



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 06:11 PM JST

PDB ID : 7FEE  
Title : Crystal Structure of protein l  
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.

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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 : 2.28.1  
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) : 2.28.1

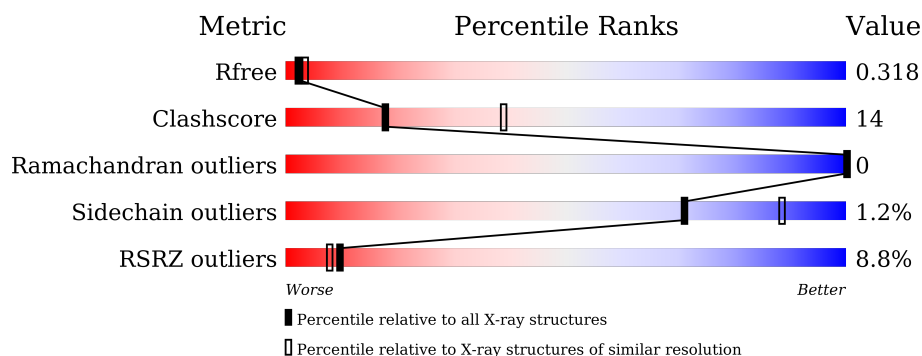
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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	

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
8	OLA	A	1215	-	-	-	X

## 2 Entry composition

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:

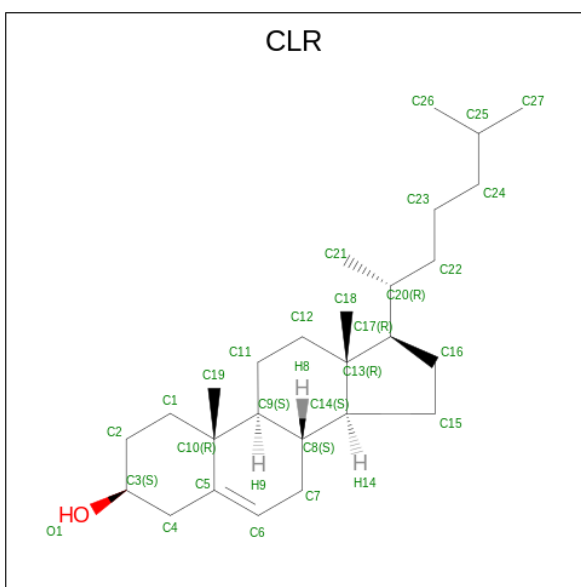
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	expression tag	UNP P21554
A	43	LYS	-	expression tag	UNP P21554
A	44	THR	-	expression tag	UNP P21554
A	45	ILE	-	expression tag	UNP P21554
A	46	ILE	-	expression tag	UNP P21554
A	47	ALA	-	expression tag	UNP P21554
A	48	LEU	-	expression tag	UNP P21554
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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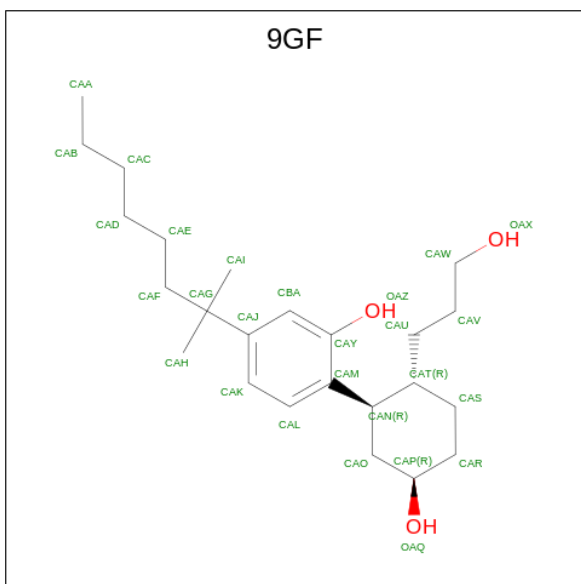
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	LEU	-	linker	UNP P21554
A	86	TYR	-	linker	UNP P21554
A	87	PHE	-	linker	UNP P21554
A	88	GLN	-	linker	UNP P21554
A	89	GLY	-	linker	UNP P21554
A	203	LYS	SER	engineered mutation	UNP P21554
A	210	ALA	THR	engineered mutation	UNP P21554
A	273	LYS	GLU	engineered 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 (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



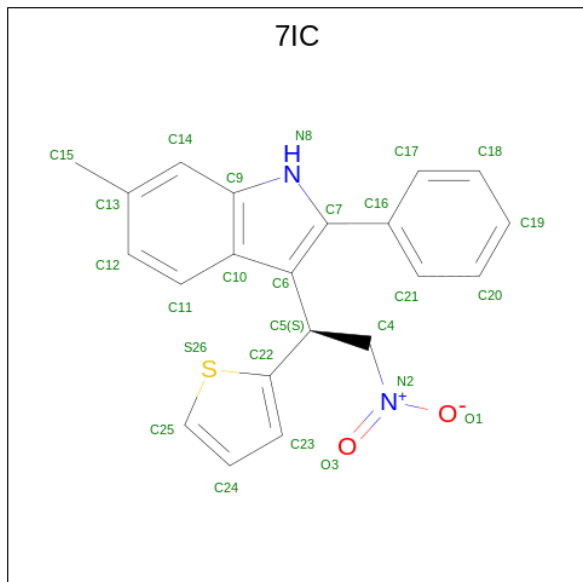
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	27	1		
2	A	1	Total	C	O	0	0
			28	27	1		

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



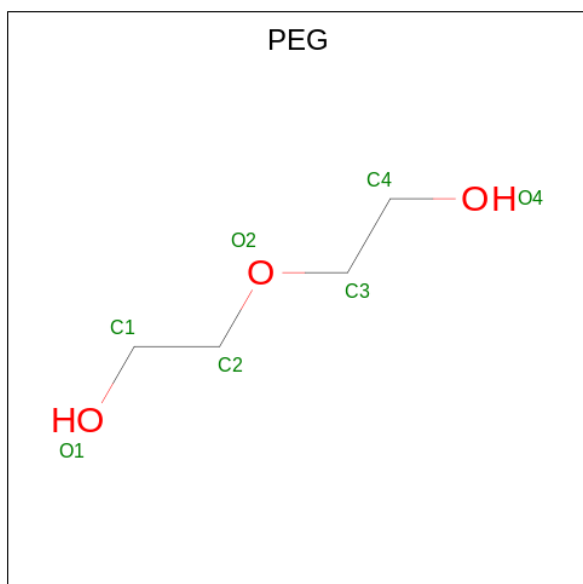
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			27	24	3		

- Molecule 4 is 6-methyl-3-[(1S)-2-nitro-1-thiophen-2-yl-ethyl]-2-phenyl-1H-indole (three-letter code: 7IC) (formula:  $C_{21}H_{18}N_2O_2S$ ).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



