



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 05:46 PM JST

PDB ID : 7WLF  
Title : Crystal structure of the HSA Fe complex  
Authors : Bai, H.H.; Xie, L.L.; Wang, W.M.; Wang, H.F.  
Deposited on : 2022-01-13  
Resolution : 2.40 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 : 2.36  
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) : 2.36

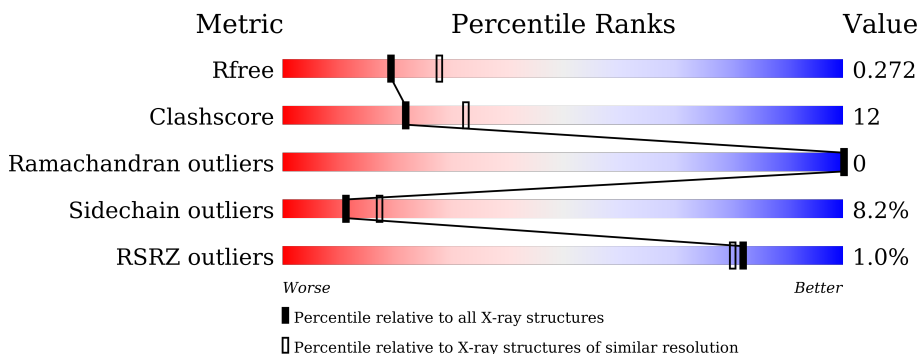
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	585	

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
5	PLM	A	614	-	-	-	X
7	CL	A	620	-	-	-	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
7	CL	A	628	-	-	X	X
7	CL	A	629	-	-	X	-

## 2 Entry composition [i](#)

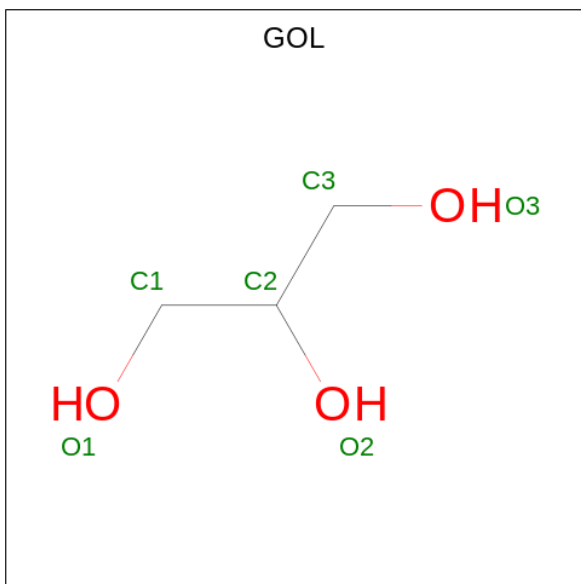
There are 8 unique types of molecules in this entry. The entry contains 4853 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

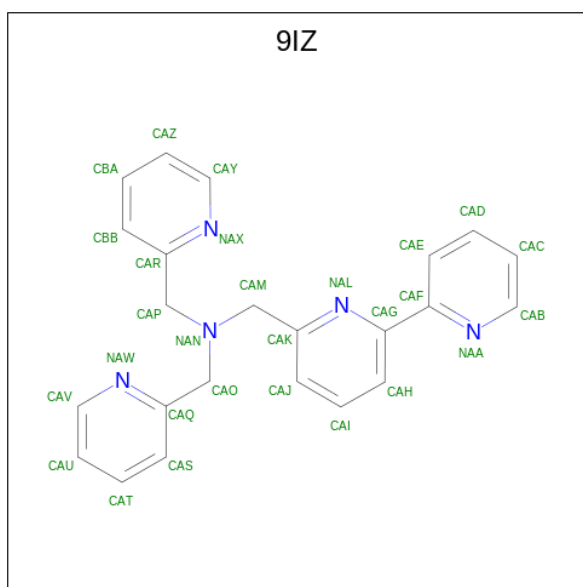
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	584	4562	2885	776	860	41	0	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is 1-pyridin-2-yl- {N}-(pyridin-2-ylmethyl)- {N}-[(6-pyridin-2-ylpyridin-2-yl)methyl]methanamine (three-letter code: 9IZ) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

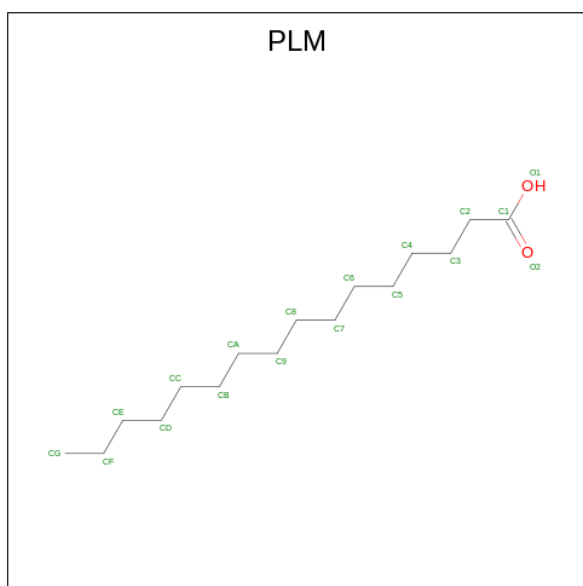


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 28 23 5	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

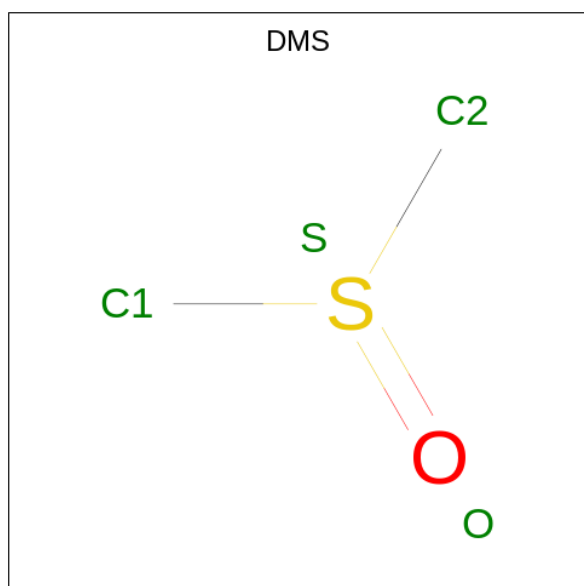
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Fe 5 5	0	0

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	16	Total Cl 16 16	0	0

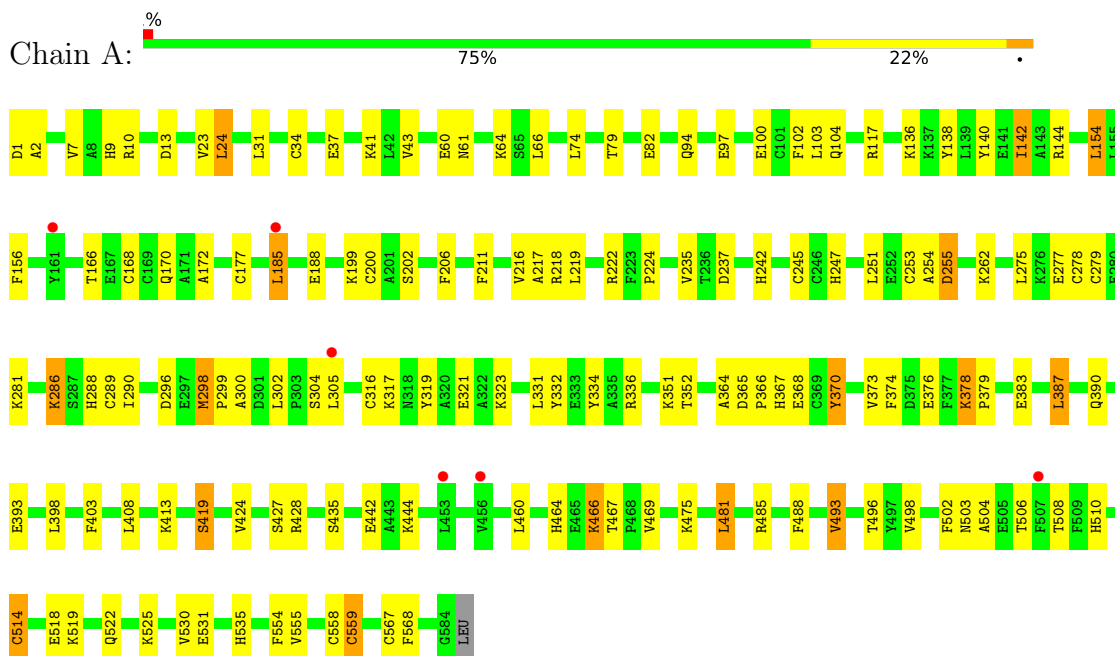
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	94	Total O 94 94	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: Serum albumin





