



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:58 AM UTC

PDB ID : 8J8E / pdb_00008j8e
Title : Human serum albumin-palladium(II) agent complex
Authors : Zhang, Z.L.; Zhang, J.Z.
Deposited on : 2023-05-01
Resolution : 2.50 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

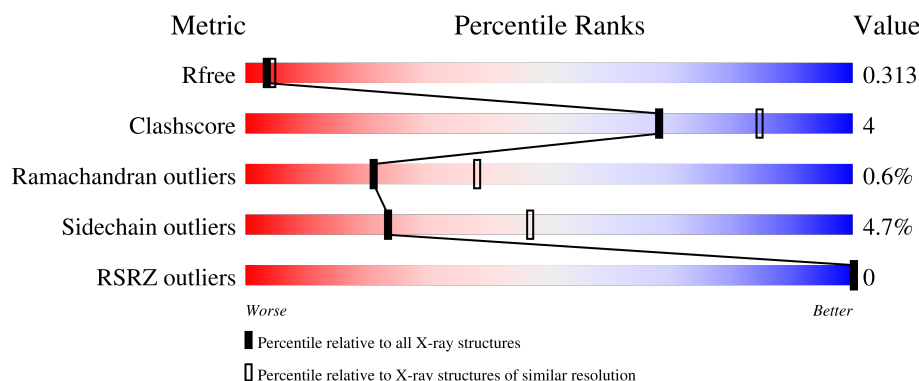
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	 89% 10% ..
1	I	585	 87% 11% ..

2 Entry composition [i](#)

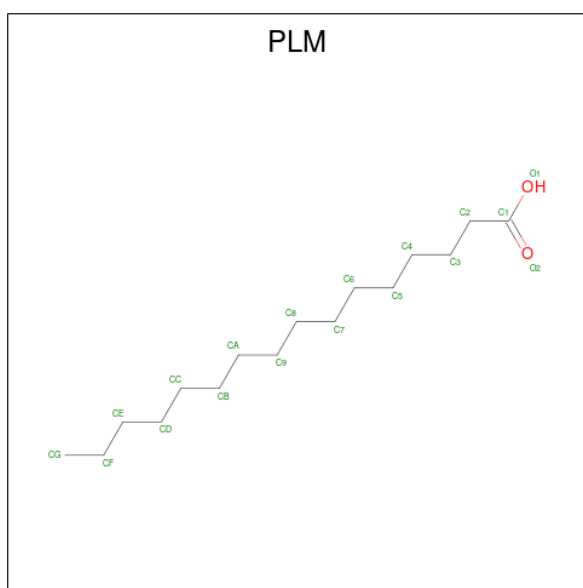
There are 4 unique types of molecules in this entry. The entry contains 9306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	581	Total	C	N	O	S	0	0	0
			4443	2819	744	839	41			
1	I	581	Total	C	N	O	S	0	0	0
			4443	2819	744	839	41			

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



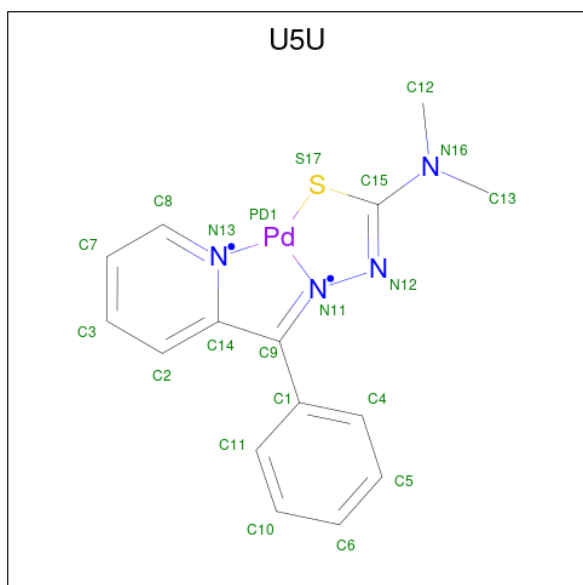
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			18	16	2		
2	A	1	Total	C	O	0	0
			17	15	2		
2	A	1	Total	C	O	0	0
			18	16	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	15	2		
2	A	1	Total	C	O	0	0
			18	16	2		
2	I	1	Total	C	O	0	0
			13	11	2		
2	I	1	Total	C	O	0	0
			18	16	2		
2	I	1	Total	C	O	0	0
			17	15	2		
2	I	1	Total	C	O	0	0
			18	16	2		
2	I	1	Total	C	O	0	0
			17	15	2		
2	I	1	Total	C	O	0	0
			18	16	2		