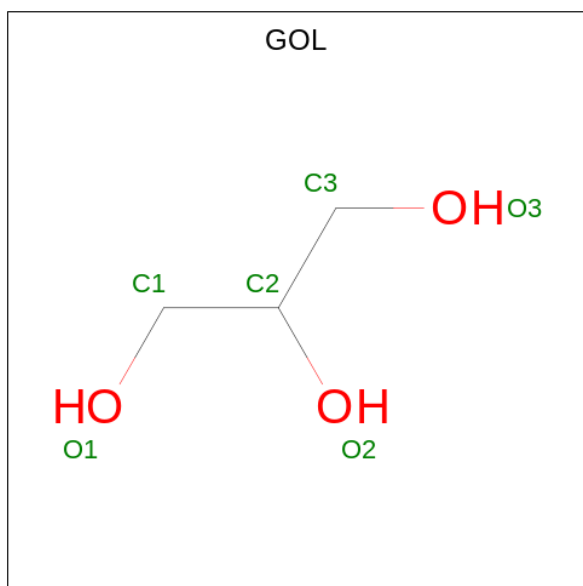
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

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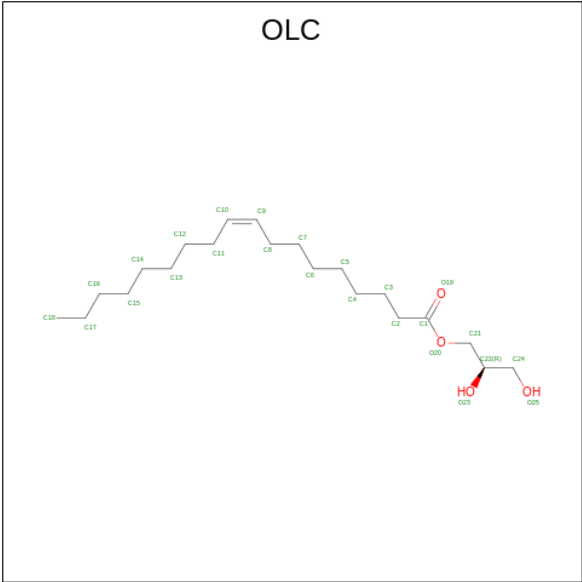
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



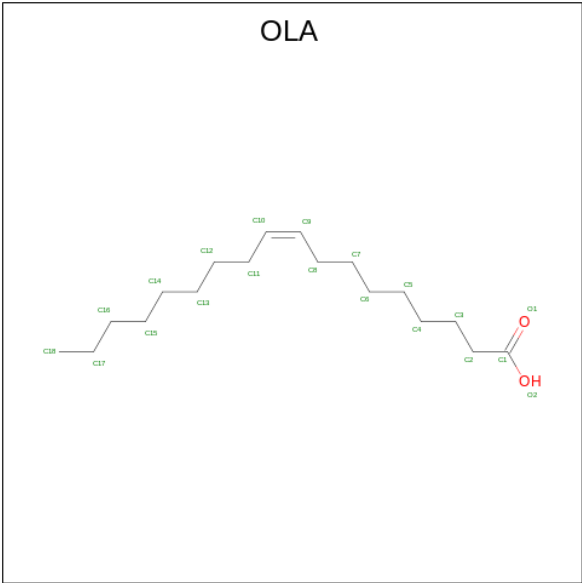
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: 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 (three-letter code: OLA) (formula: C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>).



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

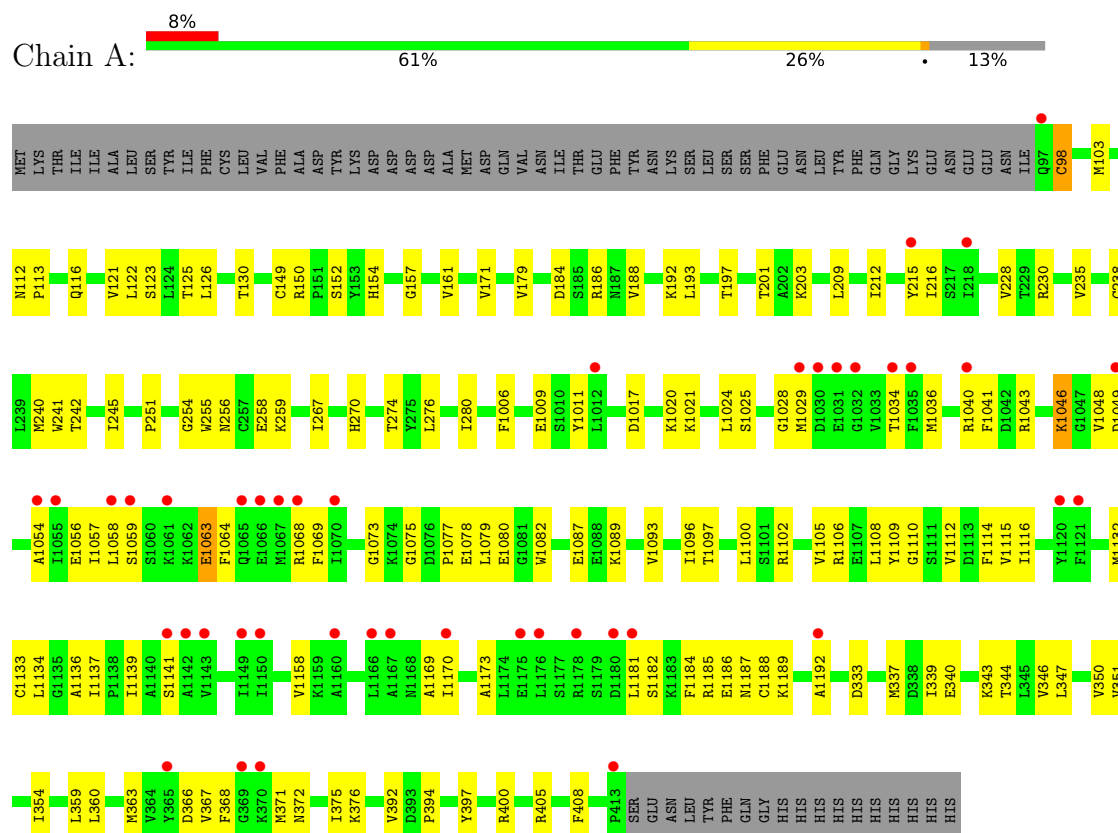
- Molecule 9 is water.

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

### 3 Residue-property plots

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) 99.8 (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)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.293 , 0.319 0.290 , 0.318	Depositor DCC
$R_{free}$ test set	1597 reflections (9.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.9	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 77.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	107.0	wwPDB-VP

Xtriage'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, 9GF, PEG, GOL, OLC, OLA, CLR

