



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 04:40 AM EDT

PDB ID : 5LPK  
Title : Crystal structure of the bromodomain of human EP300 bound to the inhibitor XDM1  
Authors : Huegle, M.; Wohlwend, D.  
Deposited on : 2016-08-13  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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)	:	2.37.1

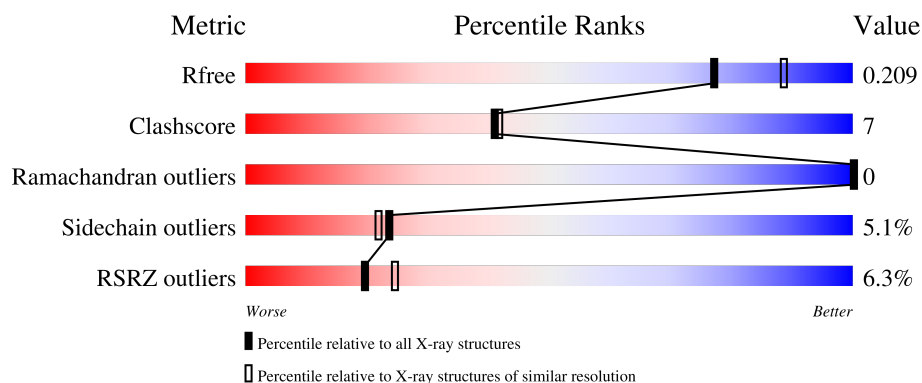
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	122	<div> <div>2%</div> <div>79% 16% • 5%</div> </div>
1	B	122	<div> <div>2%</div> <div>75% 15% • 8%</div> </div>
1	C	122	<div> <div>6%</div> <div>81% 11% • 7%</div> </div>
1	D	122	<div> <div>6%</div> <div>84% 8% • 6%</div> </div>
1	E	122	<div> <div>5%</div> <div>81% 10% • 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	122	
1	G	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	D	1204	-	-	X	-

## 2 Entry composition [i](#)

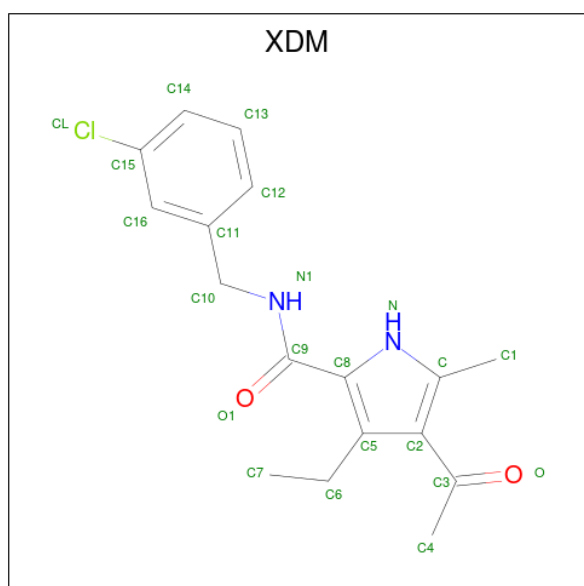
There are 6 unique types of molecules in this entry. The entry contains 7515 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 acetyltransferase p300.

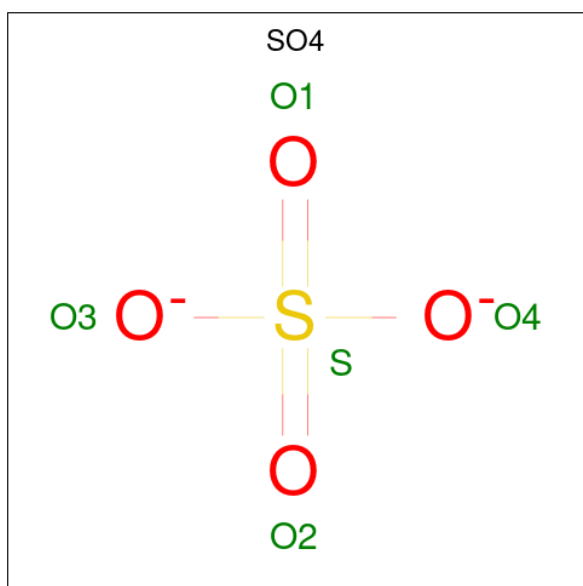
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			976	633	158	180	5			
1	B	112	Total	C	N	O	S	0	1	0
			951	613	156	177	5			
1	C	114	Total	C	N	O	S	0	0	0
			958	621	154	178	5			
1	D	115	Total	C	N	O	S	0	0	0
			967	627	156	179	5			
1	E	113	Total	C	N	O	S	0	0	0
			955	619	154	177	5			
1	F	115	Total	C	N	O	S	0	3	0
			994	641	165	183	5			
1	G	114	Total	C	N	O	S	0	0	0
			963	625	155	178	5			

- Molecule 2 is {N}-[(3-chlorophenyl)methyl]-4-ethanoyl-3-ethyl-5-methyl-1 {H}-pyrrole-2-carboxamide (three-letter code: XDM) (formula: C<sub>17</sub>H<sub>19</sub>ClN<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		
2	B	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		
2	C	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		
2	D	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		
2	E	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		
2	E	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		
2	F	1	Total	C	Cl	N	O	0	0
			22	17	1	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



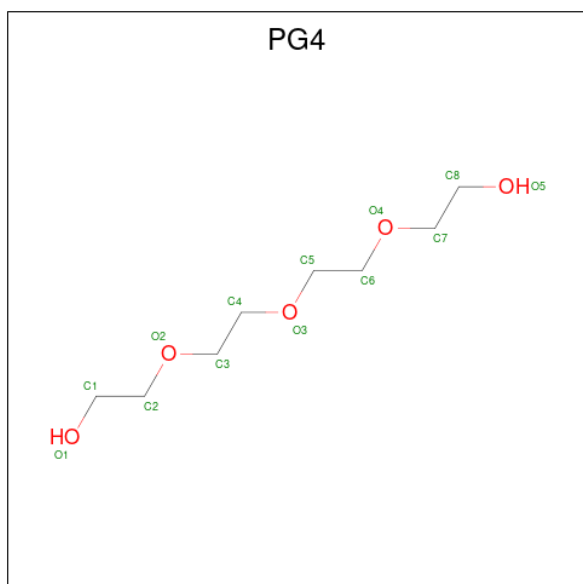
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total	O	0	0
			89	89		
6	B	74	Total	O	0	0
			74	74		

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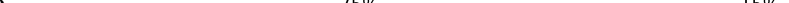
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	82	Total 82	O 82	0	0
6	D	67	Total 67	O 67	0	0
6	E	64	Total 64	O 64	0	0
6	F	63	Total 63	O 63	0	0
6	G	44	Total 44	O 44	0	0

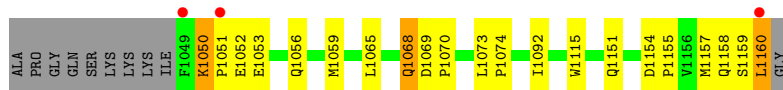


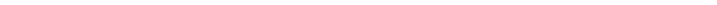


- Molecule 1: Histone acetyltransferase p300

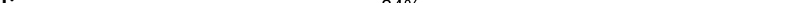


- Chain B:  2% 75% 15% 8%

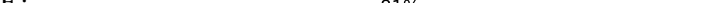


- Chain C:  6% 81% 11% 2%



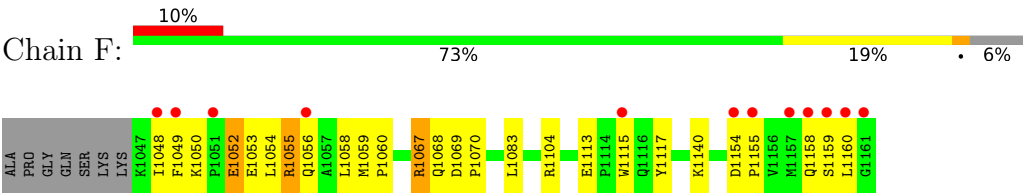
- Chain D:  6% 84% 8% 6%



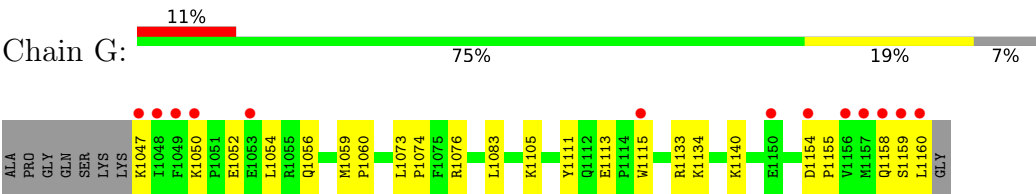
- Chain E:  5% 81% 10% 7%



● Molecule 1: Histone acetyltransferase p300



● Molecule 1: Histone acetyltransferase p300



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.60Å 61.04Å 135.68Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	41.52 – 2.10 41.52 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.52-2.10) 99.9 (41.52-1.78)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.176 , 0.203 0.184 , 0.209	Depositor DCC
$R_{free}$ test set	5114 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.9	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	0.96	EDS
Total number of atoms	7515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: EDO, PG4, XDM, SO4

