



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:00 PM UTC

PDB ID : 7FEE / pdb\_00007fee  
Title : Crystal structure of the allosteric modulator ZCZ011 binding to CP55940-bound cannabinoid receptor 1  
Authors : Wang, X.; Zhao, C.; Shao, Z.  
Deposited on : 2021-07-19  
Resolution : 2.70 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

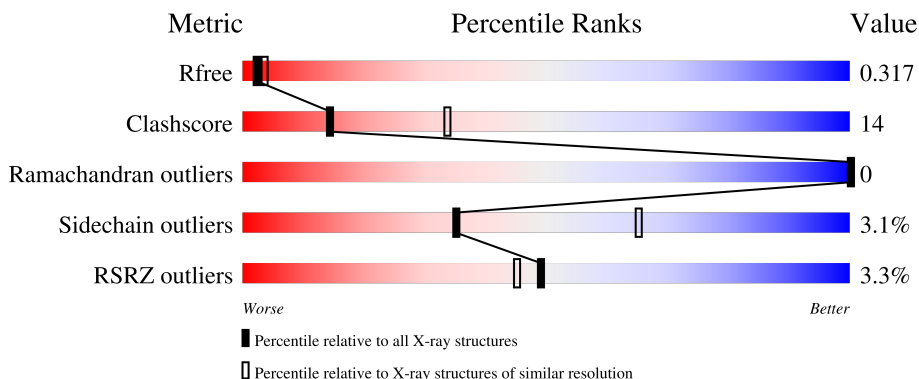
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	559	 3% 59% 27% 13%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4060 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 Cannabinoid receptor 1, GlgA glycogen synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	486	3815	2503	623	661	28	0	0	0

There are 55 discrepancies between the modelled and reference sequences:

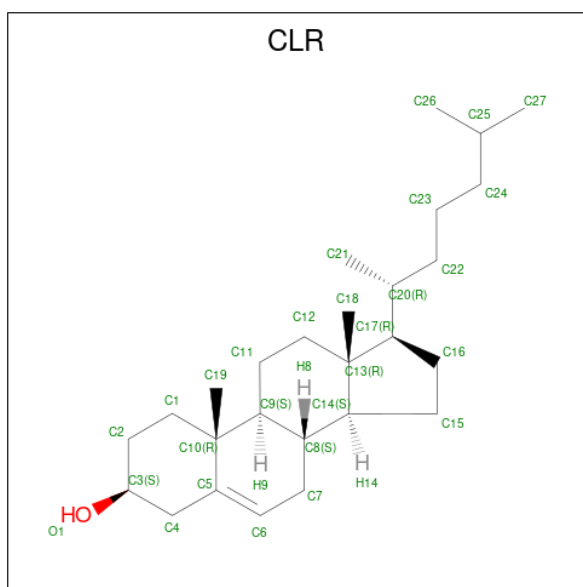
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	expression tag	UNP P21554
A	43	LYS	-	expression tag	UNP P21554
A	44	THR	-	expression tag	UNP P21554
A	45	ILE	-	expression tag	UNP P21554
A	46	ILE	-	expression tag	UNP P21554
A	47	ALA	-	expression tag	UNP P21554
A	48	LEU	-	expression tag	UNP P21554
A	49	SER	-	expression tag	UNP P21554
A	50	TYR	-	expression tag	UNP P21554
A	51	ILE	-	expression tag	UNP P21554
A	52	PHE	-	expression tag	UNP P21554
A	53	CYS	-	expression tag	UNP P21554
A	54	LEU	-	expression tag	UNP P21554
A	55	VAL	-	expression tag	UNP P21554
A	56	PHE	-	expression tag	UNP P21554
A	57	ALA	-	expression tag	UNP P21554
A	58	ASP	-	expression tag	UNP P21554
A	59	TYR	-	expression tag	UNP P21554
A	60	LYS	-	expression tag	UNP P21554
A	61	ASP	-	expression tag	UNP P21554
A	62	ASP	-	expression tag	UNP P21554
A	63	ASP	-	expression tag	UNP P21554
A	64	ASP	-	expression tag	UNP P21554
A	65	ALA	-	expression tag	UNP P21554
A	66	MET	-	expression tag	UNP P21554
A	83	GLU	-	linker	UNP P21554
A	84	ASN	-	linker	UNP P21554

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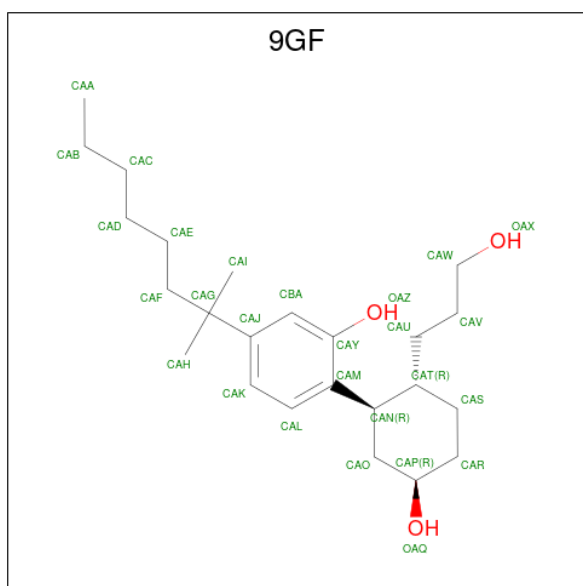
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	-	linker	UNP P21554
A	86	TYR	-	linker	UNP P21554
A	87	PHE	-	linker	UNP P21554
A	88	GLN	-	linker	UNP P21554
A	89	GLY	-	linker	UNP P21554
A	203	LYS	SER	engineered mutation	UNP P21554
A	210	ALA	THR	engineered mutation	UNP P21554
A	273	LYS	GLU	engineered mutation	UNP P21554
A	283	VAL	THR	engineered mutation	UNP P21554
A	340	GLU	ARG	engineered mutation	UNP P21554
A	393	ASP	ASN	engineered mutation	UNP P21554
A	415	GLU	-	expression tag	UNP P21554
A	416	ASN	-	expression tag	UNP P21554
A	417	LEU	-	expression tag	UNP P21554
A	418	TYR	-	expression tag	UNP P21554
A	419	PHE	-	expression tag	UNP P21554
A	420	GLN	-	expression tag	UNP P21554
A	421	GLY	-	expression tag	UNP P21554
A	422	HIS	-	expression tag	UNP P21554
A	423	HIS	-	expression tag	UNP P21554
A	424	HIS	-	expression tag	UNP P21554
A	425	HIS	-	expression tag	UNP P21554
A	426	HIS	-	expression tag	UNP P21554
A	427	HIS	-	expression tag	UNP P21554
A	428	HIS	-	expression tag	UNP P21554
A	429	HIS	-	expression tag	UNP P21554
A	430	HIS	-	expression tag	UNP P21554
A	431	HIS	-	expression tag	UNP P21554

- Molecule 2 is CHOLESTEROL (CCD ID: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



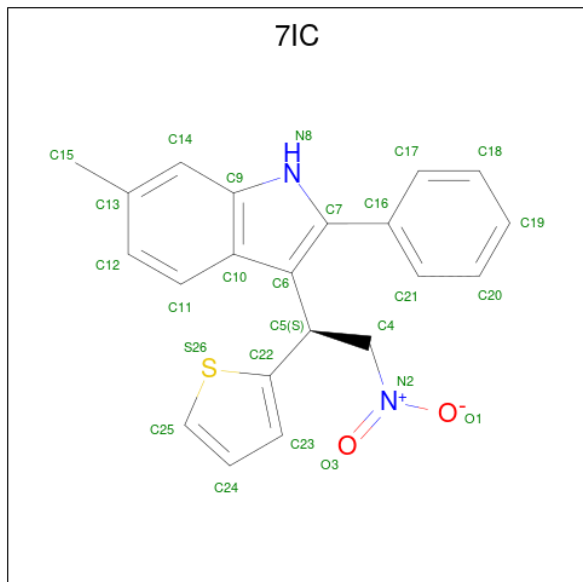
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	A	1	Total	C	O	0	0
			28	27	1		
2	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 3 is 2-[(1R,2R,5R)-5-hydroxy-2-(3-hydroxypropyl)cyclohexyl]-5-(2-methyloctan-2-yl)phenol (CCD ID: 9GF) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>3</sub>).