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	0.30	0/3899	0.51	0/5274

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	3815	0	3920	111	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	112	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 (112) 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: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:366:ASP:HA	1:A:371:MET:HE1	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1110:GLY:HA2	1:A:1134:LEU:O	2.13	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:98:CYS:HB3	1:A:103:MET:HE2	1.95	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: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
1:A:1063:GLU:H	1:A:1063:GLU:CD	2.19	0.44
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:256:ASN:HD21	1:A:259:LYS:HD3	1.83	0.44
1:A:267:ILE:O	3:A:1203:9GF:OAO	2.35	0.44
1:A:1059:SER:HA	1:A:1064:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:GLY:O	1:A:1097:THR:HA	2.17	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:212:ILE:O	1:A:216:ILE:HG23	2.20	0.41
1:A:366:ASP:CA	1:A:371:MET:HE1	2.50	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%)	411 (99%)	5 (1%)	71	88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	215	TYR
1	A	1046	LYS
1	A	1063	GLU
1	A	1184	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	HIS
1	A	1187	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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
3	9GF	A	1203	-	28,28,28	0.63	1 (3%)	37,38,38	0.83	1 (2%)
7	OLC	A	1211	-	24,24,24	1.14	1 (4%)	25,25,25	1.27	2 (8%)
8	OLA	A	1213	-	7,7,19	0.27	0	6,6,19	0.50	0
6	GOL	A	1209	-	5,5,5	0.94	0	5,5,5	1.01	0
8	OLA	A	1216	-	6,6,19	0.28	0	5,5,19	0.42	0
6	GOL	A	1210	-	5,5,5	0.92	0	5,5,5	1.04	0
2	CLR	A	1202	-	31,31,31	0.27	0	48,48,48	0.39	0
4	7IC	A	1204	-	25,29,29	2.23	6 (24%)	24,41,41	2.18	4 (16%)
8	OLA	A	1214	-	6,6,19	0.26	0	5,5,19	0.48	0
8	OLA	A	1215	-	7,7,19	0.26	0	6,6,19	0.49	0
5	PEG	A	1205	-	6,6,6	0.10	0	5,5,5	0.09	0
5	PEG	A	1206	-	6,6,6	0.11	0	5,5,5	0.07	0
6	GOL	A	1207	-	5,5,5	0.96	0	5,5,5	0.99	0
2	CLR	A	1201	-	31,31,31	0.29	0	48,48,48	0.44	0
6	GOL	A	1208	-	5,5,5	0.90	0	5,5,5	0.98	0
7	OLC	A	1212	-	24,24,24	1.13	1 (4%)	25,25,25	1.25	2 (8%)

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	9GF	A	1203	-	-	8/21/34/34	0/2/2/2
7	OLC	A	1211	-	-	8/24/24/24	-
8	OLA	A	1213	-	-	2/5/5/17	-
6	GOL	A	1209	-	-	0/4/4/4	-
8	OLA	A	1216	-	-	3/4/4/17	-
6	GOL	A	1210	-	-	4/4/4/4	-
2	CLR	A	1202	-	-	2/10/68/68	0/4/4/4
4	7IC	A	1204	-	-	1/8/28/28	0/4/4/4
8	OLA	A	1214	-	-	0/4/4/17	-
8	OLA	A	1215	-	-	1/5/5/17	-
5	PEG	A	1205	-	-	2/4/4/4	-
5	PEG	A	1206	-	-	2/4/4/4	-
6	GOL	A	1207	-	-	0/4/4/4	-
2	CLR	A	1201	-	-	1/10/68/68	0/4/4/4
6	GOL	A	1208	-	-	1/4/4/4	-
7	OLC	A	1212	-	-	12/24/24/24	-

All (9) 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	C16-C7	4.27	1.53	1.49
4	A	1204	7IC	C6-C10	3.38	1.44	1.40
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-N8	-2.63	1.32	1.37
3	A	1203	9GF	OAZ-CAY	2.13	1.40	1.36
4	A	1204	7IC	C24-C25	2.08	1.40	1.34
4	A	1204	7IC	C22-S26	-2.01	1.69	1.73

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1204	7IC	C24-C25-S26	-8.84	105.80	112.98
7	A	1212	OLC	C8-C9-C10	3.68	152.96	124.73
7	A	1211	OLC	C8-C9-C10	3.66	152.80	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1204	7IC	C7-N8-C9	3.64	111.38	103.90
7	A	1211	OLC	O20-C1-C2	2.82	120.76	111.91
4	A	1204	7IC	C23-C22-S26	-2.82	104.77	111.36
7	A	1212	OLC	O20-C1-C2	2.62	120.12	111.91
4	A	1204	7IC	C6-C5-C22	-2.28	107.86	111.17
3	A	1203	9GF	CAU-CAT-CAS	-2.27	106.76	112.57

There are no chirality outliers.

All (47) 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
7	A	1212	OLC	C21-C22-C24-O25
7	A	1212	OLC	O20-C21-C22-C24
7	A	1212	OLC	O20-C21-C22-O23
3	A	1203	9GF	CAC-CAD-CAE-CAF
7	A	1211	OLC	C14-C15-C16-C17
7	A	1212	OLC	C3-C4-C5-C6
6	A	1210	GOL	O1-C1-C2-C3
6	A	1210	GOL	C1-C2-C3-O3
7	A	1211	OLC	C3-C4-C5-C6
8	A	1213	OLA	C13-C14-C15-C16
7	A	1212	OLC	O23-C22-C24-O25
7	A	1212	OLC	C6-C7-C8-C9
3	A	1203	9GF	CAF-CAG-CAJ-CAK
3	A	1203	9GF	CAF-CAG-CAJ-CBA
8	A	1213	OLA	C12-C13-C14-C15
8	A	1216	OLA	C14-C15-C16-C17
7	A	1211	OLC	C10-C11-C12-C13
8	A	1215	OLA	C12-C13-C14-C15
2	A	1202	CLR	C20-C22-C23-C24
3	A	1203	9GF	CAA-CAB-CAC-CAD
7	A	1212	OLC	C13-C14-C15-C16
5	A	1206	PEG	C1-C2-O2-C3
8	A	1216	OLA	C13-C14-C15-C16
8	A	1216	OLA	C12-C13-C14-C15
7	A	1211	OLC	C5-C6-C7-C8
6	A	1208	GOL	O1-C1-C2-C3
7	A	1211	OLC	C11-C12-C13-C14
2	A	1202	CLR	C21-C20-C22-C23

