



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 01:00 PM BST

PDB ID : 5GIX  
Title : Human serum albumin-Palmitic acid-Fe(Hn3piT)Cl2  
Authors : Yang, F.; Qi, J.; Wang, T.  
Deposited on : 2016-06-25  
Resolution : 2.80 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 : 2.13.1  
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) : 2.13.1

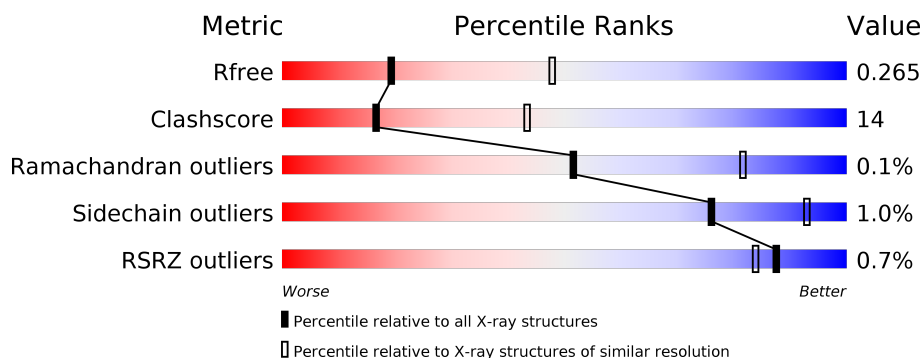
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	581	<div> <div></div> <div>69%</div> <div>30%</div> </div>
1	B	581	<div> <div>%</div> <div>69%</div> <div>30%</div> </div>

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
3	PLM	A	602	-	-	-	X
3	PLM	B	602	-	-	-	X

## 2 Entry composition [i](#)

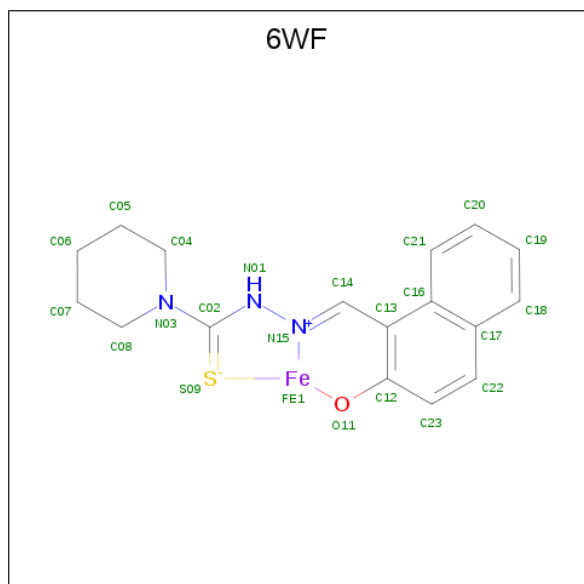
There are 4 unique types of molecules in this entry. The entry contains 9498 atoms, of which 36 are hydrogens and 0 are deuteriums.

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.

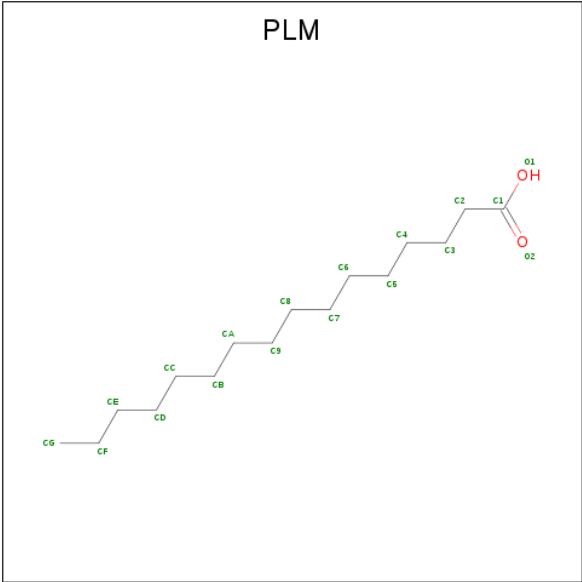
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4606	2909	776	880	41			
1	B	581	Total	C	N	O	S	0	0	0
			4606	2909	776	880	41			

- Molecule 2 is 14-piperidin-1-yl-11-oxa-13 $\lambda$ <sup>3</sup>-thia-15,16 $\lambda$ <sup>4</sup>-diaz-12 $\lambda$ <sup>3</sup>-ferratetracyclo[8.7.0.0<sup>2,7</sup>.0<sup>12,16</sup>]heptadeca-1(10),2(7),3,5,8,13,16-heptaene (three-letter code: 6WF) (formula: C<sub>17</sub>H<sub>18</sub>FeN<sub>3</sub>OS).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Fe	H	N	O	S	0	0
			41	17	1	18	3	1	1		
2	B	1	Total	C	Fe	H	N	O	S	0	0
			41	17	1	18	3	1	1		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			13	11	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C	O	0	0
			17	15	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C	O	0	0
			17	15	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			13	11	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			17	15	2		
3	B	1	Total	C	O	0	0
			18	16	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.47Å 94.55Å 96.11Å 104.90° 89.90° 100.86°	Depositor
Resolution (Å)	27.13 – 2.80 35.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (27.13-2.80) 95.3 (35.51-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.54 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.209 , 0.268 0.212 , 0.265	Depositor DCC
$R_{free}$ test set	1995 reflections (6.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 21.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.258 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6WF, PLM

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	0.29	0/4696	0.40	0/6339
1	B	0.23	0/4696	0.38	0/6339
All	All	0.26	0/9392	0.39	0/12678

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

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	4606	0	4501	127	0
1	B	4606	0	4499	128	0
2	A	23	18	0	6	0
2	B	23	18	0	8	0
3	A	101	0	163	16	0
3	B	101	0	163	18	0
4	A	2	0	0	0	0
All	All	9462	36	9326	267	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 14.