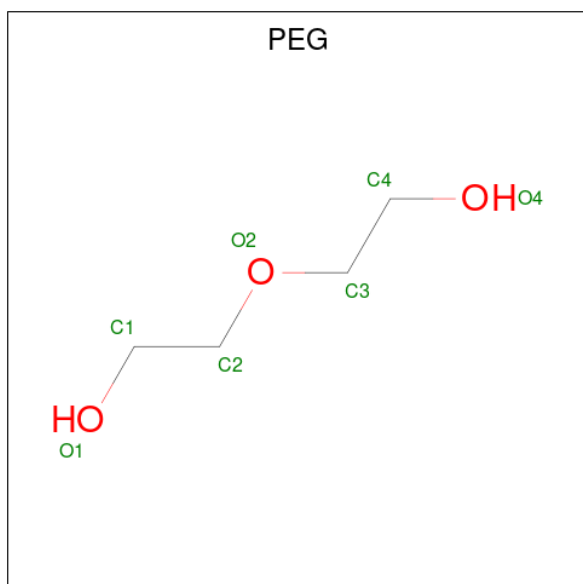
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total	C	O	0	0
			27	24	3		

- Molecule 4 is 6-methyl-3-[(1S)-2-nitro-1-thiophen-2-yl-ethyl]-2-phenyl-1H-indole (CCD ID: 7IC) (formula: C<sub>21</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	26	21	2	2	1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



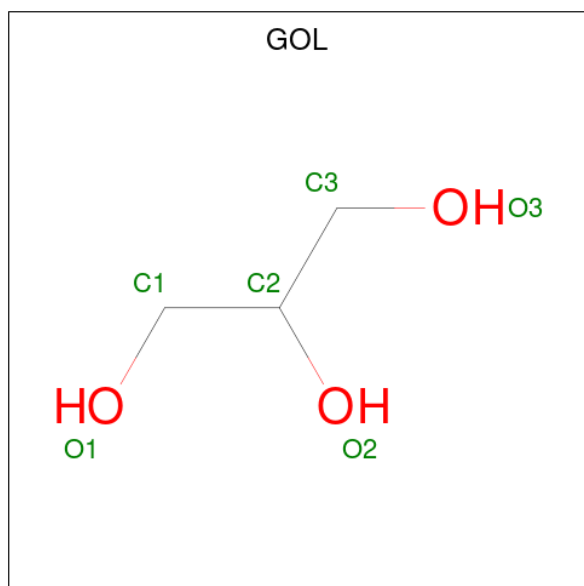
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	7	4	3	0	0

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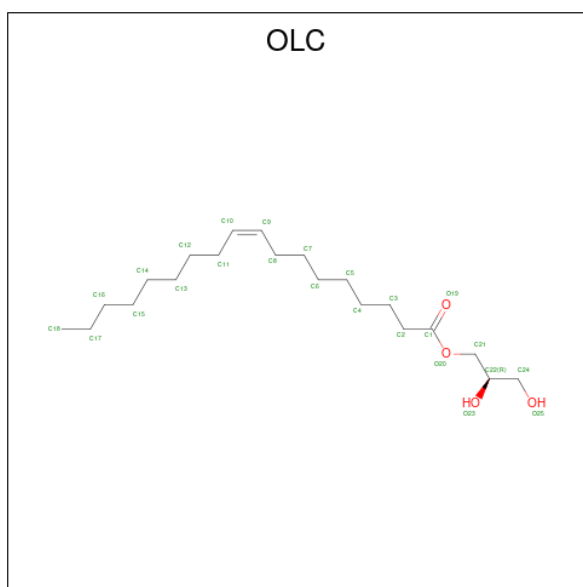
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



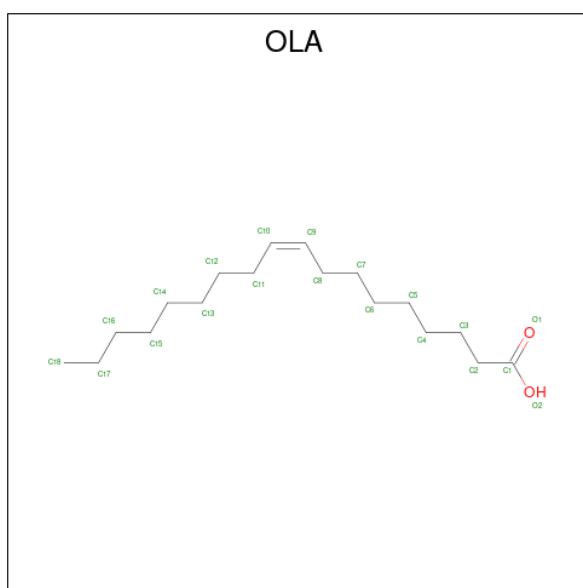
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula:  $C_{21}H_{40}O_4$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C O	0	0
			25	21 4		
7	A	1	Total	C O	0	0
			25	21 4		

- Molecule 8 is OLEIC ACID (CCD ID: OLA) (formula:  $C_{18}H_{34}O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			8	8		
8	A	1	Total	C	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 8 8	0	0
8	A	1	Total C 7 7	0	0

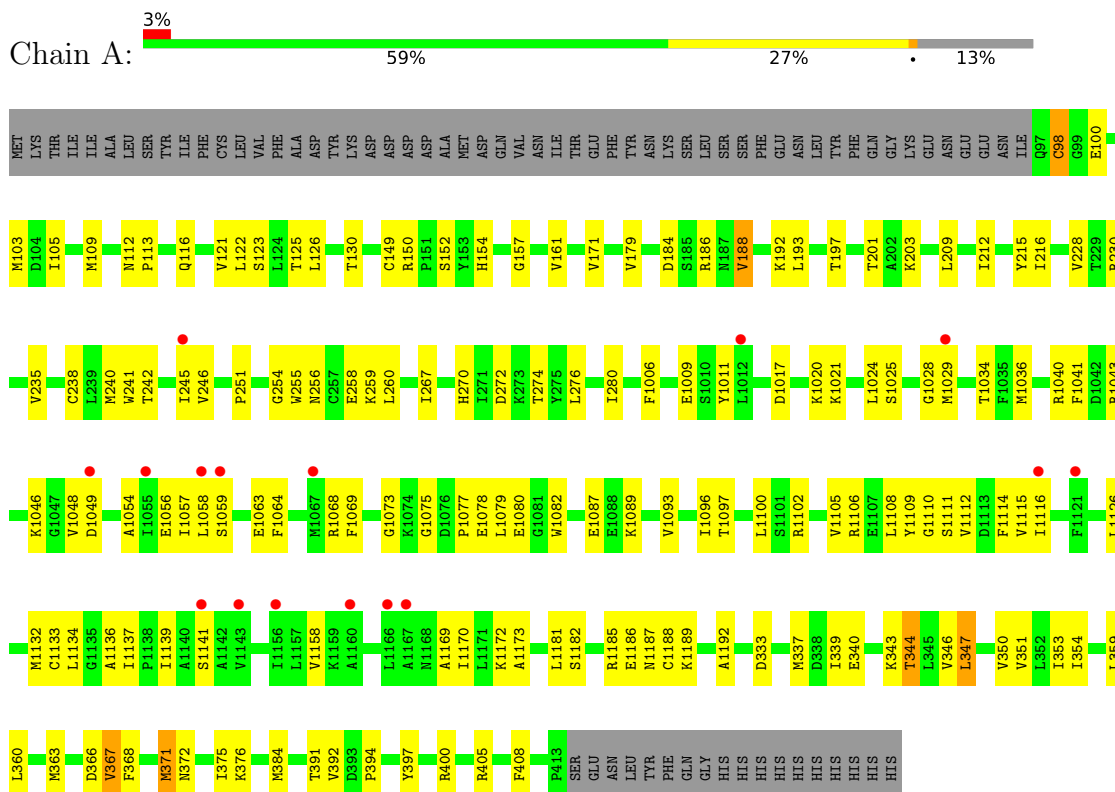
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	18	Total O 18 18	0	0

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

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

- Molecule 1: Cannabinoid receptor 1, GlgA glycogen synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.79Å 74.33Å 184.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.60 – 2.70 42.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.60-2.70) 99.7 (42.60-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.293 , 0.319 0.292 , 0.317	Depositor DCC
$R_{free}$ test set	1597 reflections (9.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.9	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% 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: 7IC, PEG, OLC, OLA, 9GF, CLR, GOL

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	0.28	0/3899	0.50	1/5274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1172	LYS	N-CA-C	-5.00	106.01	111.82

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	3815	0	3920	115	1
2	A	56	0	92	1	0
3	A	27	0	0	1	0
4	A	26	0	0	1	0
5	A	14	0	20	0	0
6	A	24	0	32	1	0
7	A	50	0	80	5	0
8	A	30	0	56	1	0
9	A	18	0	0	1	0
All	All	4060	0	4200	116	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 14.