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	0.56	1/1003 (0.1%)	0.67	1/1360 (0.1%)
1	B	0.48	0/977	0.62	0/1327
1	C	0.48	0/985	0.60	0/1338
1	D	0.46	0/994	0.56	0/1349
1	E	0.47	0/982	0.59	0/1333
1	F	0.46	0/1021	0.65	1/1385 (0.1%)
1	G	0.45	0/990	0.58	0/1344
All	All	0.48	1/6952 (0.0%)	0.61	2/9436 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1154	ASP	CB-CG	5.44	1.63	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1154	ASP	CB-CG-OD1	8.02	125.52	118.30
1	F	1104	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	976	0	967	15	0
1	B	951	0	932	13	0
1	C	958	0	941	13	0
1	D	967	0	954	15	0
1	E	955	0	940	9	1
1	F	994	0	974	22	0
1	G	963	0	951	12	0
2	A	22	0	0	0	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
2	E	44	0	0	1	0
2	F	22	0	0	0	0
3	A	10	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	1	0
3	F	5	0	0	0	0
4	A	20	0	30	4	0
4	B	24	0	36	0	0
4	C	4	0	6	1	0
4	D	12	0	18	8	0
4	E	4	0	6	0	0
4	F	8	0	12	0	0
4	G	4	0	6	0	0
5	B	13	0	18	4	0
6	A	89	0	0	0	0
6	B	74	0	0	0	0
6	C	82	0	0	0	0
6	D	67	0	0	3	0
6	E	64	0	0	1	0
6	F	63	0	0	0	0
6	G	44	0	0	1	0
All	All	7515	0	6791	98	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (98) 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:C:1050:LYS:HB2	1:C:1053:GLU:HG2	1.26	1.08
1:C:1050:LYS:HB2	1:C:1053:GLU:CG	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1050:LYS:CB	1:C:1053:GLU:HG2	1.90	1.00
1:F:1113:GLU:HG3	1:F:1115:TRP:HE1	1.41	0.83
1:F:1067[A]:ARG:HH11	1:F:1067[A]:ARG:CG	1.94	0.80
1:D:1104:ARG:HE	4:D:1204:EDO:C2	1.99	0.74
1:F:1113:GLU:HB3	1:F:1115:TRP:CD1	2.24	0.72
1:F:1067[A]:ARG:HG3	1:F:1067[A]:ARG:NH1	2.03	0.71
4:C:1203:EDO:O2	3:E:1203:SO4:O2	2.08	0.71
1:F:1067[A]:ARG:HH11	1:F:1067[A]:ARG:HG3	1.57	0.68
1:D:1104:ARG:NE	4:D:1204:EDO:H22	2.09	0.68
1:E:1112:GLN:NE2	1:E:1116:GLN:HE22	1.94	0.65
1:A:1055:ARG:HH22	4:A:1204:EDO:C1	2.11	0.64
1:F:1067[A]:ARG:CG	1:F:1067[A]:ARG:NH1	2.57	0.61
1:G:1052:GLU:O	1:G:1056:GLN:HG2	2.01	0.60
1:F:1113:GLU:HG3	1:F:1115:TRP:NE1	2.15	0.59
1:G:1159:SER:O	1:G:1160:LEU:HD23	2.02	0.58
1:F:1113:GLU:HA	1:F:1113:GLU:OE1	2.04	0.57
1:D:1104:ARG:NE	4:D:1204:EDO:C2	2.67	0.57
1:F:1055[A]:ARG:O	1:F:1059:MET:HB2	2.04	0.57
1:E:1112:GLN:HE21	1:E:1116:GLN:HE22	1.51	0.56
1:F:1055[B]:ARG:O	1:F:1059:MET:HB2	2.05	0.56
1:B:1092:ILE:CD1	5:B:1208:PG4:H32	2.36	0.55
1:F:1059:MET:N	1:F:1060:PRO:CD	2.70	0.55
1:D:1104:ARG:HD3	4:D:1204:EDO:H22	1.90	0.54
1:F:1154:ASP:HB3	1:F:1155:PRO:HD3	1.88	0.54
1:B:1160:LEU:C	1:B:1160:LEU:HD23	2.28	0.54
1:D:1052:GLU:HG2	6:D:1355:HOH:O	2.08	0.53
1:D:1104:ARG:CD	4:D:1204:EDO:H22	2.38	0.53
1:E:1159:SER:HA	6:E:1353:HOH:O	2.08	0.53
1:G:1059:MET:N	1:G:1060:PRO:CD	2.72	0.53
1:A:1055:ARG:HH22	4:A:1204:EDO:H11	1.74	0.52
1:D:1066:TYR:CZ	1:D:1076:ARG:HG2	2.43	0.52
1:F:1050:LYS:HB2	1:F:1053:GLU:HG3	1.91	0.52
1:G:1154:ASP:O	1:G:1158:GLN:HG2	2.10	0.52
1:B:1154:ASP:O	1:B:1158:GLN:HG2	2.09	0.51
1:D:1137:ARG:NH1	6:D:1302:HOH:O	2.26	0.51
1:D:1155:PRO:O	1:D:1159:SER:OG	2.28	0.51
1:G:1154:ASP:HB3	1:G:1155:PRO:HD3	1.92	0.50
1:A:1050:LYS:O	1:A:1053:GLU:HG2	2.12	0.50
1:G:1133:ARG:NH2	6:G:1301:HOH:O	2.44	0.49
1:D:1049:PHE:HZ	1:D:1160:LEU:O	1.95	0.49
1:F:1052:GLU:O	1:F:1056:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1049:PHE:CD1	1:C:1049:PHE:N	2.81	0.48
1:A:1108:THR:CG2	4:D:1204:EDO:H12	2.43	0.48
1:A:1055:ARG:HH22	4:A:1204:EDO:H12	1.77	0.48
1:A:1050:LYS:N	1:A:1053:GLU:OE2	2.40	0.47
1:B:1092:ILE:HD13	5:B:1208:PG4:C3	2.44	0.47
1:B:1092:ILE:HD13	5:B:1208:PG4:H32	1.96	0.47
1:G:1113:GLU:HB2	1:G:1115:TRP:NE1	2.29	0.47
1:F:1154:ASP:O	1:F:1158:GLN:HG3	2.16	0.46
1:A:1069:ASP:OD1	4:A:1206:EDO:O1	2.27	0.46
1:F:1049:PHE:CE1	1:F:1113:GLU:OE1	2.69	0.46
1:A:1049:PHE:N	1:A:1049:PHE:CD1	2.84	0.45
1:B:1050:LYS:HG2	1:B:1051:PRO:N	2.30	0.45
1:B:1065:LEU:O	1:B:1068:GLN:HB2	2.17	0.45
1:D:1104:ARG:HA	4:D:1204:EDO:H21	1.98	0.45
1:D:1154:ASP:HB3	1:D:1155:PRO:HD3	1.99	0.45
1:B:1115:TRP:CZ2	1:C:1137:ARG:HA	2.52	0.44
1:B:1073:LEU:N	1:B:1074:PRO:CD	2.81	0.44
1:D:1052:GLU:HA	1:D:1052:GLU:OE1	2.18	0.44
1:C:1050:LYS:HB2	1:C:1053:GLU:HG3	1.91	0.44
1:C:1050:LYS:HB3	1:C:1053:GLU:HG2	1.93	0.44
1:C:1156:VAL:HG12	1:C:1160:LEU:HD12	1.99	0.44
1:B:1154:ASP:HB3	1:B:1155:PRO:CD	2.47	0.43
1:F:1055[A]:ARG:O	1:F:1059:MET:CB	2.65	0.43
1:F:1058:LEU:HD13	1:F:1117:TYR:CG	2.54	0.43
1:C:1134:LYS:HA	1:C:1139:TYR:CG	2.54	0.43
1:A:1050:LYS:HB2	1:A:1053:GLU:HG2	2.00	0.43
1:C:1059:MET:N	1:C:1060:PRO:CD	2.82	0.43
1:E:1094:LYS:HA	1:E:1094:LYS:HD3	1.81	0.43
1:G:1105:LYS:HE2	1:G:1111:TYR:CE1	2.54	0.42
1:F:1055[B]:ARG:O	1:F:1059:MET:CB	2.66	0.42
1:G:1159:SER:C	1:G:1160:LEU:HD23	2.40	0.42
1:A:1059:MET:N	1:A:1060:PRO:CD	2.82	0.42
1:E:1063:GLU:O	1:E:1067:ARG:HD3	2.20	0.42
1:F:1049:PHE:CD1	1:F:1113:GLU:OE1	2.73	0.42
1:F:1055[A]:ARG:O	1:F:1059:MET:N	2.47	0.42
1:E:1077:GLN:OE1	2:E:1202:XDM:C13	2.68	0.42
1:B:1052:GLU:OE2	1:B:1052:GLU:HA	2.20	0.42
1:F:1069:ASP:HA	1:F:1070:PRO:HA	1.76	0.42
1:A:1081:PRO:HG2	1:A:1090:PHE:CE2	2.55	0.41
1:B:1069:ASP:HA	1:B:1070:PRO:HA	1.78	0.41
1:B:1092:ILE:HD11	5:B:1208:PG4:H32	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:LEU:N	1:A:1074:PRO:CD	2.83	0.41
1:A:1104:ARG:CD	4:D:1204:EDO:H11	2.51	0.41
1:C:1134:LYS:HA	1:C:1139:TYR:CD2	2.55	0.41
1:E:1073:LEU:N	1:E:1074:PRO:CD	2.83	0.41
1:A:1094:LYS:HA	1:A:1094:LYS:HD3	1.93	0.41
1:C:1069:ASP:HA	1:C:1070:PRO:HA	1.84	0.41
1:A:1049:PHE:CE1	1:A:1114:PRO:HD3	2.56	0.41
1:C:1082:GLN:HE21	1:D:1051:PRO:HG2	1.84	0.41
1:D:1050:LYS:N	6:D:1304:HOH:O	2.46	0.41
1:E:1059:MET:N	1:E:1060:PRO:CD	2.84	0.41
1:G:1073:LEU:HA	1:G:1076:ARG:HD2	2.03	0.41
1:E:1158:GLN:CA	1:E:1158:GLN:NE2	2.84	0.41
1:G:1054:LEU:HD23	1:G:1054:LEU:HA	1.93	0.40
1:G:1073:LEU:N	1:G:1074:PRO:CD	2.84	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1052:GLU:OE2	1:E:1052:GLU:OE2[2_858]	1.54	0.66