All (267) 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)
2:B:601:6WF:C13	2:B:601:6WF:C14	1.75	1.59
2:A:601:6WF:N15	2:A:601:6WF:N01	1.77	1.30
2:B:601:6WF:N15	2:B:601:6WF:N01	1.81	1.28
1:A:242:HIS:NE2	2:A:601:6WF:S09	2.25	1.05
1:B:199:LYS:NZ	2:B:601:6WF:S09	2.30	1.03
1:A:460:LEU:HD21	3:A:605:PLM:HC2	1.50	0.92
1:A:242:HIS:CD2	2:A:601:6WF:S09	2.67	0.88
1:B:460:LEU:HD21	3:B:605:PLM:HC2	1.54	0.86
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.43	0.84
1:B:222:ARG:HG3	1:B:222:ARG:HH11	1.43	0.83
1:B:418:VAL:HG21	3:B:605:PLM:HD2	1.62	0.80
1:A:316:CYS:SG	1:A:370:TYR:OH	2.40	0.80
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.22	0.80
2:A:601:6WF:C02	2:A:601:6WF:N15	2.40	0.79
1:B:119:GLU:HB2	1:B:122:VAL:HG23	1.68	0.76
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.26	0.75
2:B:601:6WF:N15	2:B:601:6WF:C02	2.50	0.74
2:B:601:6WF:FE1	2:B:601:6WF:S09	1.79	0.74
1:A:138:TYR:O	1:A:142:ILE:HG12	1.87	0.73
1:A:138:TYR:HB3	3:A:602:PLM:H81	1.69	0.72
3:B:604:PLM:H81	3:B:605:PLM:H22	1.72	0.71
1:A:191:ALA:O	1:A:195:LYS:HG3	1.91	0.71
1:A:198:LEU:O	1:A:198:LEU:HD12	1.90	0.70
2:B:601:6WF:N15	2:B:601:6WF:S09	2.66	0.69
1:A:115:LEU:HD11	1:A:141:GLU:HB3	1.74	0.69
1:B:138:TYR:O	1:B:142:ILE:HG12	1.93	0.69
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.73	0.68
1:A:119:GLU:HB2	1:A:122:VAL:HG23	1.75	0.67
1:A:424:VAL:O	1:A:428:ARG:HG3	1.94	0.67
1:B:108:ASP:OD2	1:B:197:ARG:NH1	2.27	0.67
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.77	0.66
1:B:310:VAL:HG13	1:B:370:TYR:HB3	1.77	0.65
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.78	0.65
1:A:153:GLU:OE2	1:A:288:HIS:ND1	2.29	0.65
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.78	0.64
1:A:138:TYR:CB	3:A:602:PLM:H81	2.27	0.64
1:B:417:GLN:NE2	1:B:494:ASP:OD2	2.31	0.63
1:A:117:ARG:HG3	3:A:602:PLM:H32	1.80	0.63
1:A:138:TYR:CD2	3:A:602:PLM:H61	2.34	0.63
1:A:417:GLN:NE2	1:A:494:ASP:OD2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:O	1:B:45:GLU:HG3	1.99	0.62
1:B:424:VAL:O	1:B:428:ARG:HG3	1.99	0.62
1:A:161:TYR:CD1	1:A:185:LEU:HD23	2.35	0.61
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.15	0.61
1:A:10:ARG:HG3	1:A:66:LEU:HD11	1.83	0.61
1:A:72:ASP:O	1:A:76:THR:HG23	1.99	0.61
1:A:225:LYS:HE3	1:A:297:GLU:O	2.01	0.60
1:B:284:LEU:HD12	3:B:603:PLM:H31	1.83	0.60
1:A:81:ARG:NH2	1:A:89:ASP:OD1	2.35	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.85	0.59
1:B:115:LEU:HD11	1:B:141:GLU:HB3	1.83	0.59
1:B:10:ARG:HG3	1:B:66:LEU:HD11	1.85	0.59
1:B:372:LYS:O	1:B:376:GLU:HG3	2.03	0.59
1:B:457:LEU:HD21	3:B:605:PLM:H51	1.86	0.58
1:B:72:ASP:O	1:B:76:THR:HG23	2.03	0.58
1:A:408:LEU:HD23	1:A:529:LEU:HD23	1.86	0.58
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.86	0.58
1:A:95:GLU:OE2	1:A:99:ASN:HB2	2.03	0.57
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.85	0.57
1:B:6:GLU:HB3	1:B:66:LEU:HG	1.86	0.57
1:B:436:LYS:HE2	1:B:452:TYR:OH	2.05	0.57
1:A:422:THR:O	1:A:426:VAL:HG13	2.04	0.57
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.87	0.57
1:A:41:LYS:O	1:A:45:GLU:HG3	2.04	0.57
1:B:551:PHE:CD1	3:B:606:PLM:H91	2.40	0.57
1:B:411:TYR:HB3	3:B:605:PLM:HA1	1.87	0.57
1:A:108:ASP:OD2	1:A:197:ARG:NH1	2.38	0.56
1:B:225:LYS:HE3	1:B:297:GLU:O	2.06	0.56
1:A:464:HIS:CD2	1:A:468:PRO:HA	2.40	0.56
1:B:254:ALA:HB1	3:B:603:PLM:H42	1.85	0.56
1:A:25:ILE:O	1:A:29:GLN:HG3	2.05	0.56
1:B:5:SER:HB3	1:B:8:ALA:HB3	1.87	0.56
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.88	0.56
1:B:418:VAL:HG22	3:B:605:PLM:HF2	1.88	0.56
1:A:117:ARG:HG3	3:A:602:PLM:C3	2.36	0.56
1:B:25:ILE:O	1:B:29:GLN:HG3	2.05	0.55
1:B:191:ALA:O	1:B:195:LYS:HG3	2.07	0.55
1:A:569:ALA:O	1:A:573:LYS:HG3	2.07	0.55
1:B:138:TYR:HB3	3:B:602:PLM:HA1	1.88	0.55
1:B:137:LYS:O	1:B:141:GLU:HG2	2.07	0.55
1:B:155:LEU:HD23	1:B:284:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TYR:CD1	1:B:185:LEU:HD23	2.43	0.54
1:B:214:TRP:CH2	1:B:218:ARG:HD2	2.42	0.54
1:A:418:VAL:HG22	3:A:605:PLM:HF2	1.89	0.54
1:B:473:VAL:HG11	3:B:605:PLM:HF1	1.90	0.54
1:B:81:ARG:NH2	1:B:89:ASP:OD1	2.40	0.54
2:B:601:6WF:N15	2:B:601:6WF:C13	2.65	0.54
1:A:563:ASP:OD1	1:A:564:LYS:N	2.41	0.54
1:B:14:LEU:HD11	3:B:603:PLM:H72	1.90	0.54
1:A:420:THR:HB	1:A:421:PRO:HD3	1.90	0.53
1:B:370:TYR:O	1:B:373:VAL:HB	2.08	0.53
1:B:175:ALA:O	1:B:179:LEU:HB2	2.06	0.53
1:A:460:LEU:HG	3:A:605:PLM:HE2	1.89	0.53
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.90	0.53
1:B:238:LEU:HD22	1:B:242:HIS:CE1	2.43	0.53
1:B:378:LYS:N	1:B:379:PRO:HD2	2.24	0.53
1:B:441:PRO:O	1:B:445:ARG:HG3	2.08	0.53
1:A:411:TYR:HB3	3:A:605:PLM:HA1	1.91	0.53
1:B:446:MET:N	1:B:447:PRO:HD2	2.24	0.53
1:B:420:THR:HB	1:B:421:PRO:HD3	1.91	0.53
1:A:137:LYS:O	1:A:141:GLU:HG2	2.09	0.52
1:A:539:ALA:HB1	1:A:544:LEU:HD13	1.90	0.52
1:A:441:PRO:O	1:A:445:ARG:HG3	2.09	0.52
1:B:216:VAL:CG2	1:B:235:VAL:HG21	2.40	0.52
1:A:214:TRP:CH2	1:A:218:ARG:HD2	2.45	0.52
1:B:457:LEU:HD21	3:B:605:PLM:H62	1.90	0.52
1:B:563:ASP:OD1	1:B:564:LYS:N	2.43	0.52
1:A:378:LYS:N	1:A:379:PRO:HD2	2.25	0.52
1:A:539:ALA:CB	1:A:544:LEU:HD13	2.41	0.51
1:B:550:ASP:HB3	1:B:575:LEU:HD11	1.92	0.51
1:A:446:MET:N	1:A:447:PRO:HD2	2.25	0.51
1:A:372:LYS:O	1:A:376:GLU:HG3	2.11	0.51
1:B:464:HIS:CD2	1:B:468:PRO:HA	2.46	0.51
1:A:264:ILE:CG2	1:A:275:LEU:HD21	2.41	0.50
1:A:393:GLU:O	1:A:397:GLN:HG3	2.11	0.50
1:B:426:VAL:HG11	1:B:460:LEU:HD13	1.93	0.50
1:A:49:PHE:O	1:A:52:THR:HB	2.10	0.50
1:A:95:GLU:HG3	1:A:96:PRO:HA	1.92	0.50
1:B:378:LYS:HE3	1:B:382:GLU:OE2	2.11	0.50
1:A:344:VAL:HA	1:A:347:LEU:HD12	1.93	0.50
1:A:370:TYR:O	1:A:373:VAL:HB	2.11	0.50
1:A:551:PHE:CD1	3:A:606:PLM:H82	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PHE:O	1:B:52:THR:HB	2.11	0.50
1:A:208:GLU:O	1:A:212:LYS:HG3	2.12	0.49
1:A:66:LEU:HD22	3:A:603:PLM:HF2	1.94	0.49
1:A:550:ASP:HB3	1:A:575:LEU:CD1	2.42	0.49
1:A:556:GLU:O	1:A:560:LYS:HB2	2.11	0.49
1:B:529:LEU:O	1:B:533:VAL:HG23	2.12	0.49
1:B:264:ILE:CG2	1:B:275:LEU:HD21	2.42	0.49
1:B:550:ASP:HB3	1:B:575:LEU:CD1	2.41	0.49
3:A:604:PLM:HA1	3:A:605:PLM:H21	1.95	0.49
1:B:150:TYR:CD2	1:B:152:PRO:HD2	2.48	0.49
1:B:408:LEU:HD11	1:B:530:VAL:CG2	2.42	0.49
1:B:422:THR:O	1:B:426:VAL:HG13	2.12	0.48
1:A:217:ALA:HB3	1:A:343:VAL:HG13	1.94	0.48
1:A:307:ALA:O	1:A:312:SER:HB2	2.12	0.48
1:B:140:TYR:O	1:B:144:ARG:HG2	2.13	0.48
1:B:205:LYS:HD3	1:B:206:PHE:CE2	2.48	0.48
1:A:553:ALA:O	1:A:557:LYS:HG3	2.13	0.48
1:A:426:VAL:HG11	1:A:460:LEU:HD13	1.95	0.48
1:B:393:GLU:O	1:B:397:GLN:HG3	2.14	0.48
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.43	0.48
1:A:436:LYS:HE2	1:A:452:TYR:OH	2.12	0.48
1:B:333:GLU:HA	1:B:336:ARG:HD3	1.94	0.48
1:B:521:ARG:HB2	1:B:521:ARG:NH2	2.29	0.48
1:B:539:ALA:CB	1:B:544:LEU:HD13	2.43	0.48
1:A:378:LYS:HE3	1:A:382:GLU:OE2	2.12	0.48
1:B:569:ALA:O	1:B:573:LYS:HG3	2.14	0.48
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.44	0.47
1:A:313:LYS:HG2	1:A:314:ASP:H	1.80	0.47
1:A:452:TYR:O	1:A:455:VAL:HG22	2.14	0.47
1:A:150:TYR:CD2	1:A:152:PRO:HD2	2.50	0.47
1:B:556:GLU:O	1:B:560:LYS:HB2	2.14	0.47
1:A:400:GLU:O	1:A:404:GLN:HG3	2.13	0.47
1:A:408:LEU:HD11	1:A:530:VAL:CG2	2.44	0.47
1:B:217:ALA:HB3	1:B:343:VAL:HG13	1.97	0.47
1:B:222:ARG:NH1	1:B:222:ARG:HG3	2.17	0.47
1:B:576:VAL:O	1:B:580:GLN:HG3	2.15	0.47
1:B:452:TYR:O	1:B:455:VAL:HG22	2.14	0.47
1:B:477:CYS:O	1:B:484:ARG:NH2	2.48	0.47
1:A:175:ALA:O	1:A:179:LEU:HB2	2.14	0.47
1:B:313:LYS:HG2	1:B:314:ASP:H	1.80	0.46
1:A:223:PHE:CD1	1:A:272:SER:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:LYS:HE3	1:A:542:GLU:OE2	2.15	0.46
1:A:576:VAL:O	1:A:580:GLN:HG3	2.15	0.46
1:A:171:ALA:O	1:A:174:LYS:HG2	2.14	0.46
1:A:180:PRO:O	1:A:184:GLU:HG3	2.16	0.46
1:A:556:GLU:O	1:A:560:LYS:HE3	2.15	0.46
1:B:400:GLU:O	1:B:404:GLN:HG3	2.15	0.46
1:B:153:GLU:OE2	1:B:288:HIS:ND1	2.40	0.46
1:A:257:ARG:NH1	1:A:287:SER:OG	2.48	0.46
1:B:258:ALA:O	1:B:262:LYS:HB2	2.16	0.46
1:A:504:ALA:O	1:A:508:THR:OG1	2.24	0.46
1:B:307:ALA:O	1:B:312:SER:HB2	2.15	0.46
1:B:330:PHE:HZ	1:B:377:PHE:CE2	2.34	0.46
1:A:462:VAL:O	1:A:465:GLU:HB3	2.16	0.45
1:B:199:LYS:HD3	1:B:242:HIS:CD2	2.51	0.45
1:B:504:ALA:O	1:B:508:THR:OG1	2.26	0.45
1:A:133:THR:O	1:A:137:LYS:HB2	2.15	0.45
1:B:525:LYS:HG2	1:B:551:PHE:HE2	1.82	0.45
1:B:138:TYR:CE2	3:B:602:PLM:H51	2.51	0.45
1:B:161:TYR:CD1	3:B:602:PLM:H72	2.52	0.45
1:B:302:LEU:HA	1:B:303:PRO:HD3	1.82	0.45
1:B:513:ILE:HA	1:B:516:LEU:HD12	1.98	0.45
1:A:395:PHE:CZ	1:A:435:SER:HA	2.51	0.45
1:A:521:ARG:NH2	1:A:521:ARG:HB2	2.32	0.45
1:A:205:LYS:HD3	1:A:206:PHE:CE2	2.52	0.45
1:A:416:PRO:HB2	1:A:497:TYR:CD1	2.52	0.45
1:A:513:ILE:O	1:A:521:ARG:NH2	2.50	0.45
1:B:344:VAL:O	1:B:348:ARG:HG3	2.16	0.45
1:A:453:LEU:CD1	3:A:604:PLM:H62	2.47	0.45
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.82	0.44
1:B:377:PHE:O	1:B:381:VAL:HG23	2.16	0.44
1:A:373:VAL:HG12	1:A:374:PHE:N	2.31	0.44
1:B:180:PRO:O	1:B:184:GLU:HG3	2.18	0.44
1:B:408:LEU:HD23	1:B:529:LEU:HD23	1.98	0.44
1:B:464:HIS:CE1	1:B:473:VAL:HB	2.52	0.44
1:A:196:GLN:HG3	2:A:601:6WF:C07	2.47	0.44
1:B:455:VAL:HG23	1:B:456:VAL:N	2.33	0.44
1:A:198:LEU:HD12	1:A:198:LEU:C	2.35	0.44
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.80	0.44
1:A:529:LEU:O	1:A:533:VAL:HG23	2.17	0.44
1:B:171:ALA:O	1:B:174:LYS:HG2	2.17	0.44
1:A:115:LEU:HD11	1:A:141:GLU:CB	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HD22	1:B:242:HIS:HE1	1.81	0.44
1:B:471:ASP:N	1:B:471:ASP:OD1	2.46	0.44
1:B:387:LEU:HD13	3:B:604:PLM:H71	2.00	0.44
1:A:550:ASP:HB3	1:A:575:LEU:HD11	1.99	0.44
1:A:140:TYR:O	1:A:144:ARG:HG2	2.18	0.43
1:B:373:VAL:HG12	1:B:374:PHE:N	2.32	0.43
1:B:419:SER:OG	1:B:421:PRO:HD2	2.18	0.43
1:A:464:HIS:CE1	1:A:473:VAL:HB	2.53	0.43
1:A:455:VAL:HG23	1:A:456:VAL:N	2.34	0.43
1:B:155:LEU:HG	1:B:159:LYS:HE2	2.00	0.43
1:B:369:CYS:HA	1:B:372:LYS:CG	2.49	0.43
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.83	0.43
1:A:333:GLU:HA	1:A:336:ARG:HD3	2.00	0.43
1:B:395:PHE:CZ	1:B:435:SER:HA	2.52	0.43
1:A:337:ARG:HH11	1:A:337:ARG:HG3	1.83	0.43
1:A:471:ASP:N	1:A:471:ASP:OD1	2.46	0.43
1:A:161:TYR:CE1	1:A:185:LEU:HD23	2.52	0.43
1:B:539:ALA:HB1	1:B:544:LEU:HD13	2.01	0.43
1:B:133:THR:O	1:B:137:LYS:HB2	2.17	0.43
1:A:268:GLN:HG3	1:A:275:LEU:HB3	2.01	0.43
1:A:551:PHE:O	1:A:555:VAL:HG23	2.19	0.43
1:B:357:LEU:O	1:B:361:CYS:HB2	2.19	0.43
1:A:254:ALA:HB1	3:A:603:PLM:H42	2.01	0.42
1:B:541:LYS:HE3	1:B:542:GLU:OE2	2.17	0.42
1:A:343:VAL:O	1:A:347:LEU:HG	2.18	0.42
1:A:426:VAL:HG11	1:A:460:LEU:CD1	2.48	0.42
1:B:553:ALA:O	1:B:557:LYS:HG3	2.19	0.42
2:B:601:6WF:C16	2:B:601:6WF:C14	2.74	0.42
1:A:245:CYS:HB3	2:A:601:6WF:C06	2.49	0.42
1:B:24:LEU:HD23	1:B:139:LEU:HD23	2.01	0.42
1:A:6:GLU:HB3	1:A:66:LEU:HG	2.01	0.42
1:B:372:LYS:HG2	1:B:372:LYS:H	1.68	0.42
1:A:114:ARG:NH1	1:A:116:VAL:HG12	2.34	0.42
1:B:429:ASN:O	1:B:433:VAL:HG23	2.20	0.42
3:B:604:PLM:H92	3:B:604:PLM:H61	1.81	0.42
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.90	0.41
1:B:369:CYS:HA	1:B:372:LYS:HG3	2.02	0.41
1:A:417:GLN:HB2	1:A:469:VAL:CG1	2.49	0.41
1:A:418:VAL:HG21	3:A:605:PLM:HD2	2.01	0.41
1:B:35:PRO:HG2	1:B:38:ASP:CG	2.40	0.41
1:B:345:LEU:O	1:B:349:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:PHE:O	1:B:555:VAL:HG23	2.21	0.41
1:A:22:LEU:HD13	3:A:603:PLM:H72	2.03	0.41
1:B:222:ARG:NH1	1:B:222:ARG:CG	2.81	0.41
1:B:353:TYR:CZ	1:B:357:LEU:HD11	2.56	0.41
1:B:10:ARG:NH2	1:B:255:ASP:OD1	2.54	0.41
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.56	0.41
1:B:138:TYR:CB	3:B:602:PLM:HA1	2.50	0.41
1:A:330:PHE:HZ	1:A:377:PHE:CE2	2.39	0.41
1:A:513:ILE:HA	1:A:516:LEU:HD12	2.01	0.41
1:B:343:VAL:O	1:B:347:LEU:HG	2.20	0.41
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.56	0.41
1:A:345:LEU:O	1:A:349:LEU:HG	2.21	0.41
1:A:416:PRO:HB2	1:A:497:TYR:CE1	2.56	0.41
1:A:477:CYS:O	1:A:484:ARG:NH2	2.54	0.41
1:B:32:GLN:H	1:B:32:GLN:HG3	1.71	0.41
1:A:458:ASN:O	1:A:462:VAL:HG23	2.21	0.40
1:B:415:VAL:HG12	1:B:418:VAL:HG23	2.03	0.40
1:A:24:LEU:HD23	1:A:139:LEU:HD23	2.04	0.40
1:A:373:VAL:HA	1:A:376:GLU:OE1	2.22	0.40
1:B:203:LEU:O	1:B:203:LEU:HD23	2.20	0.40
1:A:119:GLU:HB2	1:A:122:VAL:CG2	2.47	0.40
1:B:344:VAL:HA	1:B:347:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/581 (100%)	565 (98%)	13 (2%)	1 (0%)	47	78
1	B	579/581 (100%)	565 (98%)	14 (2%)	0	100	100
All	All	1158/1162 (100%)	1130 (98%)	27 (2%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLY

### 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	503/509 (99%)	496 (99%)	7 (1%)	67	90
1	B	503/509 (99%)	500 (99%)	3 (1%)	86	96
All	All	1006/1018 (99%)	996 (99%)	10 (1%)	76	93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	94	GLN
1	A	197	ARG
1	A	199	LYS
1	A	203	LEU
1	A	262	LYS
1	A	544	LEU
1	B	3	HIS
1	B	262	LYS
1	B	544	LEU

Some 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](#)

14 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	PLM	B	603	-	14,17,17	0.07	0	13,17,17	0.38	0
3	PLM	B	604	-	13,16,17	0.07	0	12,16,17	0.47	0
3	PLM	A	602	1	9,12,17	0.09	0	8,12,17	0.32	0
3	PLM	A	607	-	14,17,17	0.07	0	13,17,17	0.40	0
3	PLM	B	607	1	14,17,17	0.08	0	13,17,17	0.41	0
3	PLM	A	603	-	14,17,17	0.06	0	13,17,17	0.42	0
3	PLM	B	606	-	13,16,17	0.07	0	12,16,17	0.39	0
3	PLM	B	602	-	9,12,17	0.08	0	8,12,17	0.35	0
3	PLM	A	604	-	13,16,17	0.07	0	12,16,17	0.43	0
3	PLM	B	605	-	14,17,17	0.07	0	13,17,17	0.40	0
3	PLM	A	605	-	14,17,17	0.07	0	13,17,17	0.41	0
2	6WF	B	601	1	23,27,27	6.57	11 (47%)	30,39,39	5.88	11 (36%)
2	6WF	A	601	1	23,27,27	6.02	12 (52%)	30,39,39	7.54	9 (30%)
3	PLM	A	606	-	13,16,17	0.07	0	12,16,17	0.40	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
3	PLM	B	603	-	-	6/13/15/15	-
3	PLM	B	604	-	-	8/12/14/15	-
3	PLM	A	602	1	-	3/8/10/15	-
3	PLM	A	607	-	-	6/13/15/15	-
3	PLM	B	607	1	-	5/13/15/15	-
3	PLM	A	603	-	-	9/13/15/15	-
3	PLM	B	606	-	-	6/12/14/15	-
3	PLM	B	602	-	-	6/8/10/15	-
3	PLM	A	604	-	-	5/12/14/15	-
3	PLM	B	605	-	-	6/13/15/15	-
3	PLM	A	605	-	-	5/13/15/15	-
2	6WF	B	601	1	-	3/4/32/32	0/5/5/5
2	6WF	A	601	1	-	3/4/32/32	0/5/5/5
3	PLM	A	606	-	-	7/12/14/15	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6WF	N01-N15	16.08	1.81	1.37
2	A	601	6WF	N01-N15	14.71	1.77	1.37
2	B	601	6WF	C13-C14	14.25	1.75	1.43
2	B	601	6WF	C02-N01	13.84	1.58	1.35
2	A	601	6WF	C13-C14	12.70	1.71	1.43
2	A	601	6WF	C02-N01	10.84	1.53	1.35
2	B	601	6WF	C13-C12	9.12	1.60	1.41
2	A	601	6WF	C13-C12	8.97	1.59	1.41
2	A	601	6WF	C02-S09	8.47	1.85	1.70
2	B	601	6WF	O11-C12	8.42	1.44	1.32
2	A	601	6WF	O11-C12	8.24	1.43	1.32
2	B	601	6WF	C02-S09	8.13	1.84	1.70
2	A	601	6WF	C02-N03	6.14	1.44	1.33
2	B	601	6WF	C02-N03	6.12	1.44	1.33
2	B	601	6WF	C22-C17	5.98	1.56	1.41
2	B	601	6WF	C22-C23	5.14	1.47	1.36
2	A	601	6WF	C22-C17	4.73	1.53	1.41
2	A	601	6WF	C22-C23	4.63	1.46	1.36
2	A	601	6WF	C13-C16	-3.07	1.39	1.45
2	A	601	6WF	C16-C17	-2.80	1.37	1.43
2	A	601	6WF	C23-C12	-2.03	1.35	1.39
2	B	601	6WF	C20-C21	2.01	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6WF	C19-C18	2.00	1.41	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	6WF	S09-C02-N01	-29.77	88.12	120.97
2	A	601	6WF	C02-N01-N15	-25.49	92.74	119.36
2	B	601	6WF	C02-N01-N15	-23.48	94.83	119.36
2	B	601	6WF	S09-C02-N01	-18.21	100.87	120.97
2	B	601	6WF	C04-N03-C02	-7.40	108.58	123.33
2	A	601	6WF	C14-N15-N01	7.08	128.48	115.36
2	A	601	6WF	C04-N03-C02	-6.34	110.69	123.33
2	B	601	6WF	C14-N15-N01	5.61	125.76	115.36
2	A	601	6WF	C08-N03-C02	-4.71	113.95	123.33
2	A	601	6WF	C12-C13-C16	4.41	124.51	119.60
2	B	601	6WF	C08-N03-C02	-3.67	116.02	123.33
2	B	601	6WF	N01-C02-N03	-3.27	112.16	117.53
2	A	601	6WF	C05-C04-N03	3.04	116.65	110.66
2	B	601	6WF	O11-C12-C13	-2.85	119.46	124.36
2	A	601	6WF	C16-C13-C14	-2.70	115.02	119.32
2	B	601	6WF	C21-C16-C13	-2.57	120.13	123.42
2	A	601	6WF	C21-C16-C17	2.36	120.94	117.89
2	B	601	6WF	C21-C16-C17	2.23	120.77	117.89
2	B	601	6WF	O11-C12-C23	2.09	121.78	118.66
2	B	601	6WF	C12-C13-C16	2.07	121.90	119.60

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	603	PLM	C1-C2-C3-C4
3	A	602	PLM	C1-C2-C3-C4
3	A	607	PLM	C1-C2-C3-C4
3	A	603	PLM	C1-C2-C3-C4
3	B	606	PLM	C1-C2-C3-C4
3	B	602	PLM	C1-C2-C3-C4
3	B	605	PLM	C1-C2-C3-C4
2	B	601	6WF	N01-C02-N03-C04
2	B	601	6WF	N01-C02-N03-C08
2	B	601	6WF	S09-C02-N03-C04
2	A	601	6WF	N01-C02-N03-C04
2	A	601	6WF	N01-C02-N03-C08