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.50Å 38.16Å 95.78Å 90.00° 105.08° 90.00°	Depositor
Resolution (Å)	36.99 – 2.40 36.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.99-2.40) 97.8 (36.99-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.209 , 0.282 0.221 , 0.272	Depositor DCC
$R_{free}$ test set	1203 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtrriage
Anisotropy	0.510	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: PLM, CL, FE, DMS, GOL, 9IZ

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	0.50	0/4655	0.67	3/6295 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ALA	CB-CA-C	-6.40	100.49	110.10
1	A	300	ALA	N-CA-C	5.83	126.74	111.00
1	A	172	ALA	CB-CA-C	-5.55	101.77	110.10

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	4562	0	4433	104	0
2	A	6	0	8	0	0
3	A	28	0	0	4	0
4	A	5	0	0	0	0
5	A	126	0	217	21	0
6	A	16	0	24	0	0
7	A	16	0	0	6	0
8	A	94	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4853	0	4682	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (111) 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:211:PHE:HZ	1:A:242:HIS:HD1	1.18	0.91
1:A:275:LEU:O	8:A:701:HOH:O	1.93	0.85
7:A:629:CL:CL	8:A:772:HOH:O	2.36	0.81
7:A:628:CL:CL	8:A:740:HOH:O	2.37	0.79
1:A:275:LEU:HD21	1:A:290:ILE:HG23	1.69	0.74
1:A:217:ALA:HB2	1:A:331:LEU:HD21	1.70	0.72
1:A:519:LYS:NZ	8:A:705:HOH:O	2.22	0.71
1:A:378:LYS:HD2	1:A:379:PRO:HD3	1.72	0.70
1:A:279:CYS:N	8:A:701:HOH:O	2.24	0.70
1:A:525:LYS:NZ	8:A:706:HOH:O	2.24	0.70
1:A:387[B]:LEU:HD11	5:A:608:PLM:H52	1.75	0.69
1:A:66:LEU:HB2	1:A:251:LEU:HD21	1.77	0.67
1:A:387[A]:LEU:HD22	5:A:608:PLM:H82	1.77	0.67
1:A:142:ILE:HG21	5:A:614:PLM:H42	1.78	0.65
1:A:316:CYS:O	8:A:702:HOH:O	2.15	0.65
1:A:138:TYR:HB3	5:A:614:PLM:H81	1.77	0.64
1:A:288:HIS:CD2	3:A:602:9IZ:NAW	2.66	0.64
1:A:288:HIS:CE1	3:A:602:9IZ:NAX	2.65	0.64
1:A:514:CYS:HB2	8:A:712:HOH:O	1.99	0.63
1:A:1:ASP:OD1	1:A:2:ALA:N	2.32	0.62
1:A:41:LYS:H	1:A:41:LYS:HD2	1.65	0.62
1:A:185:LEU:HA	1:A:188:GLU:HB2	1.82	0.61
1:A:9:HIS:O	1:A:13:ASP:HB2	1.99	0.61
1:A:387[B]:LEU:HD13	5:A:608:PLM:H71	1.82	0.60
1:A:199:LYS:HG3	1:A:200:CYS:N	2.17	0.59
1:A:352:THR:HG21	1:A:376:GLU:HG2	1.83	0.59
1:A:7:VAL:HG13	8:A:720:HOH:O	2.02	0.58
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.85	0.58
1:A:319:TYR:CZ	1:A:323:LYS:HG2	2.39	0.58
1:A:37:GLU:HG2	1:A:41:LYS:NZ	2.19	0.57
1:A:254:ALA:HB1	5:A:610:PLM:H61	1.86	0.57
1:A:373:VAL:O	1:A:376:GLU:HB3	2.05	0.56
1:A:502:PHE:HB2	1:A:535:HIS:NE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:HIS:HA	1:A:370:TYR:CE1	2.41	0.56
7:A:629:CL:CL	8:A:751:HOH:O	2.55	0.56
1:A:218:ARG:NH2	1:A:222:ARG:HE	2.03	0.55
1:A:24:LEU:HB2	1:A:43:VAL:HG21	1.88	0.54
5:A:612:PLM:H62	5:A:612:PLM:H21	1.90	0.54
1:A:156:PHE:HB3	3:A:602:9IZ:CAY	2.38	0.54
1:A:444:LYS:O	1:A:444:LYS:HD3	2.08	0.54
1:A:504:ALA:O	1:A:508:THR:HG23	2.08	0.54
1:A:23:VAL:HG22	5:A:610:PLM:HD2	1.90	0.53
1:A:568:PHE:HE2	8:A:712:HOH:O	1.92	0.53
1:A:364:ALA:O	1:A:366:PRO:HD3	2.09	0.53
1:A:535:HIS:HD2	5:A:611:PLM:HG3	1.74	0.52
1:A:66:LEU:HD22	5:A:610:PLM:HC1	1.91	0.52
1:A:555:VAL:O	1:A:559:CYS:HB2	2.10	0.52
1:A:102:PHE:O	8:A:703:HOH:O	2.19	0.51
1:A:365:ASP:OD1	1:A:368:GLU:HB2	2.10	0.51
1:A:502:PHE:HE1	5:A:611:PLM:HE1	1.75	0.51
1:A:367:HIS:NE2	7:A:621:CL:CL	2.80	0.51
1:A:413:LYS:HB3	1:A:493:VAL:HG12	1.91	0.50
1:A:286:LYS:O	1:A:290:ILE:HG13	2.11	0.50
1:A:408:LEU:HD12	1:A:530:VAL:CG2	2.42	0.49
1:A:31:LEU:HD13	1:A:74:LEU:HD22	1.95	0.48
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.96	0.48
1:A:117:ARG:HB2	5:A:614:PLM:HG2	1.96	0.48
1:A:558:CYS:HB2	1:A:568:PHE:CE1	2.48	0.48
1:A:100:GLU:O	1:A:104:GLN:HG2	2.14	0.47
1:A:168:CYS:HB3	1:A:177:CYS:HB3	1.70	0.47
1:A:510:HIS:HE1	8:A:776:HOH:O	1.96	0.47
1:A:216:VAL:HG23	1:A:235:VAL:HG21	1.96	0.47
1:A:216:VAL:CG2	1:A:235:VAL:HG21	2.45	0.47
1:A:66:LEU:CB	1:A:251:LEU:HD21	2.45	0.47
1:A:424:VAL:O	1:A:428:ARG:HG3	2.15	0.46
1:A:299:PRO:HG2	1:A:336:ARG:HH21	1.80	0.46
3:A:602:9IZ:CAY	3:A:602:9IZ:NAA	2.78	0.46
5:A:609:PLM:H21	5:A:609:PLM:H51	1.65	0.46
1:A:503:ASN:HB3	1:A:506:THR:HG23	1.98	0.46
1:A:558:CYS:HB3	1:A:567:CYS:HB3	1.85	0.46
1:A:383:GLU:OE1	1:A:485:ARG:NH1	2.42	0.46
1:A:298:MET:HE2	1:A:298:MET:HB2	1.77	0.45
1:A:460:LEU:HG	5:A:609:PLM:HF2	1.98	0.45
1:A:488:PHE:HB3	5:A:609:PLM:H61	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:CG2	1:A:376:GLU:HG2	2.46	0.45
1:A:277:GLU:O	1:A:281:LYS:HG3	2.17	0.45
1:A:206:PHE:CE2	1:A:481:LEU:HG	2.52	0.45
1:A:103:LEU:HD11	1:A:247:HIS:O	2.17	0.44
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.82	0.44
1:A:408:LEU:HD12	1:A:530:VAL:HG22	1.99	0.44
1:A:317:LYS:O	1:A:321:GLU:HB2	2.17	0.44
1:A:154:LEU:HD12	1:A:154:LEU:HA	1.75	0.44
1:A:219:LEU:HD21	5:A:612:PLM:H61	1.99	0.44
1:A:442:GLU:HB2	7:A:628:CL:CL	2.54	0.44
1:A:531:GLU:O	8:A:704:HOH:O	2.21	0.44
1:A:216:VAL:HG12	1:A:331:LEU:HD22	1.99	0.43
1:A:7:VAL:HG12	1:A:66:LEU:HD23	2.00	0.43
1:A:351:LYS:HG3	8:A:784:HOH:O	2.18	0.43
1:A:390:GLN:O	1:A:393:GLU:HG2	2.19	0.43
1:A:535:HIS:CD2	5:A:611:PLM:HG3	2.53	0.43
1:A:7:VAL:HG12	1:A:66:LEU:CD2	2.49	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.85	0.42
1:A:10:ARG:NH2	1:A:255:ASP:OD1	2.53	0.42
1:A:387[B]:LEU:CD1	5:A:608:PLM:H52	2.47	0.42
1:A:464:HIS:HB2	5:A:609:PLM:HG2	2.02	0.42
1:A:245:CYS:HA	1:A:253:CYS:HB2	2.02	0.42
1:A:34:CYS:SG	8:A:708:HOH:O	2.60	0.41
1:A:61:ASN:HB3	1:A:64:LYS:HZ2	1.85	0.41
1:A:502:PHE:CE1	5:A:611:PLM:HE1	2.54	0.41
1:A:37:GLU:O	1:A:41:LYS:HD2	2.20	0.41
1:A:278:CYS:HB3	1:A:289:CYS:HB3	1.96	0.41
1:A:558:CYS:HB2	1:A:568:PHE:CD1	2.55	0.41
1:A:61:ASN:HB3	1:A:64:LYS:NZ	2.35	0.41
1:A:103:LEU:HD13	1:A:103:LEU:O	2.20	0.41
1:A:408:LEU:HD22	1:A:427:SER:HB2	2.02	0.41
1:A:518:GLU:O	1:A:522:GLN:HG3	2.21	0.41
5:A:608:PLM:HA2	5:A:608:PLM:HD2	1.82	0.41
1:A:398:LEU:HD12	1:A:403:PHE:HA	2.02	0.41
1:A:466:LYS:HB3	1:A:466:LYS:HE2	1.64	0.40
1:A:1:ASP:CG	1:A:2:ALA:H	2.23	0.40
1:A:419:SER:HB3	7:A:632:CL:CL	2.59	0.40