## 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	114/122 (93%)	113 (99%)	1 (1%)	0	100	100
1	B	111/122 (91%)	111 (100%)	0	0	100	100
1	C	112/122 (92%)	112 (100%)	0	0	100	100
1	D	113/122 (93%)	113 (100%)	0	0	100	100
1	E	111/122 (91%)	111 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	116/122 (95%)	116 (100%)	0	0	100	100
1	G	112/122 (92%)	111 (99%)	1 (1%)	0	100	100
All	All	789/854 (92%)	787 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	110/114 (96%)	105 (96%)	5 (4%)	27	27
1	B	107/114 (94%)	98 (92%)	9 (8%)	11	7
1	C	108/114 (95%)	105 (97%)	3 (3%)	43	47
1	D	109/114 (96%)	105 (96%)	4 (4%)	34	35
1	E	108/114 (95%)	105 (97%)	3 (3%)	43	47
1	F	111/114 (97%)	99 (89%)	12 (11%)	6	3
1	G	109/114 (96%)	104 (95%)	5 (5%)	27	26
All	All	762/798 (96%)	721 (95%)	41 (5%)	24	20

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1046	LYS
1	A	1047	LYS
1	A	1048	ILE
1	A	1049	PHE
1	A	1054	LEU
1	B	1050	LYS
1	B	1053	GLU
1	B	1056	GLN
1	B	1059	MET
1	B	1068	GLN

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Mol	Chain	Res	Type
1	B	1151	GLN
1	B	1157	MET
1	B	1159	SER
1	B	1160	LEU
1	C	1049	PHE
1	C	1154	ASP
1	C	1157	MET
1	D	1050	LYS
1	D	1082	GLN
1	D	1154	ASP
1	D	1159	SER
1	E	1049	PHE
1	E	1112	GLN
1	E	1158	GLN
1	F	1048	ILE
1	F	1052	GLU
1	F	1054	LEU
1	F	1055[A]	ARG
1	F	1055[B]	ARG
1	F	1067[A]	ARG
1	F	1067[B]	ARG
1	F	1068	GLN
1	F	1083	LEU
1	F	1140	LYS
1	F	1159	SER
1	F	1160	LEU
1	G	1047	LYS
1	G	1050	LYS
1	G	1083	LEU
1	G	1134	LYS
1	G	1140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1110	GLN
1	B	1082	GLN
1	B	1110	GLN
1	C	1082	GLN
1	C	1110	GLN
1	C	1112	GLN
1	D	1068	GLN

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Mol	Chain	Res	Type
1	E	1112	GLN
1	E	1158	GLN
1	G	1082	GLN

### 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](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	C	1202	-	4,4,4	0.35	0	6,6,6	0.59	0
4	EDO	D	1203	-	3,3,3	0.45	0	2,2,2	0.53	0
4	EDO	A	1208	-	3,3,3	0.42	0	2,2,2	0.65	0
2	XDM	D	1201	-	20,23,23	1.48	2 (10%)	23,32,32	2.44	4 (17%)
2	XDM	C	1201	-	20,23,23	1.17	2 (10%)	23,32,32	1.55	2 (8%)
4	EDO	E	1204	-	3,3,3	0.76	0	2,2,2	0.51	0
4	EDO	B	1205	-	3,3,3	0.42	0	2,2,2	0.28	0
3	SO4	F	1202	-	4,4,4	0.30	0	6,6,6	0.22	0
3	SO4	E	1203	-	4,4,4	0.27	0	6,6,6	0.25	0
4	EDO	D	1202	-	3,3,3	0.58	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	1207	-	3,3,3	0.54	0	2,2,2	0.24	0
4	EDO	B	1203	-	3,3,3	0.59	0	2,2,2	0.13	0
4	EDO	C	1203	-	3,3,3	0.50	0	2,2,2	0.24	0
4	EDO	B	1202	-	3,3,3	0.68	0	2,2,2	0.31	0
4	EDO	A	1205	-	3,3,3	0.39	0	2,2,2	0.37	0
4	EDO	F	1203	-	3,3,3	0.50	0	2,2,2	0.21	0
2	XDM	F	1201	-	20,23,23	1.31	2 (10%)	23,32,32	1.76	3 (13%)
4	EDO	A	1206	-	3,3,3	0.89	0	2,2,2	0.34	0
2	XDM	E	1201	-	20,23,23	1.22	1 (5%)	23,32,32	2.18	4 (17%)
4	EDO	B	1207	-	3,3,3	0.61	0	2,2,2	0.05	0
4	EDO	B	1204	-	3,3,3	0.56	0	2,2,2	0.06	0
2	XDM	A	1201	-	20,23,23	1.19	1 (5%)	23,32,32	2.44	4 (17%)
4	EDO	D	1204	-	3,3,3	0.34	0	2,2,2	0.35	0
5	PG4	B	1208	-	12,12,12	0.42	0	11,11,11	0.49	0
4	EDO	G	1201	-	3,3,3	0.44	0	2,2,2	0.43	0
2	XDM	E	1202	-	20,23,23	1.16	2 (10%)	23,32,32	1.54	3 (13%)
3	SO4	A	1203	-	4,4,4	0.39	0	6,6,6	0.48	0
4	EDO	F	1204	-	3,3,3	0.42	0	2,2,2	0.31	0
4	EDO	A	1204	-	3,3,3	0.46	0	2,2,2	0.33	0
2	XDM	B	1201	-	20,23,23	1.14	1 (5%)	23,32,32	2.47	7 (30%)
4	EDO	B	1206	-	3,3,3	0.58	0	2,2,2	0.32	0
3	SO4	A	1202	-	4,4,4	0.36	0	6,6,6	0.38	0