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Mol	Chain	Res	Type	Atoms
2	A	601	6WF	S09-C02-N03-C04
3	B	605	PLM	C4-C5-C6-C7
3	A	606	PLM	CA-CB-CC-CD
3	B	603	PLM	C2-C3-C4-C5
3	B	602	PLM	C5-C6-C7-C8
3	B	603	PLM	C9-CA-CB-CC
3	A	605	PLM	C4-C5-C6-C7
3	B	602	PLM	C4-C5-C6-C7
3	A	607	PLM	C2-C3-C4-C5
3	B	604	PLM	CA-CB-CC-CD
3	A	606	PLM	C6-C7-C8-C9
3	A	603	PLM	C7-C8-C9-CA
3	A	603	PLM	CA-CB-CC-CD
3	B	603	PLM	CA-CB-CC-CD
3	A	606	PLM	C8-C9-CA-CB
3	B	607	PLM	C5-C6-C7-C8
3	A	603	PLM	C3-C4-C5-C6
3	A	604	PLM	CA-CB-CC-CD
3	A	603	PLM	C6-C7-C8-C9
3	B	602	PLM	C3-C4-C5-C6
3	B	607	PLM	CC-CD-CE-CF
3	B	602	PLM	C2-C3-C4-C5
3	B	604	PLM	CB-CC-CD-CE
3	A	607	PLM	C5-C6-C7-C8
3	B	606	PLM	C5-C6-C7-C8
3	A	607	PLM	CC-CD-CE-CF
3	A	602	PLM	C2-C3-C4-C5
3	A	607	PLM	C4-C5-C6-C7
3	B	605	PLM	C3-C4-C5-C6
3	B	606	PLM	C8-C9-CA-CB
3	A	603	PLM	C5-C6-C7-C8
3	A	606	PLM	C5-C6-C7-C8
3	B	604	PLM	CC-CD-CE-CF
3	A	606	PLM	C2-C3-C4-C5
3	B	606	PLM	CB-CC-CD-CE
3	B	607	PLM	C2-C3-C4-C5
3	A	602	PLM	C8-C9-CA-CB
3	B	605	PLM	C9-CA-CB-CC
3	A	606	PLM	CB-CC-CD-CE
3	B	605	PLM	C2-C3-C4-C5
3	A	606	PLM	C9-CA-CB-CC
3	A	603	PLM	CB-CC-CD-CE

*Continued on next page...*

*Continued from previous page...*

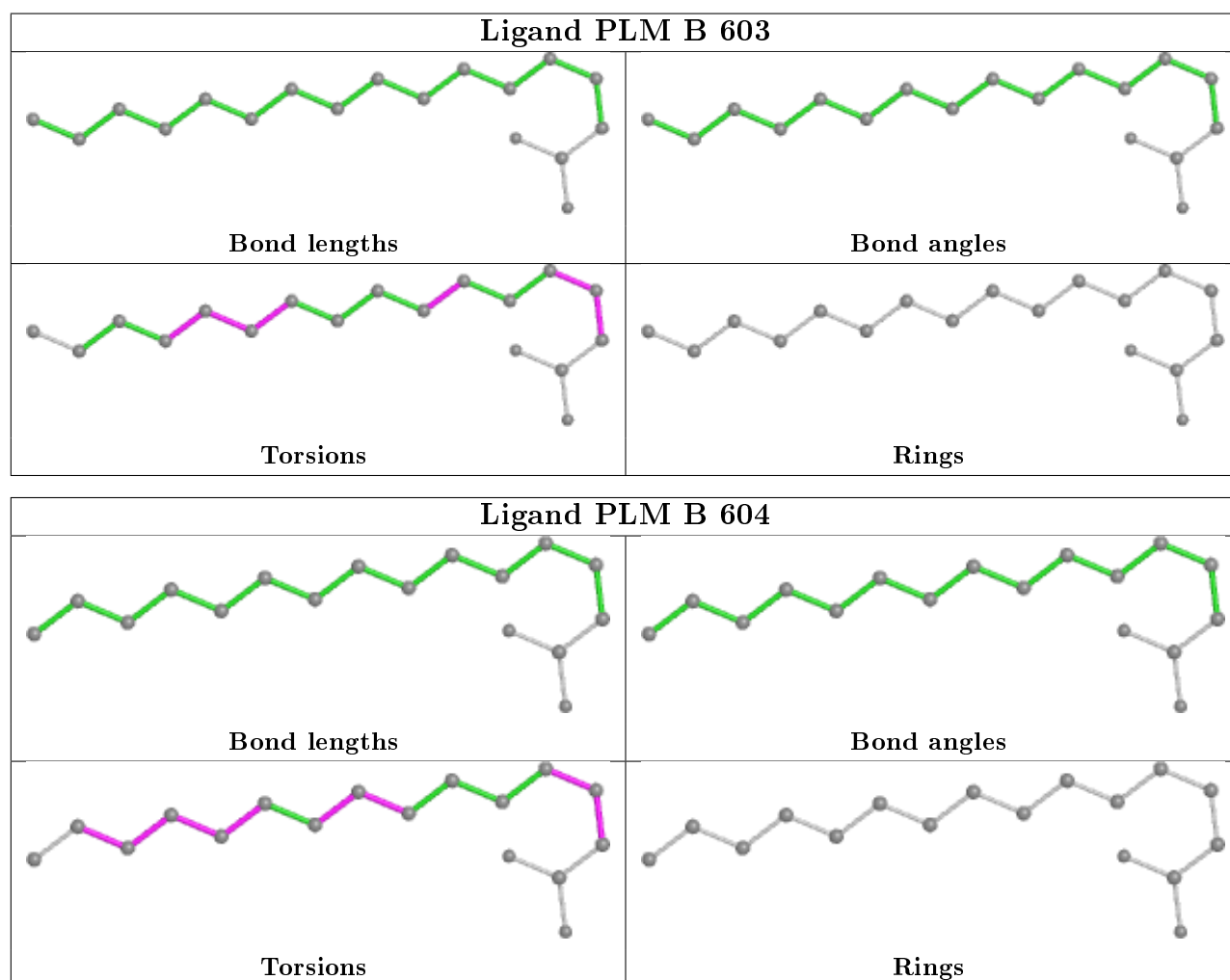
Mol	Chain	Res	Type	Atoms
3	A	604	PLM	C5-C6-C7-C8
3	B	606	PLM	C6-C7-C8-C9
3	A	604	PLM	C2-C3-C4-C5
3	B	606	PLM	C4-C5-C6-C7
3	B	604	PLM	C1-C2-C3-C4
3	B	607	PLM	C1-C2-C3-C4
3	A	604	PLM	C3-C4-C5-C6
3	B	604	PLM	C6-C7-C8-C9
3	B	604	PLM	C2-C3-C4-C5
3	A	604	PLM	CB-CC-CD-CE
3	A	603	PLM	C4-C5-C6-C7
3	A	605	PLM	C9-CA-CB-CC
3	A	605	PLM	C8-C9-CA-CB
3	B	604	PLM	C7-C8-C9-CA
3	A	607	PLM	C3-C4-C5-C6
3	A	605	PLM	CA-CB-CC-CD
3	B	603	PLM	CB-CC-CD-CE
3	B	607	PLM	C9-CA-CB-CC
3	B	603	PLM	C5-C6-C7-C8
3	A	603	PLM	C9-CA-CB-CC
3	B	604	PLM	C9-CA-CB-CC
3	A	605	PLM	C1-C2-C3-C4
3	B	602	PLM	C6-C7-C8-C9
3	B	605	PLM	C6-C7-C8-C9

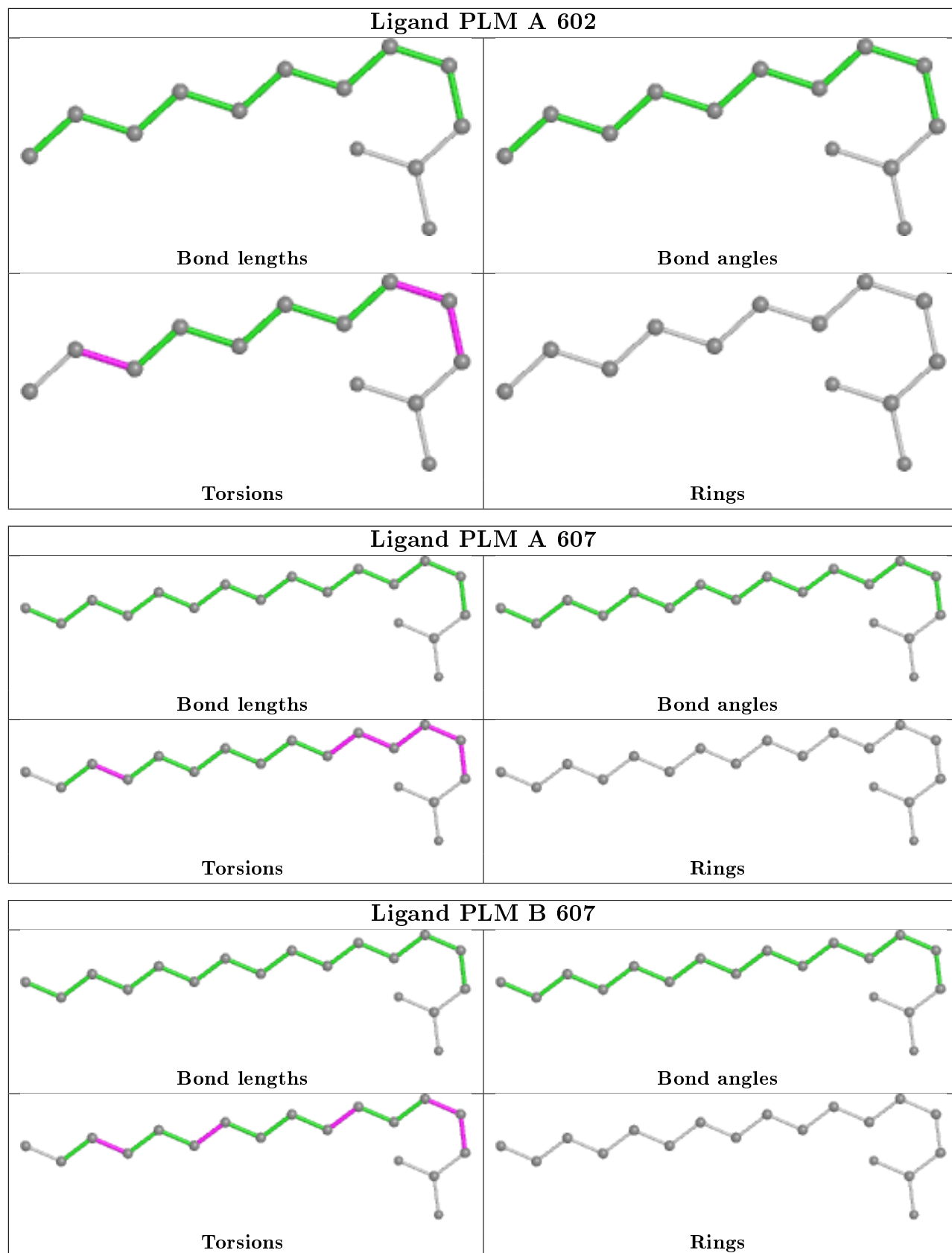
There are no ring outliers.

