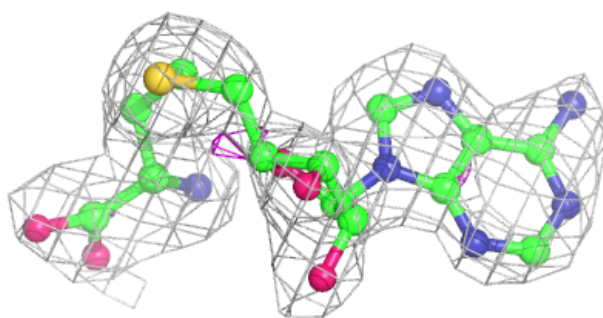
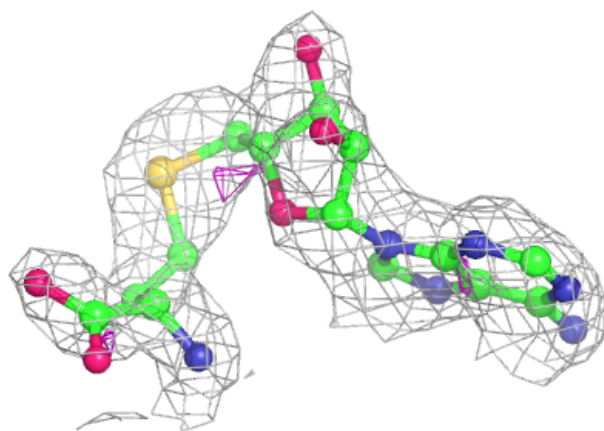
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SAH	D	104	26/26	0.76	0.23	62,68,69,70	0
3	E72	A	1236	39/39	0.80	0.19	38,43,51,52	0
3	E72	D	4	39/39	0.83	0.19	44,48,59,61	0
4	SAH	C	103	26/26	0.85	0.20	50,56,58,59	0
3	E72	C	1236	39/39	0.90	0.14	30,34,45,45	0
3	E72	B	2	39/39	0.93	0.14	31,36,45,47	0
2	ZN	D	7	1/1	0.95	0.06	39,39,39,39	0
2	ZN	D	6	1/1	0.97	0.11	34,34,34,34	0
2	ZN	D	8	1/1	0.97	0.04	49,49,49,49	0
2	ZN	C	4	1/1	0.98	0.04	39,39,39,39	0
2	ZN	C	2	1/1	0.98	0.09	28,28,28,28	0
2	ZN	B	8	1/1	0.98	0.06	41,41,41,41	0
2	ZN	A	4	1/1	0.98	0.07	41,41,41,41	0
2	ZN	A	1	1/1	0.99	0.10	22,22,22,22	0
2	ZN	D	5	1/1	0.99	0.08	35,35,35,35	0
2	ZN	B	7	1/1	0.99	0.09	28,28,28,28	0
2	ZN	B	5	1/1	0.99	0.09	28,28,28,28	0
2	ZN	A	2	1/1	0.99	0.09	18,18,18,18	0
2	ZN	C	3	1/1	0.99	0.09	28,28,28,28	0
2	ZN	B	6	1/1	1.00	0.11	27,27,27,27	0
2	ZN	C	1	1/1	1.00	0.07	27,27,27,27	0
2	ZN	A	3	1/1	1.00	0.10	20,20,20,20	0