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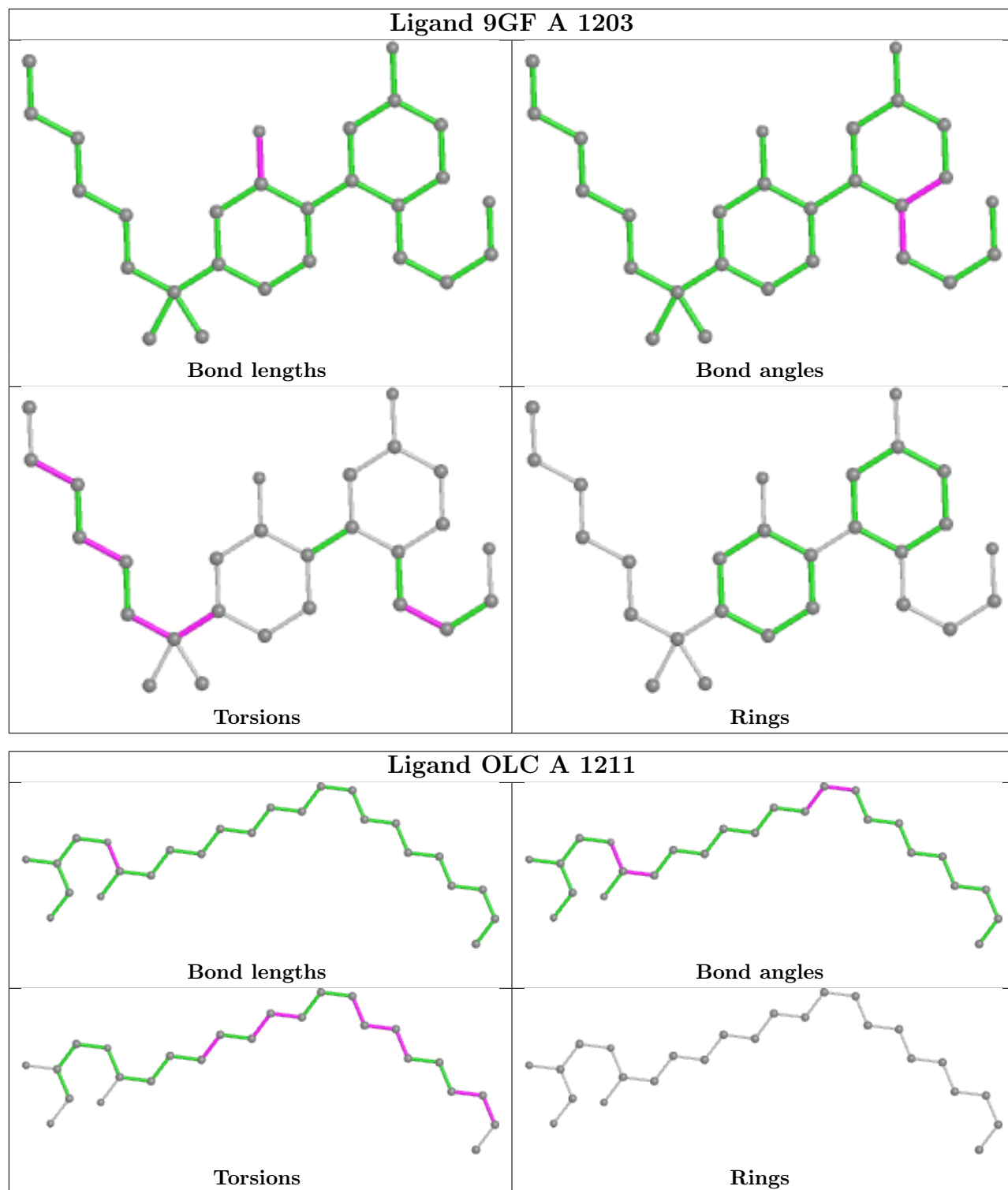
Mol	Chain	Res	Type	Atoms
7	A	1212	OLC	C15-C16-C17-C18
6	A	1210	GOL	O2-C2-C3-O3
7	A	1211	OLC	C6-C7-C8-C9
7	A	1212	OLC	C7-C8-C9-C10
7	A	1211	OLC	C15-C16-C17-C18
7	A	1212	OLC	C12-C13-C14-C15
4	A	1204	7IC	C5-C4-N2-O3
5	A	1205	PEG	O1-C1-C2-O2
5	A	1205	PEG	C1-C2-O2-C3
7	A	1212	OLC	C4-C5-C6-C7
6	A	1210	GOL	O1-C1-C2-O2
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

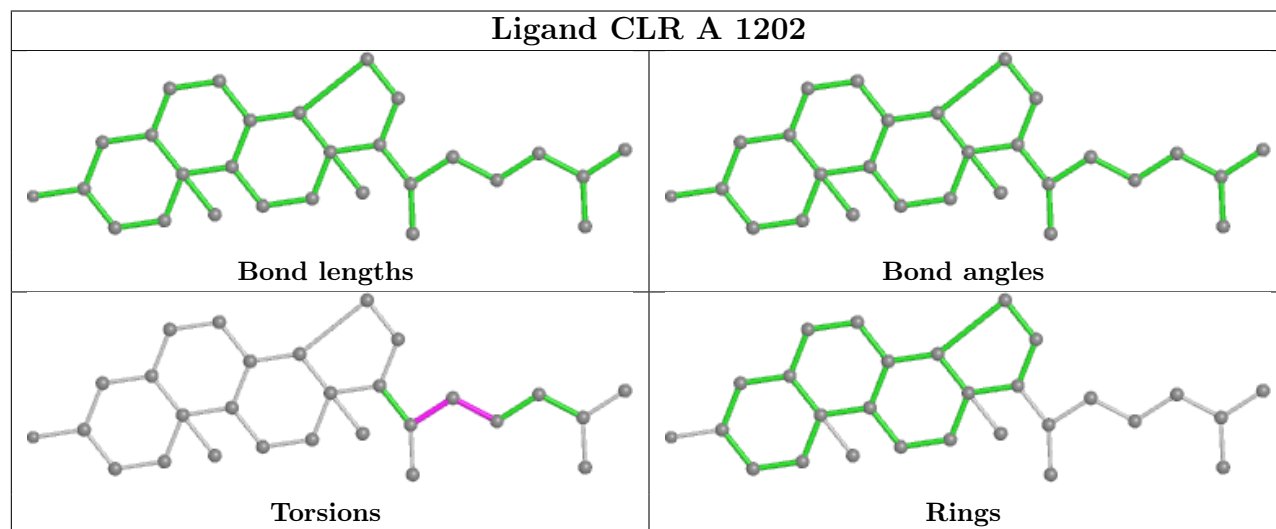
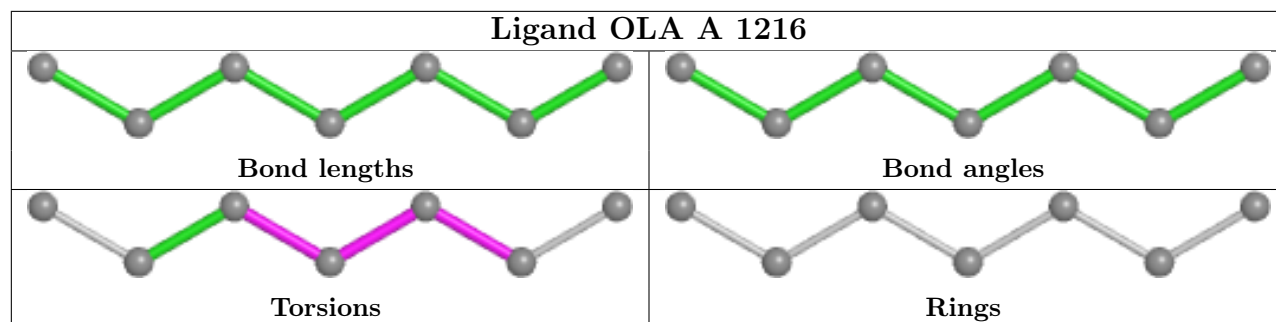
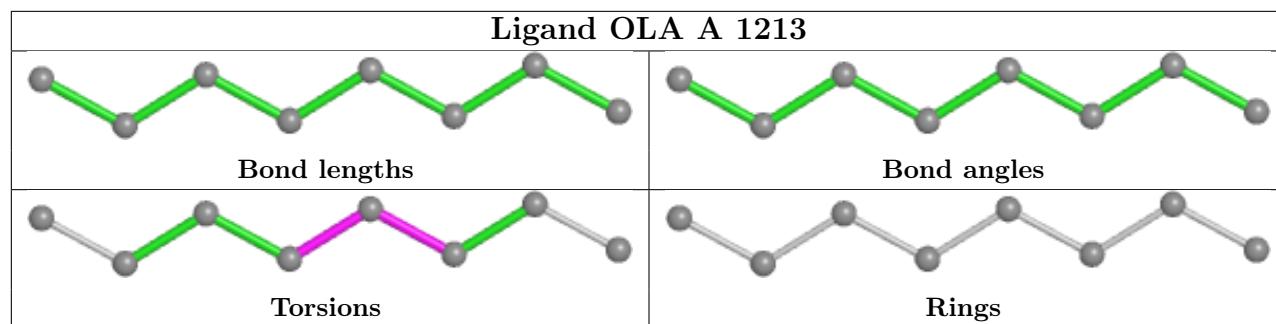
There are no ring outliers.