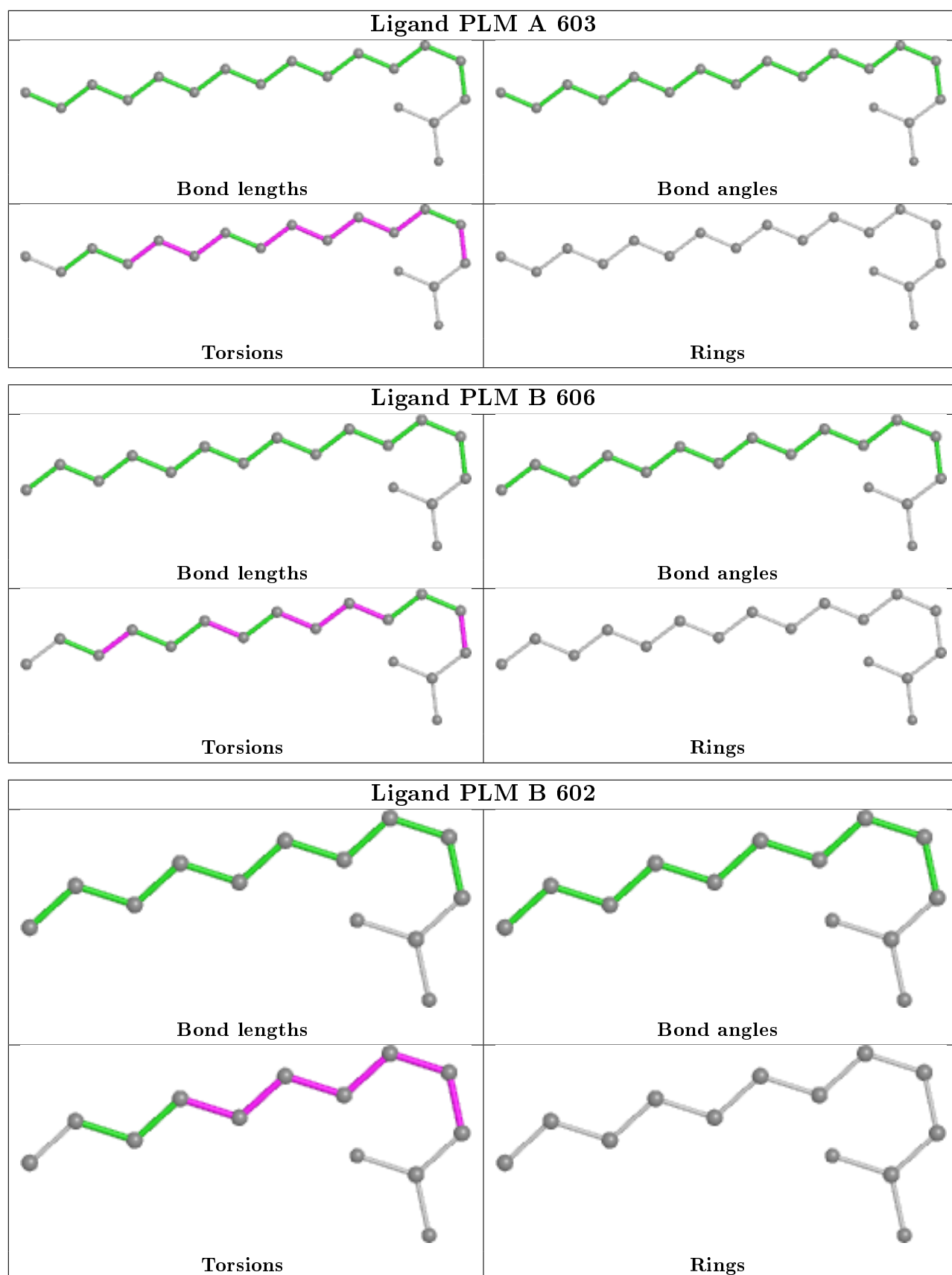
12 monomers are involved in 48 short contacts:

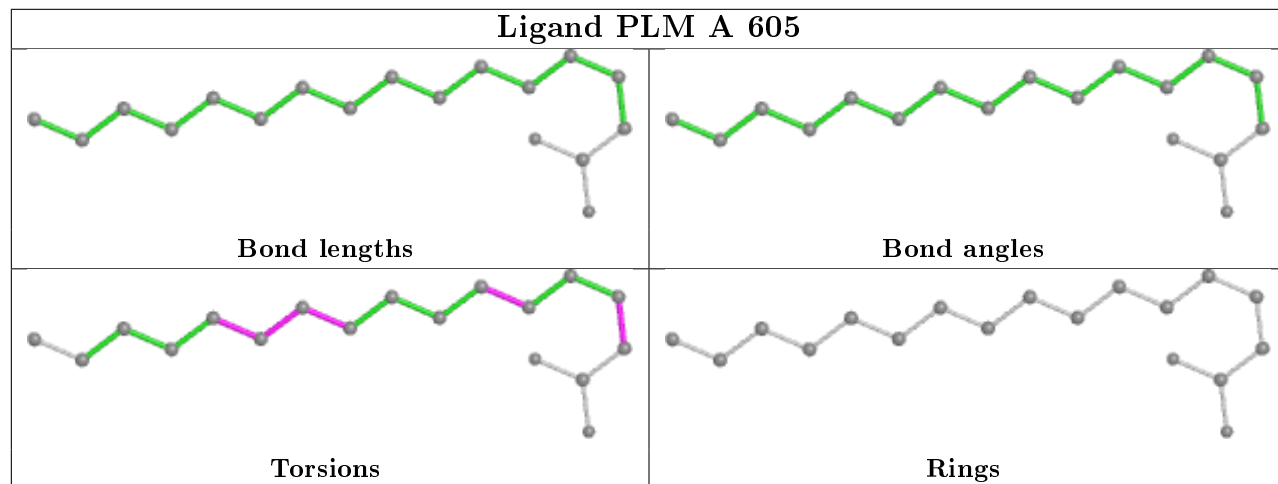
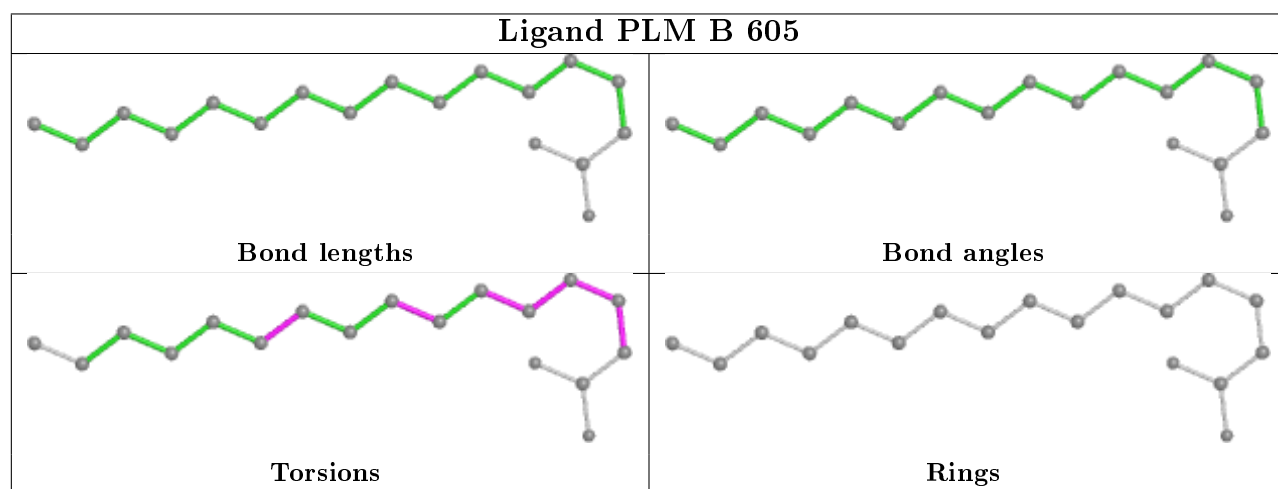
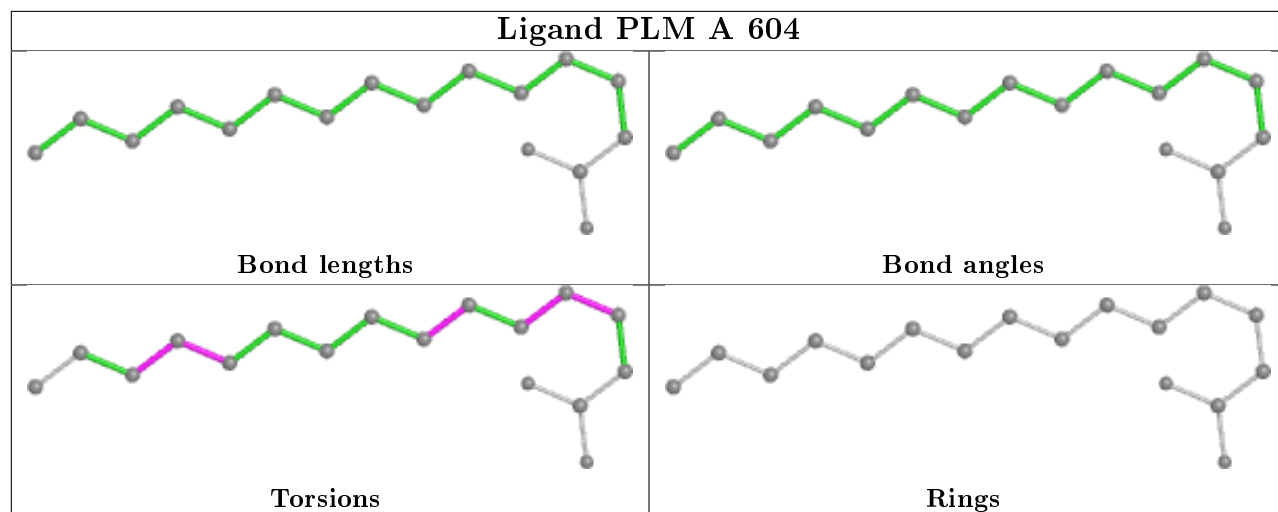
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	PLM	3	0
3	B	604	PLM	3	0
3	A	602	PLM	5	0
3	A	603	PLM	3	0
3	B	606	PLM	1	0
3	B	602	PLM	4	0
3	A	604	PLM	2	0
3	B	605	PLM	8	0
3	A	605	PLM	6	0
2	B	601	6WF	8	0
2	A	601	6WF	6	0
3	A	606	PLM	1	0