All (116) 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:116:GLN:HB3	1:A:179:VAL:HG22	1.36	1.05
1:A:245:ILE:HG23	4:A:1204:7IC:C20	1.88	1.04
1:A:1049:ASP:OD1	1:A:1079:LEU:HD22	1.78	0.83
1:A:1049:ASP:OD1	1:A:1079:LEU:CD2	2.30	0.79
1:A:405:ARG:HD2	7:A:1212:OLC:H2	1.65	0.77
1:A:1043:ARG:HA	1:A:1049:ASP:OD2	1.89	0.72
1:A:344:THR:HG22	1:A:400:ARG:HE	1.56	0.71
1:A:1158:VAL:HG21	1:A:1169:ALA:HB2	1.71	0.70
1:A:1040:ARG:HE	1:A:1046:LYS:HZ2	1.42	0.67
1:A:152:SER:HB2	6:A:1207:GOL:H2	1.77	0.66
1:A:1056:GLU:O	1:A:1059:SER:OG	2.16	0.64
1:A:230:ARG:HH22	7:A:1211:OLC:C1	2.09	0.64
1:A:1041:PHE:HB2	1:A:1075:GLY:HA3	1.79	0.63
1:A:1089:LYS:HA	1:A:1089:LYS:HE2	1.81	0.62
1:A:280:ILE:HG23	1:A:360:LEU:HD12	1.83	0.60
1:A:255:TRP:HE1	1:A:274:THR:HG23	1.67	0.60
1:A:1139:ILE:HD11	1:A:1173:ALA:HB2	1.84	0.59
1:A:1025:SER:HA	1:A:1029:MET:HA	1.83	0.59
1:A:1096:ILE:HG21	1:A:1100:LEU:HD21	1.85	0.59
1:A:184:ASP:HB3	1:A:188:VAL:HG13	1.85	0.59
1:A:1009:GLU:HB2	1:A:1189:LYS:HE2	1.84	0.59
1:A:350:VAL:O	1:A:354:ILE:HG12	2.04	0.58
1:A:154:HIS:HA	7:A:1211:OLC:H9	1.86	0.58
1:A:121:VAL:O	1:A:125:THR:HG22	2.04	0.57
1:A:1114:PHE:CE2	1:A:1139:ILE:HG13	2.39	0.57
1:A:1116:ILE:HD13	1:A:1139:ILE:HG22	1.86	0.56
1:A:184:ASP:OD2	1:A:192:LYS:NZ	2.38	0.55
1:A:340:GLU:O	1:A:344:THR:HG23	2.07	0.55
1:A:1182:SER:HA	1:A:1185:ARG:HB2	1.89	0.55
1:A:1186:GLU:OE2	1:A:1187:ASN:ND2	2.40	0.55
1:A:1105:VAL:HG23	1:A:1108:LEU:HD12	1.88	0.54
1:A:408:PHE:CD1	7:A:1212:OLC:H10	2.42	0.54
1:A:366:ASP:HA	1:A:371:MET:HE1	1.90	0.54
1:A:1069:PHE:HB2	1:A:1093:VAL:HG12	1.90	0.53
1:A:333:ASP:O	1:A:337:MET:HB2	2.09	0.53
1:A:113:PRO:HA	1:A:116:GLN:HG3	1.91	0.53
1:A:1006:PHE:HE2	1:A:1102:ARG:HE	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1077:PRO:HA	1:A:1080:GLU:HG2	1.90	0.52
1:A:258:GLU:OE2	1:A:270:HIS:ND1	2.42	0.52
1:A:1054:ALA:O	1:A:1057:ILE:HG12	2.08	0.52
1:A:1041:PHE:HA	1:A:1048:VAL:HG11	1.92	0.51
1:A:251:PRO:O	1:A:256:ASN:ND2	2.43	0.51
1:A:256:ASN:HB2	1:A:270:HIS:O	2.11	0.51
1:A:346:VAL:O	1:A:350:VAL:HG13	2.10	0.51
1:A:186:ARG:NE	1:A:259:LYS:HE3	2.26	0.51
1:A:105:ILE:HG23	1:A:109:MET:HE3	1.93	0.50
1:A:209:LEU:HD11	1:A:240:MET:HG3	1.93	0.50
1:A:276:LEU:O	1:A:280:ILE:HG12	2.11	0.50
1:A:197:THR:O	1:A:201:THR:HG23	2.12	0.49
1:A:1063:GLU:H	1:A:1063:GLU:CD	2.19	0.49
1:A:1110:GLY:HA2	1:A:1134:LEU:O	2.13	0.49
1:A:98:CYS:HB3	1:A:103:MET:HE2	1.95	0.49
1:A:149:CYS:HA	1:A:230:ARG:NH1	2.28	0.49
1:A:347:LEU:O	1:A:351:VAL:HG23	2.13	0.48
1:A:1040:ARG:HH21	1:A:1046:LYS:HZ1	1.61	0.48
1:A:157:GLY:O	1:A:161:VAL:HG23	2.14	0.48
1:A:1079:LEU:O	1:A:1082:TRP:HB3	2.13	0.48
1:A:1181:LEU:HD23	1:A:1181:LEU:H	1.79	0.48
1:A:367:VAL:HG12	1:A:368:PHE:CD2	2.49	0.48
1:A:235:VAL:HA	1:A:238:CYS:HB3	1.96	0.47
1:A:1137:ILE:HD11	1:A:1185:ARG:HG3	1.96	0.47
1:A:238:CYS:O	1:A:242:THR:HG23	2.14	0.47
1:A:359:LEU:O	1:A:363:MET:HG3	2.13	0.47
1:A:1114:PHE:HE2	1:A:1139:ILE:HG13	1.78	0.47
1:A:1006:PHE:HA	1:A:1106:ARG:HH21	1.81	0.46
1:A:203:LYS:NZ	9:A:1302:HOH:O	2.48	0.46
1:A:1132:MET:HE3	1:A:1192:ALA:HB2	1.97	0.46
1:A:344:THR:HG22	1:A:400:ARG:NE	2.27	0.46
1:A:1017:ASP:O	1:A:1021:LYS:HG3	2.16	0.46
1:A:1087:GLU:HA	1:A:1093:VAL:HG23	1.97	0.46
1:A:394:PRO:HA	1:A:397:TYR:CD2	2.51	0.45
1:A:122:LEU:O	1:A:126:LEU:HB2	2.16	0.45
1:A:193:LEU:O	1:A:197:THR:HG23	2.16	0.45
1:A:216:ILE:HD11	1:A:228:VAL:CG2	2.46	0.45
1:A:1079:LEU:HG	1:A:1082:TRP:HE3	1.80	0.45
1:A:98:CYS:SG	1:A:103:MET:HB2	2.57	0.45
1:A:123:SER:HB3	1:A:171:VAL:HG23	1.98	0.44
1:A:1170:ILE:HA	1:A:1173:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:CYS:SG	1:A:1192:ALA:HB1	2.58	0.44
1:A:339:ILE:O	1:A:343:LYS:HG2	2.17	0.44
1:A:100:GLU:H	1:A:100:GLU:CD	2.25	0.44
1:A:256:ASN:HD21	1:A:259:LYS:HD3	1.83	0.44
1:A:267:ILE:O	3:A:1203:9GF:OAQ	2.35	0.44
1:A:1059:SER:HA	1:A:1064:PHE:CD2	2.53	0.44
1:A:1073:GLY:O	1:A:1097:THR:HA	2.17	0.44
1:A:272:ASP:CG	1:A:274:THR:HG22	2.43	0.44
1:A:1132:MET:HB3	1:A:1188:CYS:HB3	2.00	0.43
1:A:112:ASN:O	1:A:116:GLN:HG3	2.18	0.43
1:A:1087:GLU:HG3	1:A:1093:VAL:O	2.18	0.43
1:A:343:LYS:HB2	1:A:400:ARG:NH2	2.34	0.43
1:A:372:ASN:OD1	1:A:375:ILE:HG12	2.18	0.43
1:A:242:THR:HG22	8:A:1216:OLA:H171	2.01	0.43
1:A:150:ARG:HA	1:A:150:ARG:HD3	1.76	0.43
1:A:1036:MET:HB2	1:A:1112:VAL:HG11	2.00	0.43
1:A:1115:VAL:HG23	1:A:1136:ALA:HB1	2.01	0.43
1:A:241:TRP:CE2	7:A:1211:OLC:H15	2.54	0.42
1:A:280:ILE:HG12	1:A:280:ILE:H	1.67	0.42
1:A:1132:MET:HB2	1:A:1192:ALA:HB2	2.01	0.42
1:A:1109:TYR:O	1:A:1136:ALA:HB2	2.20	0.42
1:A:1034:THR:HA	1:A:1068:ARG:O	2.20	0.42
1:A:1141:SER:HA	1:A:1158:VAL:O	2.20	0.42
1:A:1020:LYS:HG2	1:A:1024:LEU:HD13	2.01	0.41
1:A:1024:LEU:O	1:A:1028:GLY:N	2.53	0.41
1:A:123:SER:HA	1:A:384:MET:HE1	2.02	0.41
1:A:212:ILE:O	1:A:216:ILE:HG23	2.20	0.41
1:A:254:GLY:HA2	1:A:259:LYS:HD3	2.02	0.41
1:A:126:LEU:O	1:A:130:THR:HG23	2.20	0.41
2:A:1202:CLR:H231	2:A:1202:CLR:H211	1.76	0.41
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.84	0.41
1:A:1116:ILE:HA	1:A:1139:ILE:O	2.21	0.41
1:A:371:MET:O	1:A:376:LYS:NZ	2.53	0.41
1:A:1058:LEU:O	1:A:1064:PHE:HB2	2.21	0.40
1:A:216:ILE:HD11	1:A:228:VAL:HG22	2.03	0.40
1:A:1043:ARG:CA	1:A:1049:ASP:OD2	2.65	0.40
1:A:1187:ASN:N	1:A:1187:ASN:HD22	2.18	0.40
1:A:351:VAL:HG11	1:A:392:VAL:HG21	2.03	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:A:1011:TYR:OH	1:A:1078:GLU:OE2[1_455]	2.10	0.10