- Molecule 3 is {N}, {N}-dimethyl-7-phenyl-3-thia-1 λ^4 ,5,6 λ^4 -triazza-2 λ^3 -palladatricyclo[6.4.0.0 2,6]dodeca-1(12),4,6,8,10-pentaen-4-amine (CCD ID: U5U) (formula: C₁₅H₁₅N₄PdS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	Pd	S	0	0
			21	15	4	1	1		
3	I	1	Total	C	N	Pd	S	0	0
			21	15	4	1	1		

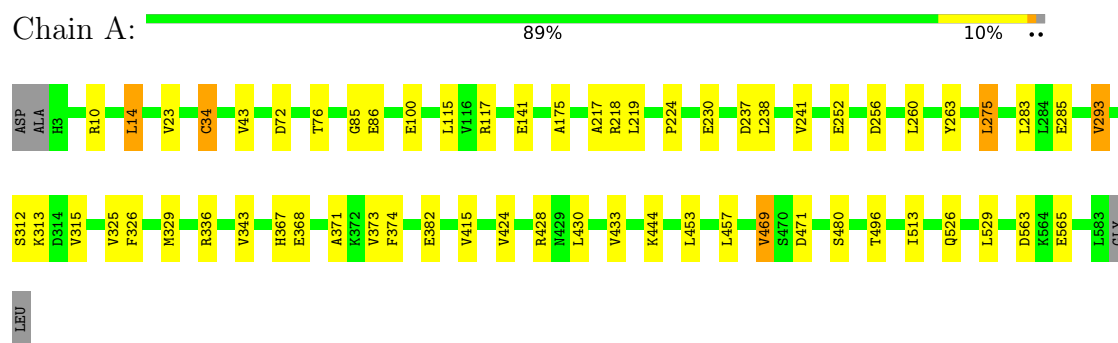
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	86	Total 86	O 86	0	0
4	I	90	Total 90	O 90	0	0

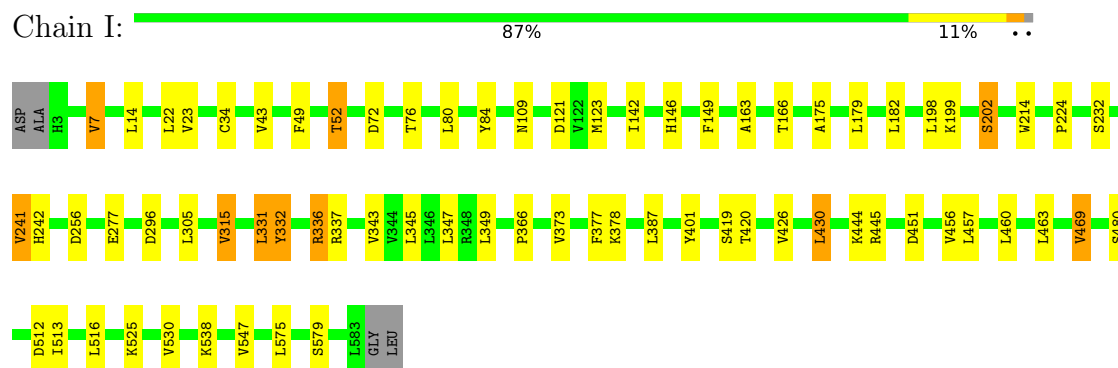
3 Residue-property plots

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



• Molecule 1: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.36Å 92.71Å 95.34Å 74.89° 89.73° 79.88°	Depositor
Resolution (Å)	91.96 – 2.50 91.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (91.96-2.50) 88.4 (91.96-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.250 , 0.316 0.250 , 0.313	Depositor DCC
R_{free} test set	2130 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.177 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9306	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, U5U