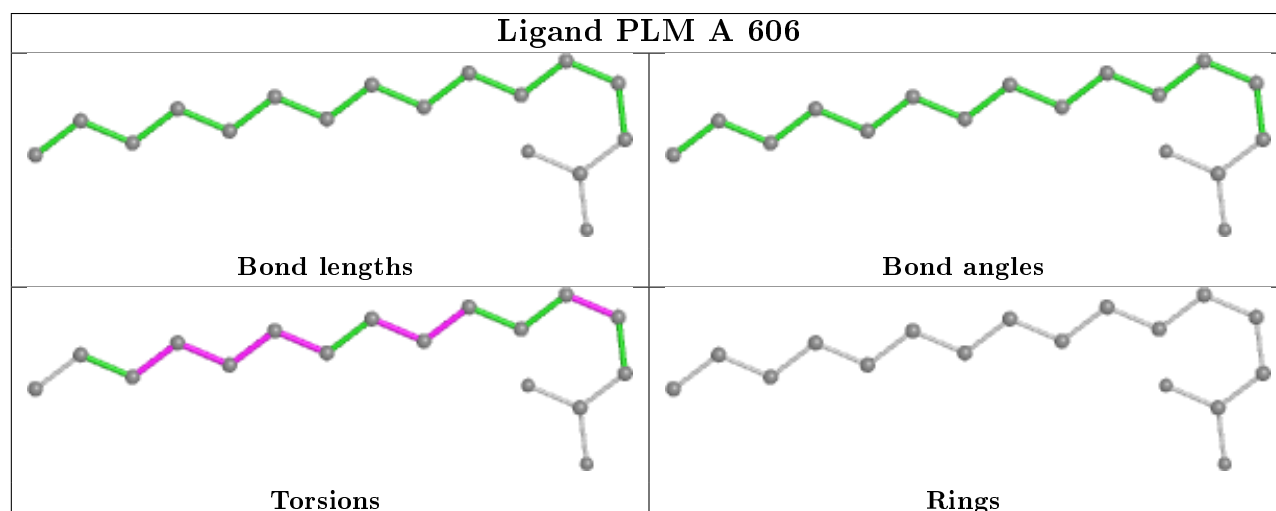
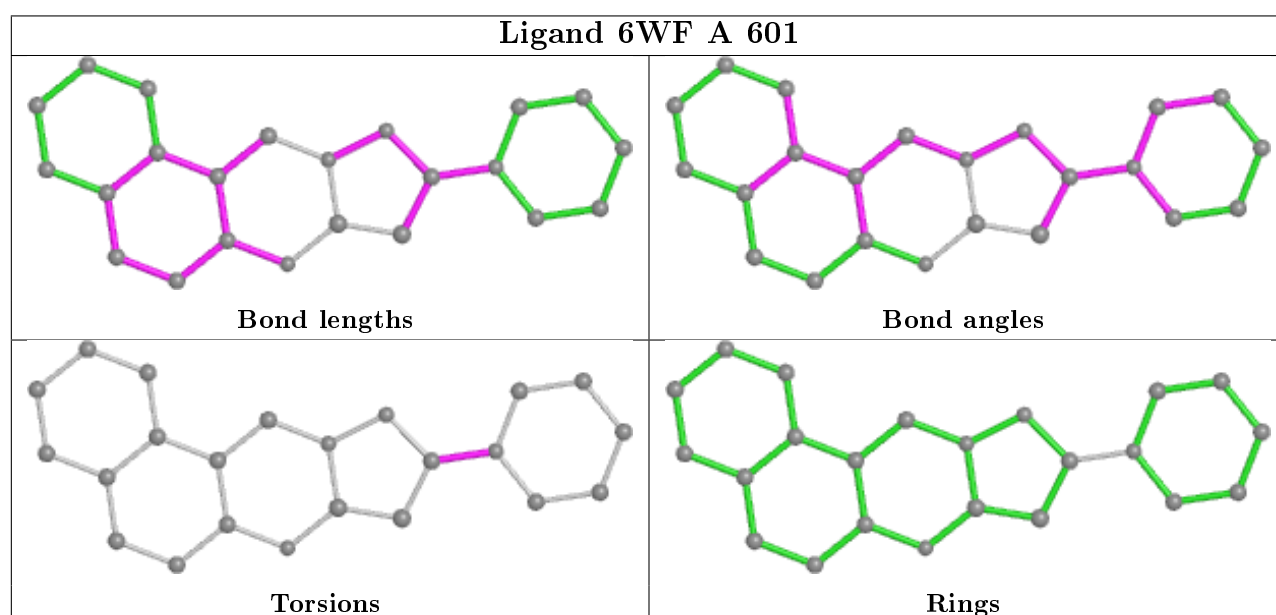
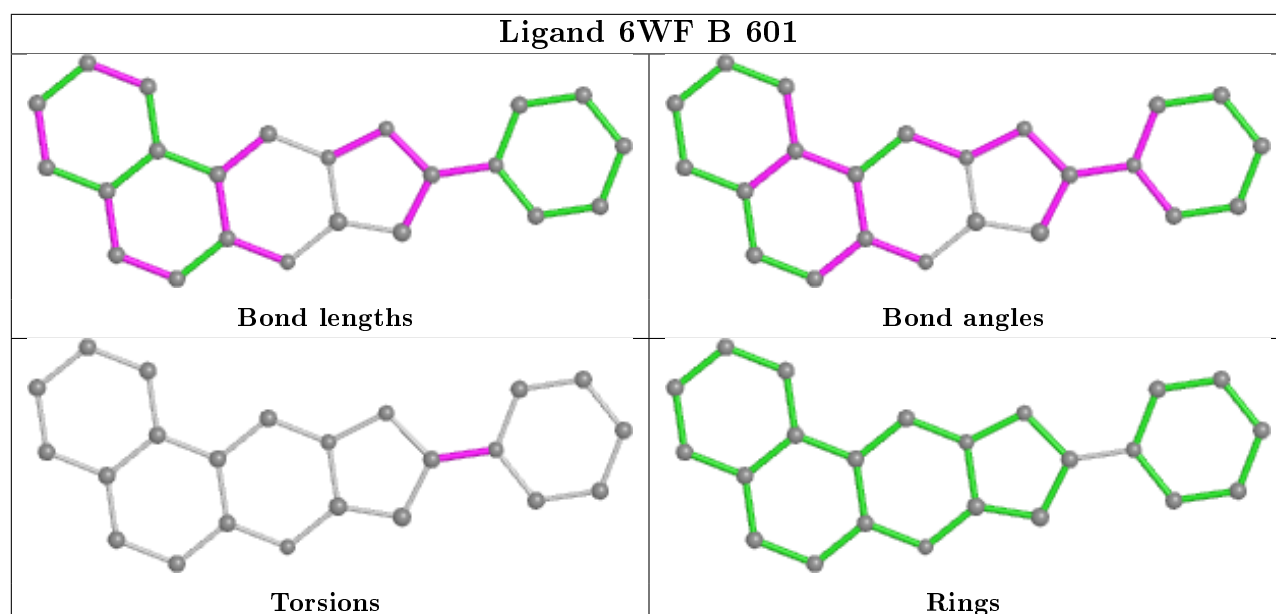
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	581/581 (100%)	-0.37	2 (0%) 94 93	32, 58, 99, 168	0
1	B	581/581 (100%)	-0.28	6 (1%) 82 77	39, 67, 106, 149	0
All	All	1162/1162 (100%)	-0.33	8 (0%) 87 84	32, 62, 102, 168	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ASP	5.2
1	B	301	ASP	3.4
1	B	481	LEU	2.8
1	B	453	LEU	2.6
1	B	109	ASN	2.5
1	B	370	TYR	2.3
1	A	370	TYR	2.3
1	B	60	GLU	2.1

### 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.

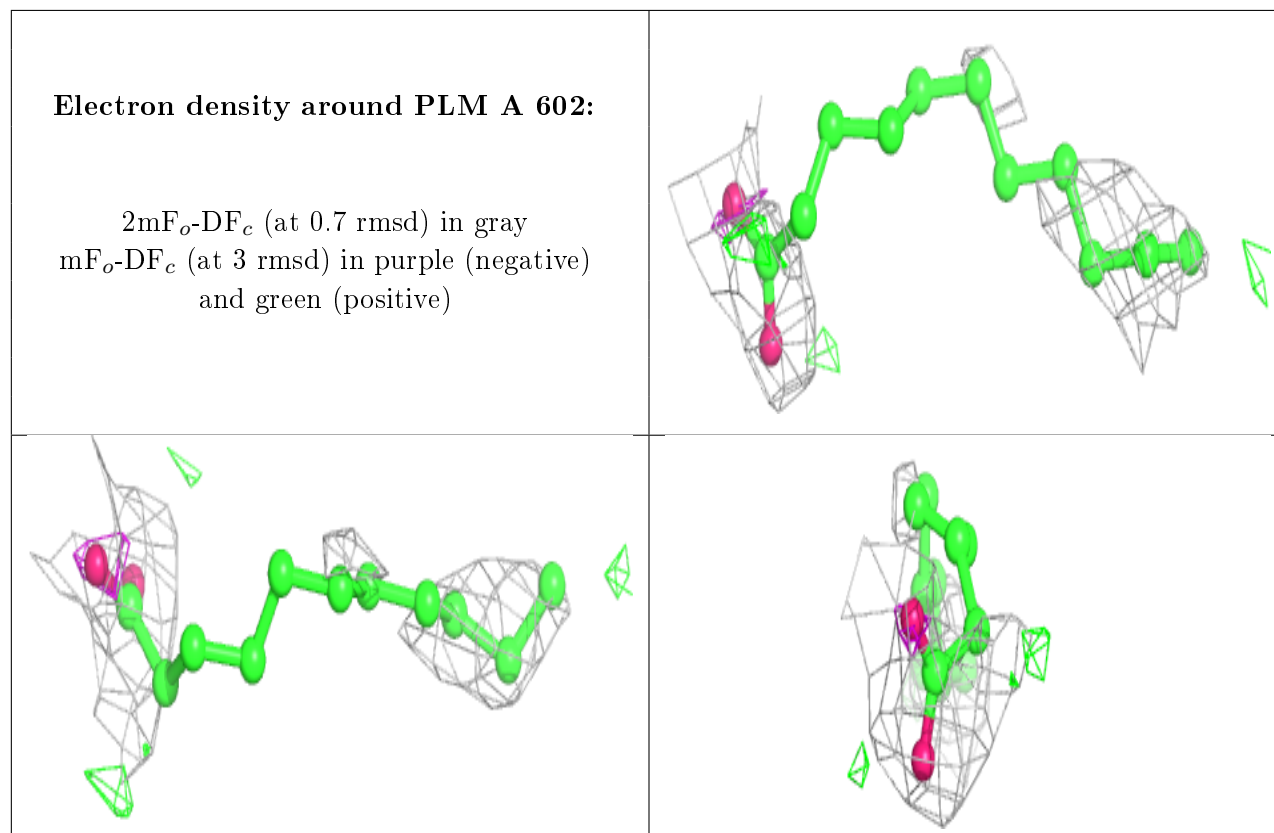
### 6.4 Ligands [i](#)

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.

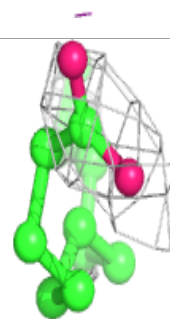
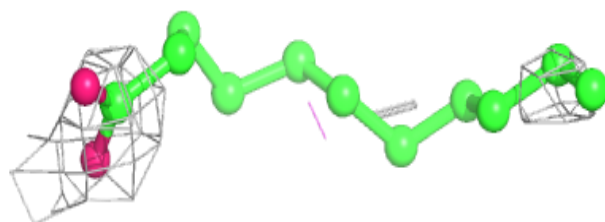
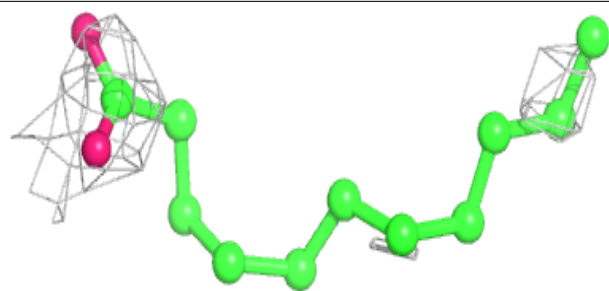
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PLM	A	602	13/18	0.69	0.53	84,90,96,96	0
3	PLM	B	602	13/18	0.70	0.82	95,105,113,114	0
3	PLM	B	605	18/18	0.81	0.35	68,82,95,95	0
3	PLM	B	607	18/18	0.84	0.34	33,51,92,93	0
3	PLM	A	605	18/18	0.86	0.34	65,81,89,91	0
3	PLM	A	607	18/18	0.87	0.35	44,59,108,111	0
3	PLM	B	603	18/18	0.89	0.38	58,66,80,81	0
3	PLM	B	606	17/18	0.90	0.36	57,60,68,72	0
3	PLM	A	603	18/18	0.91	0.36	60,67,80,84	0
3	PLM	B	604	17/18	0.92	0.29	51,63,72,72	0
2	6WF	A	601	23/23	0.92	0.18	39,54,96,223	0
2	6WF	B	601	23/23	0.93	0.19	44,64,88,202	0
3	PLM	A	606	17/18	0.93	0.26	40,49,66,74	0
3	PLM	A	604	17/18	0.94	0.28	51,59,66,66	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.