### 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	484/559 (87%)	467 (96%)	17 (4%)	0	100 100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	416/490 (85%)	403 (97%)	13 (3%)	35 65

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	188	VAL
1	A	215	TYR
1	A	246	VAL
1	A	260	LEU
1	A	1111	SER
1	A	1126	LEU
1	A	344	THR

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Mol	Chain	Res	Type
1	A	347	LEU
1	A	353	ILE
1	A	367	VAL
1	A	371	MET
1	A	391	THR

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

Mol	Chain	Res	Type
1	A	219	HIS
1	A	1187	ASN
1	A	406	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

16 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	$\# Z  > 2$
6	GOL	A	1210	-	5,5,5	0.94	0	5,5,5	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	A	1208	-	5,5,5	0.93	0	5,5,5	1.06	0
8	OLA	A	1216	-	6,6,19	0.28	0	5,5,19	0.43	0
7	OLC	A	1212	-	24,24,24	1.15	1 (4%)	25,25,25	1.27	2 (8%)
7	OLC	A	1211	-	24,24,24	1.16	1 (4%)	25,25,25	1.29	2 (8%)
2	CLR	A	1201	-	31,31,31	0.30	0	48,48,48	0.44	0
4	7IC	A	1204	-	26,29,29	2.33	5 (19%)	31,41,41	1.45	6 (19%)
5	PEG	A	1205	-	6,6,6	0.11	0	5,5,5	0.09	0
8	OLA	A	1215	-	7,7,19	0.26	0	6,6,19	0.50	0
6	GOL	A	1209	-	5,5,5	0.97	0	5,5,5	1.09	0
2	CLR	A	1202	-	31,31,31	0.28	0	48,48,48	0.40	0
5	PEG	A	1206	-	6,6,6	0.11	0	5,5,5	0.08	0
8	OLA	A	1214	-	6,6,19	0.26	0	5,5,19	0.49	0
3	9GF	A	1203	-	28,28,28	0.65	1 (3%)	37,38,38	0.80	1 (2%)
6	GOL	A	1207	-	5,5,5	0.98	0	5,5,5	1.06	0
8	OLA	A	1213	-	7,7,19	0.27	0	6,6,19	0.51	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
6	GOL	A	1210	-	-	4/4/4/4	-
6	GOL	A	1208	-	-	1/4/4/4	-
8	OLA	A	1216	-	-	3/4/4/17	-
7	OLC	A	1212	-	-	12/24/24/24	-
7	OLC	A	1211	-	-	8/24/24/24	-
2	CLR	A	1201	-	-	1/10/68/68	0/4/4/4
4	7IC	A	1204	-	-	4/15/28/28	0/4/4/4
5	PEG	A	1205	-	-	2/4/4/4	-
8	OLA	A	1215	-	-	1/5/5/17	-
6	GOL	A	1209	-	-	0/4/4/4	-
2	CLR	A	1202	-	-	2/10/68/68	0/4/4/4
5	PEG	A	1206	-	-	2/4/4/4	-
8	OLA	A	1214	-	-	0/4/4/17	-
3	9GF	A	1203	-	-	8/21/34/34	0/2/2/2
6	GOL	A	1207	-	-	0/4/4/4	-
8	OLA	A	1213	-	-	2/5/5/17	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1204	7IC	O3-N2	8.29	1.40	1.22
4	A	1204	7IC	C7-N8	-4.52	1.32	1.38
4	A	1204	7IC	C16-C7	4.12	1.53	1.47
4	A	1204	7IC	C10-C9	-3.16	1.37	1.41
7	A	1211	OLC	O20-C1	3.02	1.42	1.33
7	A	1212	OLC	O20-C1	3.01	1.42	1.33
4	A	1204	7IC	C7-C6	2.74	1.40	1.38
3	A	1203	9GF	OAZ-CAY	2.18	1.40	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1212	OLC	C8-C9-C10	3.75	152.96	124.83
7	A	1211	OLC	C8-C9-C10	3.73	152.80	124.83
4	A	1204	7IC	C25-S26-C22	3.70	100.36	92.87
4	A	1204	7IC	C24-C25-S26	-2.95	105.80	113.02
7	A	1211	OLC	O20-C1-C2	2.93	120.76	111.83
7	A	1212	OLC	O20-C1-C2	2.72	120.12	111.83
4	A	1204	7IC	C23-C22-S26	-2.67	104.77	110.94
4	A	1204	7IC	C10-C6-C7	-2.65	104.97	106.77
4	A	1204	7IC	C17-C16-C7	-2.23	118.11	120.76
3	A	1203	9GF	CAU-CAT-CAS	-2.20	106.76	112.48
4	A	1204	7IC	C14-C9-C10	-2.03	120.90	122.52

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1203	9GF	CAE-CAF-CAG-CAH
3	A	1203	9GF	CAE-CAF-CAG-CAI
3	A	1203	9GF	CAE-CAF-CAG-CAJ
4	A	1204	7IC	N2-C4-C5-C6
7	A	1212	OLC	C21-C22-C24-O25
7	A	1212	OLC	O20-C21-C22-C24
7	A	1212	OLC	O20-C21-C22-O23
6	A	1210	GOL	O1-C1-C2-C3
6	A	1210	GOL	C1-C2-C3-O3
3	A	1203	9GF	CAC-CAD-CAE-CAF
7	A	1212	OLC	O23-C22-C24-O25
7	A	1212	OLC	C3-C4-C5-C6
7	A	1211	OLC	C14-C15-C16-C17