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	0.76	0/4532	1.00	2/6148 (0.0%)
1	I	0.78	0/4532	1.03	2/6148 (0.0%)
All	All	0.77	0/9064	1.01	4/12296 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ALA	N-CA-C	5.26	117.76	111.71
1	I	7	VAL	N-CA-CB	5.22	116.65	110.55
1	I	315	VAL	N-CA-C	-5.08	105.90	110.82
1	A	315	VAL	N-CA-C	-5.02	106.90	111.67

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	4443	0	4193	29	0
1	I	4443	0	4193	32	0
2	A	101	0	163	2	0
2	I	101	0	163	3	0
3	A	21	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	21	0	0	1	0
4	A	86	0	0	3	0
4	I	90	0	0	1	0
All	All	9306	0	8712	64	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 4.

All (64) 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)
3:I:1007:U5U:PD1	3:I:1007:U5U:S17	1.83	0.99
3:A:1007:U5U:PD1	3:A:1007:U5U:S17	1.84	0.99
1:A:428:ARG:HE	1:A:526:GLN:HE22	1.31	0.76
1:I:332:TYR:OH	1:I:336:ARG:NH1	2.21	0.71
1:A:238:LEU:HD23	1:A:260:LEU:HD21	1.72	0.70
1:A:218:ARG:NH1	4:A:1101:HOH:O	2.30	0.65
1:A:10:ARG:NH1	1:A:14:LEU:HD21	2.15	0.61
1:A:428:ARG:NE	1:A:526:GLN:HE22	2.00	0.59
1:I:14:LEU:HD13	1:I:22:LEU:HD12	1.85	0.59
1:I:198:LEU:O	1:I:202:SER:OG	2.22	0.58
1:I:175:ALA:O	1:I:179:LEU:HG	2.05	0.56
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.89	0.55
1:I:80:LEU:HD12	1:I:84:TYR:CD2	2.42	0.55
1:A:424:VAL:O	1:A:428:ARG:HG3	2.07	0.54
1:A:237:ASP:O	1:A:241:VAL:HG23	2.07	0.54
1:I:445:ARG:NH1	4:I:1108:HOH:O	2.43	0.51
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.76	0.50
1:A:217:ALA:HB3	1:A:343:VAL:HG13	1.94	0.49
1:A:325:VAL:HG12	1:A:329:MET:HE2	1.95	0.49
1:I:49:PHE:O	1:I:52:THR:HB	2.13	0.49
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.94	0.49
1:I:123:MET:HE1	1:I:182:LEU:CD1	2.44	0.48
1:A:312:SER:OG	1:A:313:LYS:O	2.26	0.47
1:I:512:ASP:O	1:I:516:LEU:HD13	2.14	0.47
1:I:426:VAL:HG21	1:I:460:LEU:CD1	2.45	0.47
1:I:163:ALA:O	1:I:166:THR:HG22	2.15	0.46
1:I:163:ALA:HA	1:I:166:THR:HG22	1.98	0.46
1:I:457:LEU:HD21	2:I:1004:PLM:C5	2.45	0.46
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.51	0.46