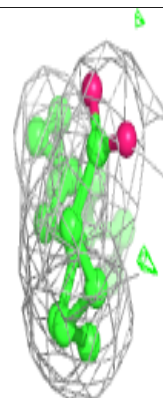
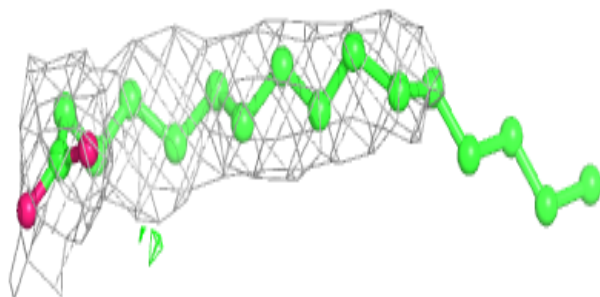
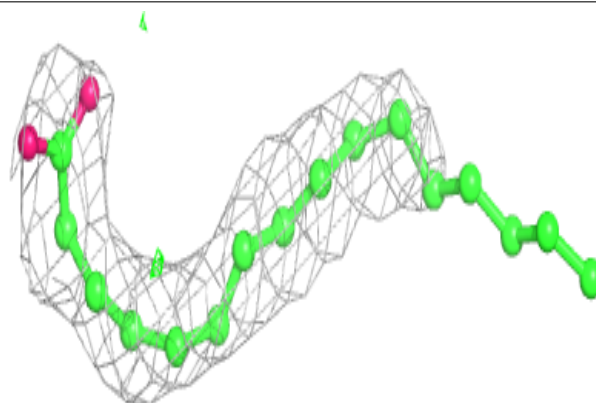


**Electron density around PLM B 602:**

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

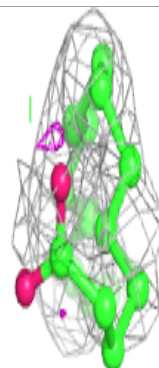
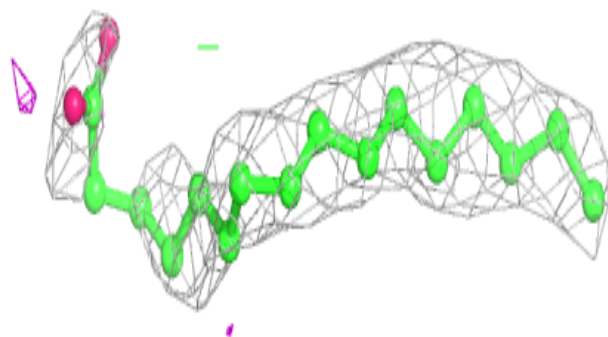
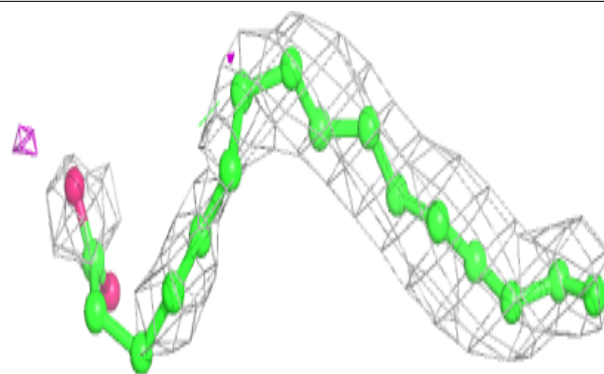
**Electron density around PLM B 605:**

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

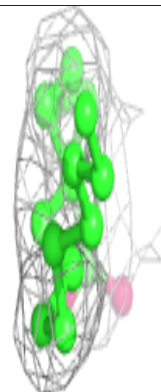
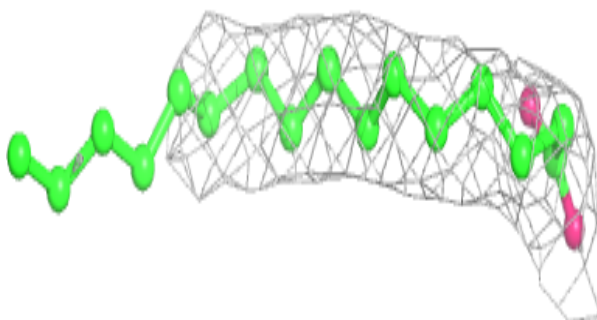
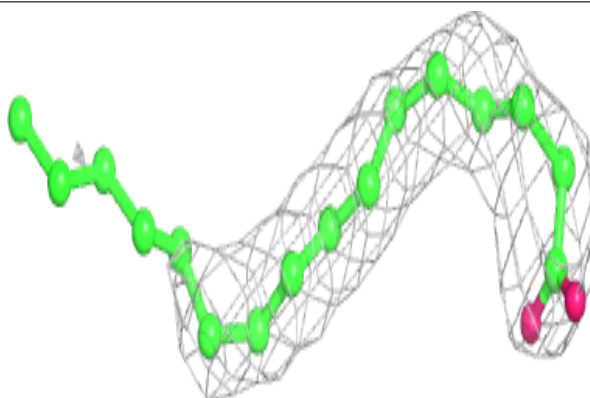


**Electron density around PLM B 607:**

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

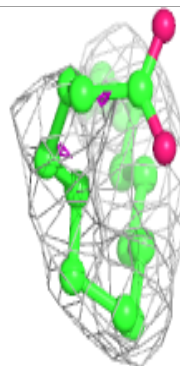
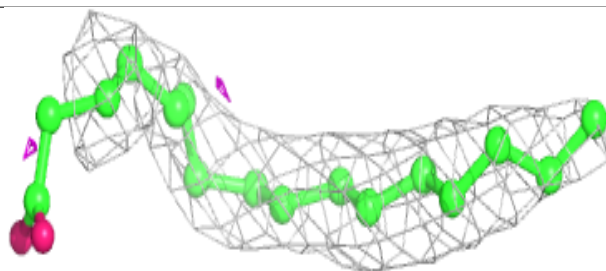
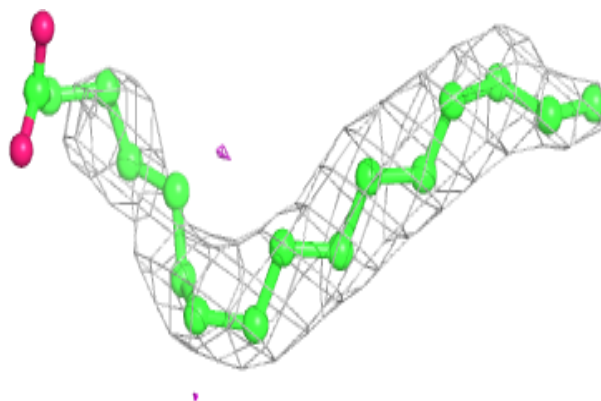
**Electron density around PLM A 605:**

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

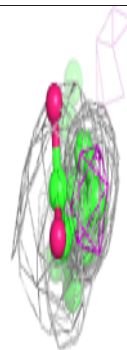
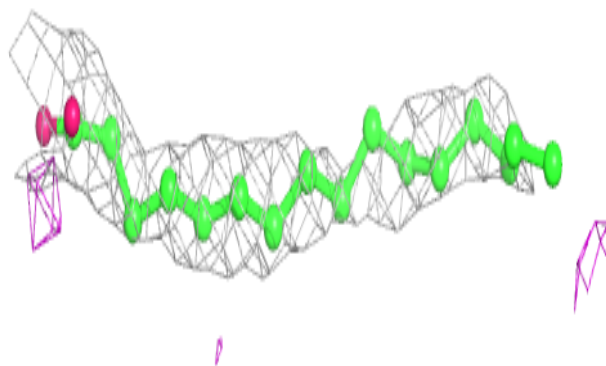
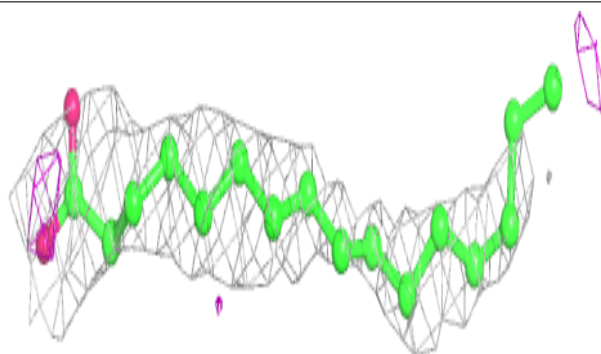


**Electron density around PLM A 607:**

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

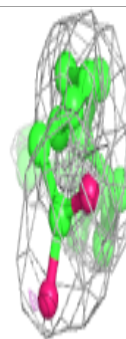
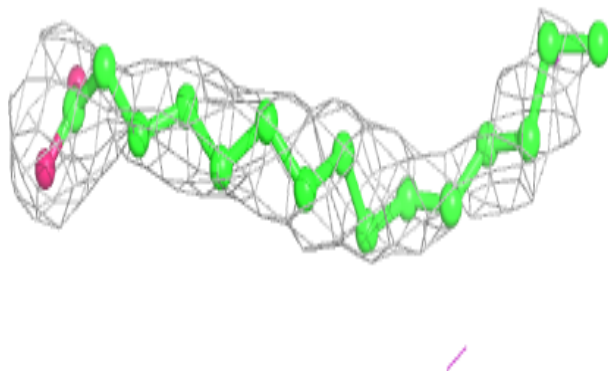
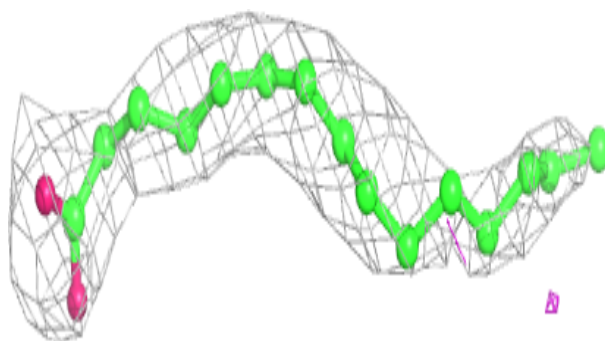
**Electron density around PLM B 603:**

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

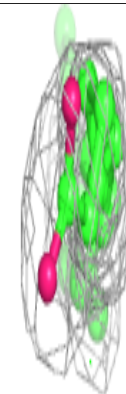
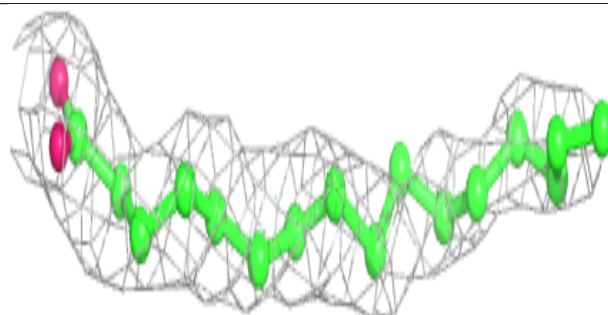
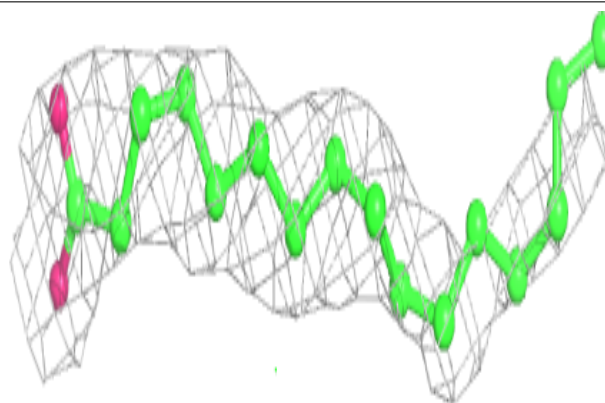