7 monomers are involved in 10 short contacts:

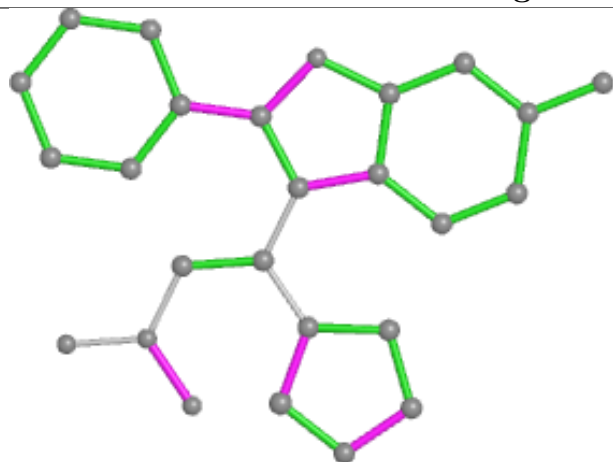
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	9GF	1	0
7	A	1211	OLC	3	0
8	A	1216	OLA	1	0
2	A	1202	CLR	1	0
4	A	1204	7IC	1	0
6	A	1207	GOL	1	0
7	A	1212	OLC	2	0

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.

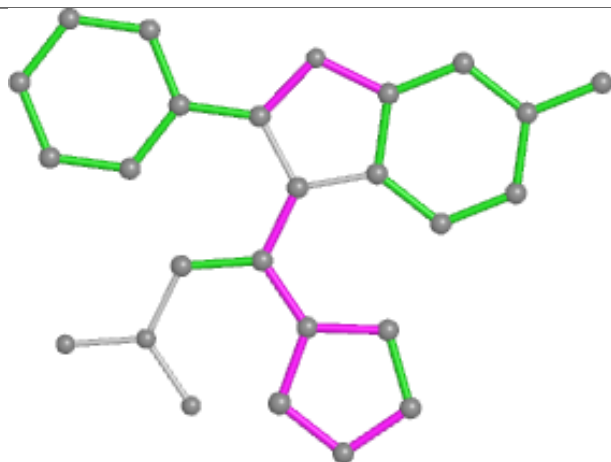




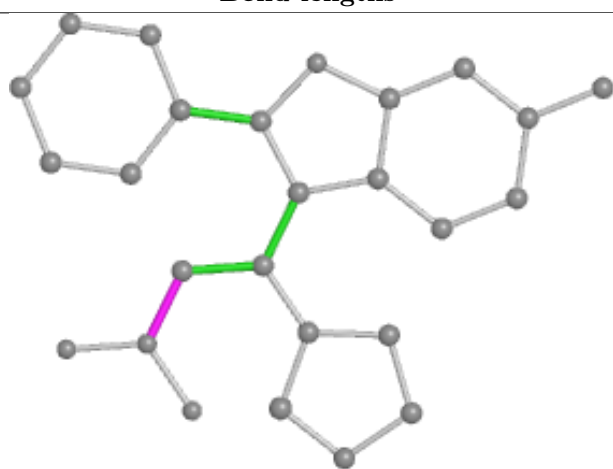
## Ligand 7IC A 1204



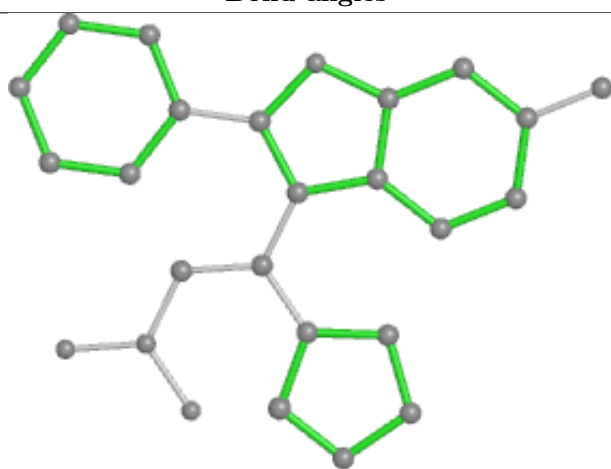
Bond lengths



Bond angles



Torsions



Rings

## Ligand OLA A 1215



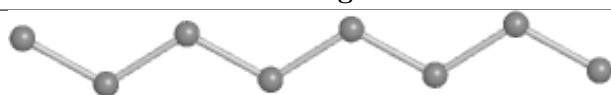
Bond lengths



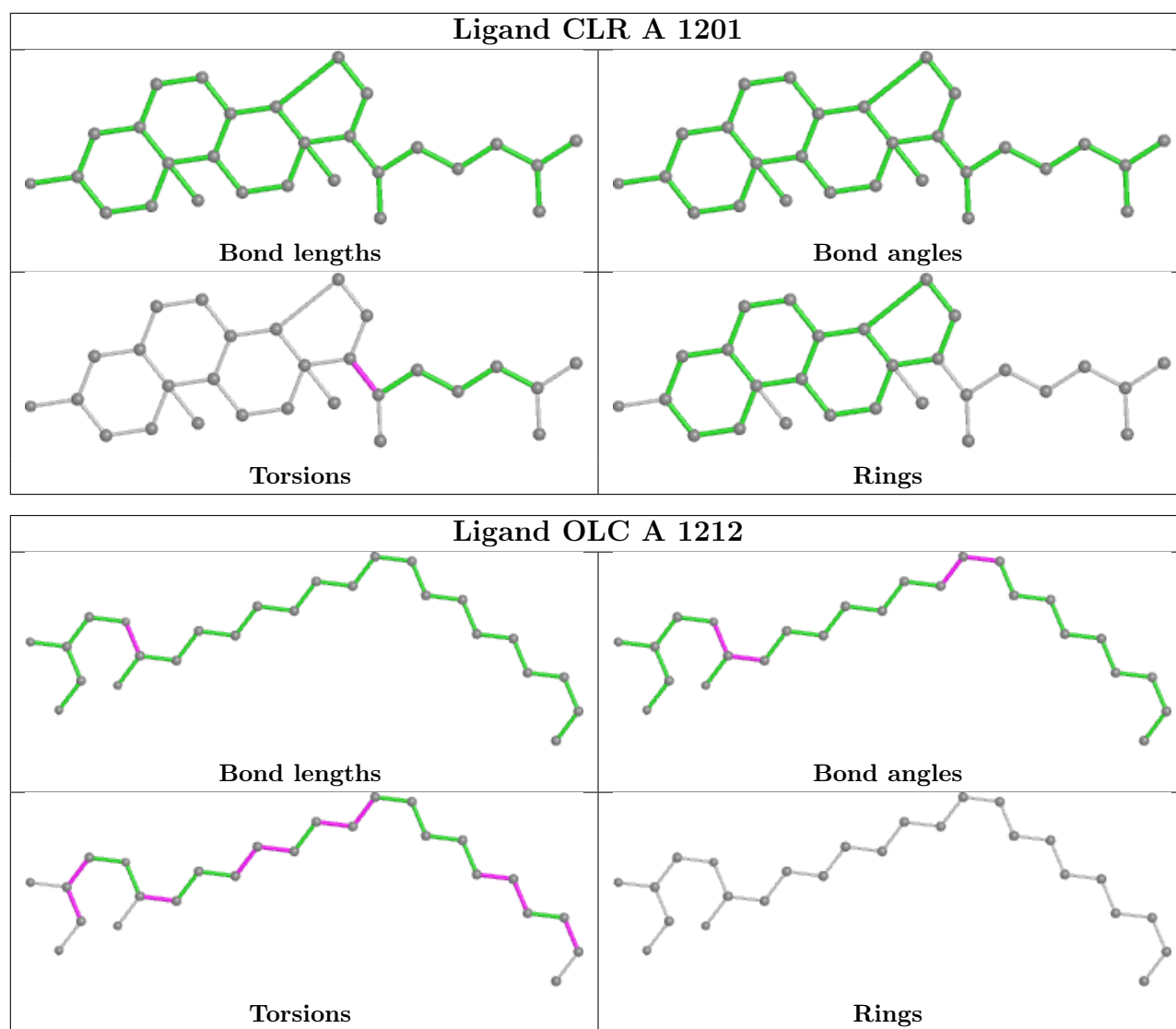
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.45	43 (8%) 10 8	63, 104, 161, 188	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1032	GLY	7.3
1	A	1058	LEU	6.8
1	A	1067	MET	5.2
1	A	1030	ASP	4.7
1	A	1068	ARG	4.3
1	A	1029	MET	4.2
1	A	1166	LEU	3.7
1	A	1143	VAL	3.6
1	A	1178	ARG	3.6
1	A	1121	PHE	3.2
1	A	1065	GLN	3.2
1	A	370	LYS	3.2
1	A	1150	ILE	3.2
1	A	1142	ALA	3.1
1	A	1120	TYR	3.0
1	A	1167	ALA	2.9
1	A	1035	PHE	2.9
1	A	1149	ILE	2.9
1	A	365	TYR	2.8
1	A	1054	ALA	2.8
1	A	1170	ILE	2.8
1	A	1180	ASP	2.7
1	A	1066	GLU	2.7
1	A	1181	LEU	2.6
1	A	1031	GLU	2.6
1	A	1059	SER	2.6
1	A	1160	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1055	ILE	2.5
1	A	1040	ARG	2.4
1	A	215	TYR	2.4
1	A	1141	SER	2.4
1	A	1175	GLU	2.4
1	A	1192	ALA	2.3
1	A	1176	LEU	2.3
1	A	1070	ILE	2.3
1	A	1012	LEU	2.2
1	A	1034	THR	2.2
1	A	1061	LYS	2.2
1	A	369	GLY	2.1
1	A	97	GLN	2.1
1	A	413	PRO	2.1
1	A	1049	ASP	2.1
1	A	218	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