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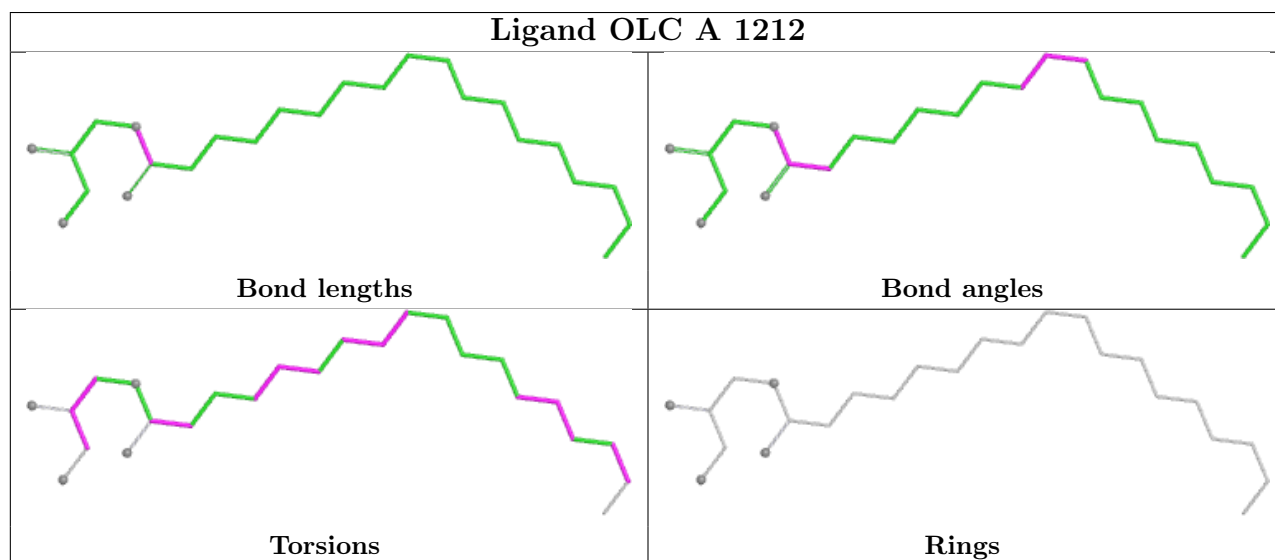
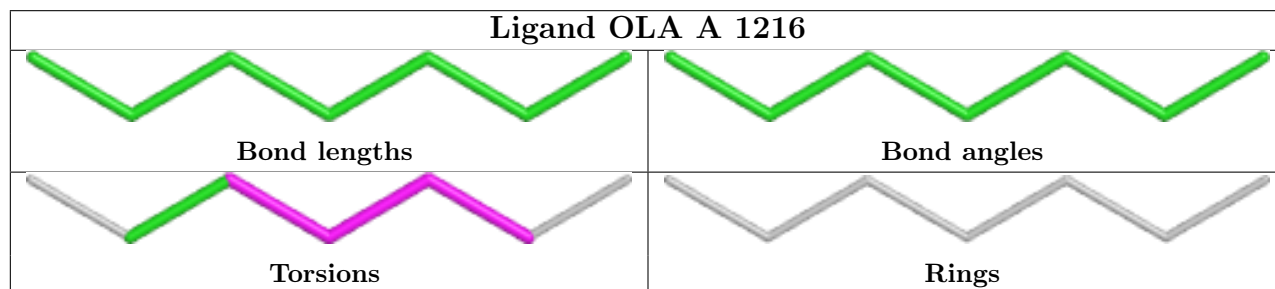
Mol	Chain	Res	Type	Atoms
8	A	1213	OLA	C12-C13-C14-C15
7	A	1212	OLC	C6-C7-C8-C9
8	A	1216	OLA	C14-C15-C16-C17
7	A	1211	OLC	C3-C4-C5-C6
7	A	1211	OLC	C10-C11-C12-C13
8	A	1213	OLA	C13-C14-C15-C16
8	A	1215	OLA	C12-C13-C14-C15
3	A	1203	9GF	CAF-CAG-CAJ-CAK
2	A	1202	CLR	C20-C22-C23-C24
3	A	1203	9GF	CAF-CAG-CAJ-CBA
8	A	1216	OLA	C12-C13-C14-C15
3	A	1203	9GF	CAA-CAB-CAC-CAD
7	A	1212	OLC	C13-C14-C15-C16
6	A	1210	GOL	O2-C2-C3-O3
8	A	1216	OLA	C13-C14-C15-C16
5	A	1206	PEG	C1-C2-O2-C3
7	A	1211	OLC	C5-C6-C7-C8
7	A	1211	OLC	C11-C12-C13-C14
7	A	1212	OLC	C15-C16-C17-C18
2	A	1202	CLR	C21-C20-C22-C23
7	A	1211	OLC	C6-C7-C8-C9
7	A	1212	OLC	C7-C8-C9-C10
6	A	1208	GOL	O1-C1-C2-C3
7	A	1211	OLC	C15-C16-C17-C18
7	A	1212	OLC	C12-C13-C14-C15
5	A	1205	PEG	O1-C1-C2-O2
4	A	1204	7IC	C4-C5-C6-C7
4	A	1204	7IC	C5-C4-N2-O3
6	A	1210	GOL	O1-C1-C2-O2
5	A	1205	PEG	C1-C2-O2-C3
7	A	1212	OLC	C4-C5-C6-C7
7	A	1212	OLC	O20-C1-C2-C3
2	A	1201	CLR	C16-C17-C20-C22
3	A	1203	9GF	CAT-CAU-CAV-CAW
7	A	1211	OLC	C9-C10-C11-C12
5	A	1206	PEG	O2-C3-C4-O4
4	A	1204	7IC	C22-C5-C6-C10

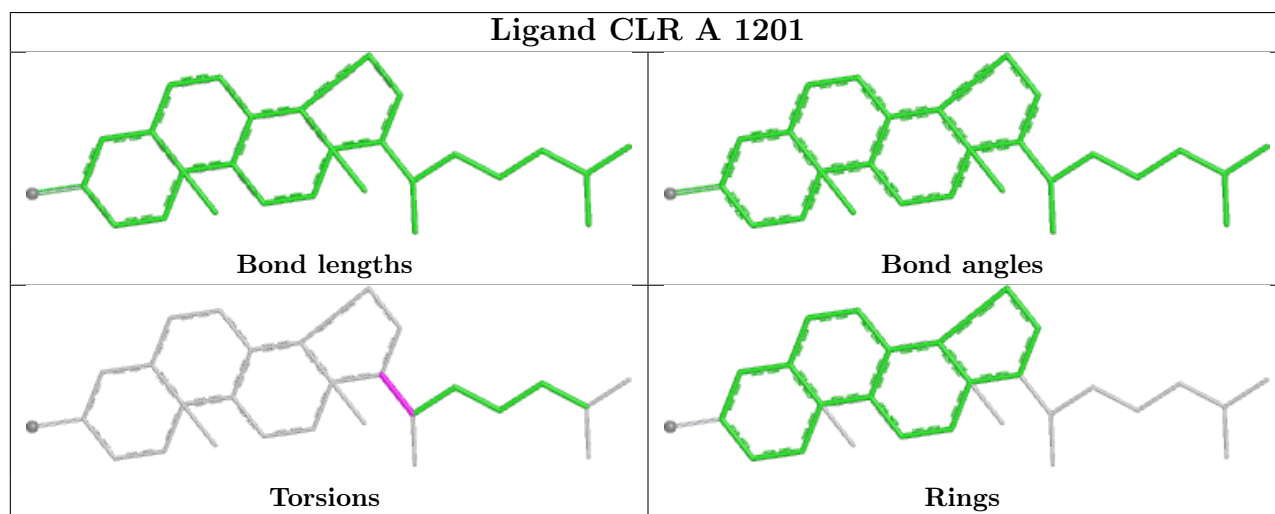
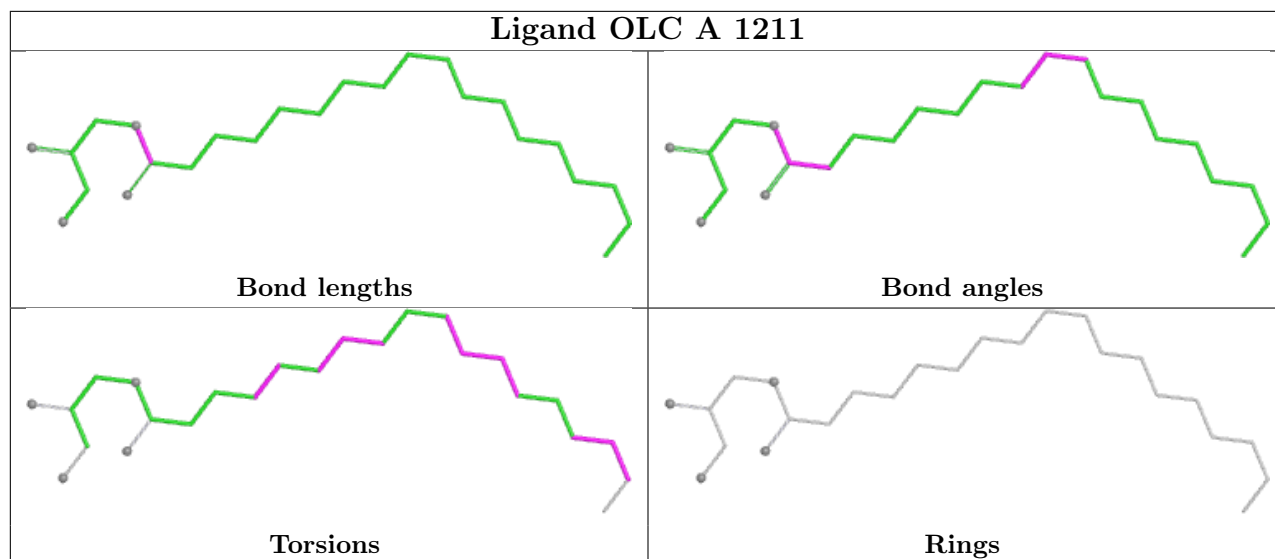
There are no ring outliers.