**Electron density around PLM B 606:**

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

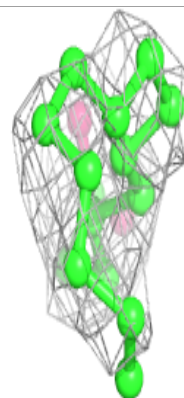
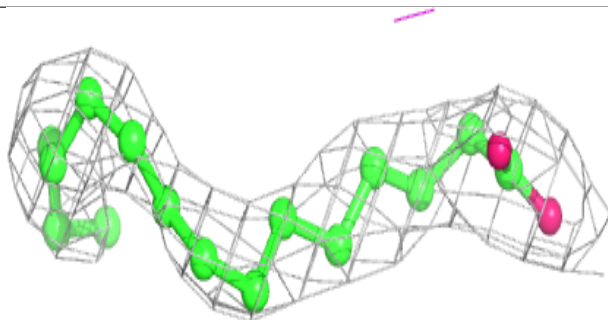
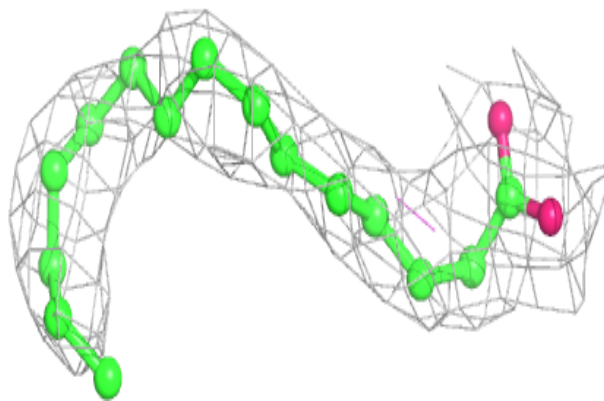
**Electron density around PLM A 603:**

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

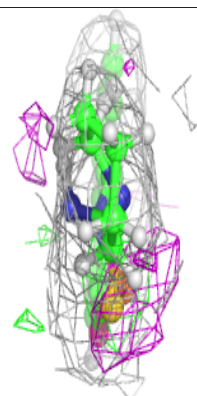
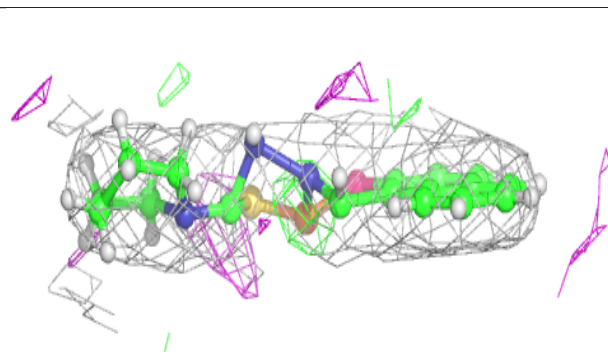
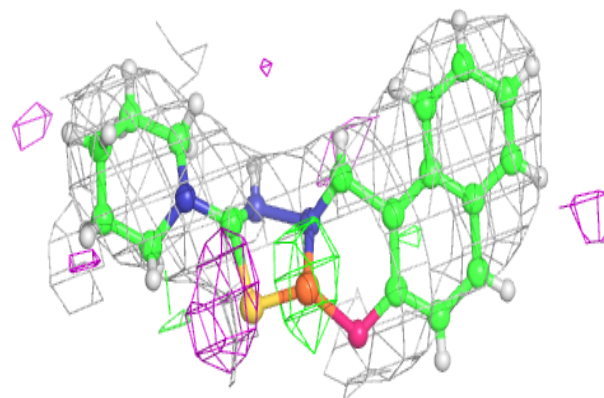


**Electron density around PLM B 604:**

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

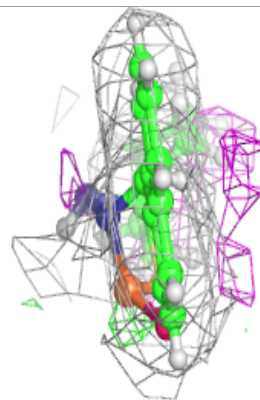
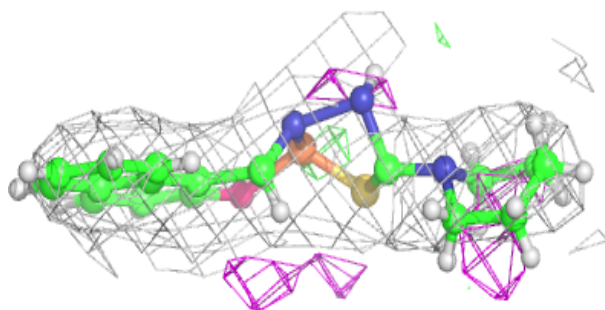
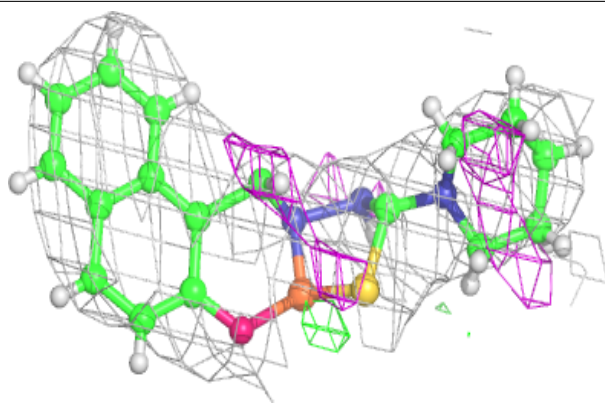
**Electron density around 6WF A 601:**

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

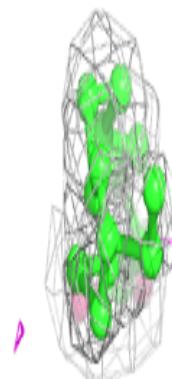
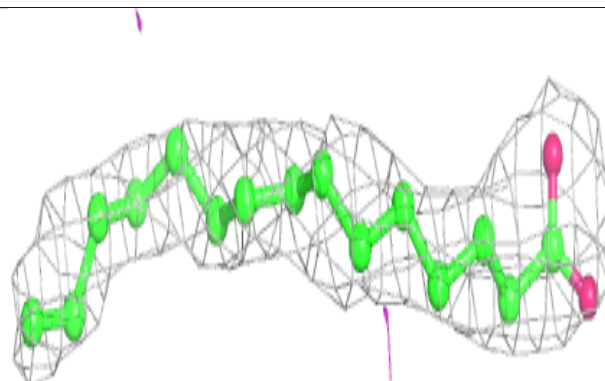
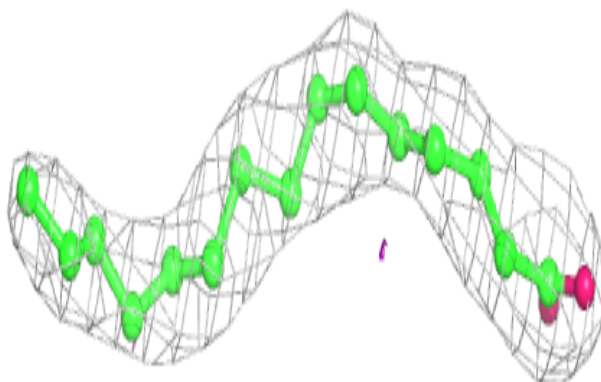


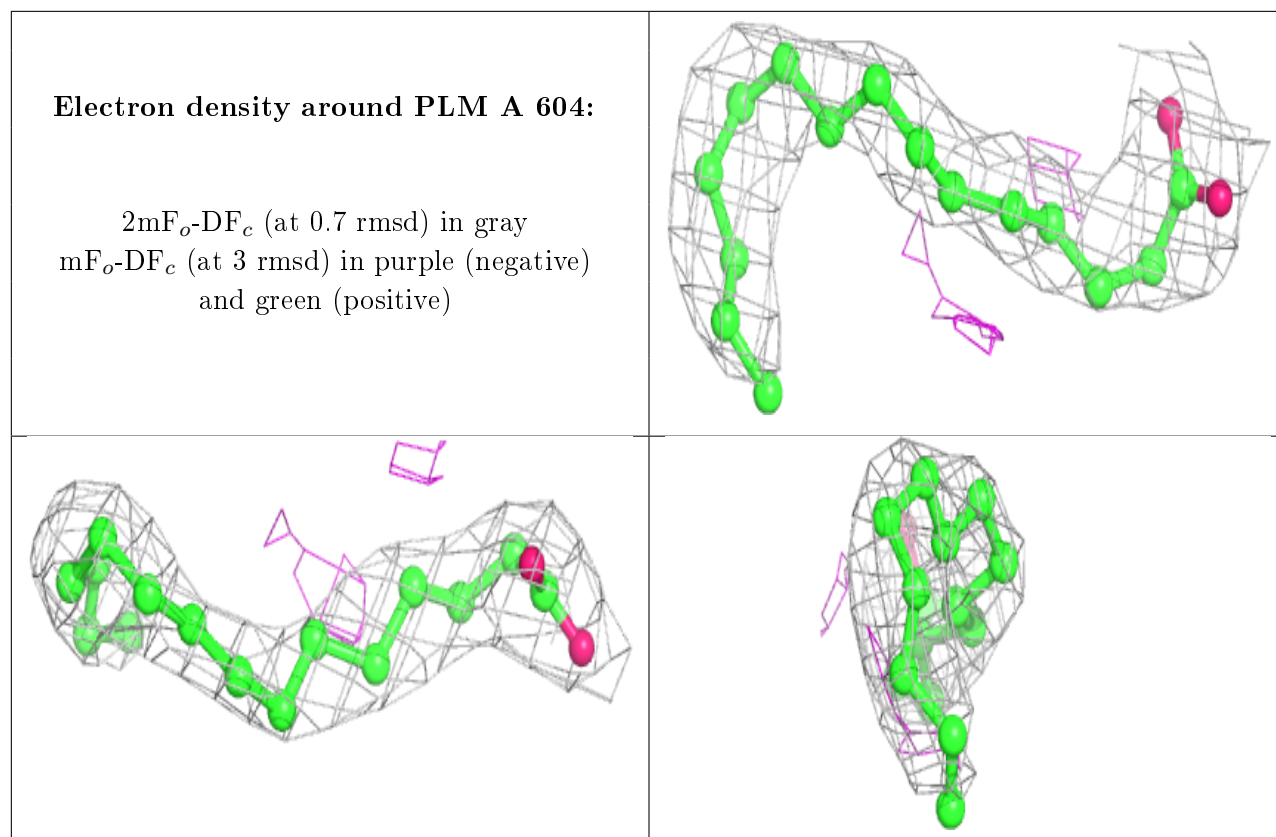
**Electron density around 6WF B 601:**

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

**Electron density around PLM A 606:**

$2mF_o-DF_c$  (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.