There are no symmetry-related clashes.

## 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	583/585 (100%)	557 (96%)	26 (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	489/511 (96%)	448 (92%)	41 (8%)	11 16

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

Mol	Chain	Res	Type
1	A	24	LEU
1	A	60	GLU
1	A	79	THR
1	A	82	GLU
1	A	94	GLN
1	A	97	GLU
1	A	136	LYS
1	A	140	TYR
1	A	142	ILE
1	A	144	ARG
1	A	154	LEU
1	A	166	THR
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	185	LEU
1	A	202	SER
1	A	237	ASP
1	A	255	ASP
1	A	262	LYS
1	A	286	LYS
1	A	298	MET
1	A	304	SER
1	A	305	LEU
1	A	332	TYR
1	A	334	TYR
1	A	370	TYR
1	A	378	LYS
1	A	387[A]	LEU
1	A	387[B]	LEU
1	A	419	SER
1	A	435	SER
1	A	466	LYS
1	A	467	THR
1	A	469	VAL
1	A	475	LYS
1	A	481	LEU
1	A	493	VAL
1	A	496	THR
1	A	498	VAL
1	A	514	CYS
1	A	554	PHE
1	A	559	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 34 ligands modelled in this entry, 21 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PLM	A	613	-	17,17,17	0.99	1 (5%)	17,17,17	0.81	1 (5%)
3	9IZ	A	602	4	31,31,31	1.24	3 (9%)	40,40,40	1.60	6 (15%)
2	GOL	A	601	-	5,5,5	1.01	0	5,5,5	0.93	0
5	PLM	A	611	-	17,17,17	1.21	1 (5%)	17,17,17	0.77	1 (5%)
5	PLM	A	610	-	17,17,17	0.94	1 (5%)	17,17,17	0.77	1 (5%)
5	PLM	A	614	-	17,17,17	1.45	1 (5%)	17,17,17	0.72	0
5	PLM	A	608	-	17,17,17	1.08	1 (5%)	17,17,17	0.81	2 (11%)
5	PLM	A	612	-	17,17,17	1.16	1 (5%)	17,17,17	0.75	2 (11%)
6	DMS	A	615	-	3,3,3	0.73	0	3,3,3	0.50	0
6	DMS	A	616	-	3,3,3	0.72	0	3,3,3	1.08	0
6	DMS	A	617	-	3,3,3	0.70	0	3,3,3	0.69	0
6	DMS	A	618	-	3,3,3	0.74	0	3,3,3	1.05	0
5	PLM	A	609	-	17,17,17	0.86	0	17,17,17	0.73	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	A	613	-	-	6/15/15/15	-
3	9IZ	A	602	4	-	7/16/16/16	0/4/4/4
2	GOL	A	601	-	-	3/4/4/4	-
5	PLM	A	611	-	-	6/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PLM	A	610	-	-	11/15/15/15	-
5	PLM	A	614	-	-	7/15/15/15	-
5	PLM	A	608	-	-	9/15/15/15	-
5	PLM	A	612	-	-	7/15/15/15	-
5	PLM	A	609	-	-	11/15/15/15	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	614	PLM	C2-C1	4.40	1.60	1.50
5	A	612	PLM	C2-C1	3.90	1.59	1.50
5	A	611	PLM	C2-C1	3.78	1.59	1.50
3	A	602	9IZ	CAP-CAR	3.33	1.56	1.51
5	A	608	PLM	C2-C1	3.26	1.58	1.50
5	A	613	PLM	C2-C1	3.18	1.58	1.50
5	A	610	PLM	C2-C1	2.69	1.56	1.50
3	A	602	9IZ	CAO-CAQ	2.55	1.55	1.51
3	A	602	9IZ	CAV-NAW	2.37	1.39	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	9IZ	CAK-CAM-NAN	-5.24	101.74	112.78
3	A	602	9IZ	CAG-NAL-CAK	3.60	122.24	118.36
3	A	602	9IZ	CAR-CAP-NAN	-2.60	107.31	112.78
5	A	613	PLM	O1-C1-O2	2.47	129.45	123.30
3	A	602	9IZ	CAU-CAV-NAW	-2.45	119.43	123.43
3	A	602	9IZ	CAQ-CAO-NAN	-2.39	107.75	112.78
5	A	610	PLM	O1-C1-O2	2.31	129.06	123.30
5	A	611	PLM	O1-C1-O2	2.25	128.91	123.30
5	A	609	PLM	O1-C1-O2	2.24	128.87	123.30
5	A	608	PLM	O1-C1-O2	2.19	128.77	123.30
5	A	612	PLM	O1-C1-O2	2.06	128.43	123.30
5	A	608	PLM	O2-C1-C2	-2.05	116.50	123.08
5	A	612	PLM	O2-C1-C2	-2.04	116.52	123.08
3	A	602	9IZ	CAV-NAW-CAQ	2.03	120.20	117.42