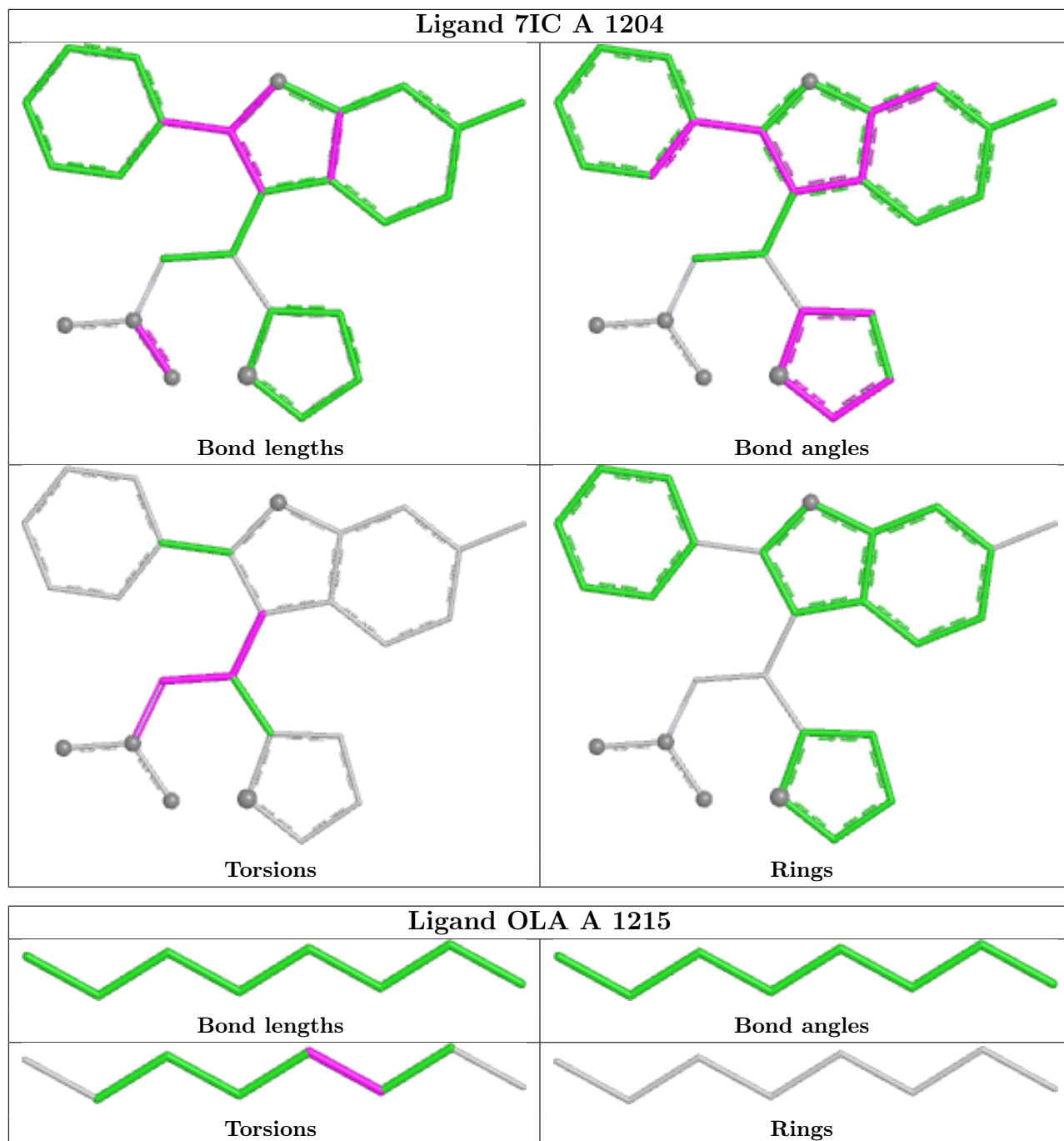
7 monomers are involved in 10 short contacts:

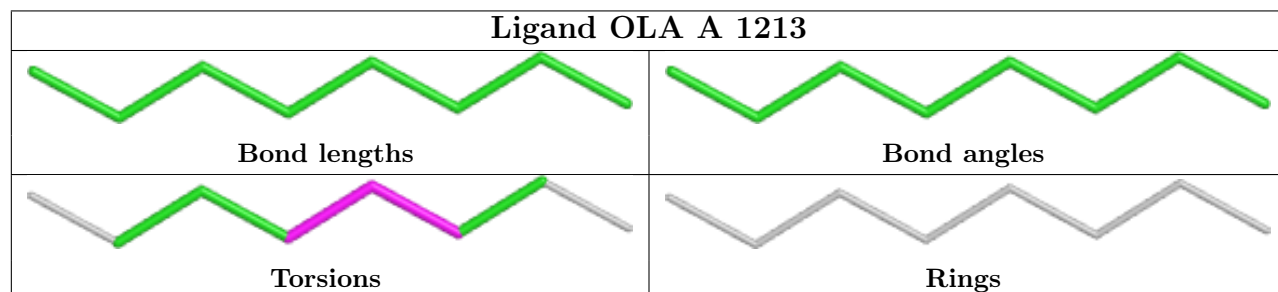
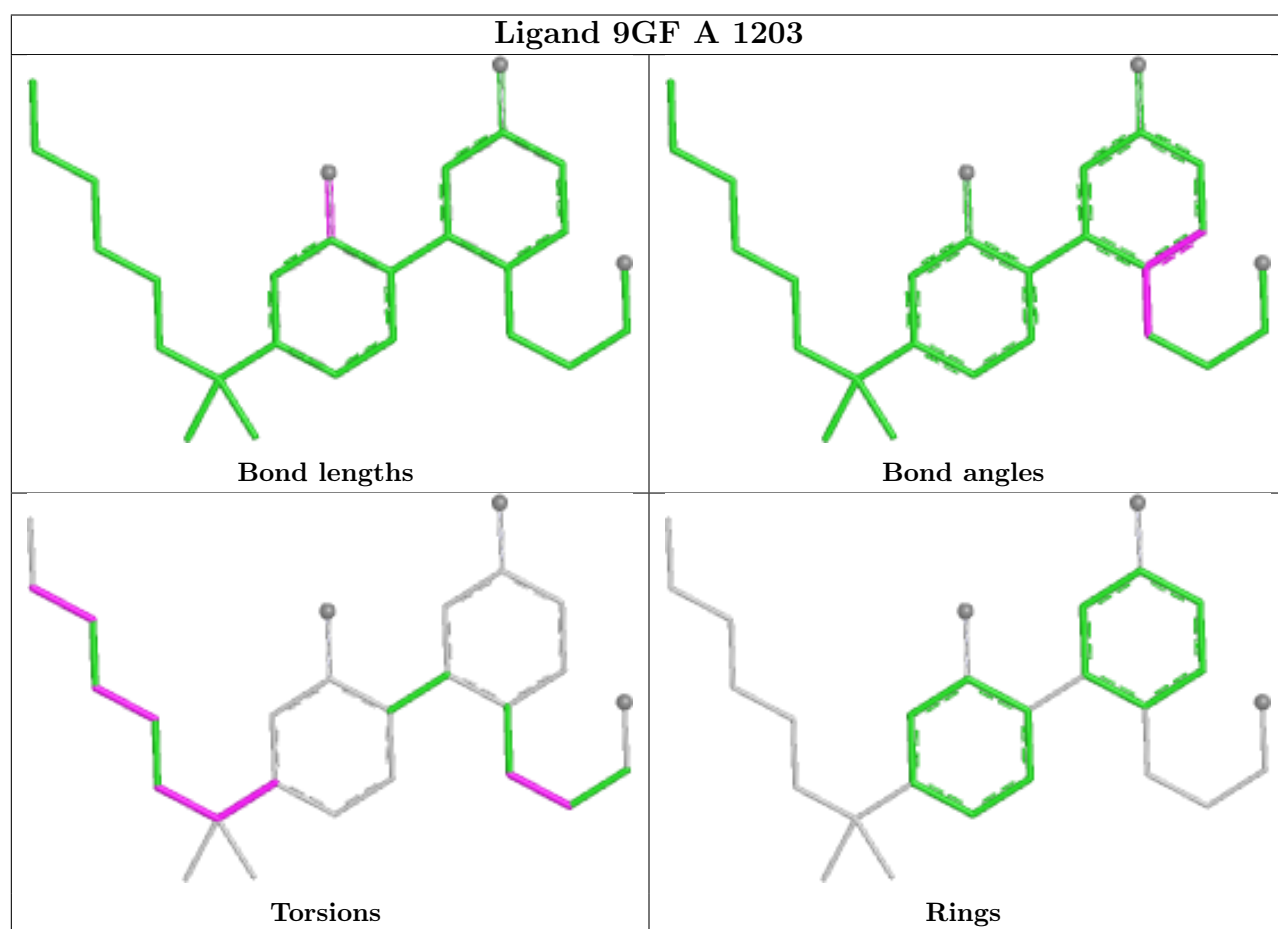
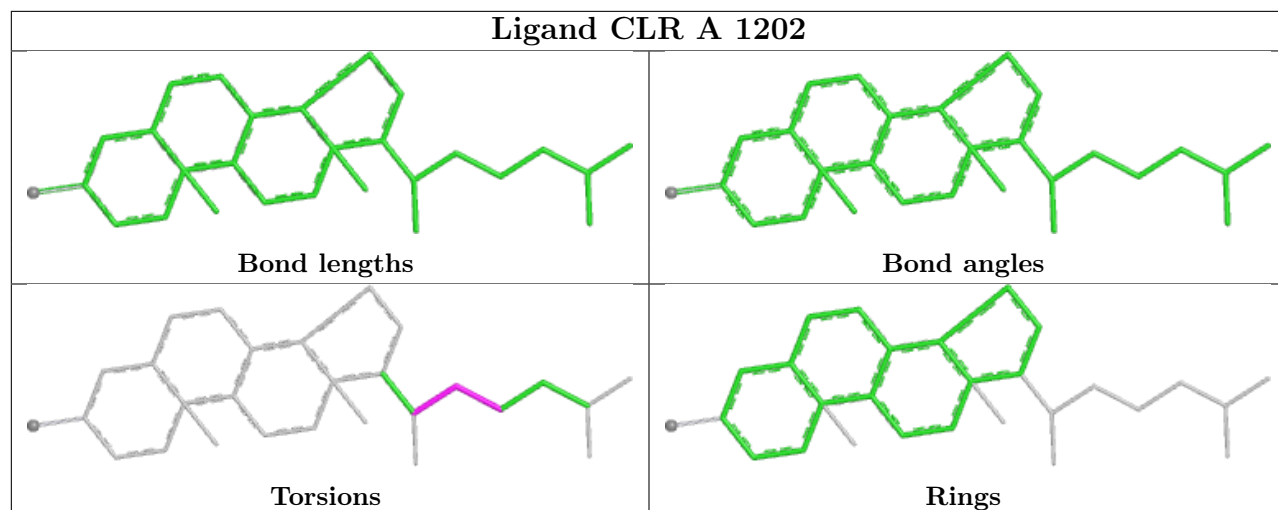
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1216	OLA	1	0
7	A	1212	OLC	2	0
7	A	1211	OLC	3	0
4	A	1204	7IC	1	0
2	A	1202	CLR	1	0
3	A	1203	9GF	1	0
6	A	1207	GOL	1	0