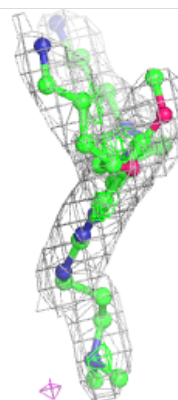
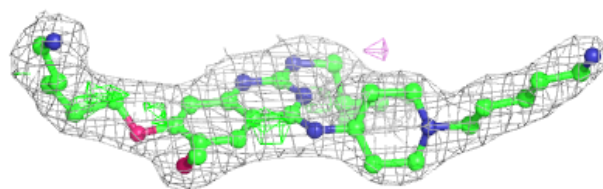
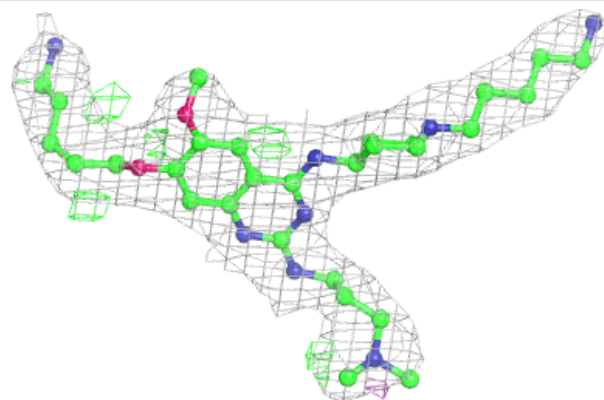
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAH 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)

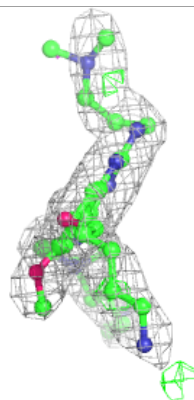
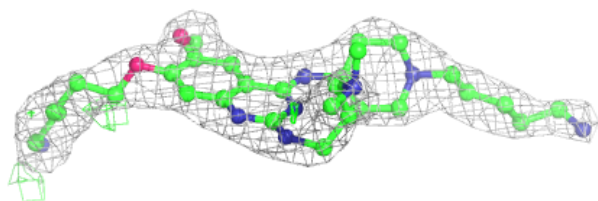
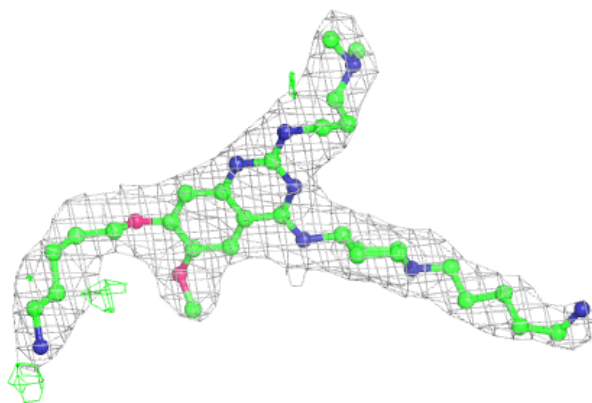
**Electron density around E72 A 1236:**

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

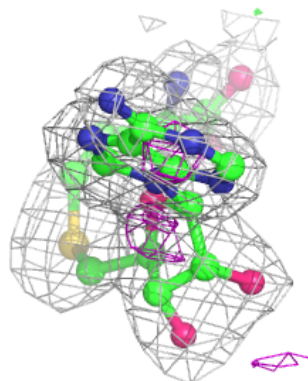
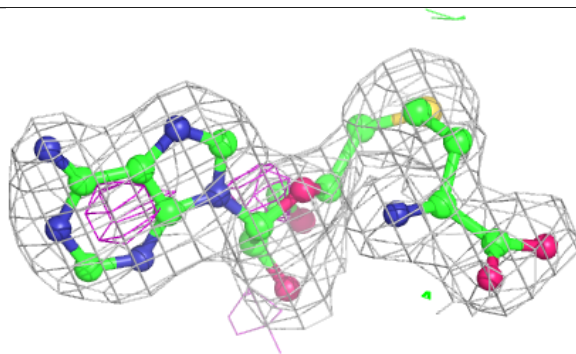
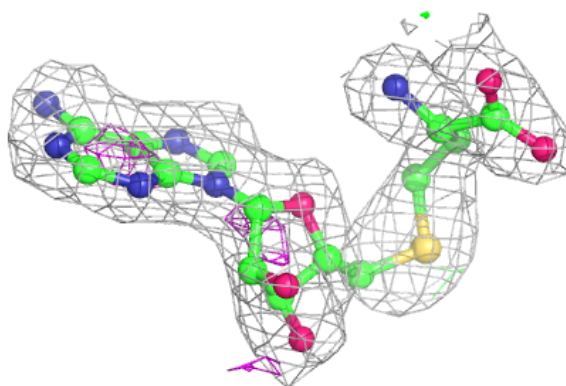