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	608	PLM	CA-CB-CC-CD
5	A	614	PLM	C5-C6-C7-C8
5	A	612	PLM	C9-CA-CB-CC
5	A	611	PLM	C1-C2-C3-C4
5	A	609	PLM	C1-C2-C3-C4
5	A	613	PLM	C6-C7-C8-C9
5	A	608	PLM	C6-C7-C8-C9
5	A	610	PLM	C1-C2-C3-C4
5	A	609	PLM	C9-CA-CB-CC
5	A	609	PLM	CA-CB-CC-CD
5	A	614	PLM	CB-CC-CD-CE
2	A	601	GOL	O1-C1-C2-C3
5	A	613	PLM	C4-C5-C6-C7
5	A	609	PLM	C2-C3-C4-C5
5	A	610	PLM	CA-CB-CC-CD
5	A	612	PLM	CB-CC-CD-CE
5	A	610	PLM	C5-C6-C7-C8
2	A	601	GOL	O1-C1-C2-O2
5	A	608	PLM	C7-C8-C9-CA
5	A	611	PLM	C5-C6-C7-C8
5	A	613	PLM	C7-C8-C9-CA
5	A	614	PLM	CA-CB-CC-CD
5	A	610	PLM	C6-C7-C8-C9
5	A	608	PLM	CC-CD-CE-CF
5	A	610	PLM	C2-C3-C4-C5
5	A	609	PLM	C3-C4-C5-C6
5	A	610	PLM	C4-C5-C6-C7
5	A	613	PLM	CD-CE-CF-CG
5	A	614	PLM	C9-CA-CB-CC
5	A	613	PLM	C2-C3-C4-C5
2	A	601	GOL	O2-C2-C3-O3
3	A	602	9IZ	CAK-CAM-NAN-CAP
5	A	614	PLM	C8-C9-CA-CB
5	A	612	PLM	C2-C3-C4-C5
5	A	608	PLM	C3-C4-C5-C6
5	A	609	PLM	C4-C5-C6-C7
5	A	609	PLM	C5-C6-C7-C8
5	A	609	PLM	C6-C7-C8-C9
5	A	608	PLM	CB-CC-CD-CE
5	A	609	PLM	CB-CC-CD-CE
5	A	612	PLM	C5-C6-C7-C8
5	A	611	PLM	C4-C5-C6-C7
3	A	602	9IZ	CAK-CAM-NAN-CAO

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Mol	Chain	Res	Type	Atoms
5	A	610	PLM	CD-CE-CF-CG
3	A	602	9IZ	CAE-CAF-CAG-CAH
5	A	612	PLM	C1-C2-C3-C4
3	A	602	9IZ	NAA-CAF-CAG-CAH
5	A	612	PLM	O2-C1-C2-C3
5	A	610	PLM	C3-C4-C5-C6
5	A	614	PLM	C1-C2-C3-C4
5	A	608	PLM	C5-C6-C7-C8
5	A	608	PLM	O2-C1-C2-C3
5	A	612	PLM	O1-C1-C2-C3
5	A	610	PLM	O1-C1-C2-C3
3	A	602	9IZ	NAA-CAF-CAG-NAL
3	A	602	9IZ	CAE-CAF-CAG-NAL
5	A	610	PLM	O2-C1-C2-C3
5	A	611	PLM	C6-C7-C8-C9
5	A	609	PLM	O1-C1-C2-C3
5	A	610	PLM	C9-CA-CB-CC
5	A	611	PLM	O2-C1-C2-C3
5	A	608	PLM	O1-C1-C2-C3
5	A	609	PLM	O2-C1-C2-C3
3	A	602	9IZ	CAQ-CAO-NAN-CAM
5	A	611	PLM	O1-C1-C2-C3
5	A	614	PLM	C6-C7-C8-C9
5	A	613	PLM	C8-C9-CA-CB

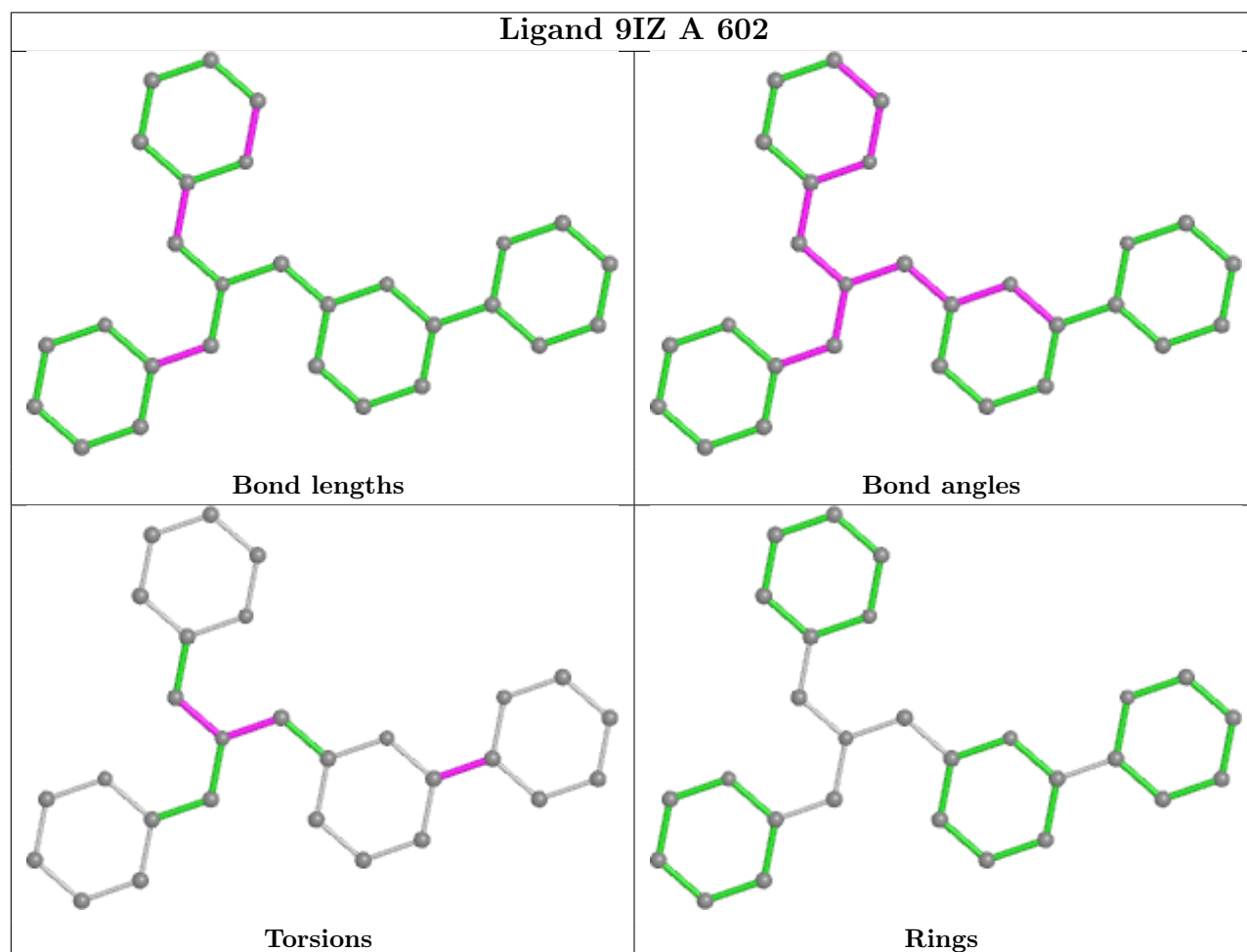
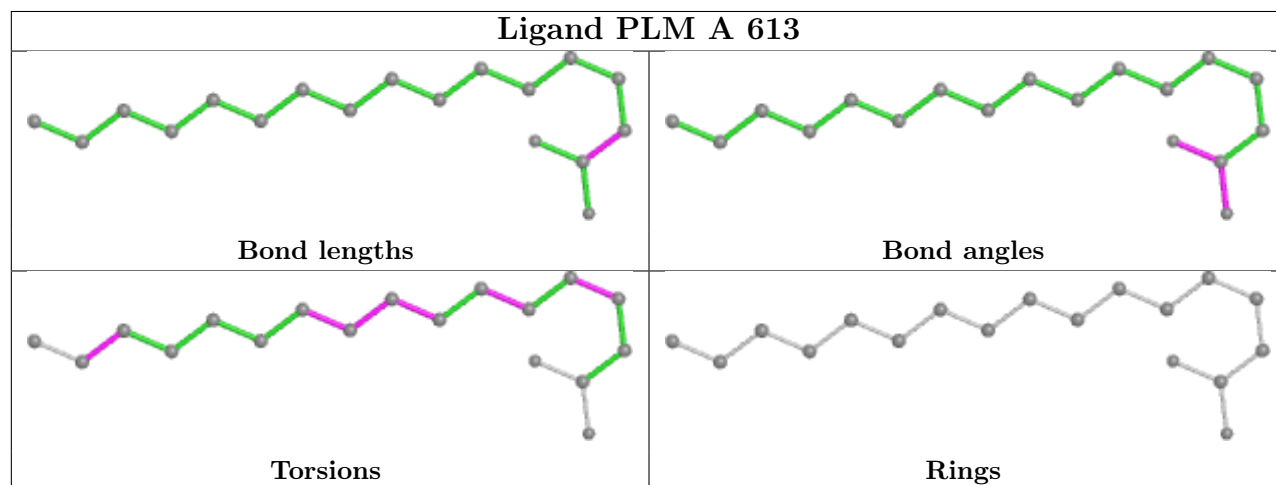
There are no ring outliers.