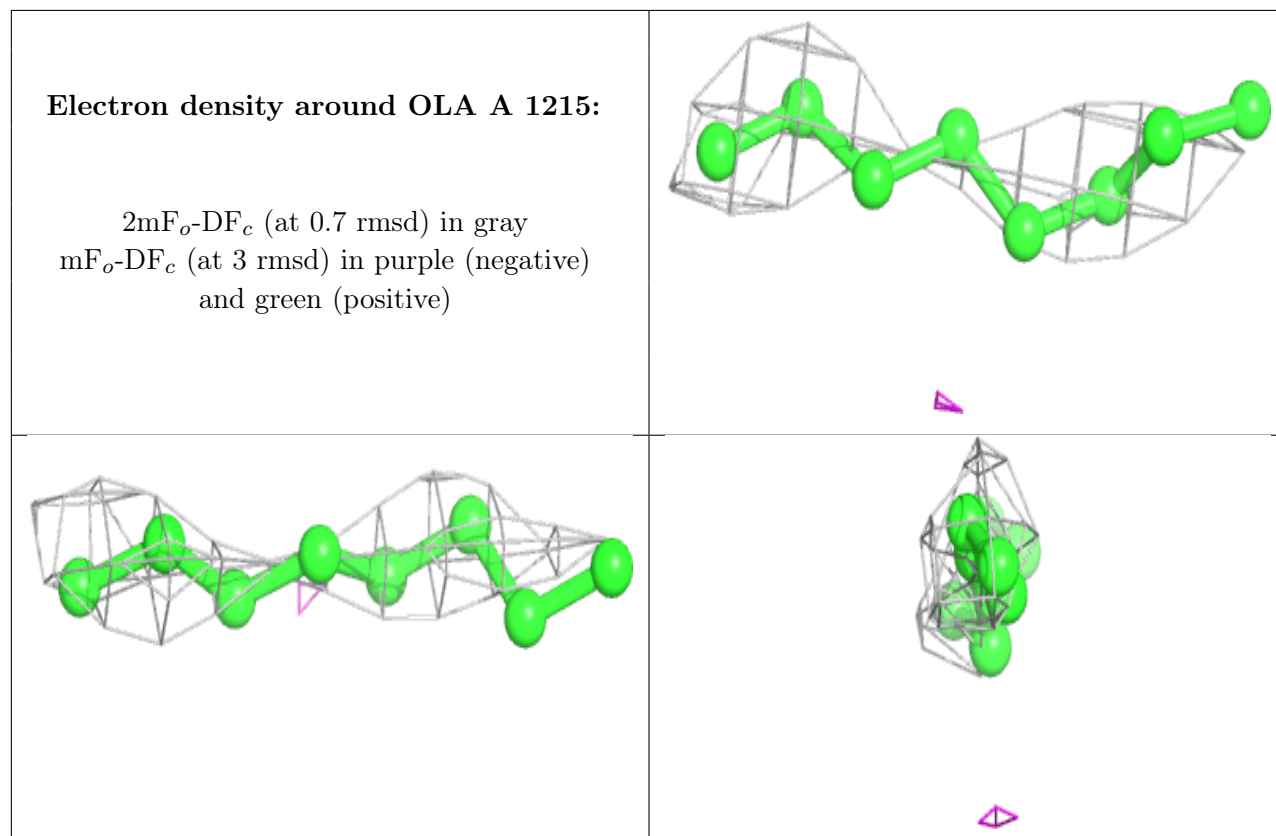
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	OLA	A	1215	8/20	0.56	0.56	85,91,95,96	0
8	OLA	A	1213	8/20	0.64	0.30	88,89,91,92	0
6	GOL	A	1210	6/6	0.65	0.19	121,123,124,124	0
7	OLC	A	1211	25/25	0.68	0.33	72,90,98,100	0
7	OLC	A	1212	25/25	0.73	0.39	87,97,109,110	0
2	CLR	A	1202	28/28	0.74	0.35	92,97,99,100	0
8	OLA	A	1214	7/20	0.77	0.28	87,90,96,98	0