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	486/559 (86%)	0.36	16 (3%) 49 45	63, 104, 161, 188	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1055	ILE	4.2
1	A	1059	SER	2.8
1	A	1058	LEU	2.8
1	A	1121	PHE	2.8
1	A	1012	LEU	2.6
1	A	1143	VAL	2.5
1	A	1067	MET	2.5
1	A	1160	ALA	2.5
1	A	1116	ILE	2.4
1	A	1141	SER	2.3
1	A	1166	LEU	2.3
1	A	1029	MET	2.2
1	A	245	ILE	2.1
1	A	1167	ALA	2.1
1	A	1156	ILE	2.0
1	A	1049	ASP	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

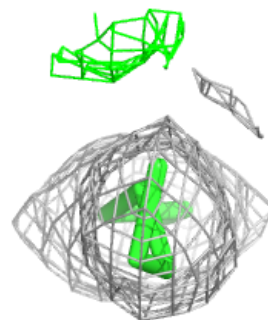
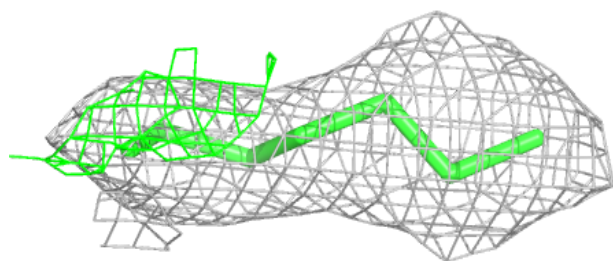
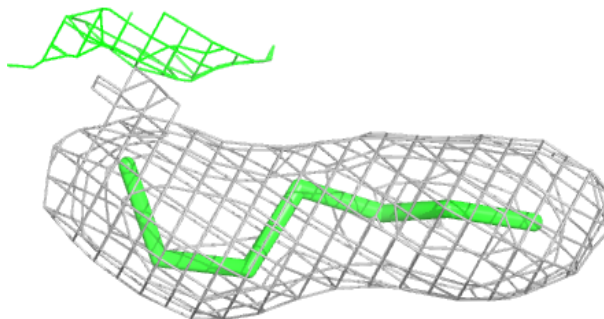
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 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
6	GOL	A	1210	6/6	0.66	0.10	121,123,124,124	0
8	OLA	A	1216	7/20	0.66	0.24	71,73,75,75	0
8	OLA	A	1213	8/20	0.70	0.15	88,89,91,92	0
2	CLR	A	1202	28/28	0.70	0.15	92,97,99,100	0
8	OLA	A	1214	7/20	0.72	0.13	87,90,96,98	0
5	PEG	A	1206	7/7	0.72	0.14	91,97,103,104	0
8	OLA	A	1215	8/20	0.73	0.22	85,91,95,96	0
7	OLC	A	1211	25/25	0.75	0.15	72,90,98,100	0
7	OLC	A	1212	25/25	0.78	0.18	87,97,109,110	0
6	GOL	A	1207	6/6	0.83	0.12	99,103,108,109	0
6	GOL	A	1208	6/6	0.88	0.11	86,88,90,91	0
6	GOL	A	1209	6/6	0.88	0.09	88,90,92,93	0
4	7IC	A	1204	26/26	0.88	0.09	68,74,82,84	0
5	PEG	A	1205	7/7	0.89	0.13	79,81,83,85	0
2	CLR	A	1201	28/28	0.92	0.14	72,81,87,89	0
3	9GF	A	1203	27/27	0.93	0.12	64,71,81,84	0

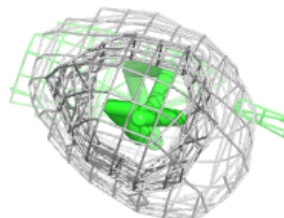
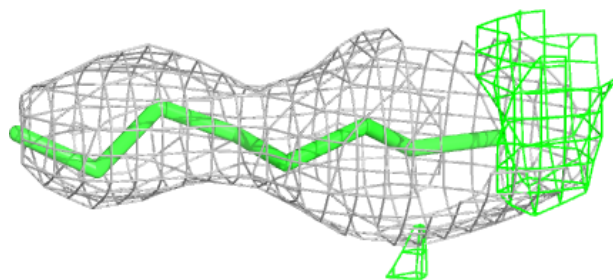
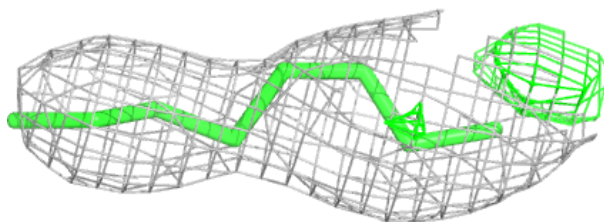
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OLA A 1216:**

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

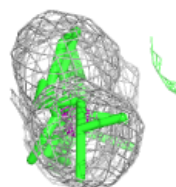
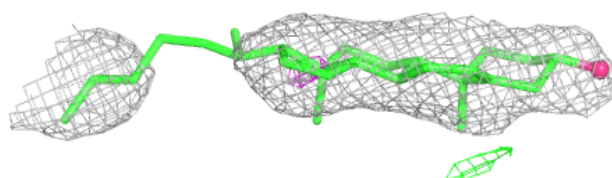
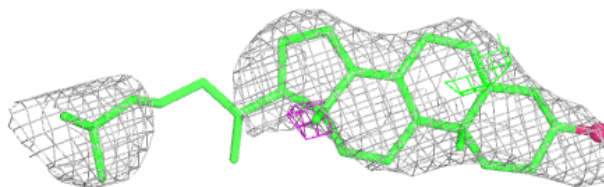
**Electron density around OLA A 1213:**

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

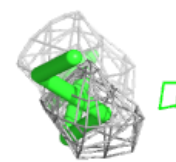
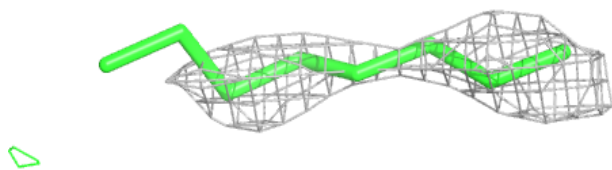
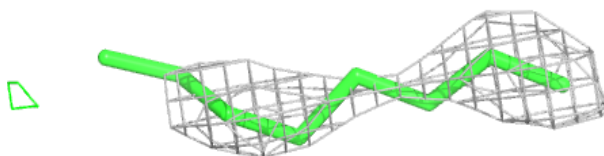