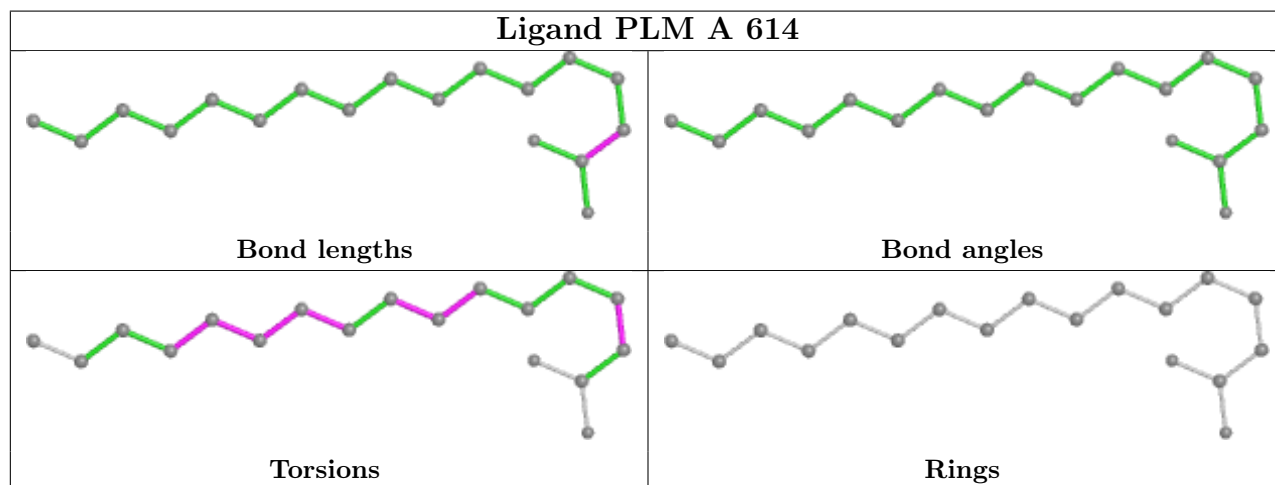
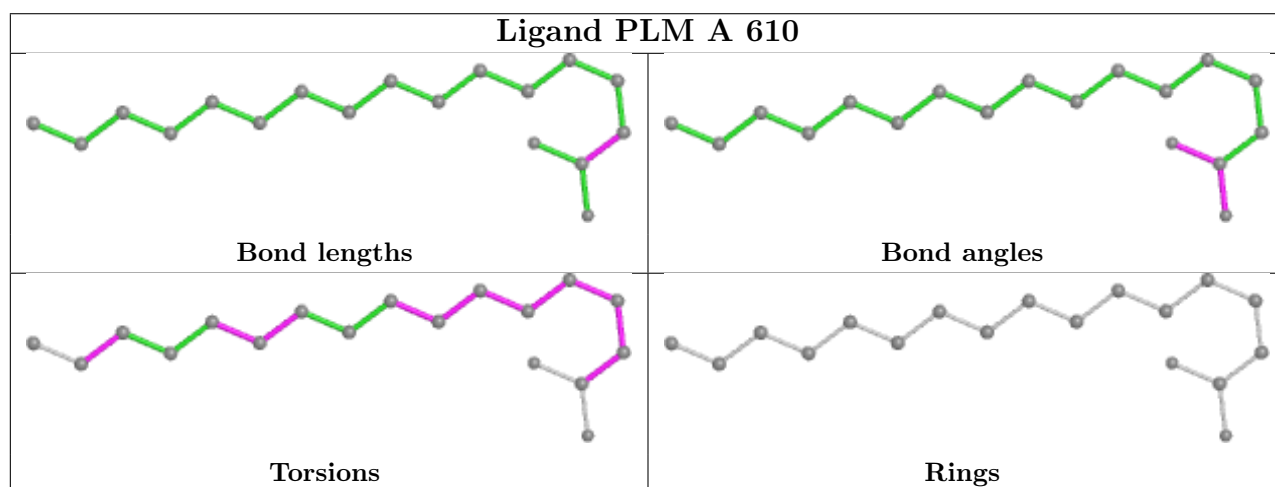
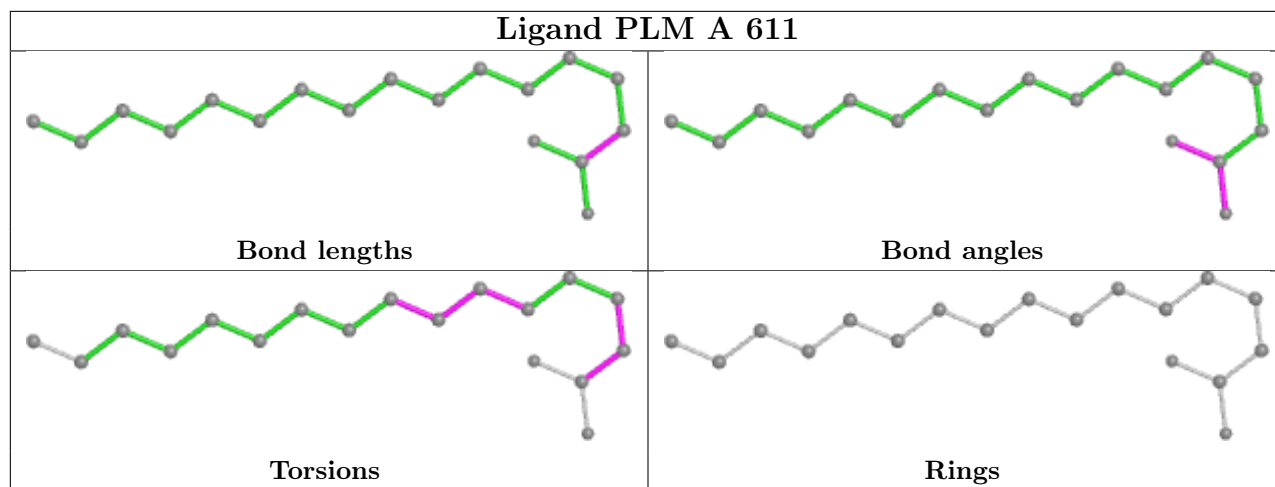
7 monomers are involved in 25 short contacts:

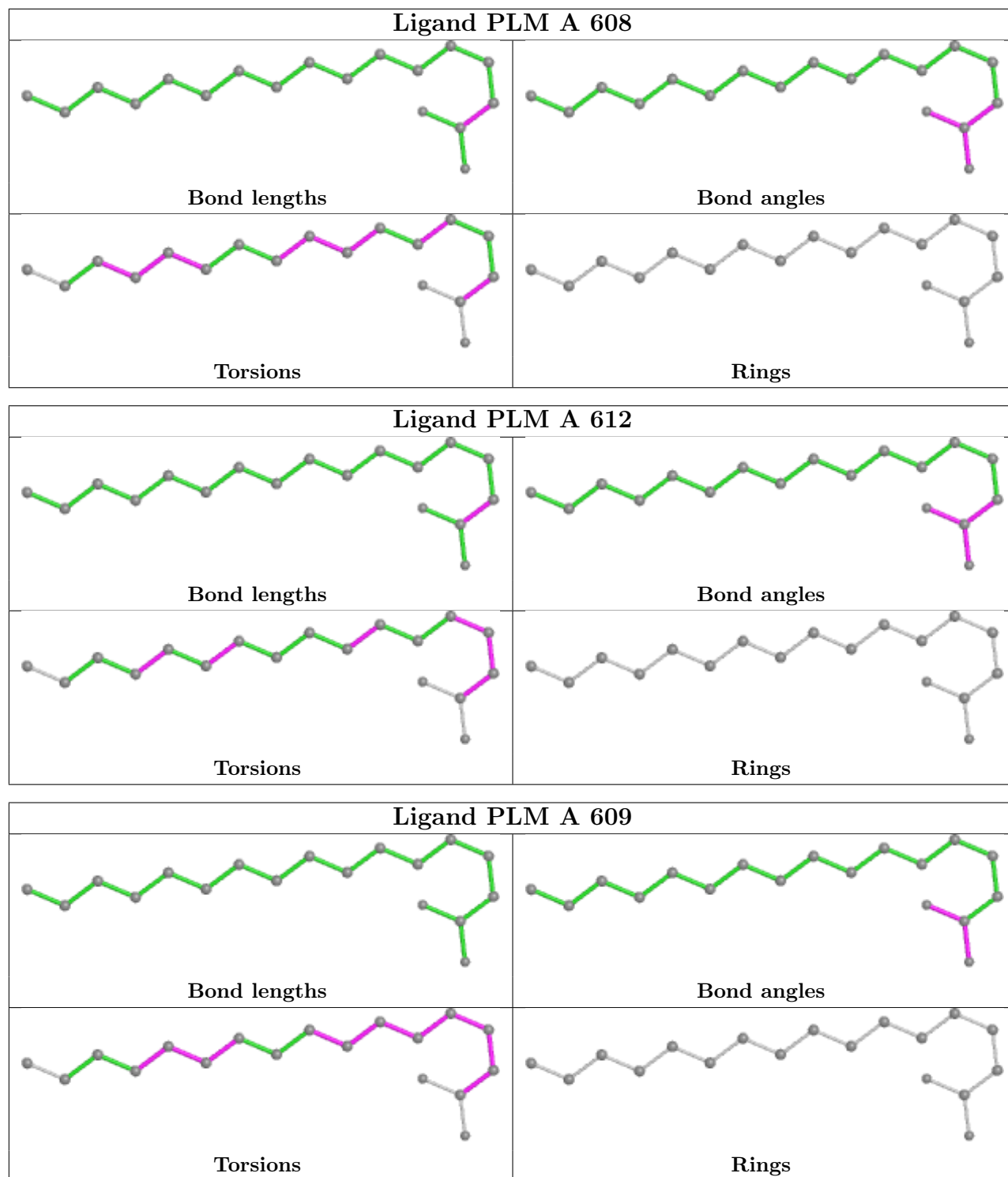
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	9IZ	4	0
5	A	611	PLM	4	0
5	A	610	PLM	3	0
5	A	614	PLM	3	0
5	A	608	PLM	5	0
5	A	612	PLM	2	0
5	A	609	PLM	4	0

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

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	584/585 (99%)	0.03	6 (1%) 82 80	57, 74, 92, 107	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	LEU	2.5
1	A	161	TYR	2.4
1	A	507	PHE	2.2
1	A	453	LEU	2.1
1	A	456	VAL	2.1
1	A	305	LEU	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(Å <sup>2</sup> )	Q<0.9
7	CL	A	628	1/1	0.53	0.41	95,95,95,95	0

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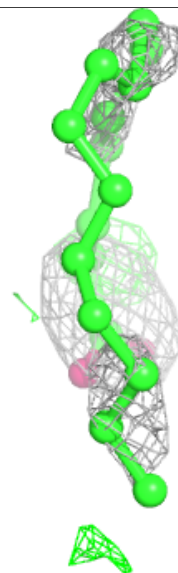
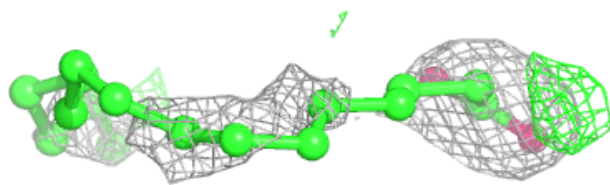
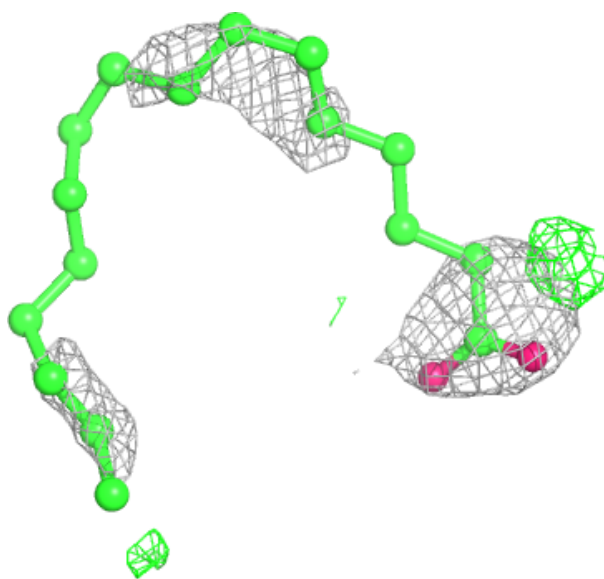
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	CL	A	634	1/1	0.57	0.14	97,97,97,97	0
7	CL	A	627	1/1	0.64	0.13	96,96,96,96	0
6	DMS	A	616	4/4	0.71	0.26	87,90,90,117	0
5	PLM	A	614	18/18	0.73	0.56	78,85,93,94	0
7	CL	A	620	1/1	0.77	0.65	95,95,95,95	0
7	CL	A	631	1/1	0.80	0.09	102,102,102,102	0
7	CL	A	621	1/1	0.81	0.14	112,112,112,112	0
6	DMS	A	618	4/4	0.82	0.35	83,89,95,100	0
5	PLM	A	611	18/18	0.86	0.28	59,66,80,83	0
5	PLM	A	612	18/18	0.86	0.37	71,78,93,94	0
5	PLM	A	613	18/18	0.86	0.39	57,68,92,94	0
2	GOL	A	601	6/6	0.86	0.23	83,88,91,92	0
5	PLM	A	610	18/18	0.87	0.41	62,72,78,79	0
7	CL	A	619	1/1	0.88	0.21	102,102,102,102	0
4	FE	A	607	1/1	0.89	0.07	120,120,120,120	0
7	CL	A	623	1/1	0.89	0.10	119,119,119,119	0
4	FE	A	604	1/1	0.89	0.06	98,98,98,98	1
7	CL	A	632	1/1	0.90	0.22	88,88,88,88	0
7	CL	A	633	1/1	0.90	0.22	87,87,87,87	0
7	CL	A	630	1/1	0.90	0.10	88,88,88,88	0
7	CL	A	625	1/1	0.91	0.07	107,107,107,107	0
7	CL	A	626	1/1	0.92	0.10	86,86,86,86	0
5	PLM	A	609	18/18	0.92	0.33	56,62,67,69	0
7	CL	A	629	1/1	0.93	0.10	91,91,91,91	0
4	FE	A	605	1/1	0.93	0.13	80,80,80,80	1
6	DMS	A	615	4/4	0.94	0.31	79,80,91,98	0
3	9IZ	A	602	28/28	0.94	0.18	73,79,86,87	0
6	DMS	A	617	4/4	0.94	0.18	74,78,82,94	0
5	PLM	A	608	18/18	0.94	0.25	60,66,69,70	0
7	CL	A	624	1/1	0.94	0.05	106,106,106,106	0
7	CL	A	622	1/1	0.95	0.07	95,95,95,95	0
4	FE	A	603	1/1	0.96	0.20	64,64,64,64	1
4	FE	A	606	1/1	0.99	0.16	71,71,71,71	1

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.