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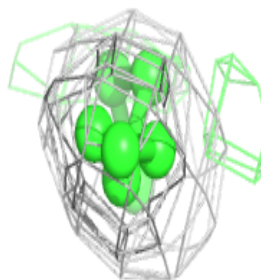
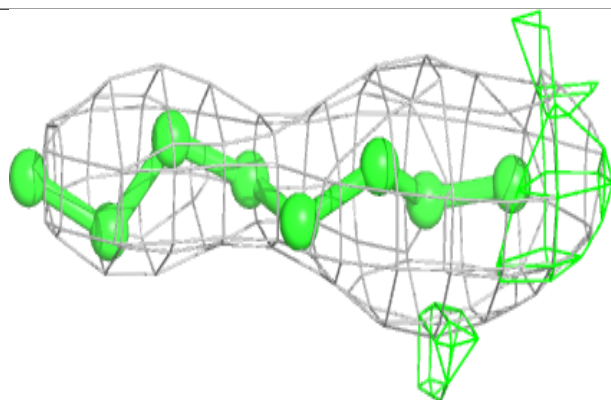
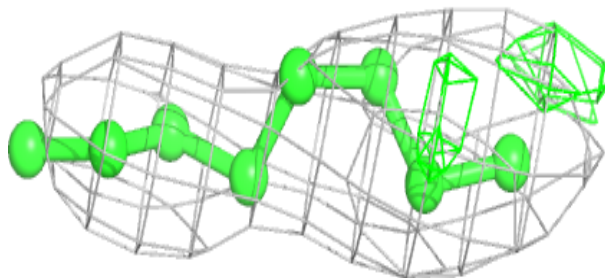
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	A	1206	7/7	0.77	0.27	91,97,103,104	0
5	PEG	A	1205	7/7	0.83	0.21	79,81,83,85	0
6	GOL	A	1209	6/6	0.84	0.20	88,90,92,93	0
8	OLA	A	1216	7/20	0.86	0.18	71,73,75,75	0
6	GOL	A	1208	6/6	0.87	0.25	86,88,90,91	0
6	GOL	A	1207	6/6	0.89	0.18	99,103,108,109	0
3	9GF	A	1203	27/27	0.91	0.28	64,71,81,84	0
2	CLR	A	1201	28/28	0.92	0.34	72,81,87,89	0
4	7IC	A	1204	26/26	0.93	0.28	68,74,82,84	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.

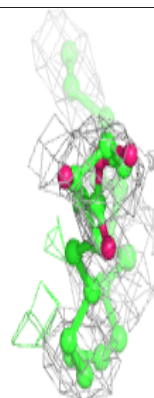
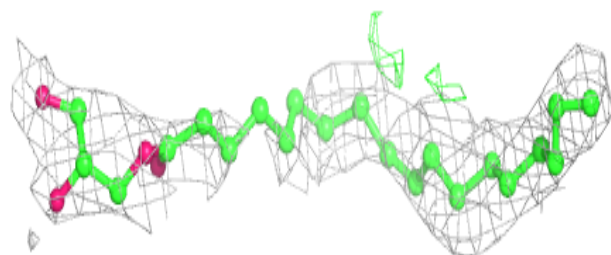
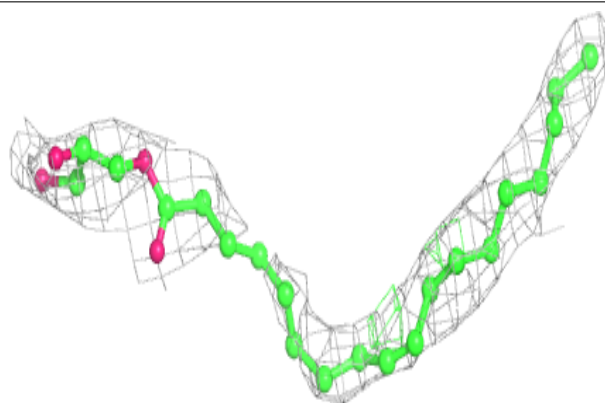


**Electron density around OLA A 1213:**

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

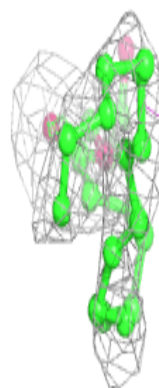
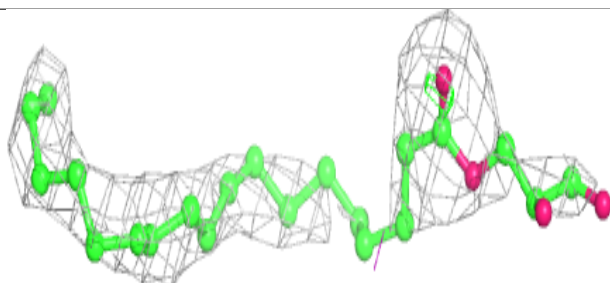
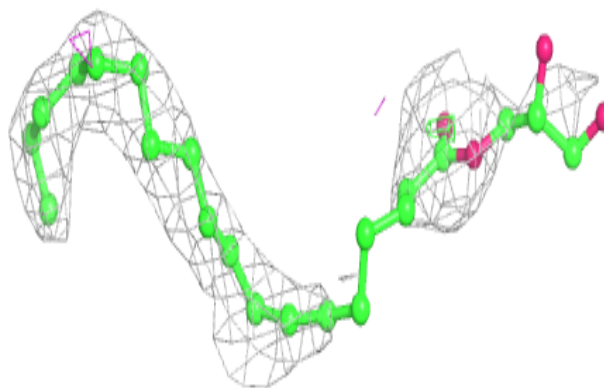
**Electron density around OLC A 1211:**

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

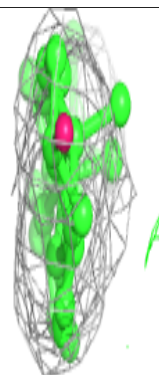
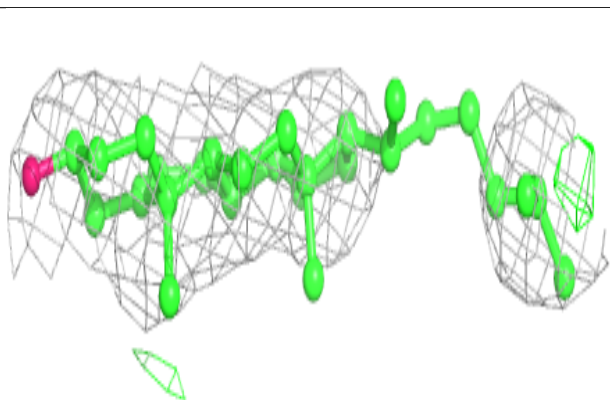
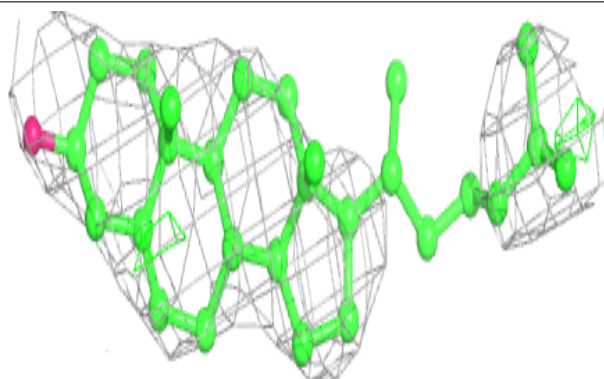