**Electron density around CLR A 1202:**

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

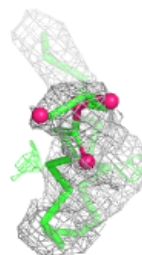
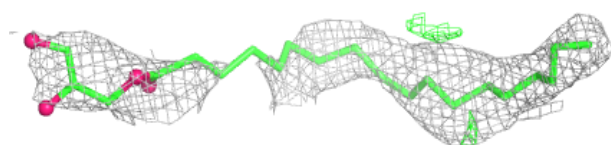
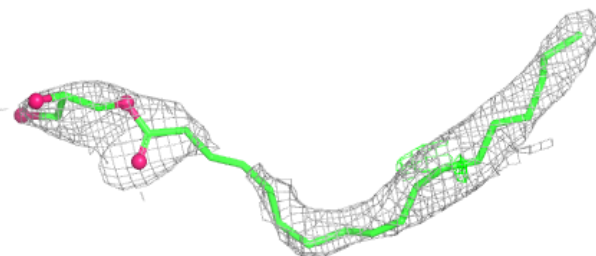
**Electron density around OLA A 1215:**

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

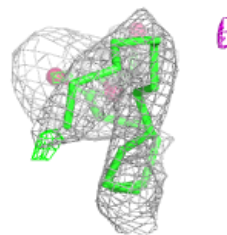
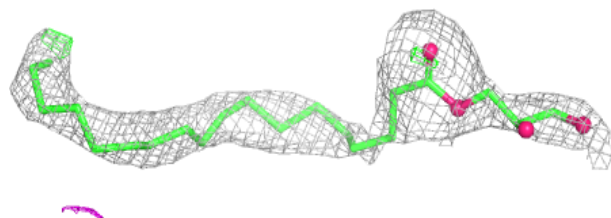
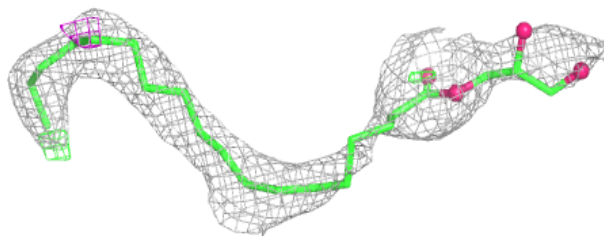


**Electron density around OLC A 1211:**

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

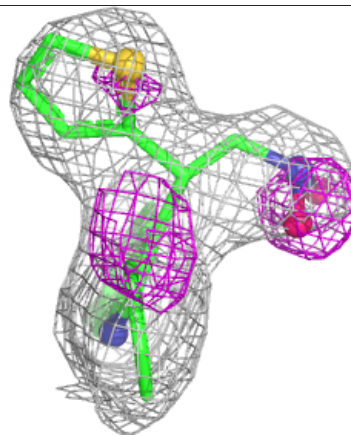
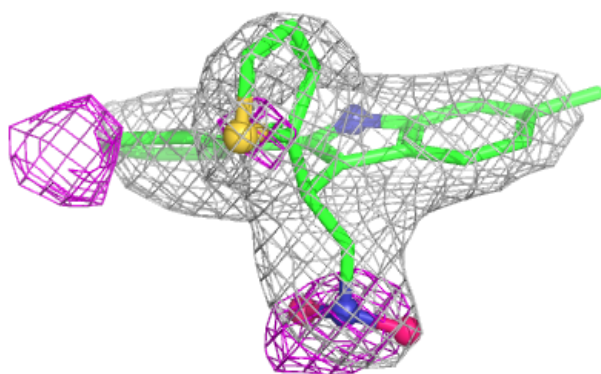
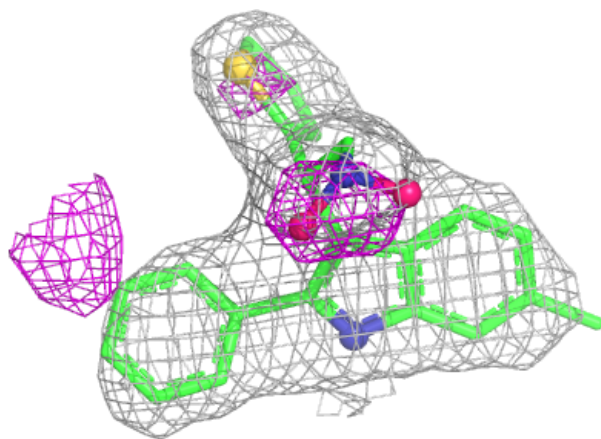
**Electron density around OLC A 1212:**

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

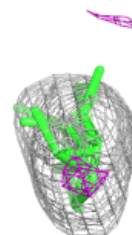
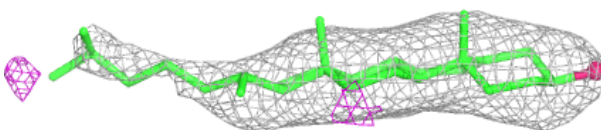
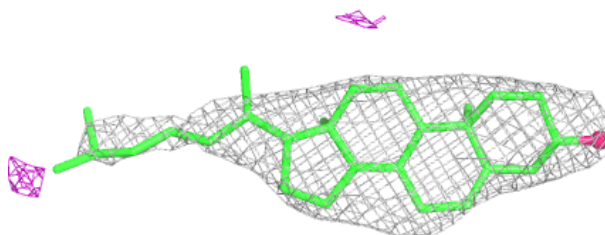


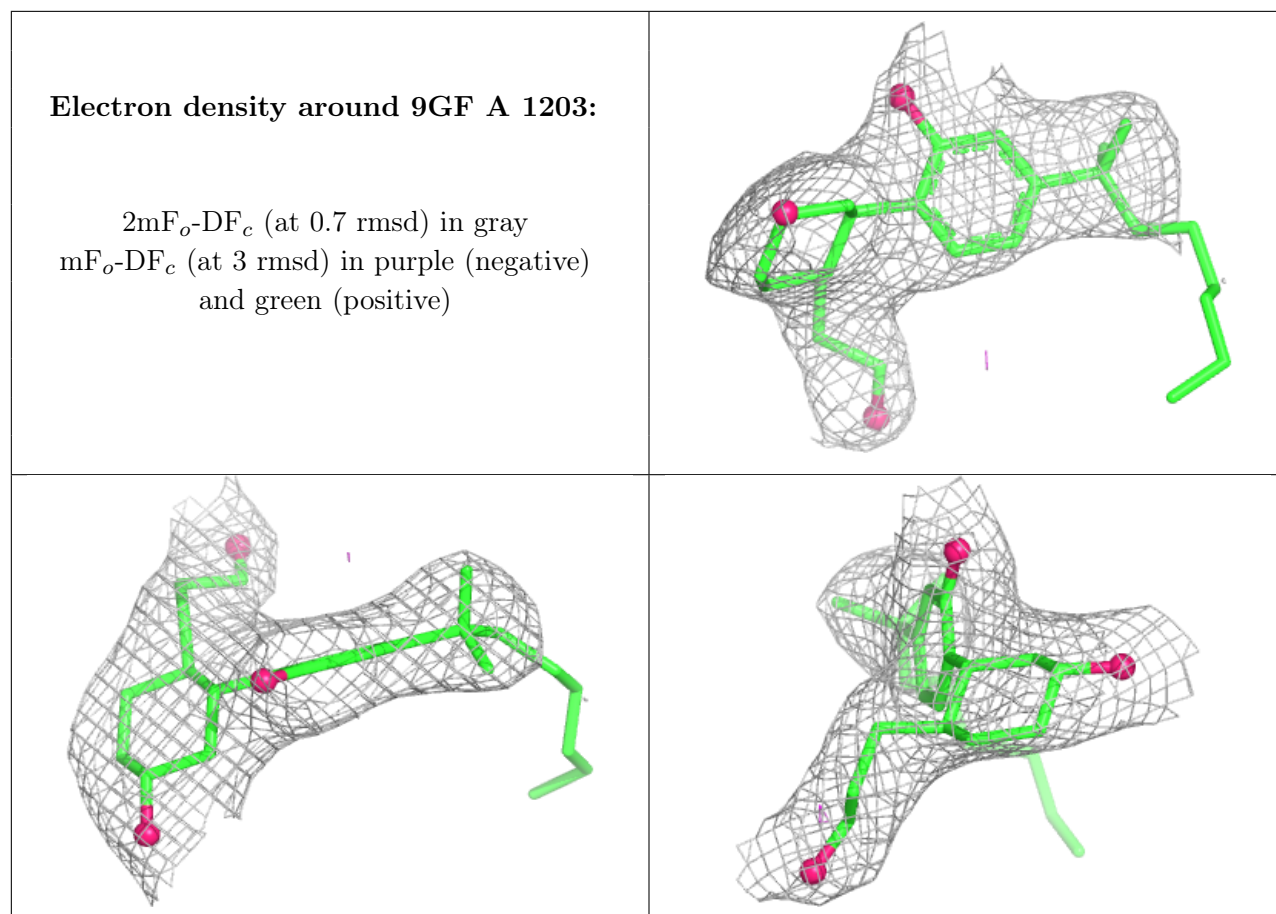
**Electron density around 7IC A 1204:**

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

**Electron density around CLR 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.