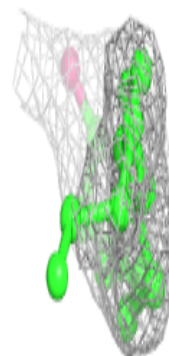
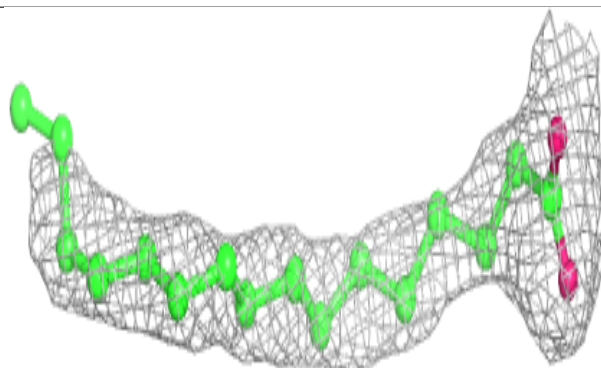
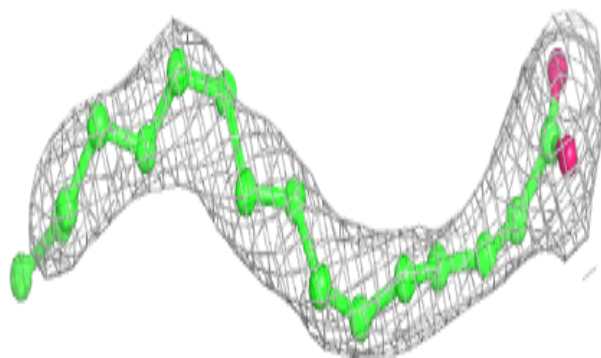
**Electron density around PLM A 614:**

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

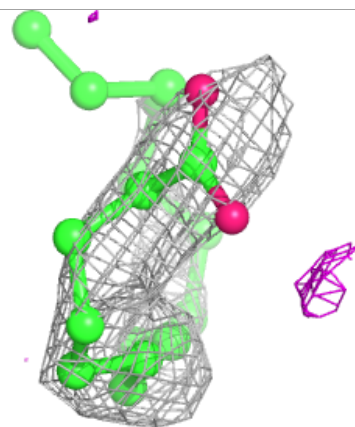
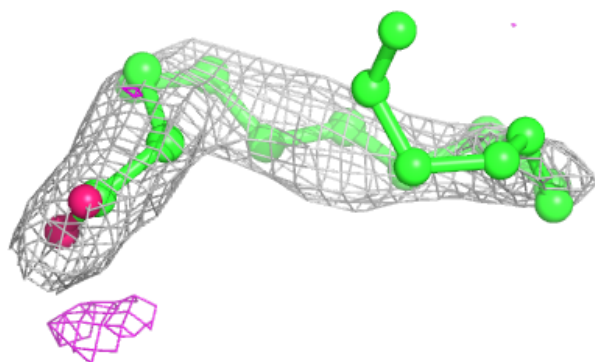
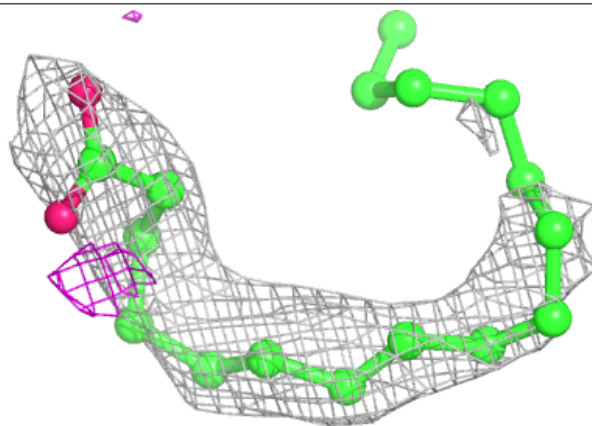