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
4	EDO	D	1203	-	-	0/1/1/1	-
4	EDO	A	1208	-	-	1/1/1/1	-
2	XDM	D	1201	-	-	0/7/15/15	0/2/2/2
2	XDM	C	1201	-	-	0/7/15/15	0/2/2/2
4	EDO	E	1204	-	-	0/1/1/1	-
4	EDO	B	1205	-	-	1/1/1/1	-
4	EDO	D	1202	-	-	1/1/1/1	-
4	EDO	A	1207	-	-	1/1/1/1	-
4	EDO	B	1203	-	-	0/1/1/1	-
4	EDO	C	1203	-	-	0/1/1/1	-
4	EDO	B	1202	-	-	0/1/1/1	-
4	EDO	A	1205	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	1203	-	-	0/1/1/1	-
2	XDM	F	1201	-	-	0/7/15/15	0/2/2/2
4	EDO	A	1206	-	-	1/1/1/1	-
2	XDM	E	1201	-	-	0/7/15/15	0/2/2/2
4	EDO	B	1207	-	-	1/1/1/1	-
4	EDO	B	1204	-	-	0/1/1/1	-
2	XDM	A	1201	-	-	0/7/15/15	0/2/2/2
4	EDO	D	1204	-	-	1/1/1/1	-
5	PG4	B	1208	-	-	3/10/10/10	-
4	EDO	G	1201	-	-	0/1/1/1	-
2	XDM	E	1202	-	-	0/7/15/15	0/2/2/2
4	EDO	F	1204	-	-	0/1/1/1	-
4	EDO	A	1204	-	-	1/1/1/1	-
2	XDM	B	1201	-	-	0/7/15/15	0/2/2/2
4	EDO	B	1206	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	XDM	C8-C5	5.14	1.49	1.41
2	E	1201	XDM	C8-C5	5.12	1.49	1.41
2	F	1201	XDM	C8-C5	4.90	1.49	1.41
2	A	1201	XDM	C8-C5	4.76	1.49	1.41
2	B	1201	XDM	C8-C5	4.46	1.48	1.41
2	C	1201	XDM	C8-C5	4.35	1.48	1.41
2	E	1202	XDM	C8-C5	4.25	1.48	1.41
2	D	1201	XDM	C15-CL	3.39	1.81	1.74
2	C	1201	XDM	C15-CL	2.20	1.79	1.74
2	F	1201	XDM	C15-CL	2.16	1.79	1.74
2	E	1202	XDM	C15-CL	2.14	1.79	1.74

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	XDM	C8-C9-N1	8.15	123.62	115.67
2	D	1201	XDM	C8-C9-N1	8.11	123.58	115.67
2	E	1201	XDM	C8-C9-N1	7.28	122.77	115.67
2	F	1201	XDM	C8-C5-C2	-6.96	101.85	106.54
2	B	1201	XDM	C8-C5-C2	-6.70	102.02	106.54
2	B	1201	XDM	C8-C9-N1	6.52	122.03	115.67
2	A	1201	XDM	C8-C5-C2	-6.37	102.24	106.54
2	C	1201	XDM	C8-C5-C2	-5.95	102.53	106.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	XDM	C8-C5-C2	-5.82	102.61	106.54
2	E	1202	XDM	C8-C5-C2	-5.33	102.95	106.54
2	E	1201	XDM	C8-C5-C2	-5.28	102.98	106.54
2	B	1201	XDM	C16-C15-CL	-3.87	114.32	119.15
2	D	1201	XDM	O1-C9-C8	-3.79	114.92	120.59
2	A	1201	XDM	O1-C9-C8	-3.70	115.06	120.59
2	E	1201	XDM	O1-C9-C8	-3.25	115.72	120.59
2	F	1201	XDM	C-C2-C5	3.24	109.86	104.34
2	B	1201	XDM	C-C2-C5	3.08	109.59	104.34
2	E	1202	XDM	C-C2-C5	2.80	109.11	104.34
2	A	1201	XDM	C-C2-C5	2.71	108.95	104.34
2	D	1201	XDM	C-C2-C5	2.64	108.83	104.34
2	C	1201	XDM	C-C2-C5	2.59	108.75	104.34
2	E	1202	XDM	C8-C9-N1	2.35	117.96	115.67
2	E	1201	XDM	C-C2-C5	2.27	108.20	104.34
2	B	1201	XDM	C14-C15-CL	2.26	122.88	119.35
2	B	1201	XDM	C-C2-C3	-2.24	120.40	127.40
2	F	1201	XDM	C-C2-C3	-2.22	120.49	127.40
2	B	1201	XDM	C10-N1-C9	-2.15	116.72	121.81

There are no chirality outliers.

All (12) torsion outliers are listed below:

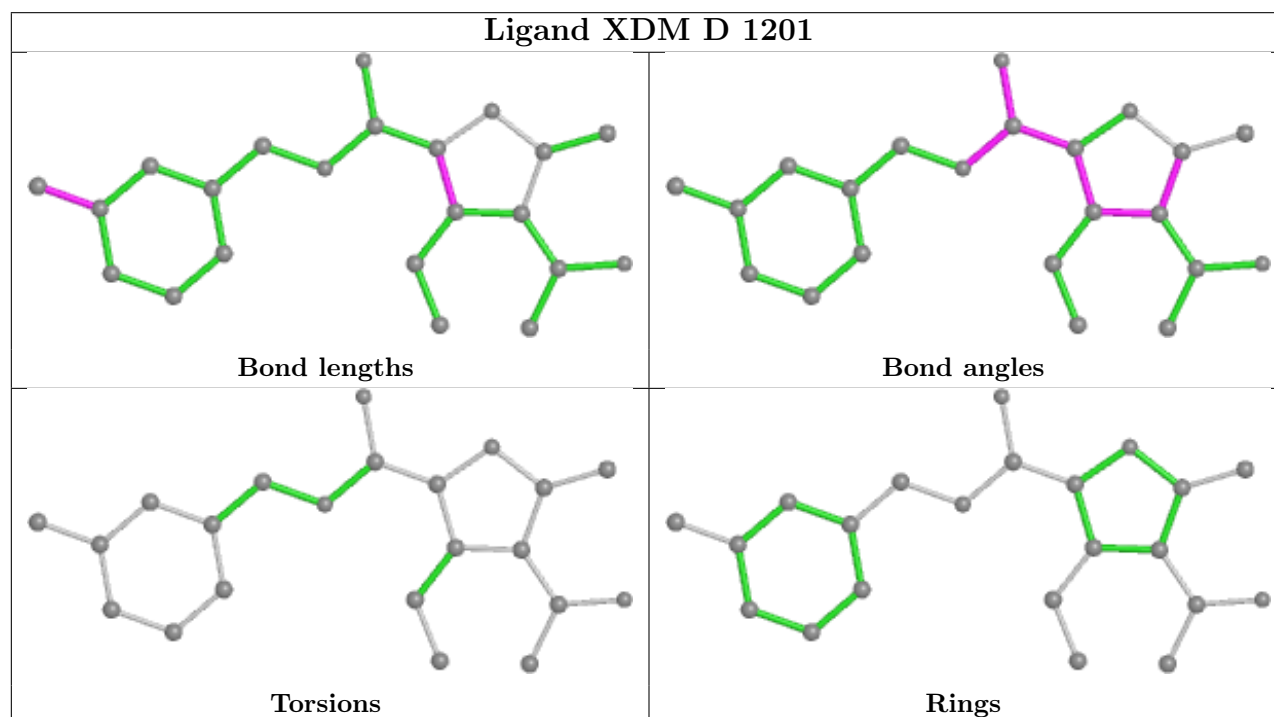
Mol	Chain	Res	Type	Atoms
4	B	1205	EDO	O1-C1-C2-O2
4	D	1204	EDO	O1-C1-C2-O2
4	A	1204	EDO	O1-C1-C2-O2
5	B	1208	PG4	O2-C3-C4-O3
4	B	1206	EDO	O1-C1-C2-O2
5	B	1208	PG4	C1-C2-O2-C3
4	B	1207	EDO	O1-C1-C2-O2
4	D	1202	EDO	O1-C1-C2-O2
4	A	1207	EDO	O1-C1-C2-O2
5	B	1208	PG4	C3-C4-O3-C5
4	A	1206	EDO	O1-C1-C2-O2
4	A	1208	EDO	O1-C1-C2-O2

There are no ring outliers.