1:I:199:LYS:HD3	1:I:242:HIS:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:MET:HE1	1:I:182:LEU:HD11	1.98	0.46
1:I:430:LEU:HD13	1:I:456:VAL:HG11	1.98	0.46
1:I:241:VAL:HG22	1:I:256:ASP:HB3	1.98	0.45
1:I:426:VAL:HG21	1:I:460:LEU:HD11	1.98	0.45
1:A:224:PRO:O	1:A:336:ARG:NH1	2.41	0.45
1:I:387:LEU:HD13	2:I:1003:PLM:H71	1.98	0.45
1:A:275:LEU:HD22	1:A:293:VAL:HG11	1.99	0.44
1:A:326:PHE:HA	1:A:329:MET:HE3	1.99	0.44
1:A:430:LEU:HA	1:A:433:VAL:HG12	2.00	0.44
1:I:23:VAL:HG12	1:I:43:VAL:HG22	1.99	0.44
1:A:238:LEU:CD2	1:A:260:LEU:HD21	2.44	0.44
1:I:305:LEU:HD11	1:I:337:ARG:HD2	2.00	0.44
1:I:72:ASP:O	1:I:76:THR:HG23	2.18	0.43
1:A:453:LEU:HD11	2:A:1003:PLM:H81	1.99	0.43
1:I:420:THR:HG23	1:I:530:VAL:HB	2.00	0.43
1:I:401:TYR:OH	1:I:525:LYS:HE2	2.18	0.43
1:A:230:GLU:OE2	1:A:263:TYR:OH	2.31	0.42
1:A:457:LEU:HD11	2:A:1004:PLM:H51	2.01	0.42
1:I:349:LEU:HD22	1:I:377:PHE:HB3	2.01	0.42
1:I:331:LEU:HD21	1:I:347:LEU:HD23	2.00	0.42
1:I:345:LEU:O	1:I:349:LEU:HG	2.19	0.42
1:A:367:HIS:ND1	1:A:368:GLU:OE1	2.49	0.42
1:A:496:THR:HG22	1:A:496:THR:O	2.19	0.42
1:I:22:LEU:HD13	2:I:1002:PLM:H72	2.01	0.42
1:I:224:PRO:HD2	1:I:296:ASP:HB3	2.02	0.42
1:A:34:CYS:CB	4:A:1120:HOH:O	2.67	0.41
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.41
1:A:115:LEU:HD11	1:A:141:GLU:HB3	2.01	0.41
1:I:146:HIS:HB3	1:I:149:PHE:HB2	2.02	0.41
1:I:214:TRP:CD1	1:I:343:VAL:HG11	2.56	0.41
1:A:34:CYS:SG	4:A:1120:HOH:O	2.62	0.41
1:A:85:GLY:O	1:A:86:GLU:C	2.64	0.41
3:A:1007:U5U:N12	3:A:1007:U5U:C4	2.84	0.41
1:I:547:VAL:HG13	1:I:579:SER:HB3	2.03	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	579/585 (99%)	551 (95%)	24 (4%)	4 (1%)	18	34
1	I	579/585 (99%)	550 (95%)	26 (4%)	3 (0%)	24	43
All	All	1158/1170 (99%)	1101 (95%)	50 (4%)	7 (1%)	21	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	LEU
1	A	469	VAL
1	A	371	ALA
1	I	366	PRO
1	I	538	LYS
1	A	563	ASP
1	I	469	VAL

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	455/511 (89%)	437 (96%)	18 (4%)	28	54
1	I	455/511 (89%)	430 (94%)	25 (6%)	19	40
All	All	910/1022 (89%)	867 (95%)	43 (5%)	23	47