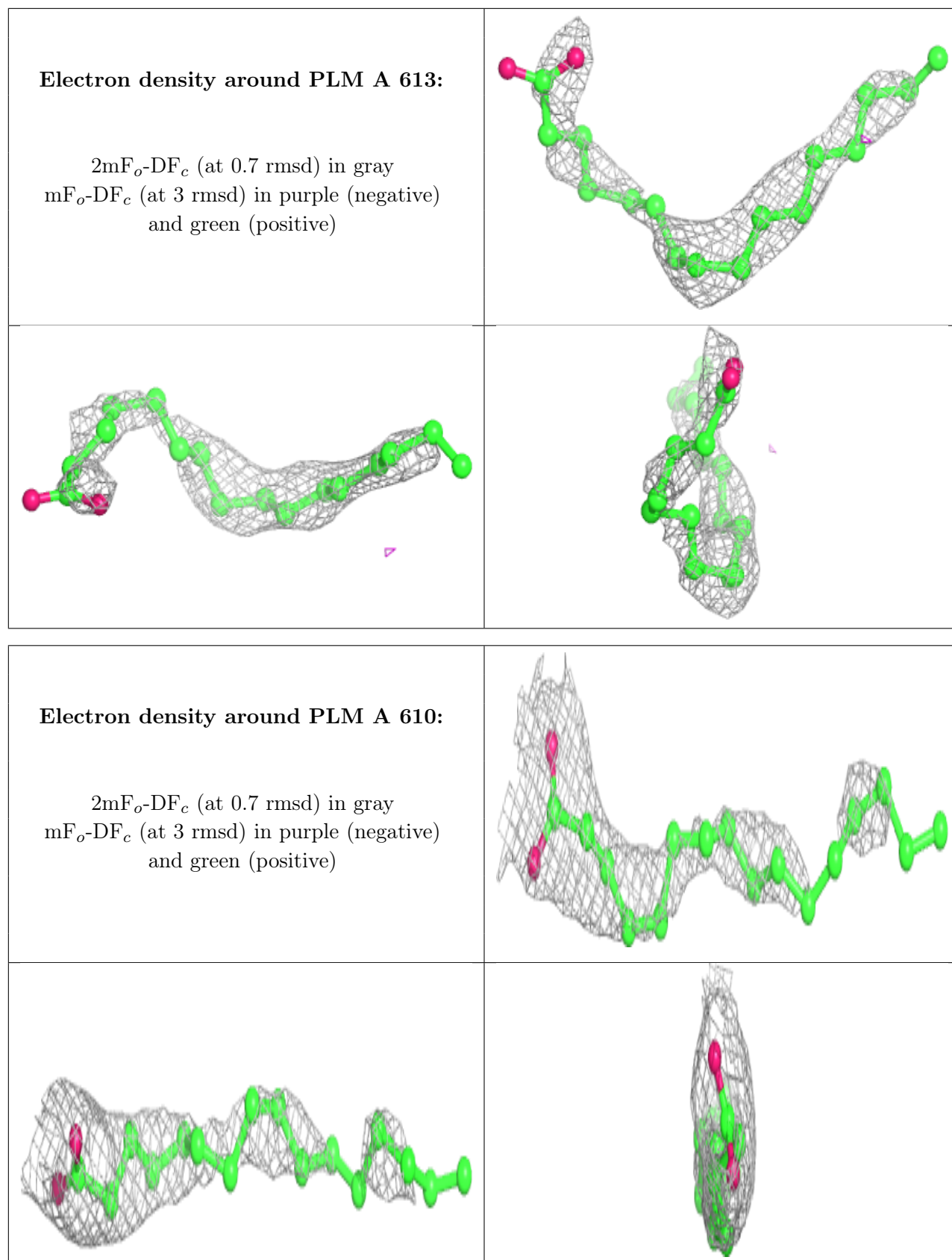
**Electron density around PLM A 611:**

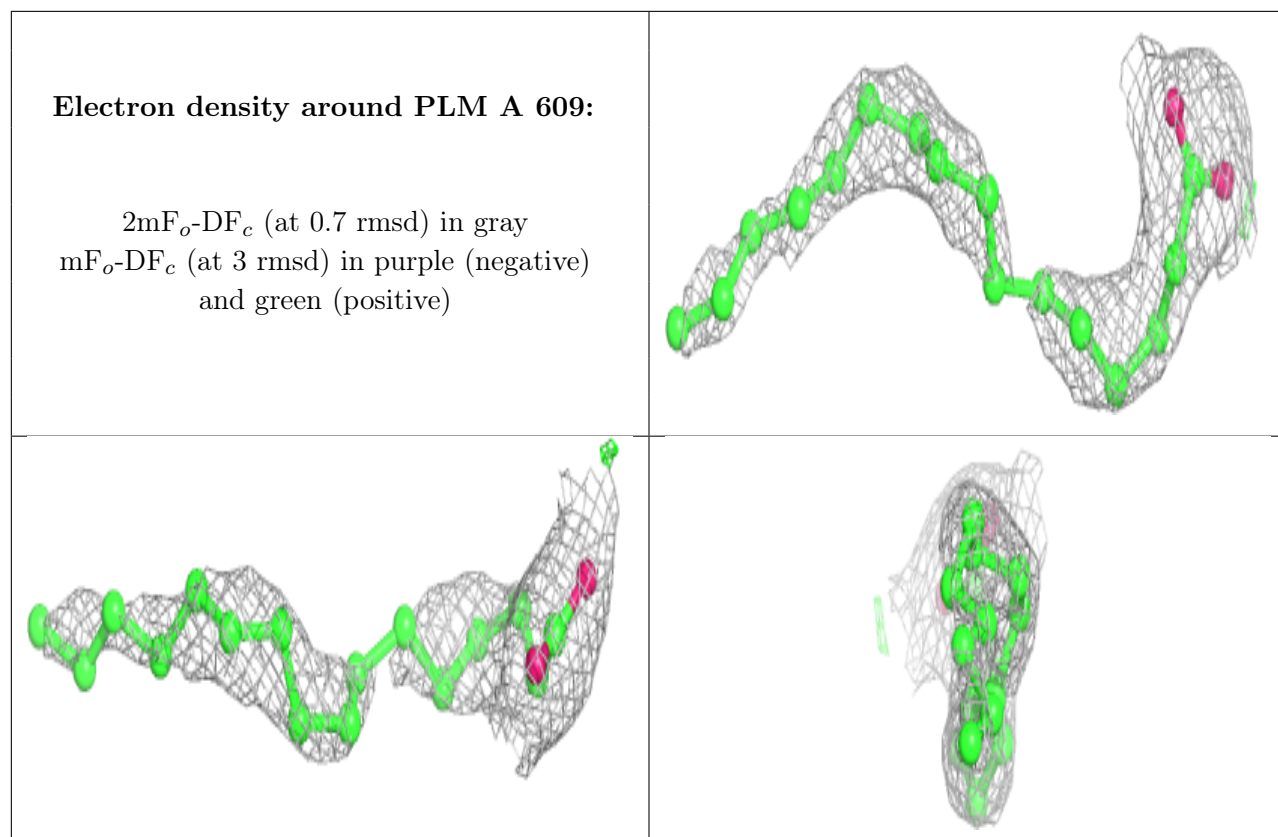
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PLM A 612:**

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

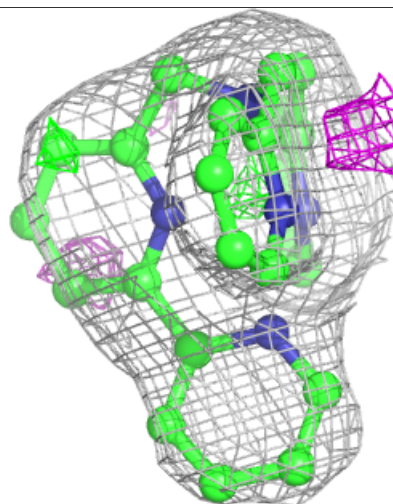
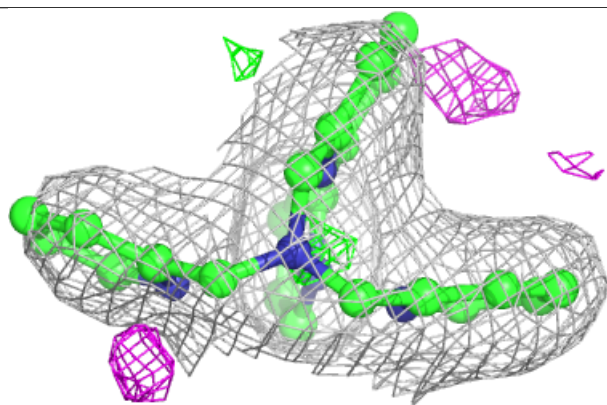
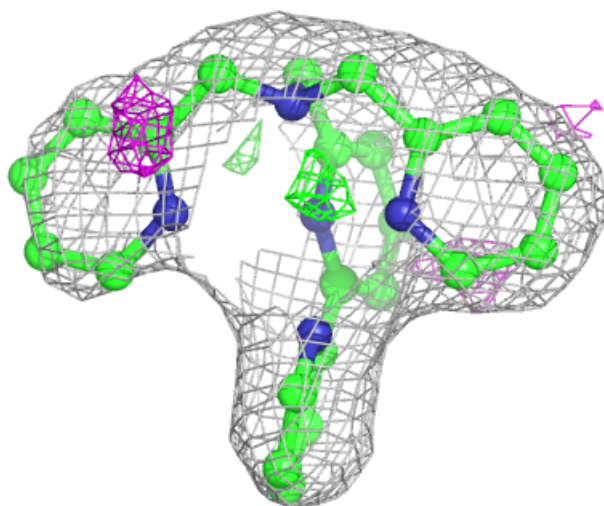


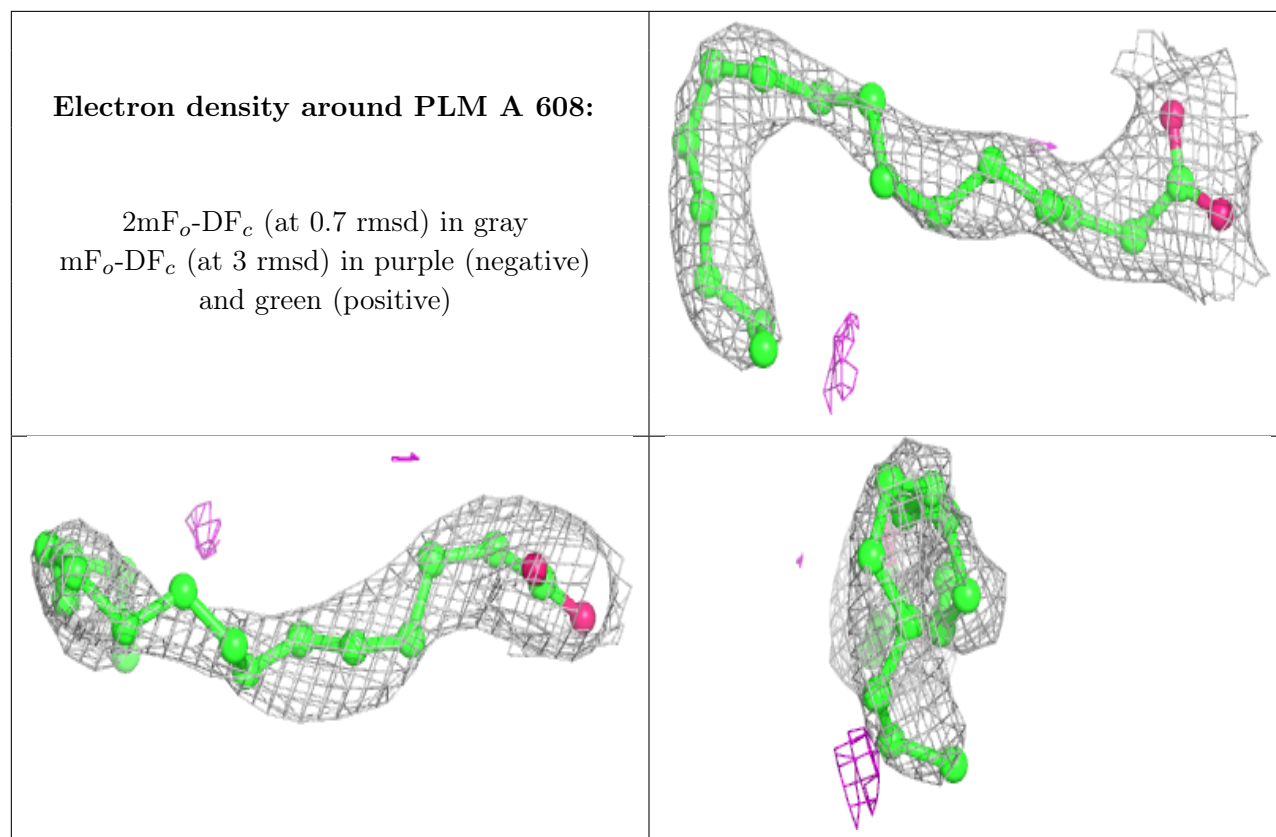




**Electron density around 9IZ A 602:**

$2mF_o-DF_c$  (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.