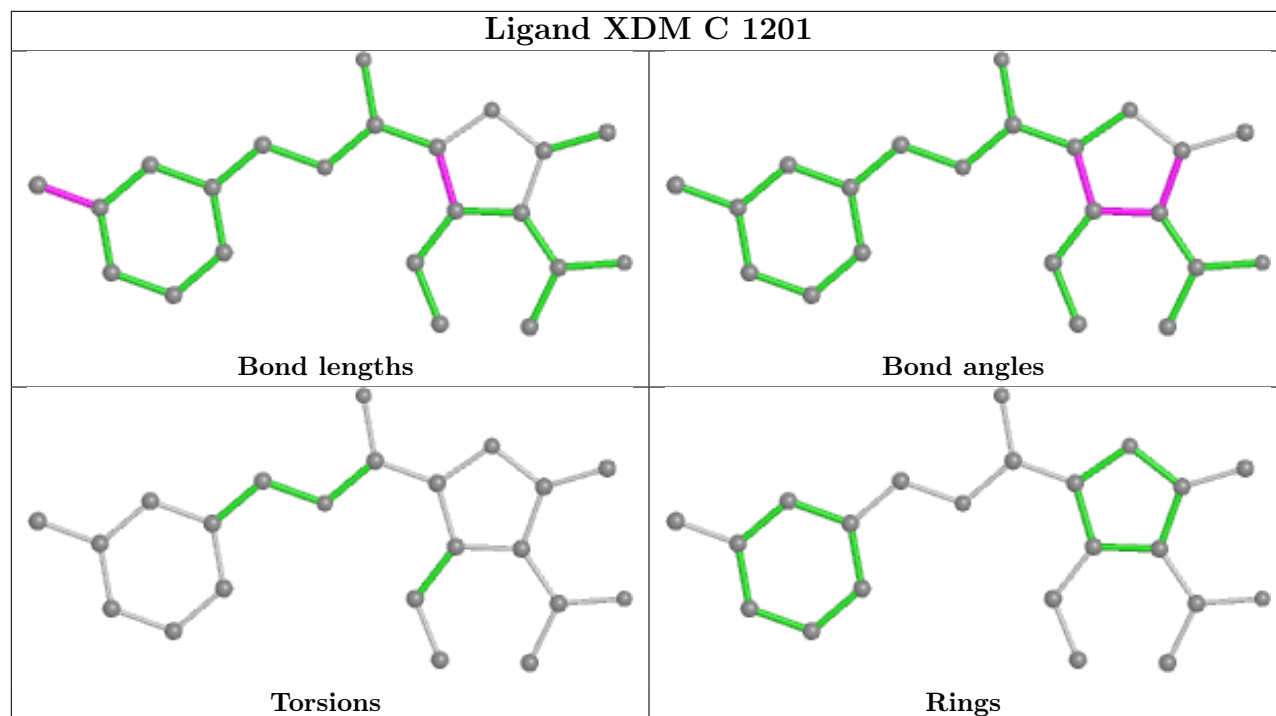
7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1203	SO4	1	0
4	C	1203	EDO	1	0
4	A	1206	EDO	1	0
4	D	1204	EDO	8	0
5	B	1208	PG4	4	0
2	E	1202	XDM	1	0
4	A	1204	EDO	3	0

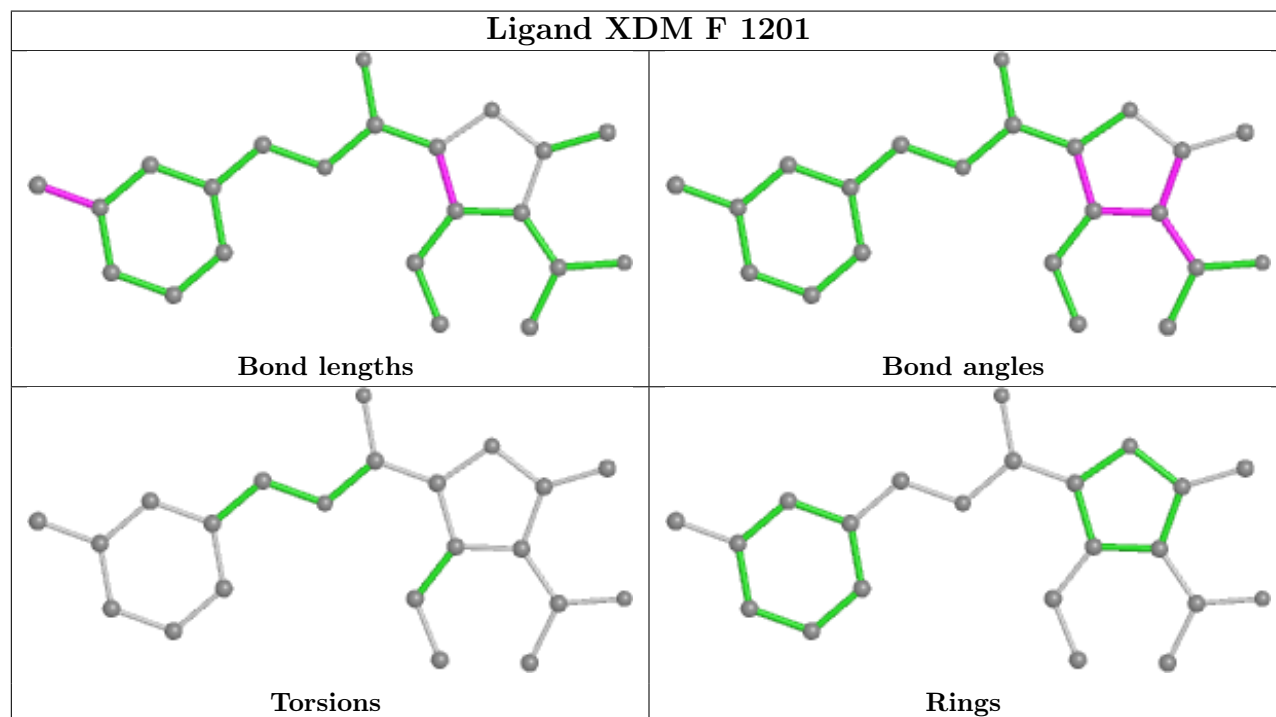
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 XDM C 1201