**Electron density around OLC A 1212:**

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

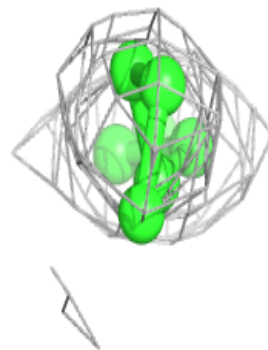
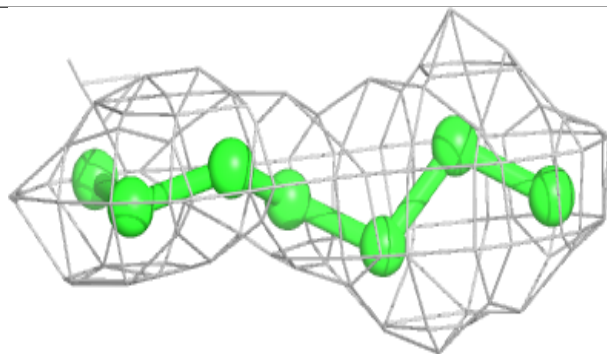
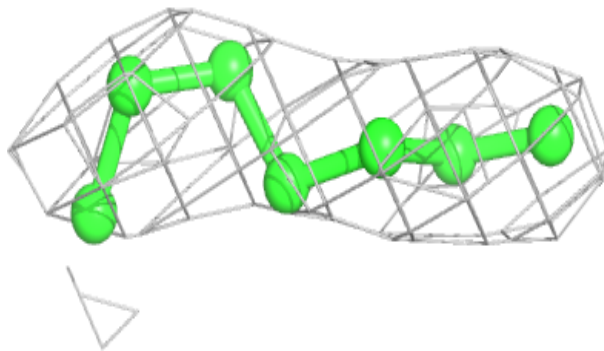
**Electron density around CLR A 1202:**

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



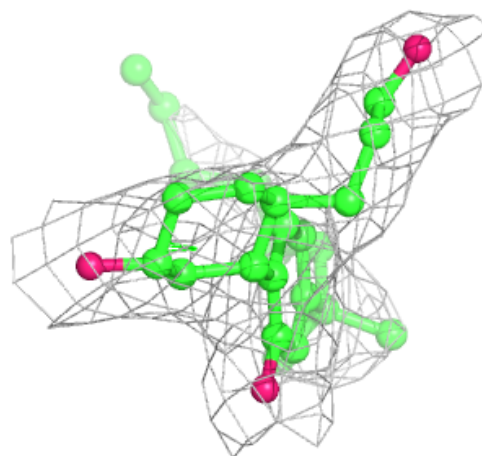
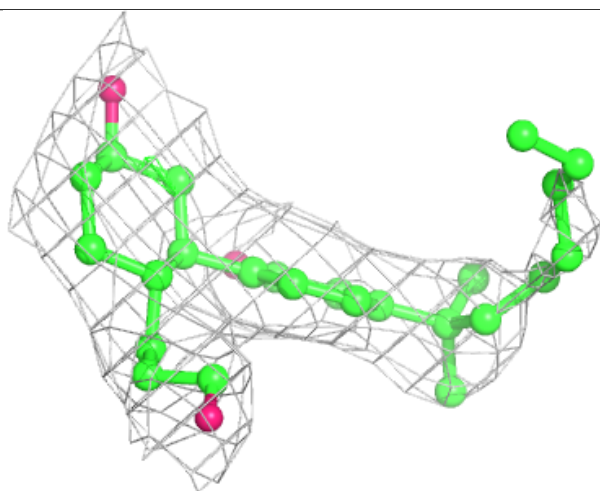
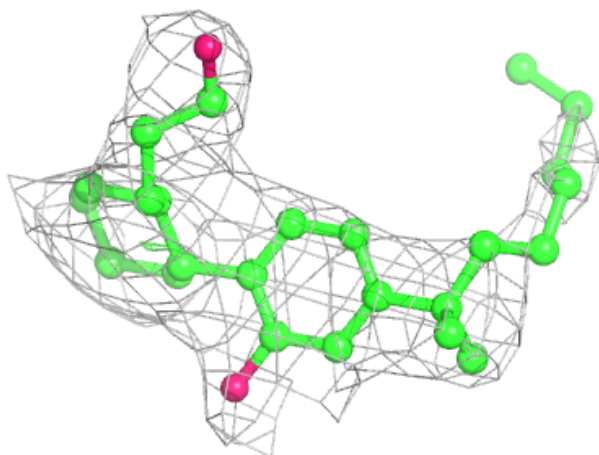
**Electron density around OLA A 1216:**

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



**Electron density around 9GF A 1203:**

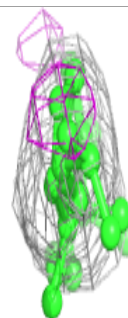
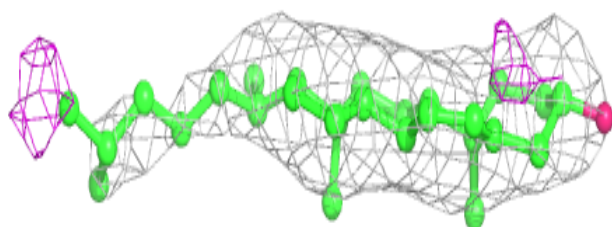
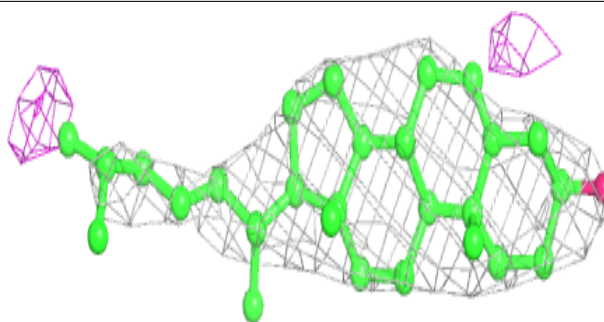
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



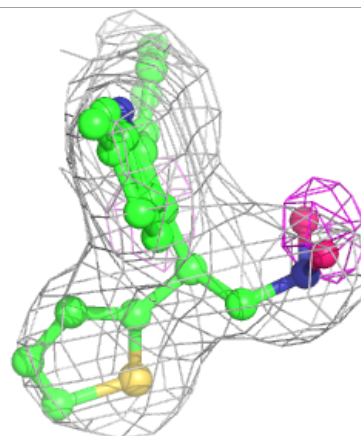
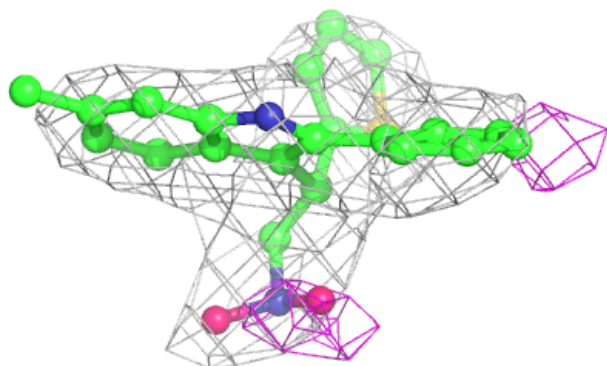
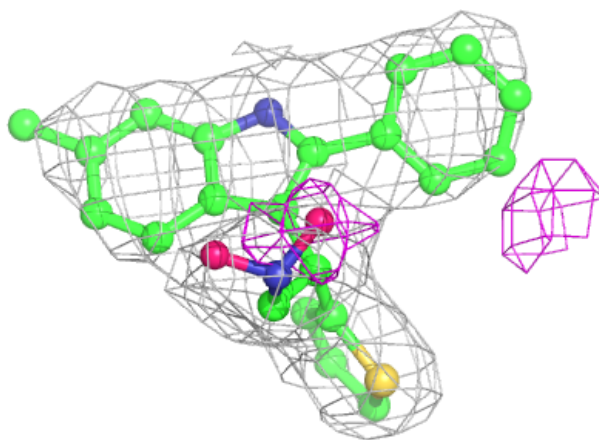


**Electron density around CLR A 1201:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.