**Electron density around E72 D 4:**

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

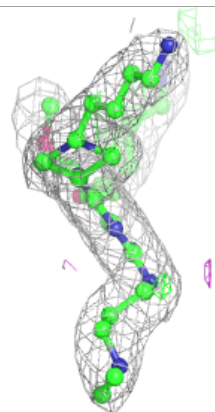
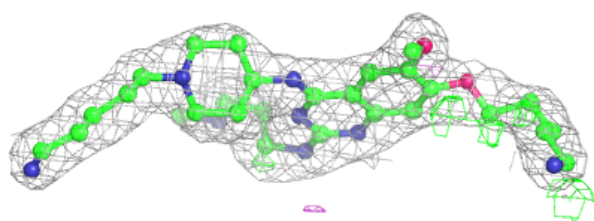
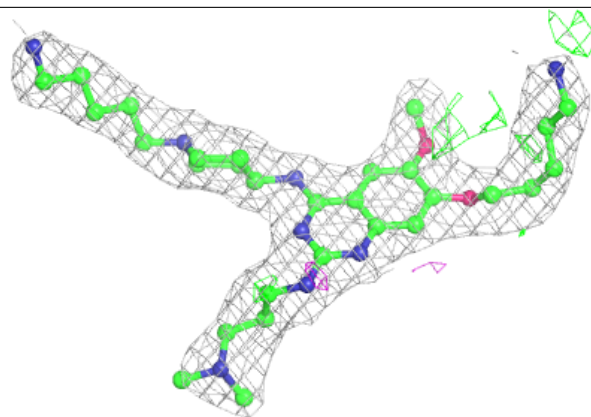
**Electron density around SAH C 103:**

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

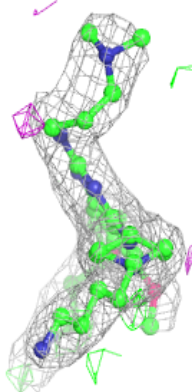
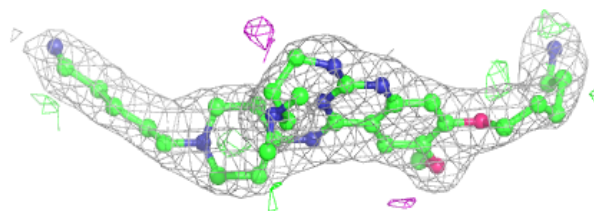
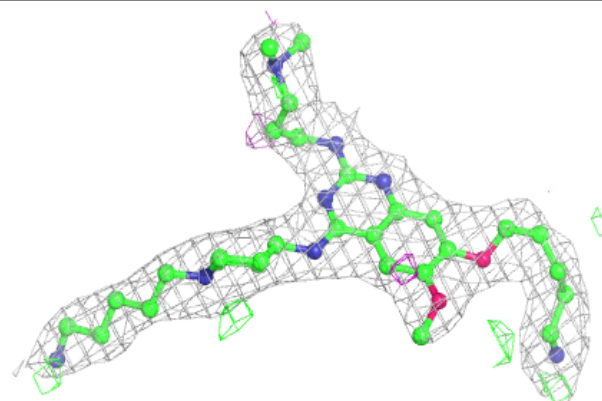


**Electron density around E72 C 1236:**

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

**Electron density around E72 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

There are no such residues in this entry.