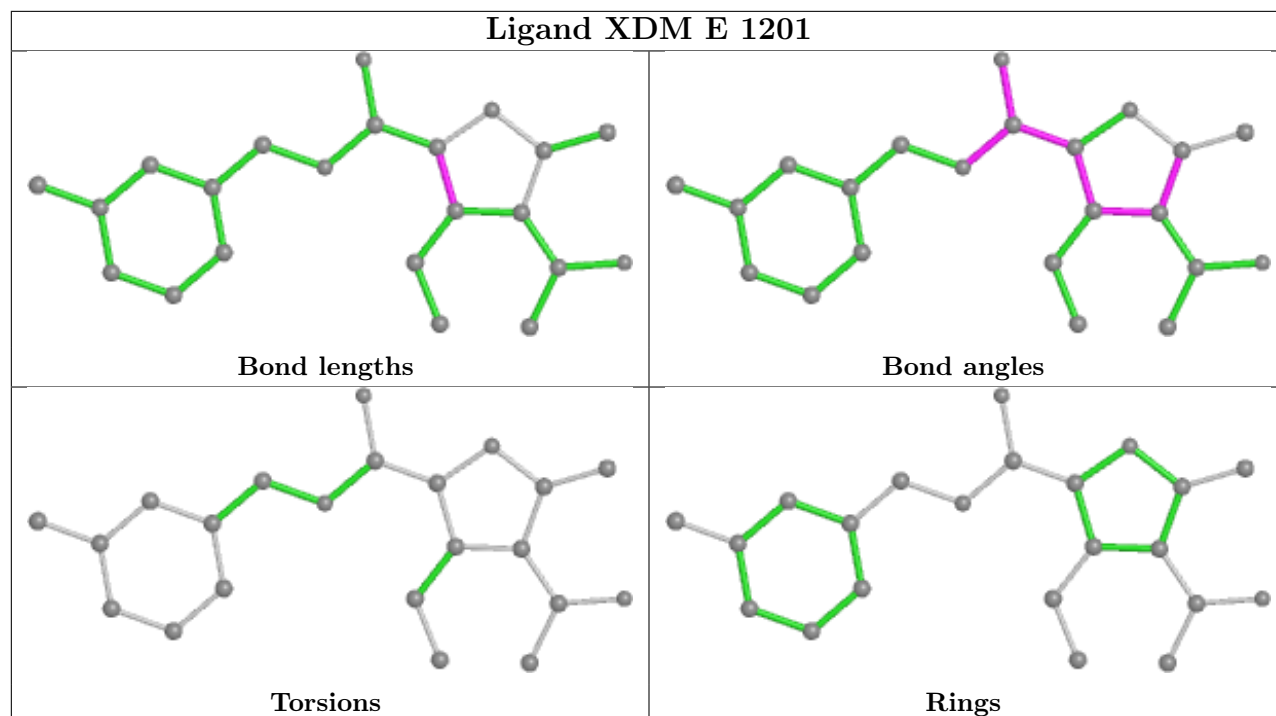


## Ligand XDM F 1201

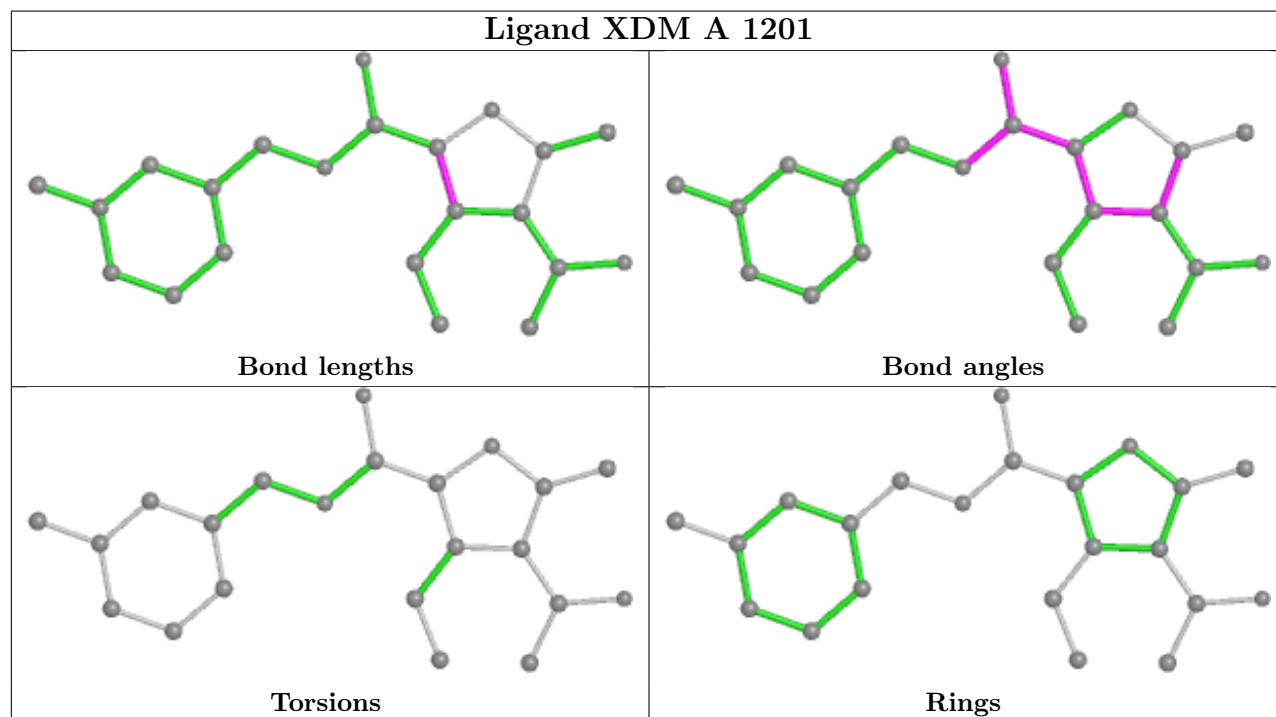


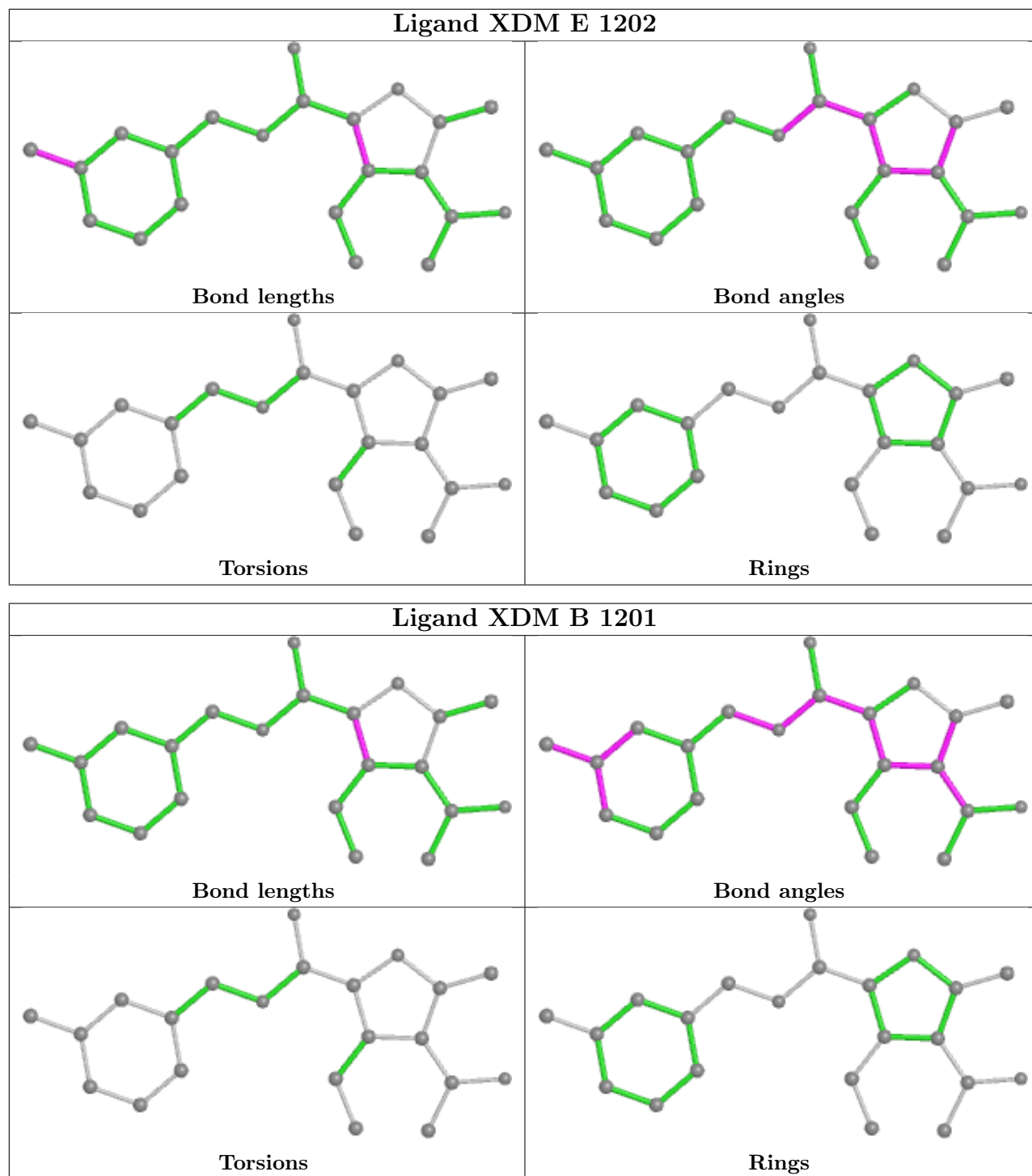


## Ligand XDM E 1201



## Ligand XDM A 1201





## 5.7 Other polymers [i](#)

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	116/122 (95%)	-0.30	2 (1%) 70 74	22, 30, 65, 101	0
1	B	112/122 (91%)	-0.49	3 (2%) 54 60	20, 32, 69, 84	0
1	C	114/122 (93%)	-0.08	7 (6%) 21 26	25, 34, 73, 88	1 (0%)
1	D	115/122 (94%)	-0.07	7 (6%) 21 26	29, 39, 67, 88	0
1	E	113/122 (92%)	-0.02	6 (5%) 26 32	29, 39, 75, 100	0
1	F	115/122 (94%)	0.14	12 (10%) 6 8	30, 40, 82, 94	0
1	G	114/122 (93%)	0.26	13 (11%) 5 6	32, 45, 86, 109	0
All	All	799/854 (93%)	-0.08	50 (6%) 20 24	20, 38, 75, 109	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1161	GLY	8.6
1	F	1048	ILE	8.3
1	F	1160	LEU	8.1
1	E	1048	ILE	5.8
1	D	1161	GLY	5.7
1	G	1160	LEU	5.7
1	G	1048	ILE	5.6
1	G	1047	LYS	4.9
1	E	1047	LYS	4.7
1	C	1159	SER	4.3
1	G	1156	VAL	4.3
1	B	1160	LEU	4.0
1	C	1161	GLY	3.9
1	G	1158	GLN	3.8
1	G	1115	TRP	3.7
1	G	1049	PHE	3.7
1	A	1046	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1048	ILE	3.6
1	F	1158	GLN	3.5
1	G	1157	MET	3.4
1	B	1049	PHE	3.3
1	C	1160	LEU	3.2
1	F	1159	SER	3.2
1	D	1160	LEU	3.1
1	F	1115	TRP	3.0
1	D	1048	ILE	2.9
1	E	1158	GLN	2.8
1	F	1157	MET	2.7
1	G	1154	ASP	2.7
1	C	1158	GLN	2.7
1	F	1051	PRO	2.7
1	E	1159	SER	2.6
1	F	1049	PHE	2.6
1	D	1159	SER	2.5
1	B	1051	PRO	2.5
1	F	1154	ASP	2.5
1	C	1049	PHE	2.5
1	G	1159	SER	2.4
1	D	1047	LYS	2.4
1	G	1053	GLU	2.3
1	C	1052	GLU	2.3
1	D	1049	PHE	2.2
1	G	1150	GLU	2.2
1	E	1157	MET	2.2
1	A	1161	GLY	2.1
1	E	1050	LYS	2.1
1	G	1050	LYS	2.1
1	F	1155	PRO	2.1
1	F	1056	GLN	2.1
1	D	1158	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

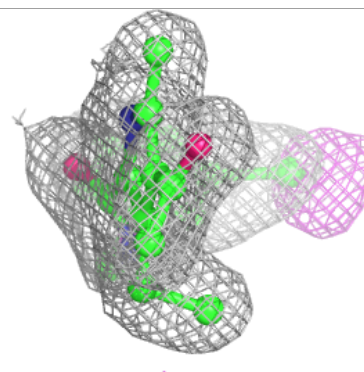
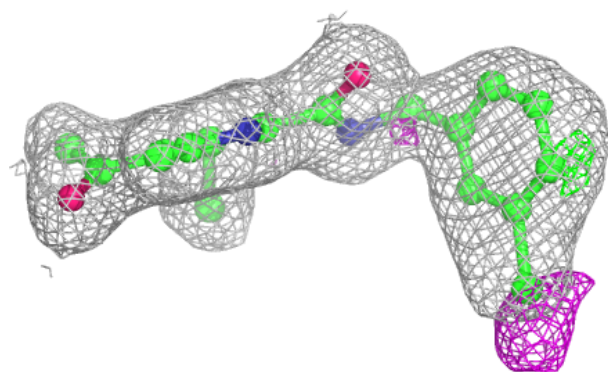
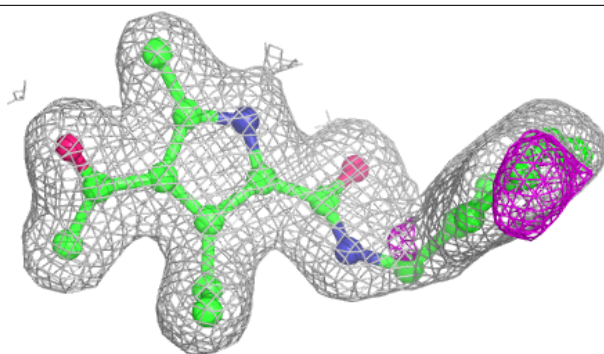
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	1207	4/4	0.48	0.26	64,65,66,67	0
4	EDO	E	1204	4/4	0.63	0.29	53,54,54,55	0
4	EDO	A	1204	4/4	0.78	0.14	45,48,50,50	0
4	EDO	B	1206	4/4	0.79	0.22	48,54,55,61	0
4	EDO	D	1202	4/4	0.80	0.12	57,60,61,61	0
4	EDO	A	1206	4/4	0.84	0.14	39,40,43,44	0
4	EDO	G	1201	4/4	0.84	0.09	57,57,57,61	0
4	EDO	F	1204	4/4	0.86	0.12	54,55,55,59	0
4	EDO	C	1203	4/4	0.88	0.12	47,48,52,54	0
4	EDO	D	1203	4/4	0.89	0.15	46,48,51,54	0
4	EDO	A	1205	4/4	0.91	0.22	43,47,49,52	0
4	EDO	D	1204	4/4	0.92	0.15	35,37,38,39	0
4	EDO	B	1205	4/4	0.92	0.13	47,48,48,54	0
3	SO4	A	1202	5/5	0.93	0.19	72,74,77,79	0
4	EDO	A	1207	4/4	0.93	0.13	28,36,36,39	0
2	XDM	B	1201	22/22	0.93	0.10	22,27,44,63	0
2	XDM	E	1202	22/22	0.93	0.12	32,38,43,53	0
5	PG4	B	1208	13/13	0.93	0.11	34,37,48,55	0
4	EDO	A	1208	4/4	0.94	0.11	43,44,45,45	0
2	XDM	F	1201	22/22	0.94	0.10	31,37,44,53	0
2	XDM	E	1201	22/22	0.94	0.12	30,34,50,72	0
2	XDM	D	1201	22/22	0.94	0.12	29,36,53,70	0
4	EDO	B	1204	4/4	0.95	0.12	30,33,34,34	0
3	SO4	E	1203	5/5	0.95	0.11	51,56,63,68	0
2	XDM	C	1201	22/22	0.95	0.12	26,29,33,45	0
2	XDM	A	1201	22/22	0.95	0.10	25,29,39,48	0
4	EDO	F	1203	4/4	0.97	0.16	36,43,43,45	0
3	SO4	F	1202	5/5	0.97	0.12	61,64,66,67	0
3	SO4	A	1203	5/5	0.97	0.08	40,43,45,45	0
4	EDO	B	1202	4/4	0.97	0.08	22,24,25,26	0
4	EDO	B	1203	4/4	0.98	0.07	26,27,27,27	0
3	SO4	C	1202	5/5	0.98	0.09	45,46,48,51	0

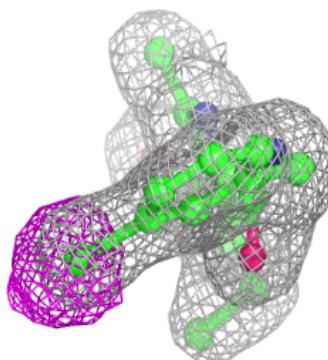
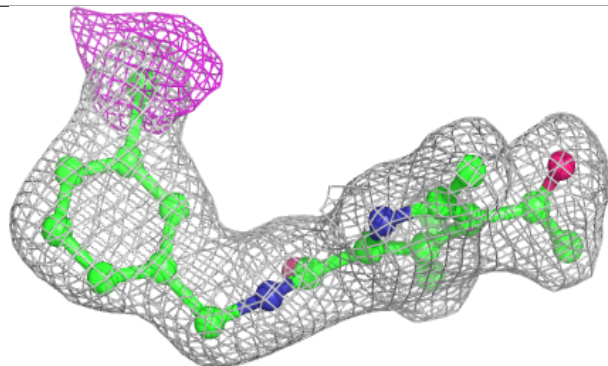
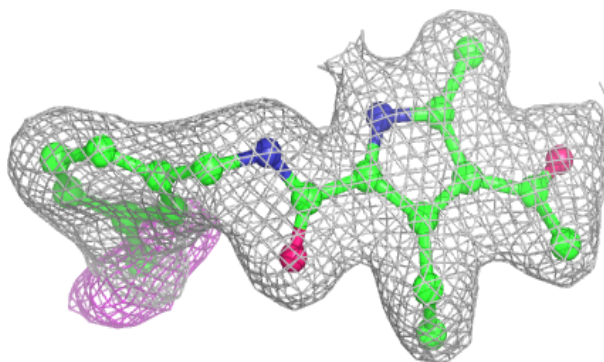
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XDM B 1201:**

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

**Electron density around XDM E 1202:**

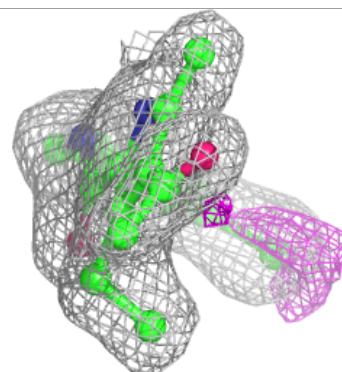
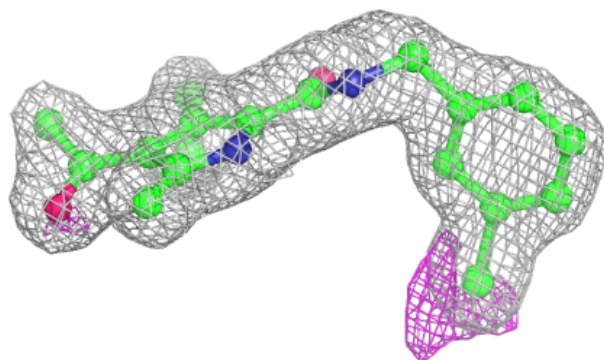
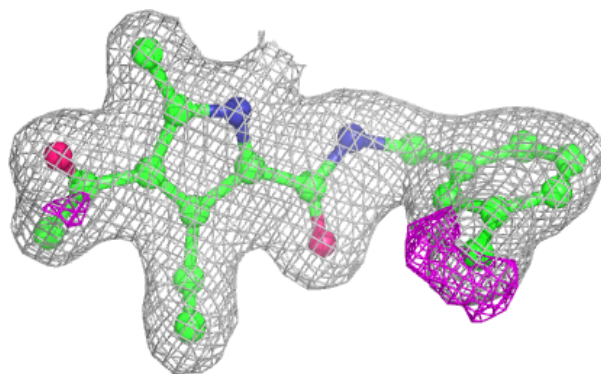
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



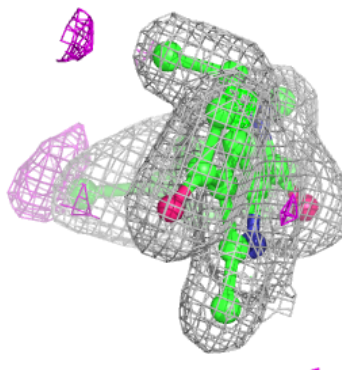
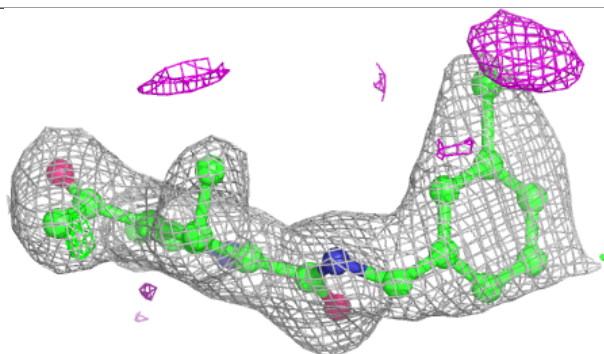
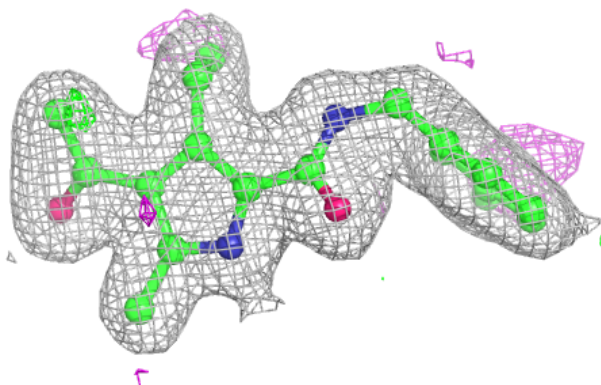


**Electron density around XDM F 1201:**

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

**Electron density around XDM E 1201:**

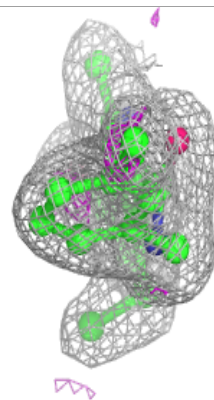
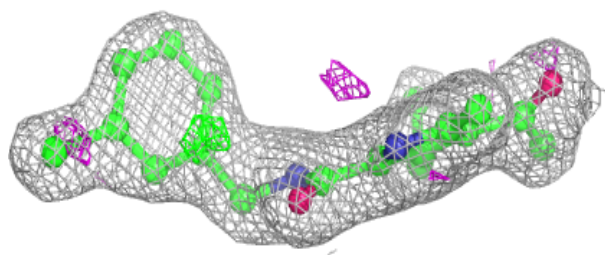
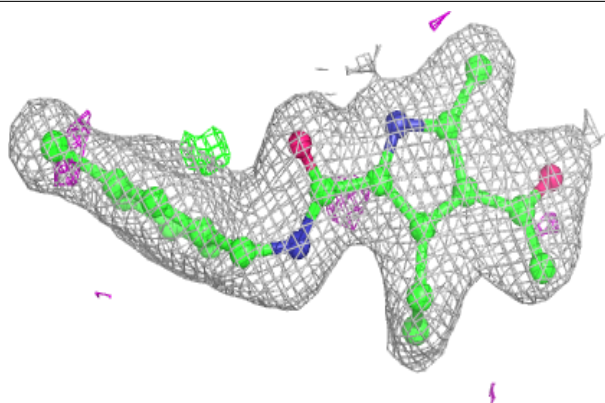
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





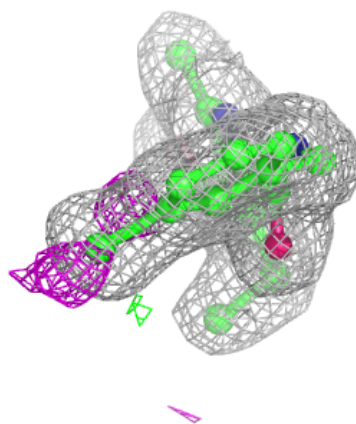
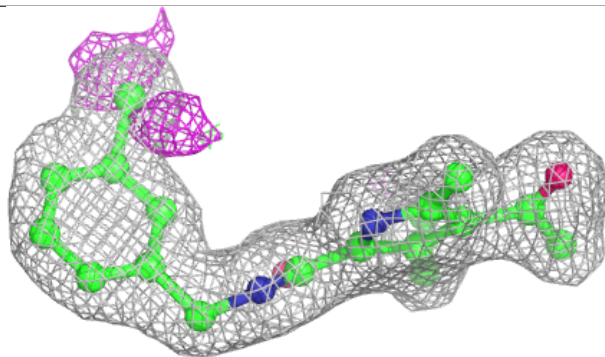
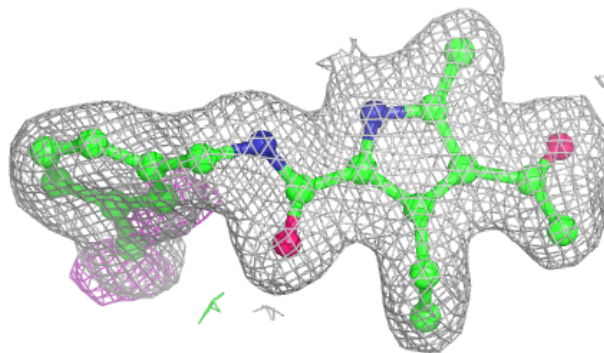
**Electron density around XDM D 1201:**

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



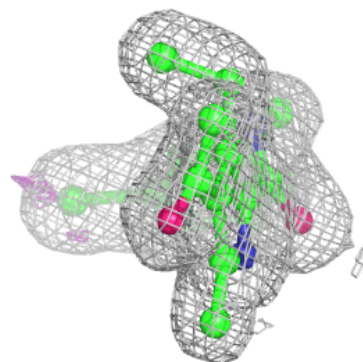
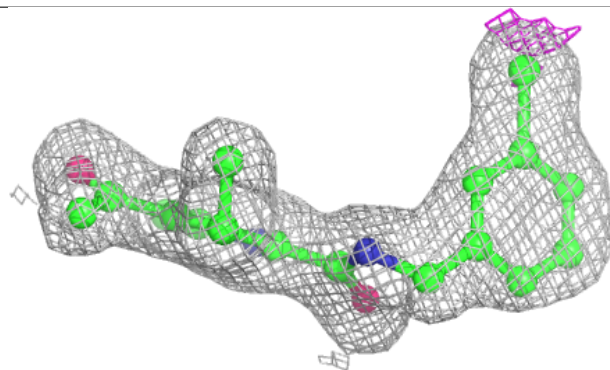
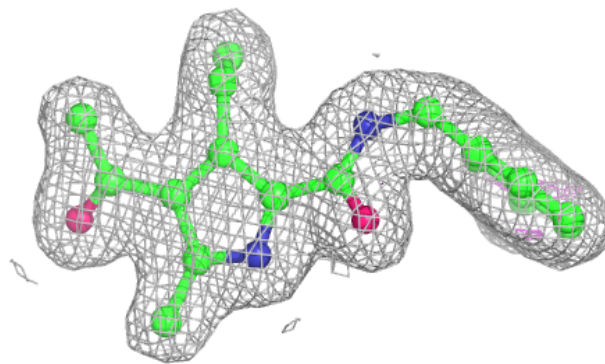
**Electron density around XDM C 1201:**

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



**Electron density around XDM A 1201:**

$2mF_o - DF_c$  (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.