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	34	CYS
1	A	100	GLU
1	A	117	ARG
1	A	219	LEU
1	A	252	GLU
1	A	275	LEU
1	A	285	GLU
1	A	293	VAL
1	A	382	GLU
1	A	415	VAL
1	A	444	LYS
1	A	469	VAL
1	A	471	ASP
1	A	480	SER
1	A	513	ILE
1	A	529	LEU
1	A	565	GLU
1	I	7	VAL
1	I	34	CYS
1	I	52	THR
1	I	109	ASN
1	I	121	ASP
1	I	142	ILE
1	I	202	SER
1	I	232	SER
1	I	241	VAL
1	I	277	GLU
1	I	315	VAL
1	I	331	LEU
1	I	332	TYR
1	I	336	ARG
1	I	373	VAL
1	I	378	LYS
1	I	419	SER
1	I	430	LEU
1	I	444	LYS
1	I	451	ASP
1	I	463	LEU
1	I	469	VAL
1	I	480	SER
1	I	513	ILE
1	I	575	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	221	GLN
1	A	268	GLN
1	A	397	GLN
1	A	503	ASN
1	A	526	GLN
1	I	99	ASN
1	I	221	GLN
1	I	267	ASN
1	I	503	ASN
1	I	543	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
2	PLM	I	1002	-	17,17,17	0.48	0	17,17,17	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLM	A	1006	-	17,17,17	0.60	0	17,17,17	0.63	0
2	PLM	A	1001	-	12,12,17	0.68	0	12,12,17	0.51	0
2	PLM	A	1003	-	16,16,17	0.60	0	16,16,17	0.61	0
2	PLM	A	1004	-	17,17,17	0.55	0	17,17,17	0.70	0
2	PLM	I	1001	-	12,12,17	0.67	0	12,12,17	0.75	0
3	U5U	A	1007	1	21,24,24	2.24	4 (19%)	22,35,35	3.94	6 (27%)
2	PLM	A	1005	-	16,16,17	0.57	0	16,16,17	0.70	0
3	U5U	I	1007	1	21,24,24	1.64	2 (9%)	22,35,35	3.65	7 (31%)
2	PLM	I	1003	-	16,16,17	0.62	0	16,16,17	0.81	0
2	PLM	I	1006	-	17,17,17	0.68	0	17,17,17	0.62	0
2	PLM	I	1004	-	17,17,17	0.49	0	17,17,17	0.83	0
2	PLM	I	1005	-	16,16,17	0.58	0	16,16,17	0.64	0
2	PLM	A	1002	-	17,17,17	0.62	0	17,17,17	0.66	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
2	PLM	I	1002	-	-	9/15/15/15	-
2	PLM	A	1006	-	-	9/15/15/15	-
2	PLM	A	1001	-	-	6/10/10/15	-
2	PLM	A	1003	-	-	8/14/14/15	-
2	PLM	A	1004	-	-	7/15/15/15	-
2	PLM	I	1001	-	-	3/10/10/15	-
3	U5U	A	1007	1	-	8/8/43/43	0/4/4/4
2	PLM	A	1005	-	-	6/14/14/15	-
3	U5U	I	1007	1	-	4/8/43/43	0/4/4/4
2	PLM	I	1003	-	-	11/14/14/15	-
2	PLM	I	1006	-	-	8/15/15/15	-
2	PLM	I	1004	-	-	10/15/15/15	-
2	PLM	I	1005	-	-	6/14/14/15	-
2	PLM	A	1002	-	-	9/15/15/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	U5U	C15-S17	-6.04	1.66	1.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	U5U	C9-N11	5.31	1.37	1.31
3	I	1007	U5U	C15-S17	-5.16	1.68	1.75
3	A	1007	U5U	C15-N12	-4.09	1.24	1.32
3	A	1007	U5U	C1-C9	3.45	1.53	1.48
3	I	1007	U5U	C15-N12	-3.08	1.26	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1007	U5U	S17-C15-N12	-14.09	111.91	124.65
3	I	1007	U5U	S17-C15-N12	-13.18	112.73	124.65
3	A	1007	U5U	S17-C15-N16	9.21	126.49	118.42
3	I	1007	U5U	S17-C15-N16	6.57	124.17	118.42
3	I	1007	U5U	C2-C14-N13	-4.94	116.02	124.08
3	I	1007	U5U	C1-C9-C14	3.92	131.75	120.98
3	I	1007	U5U	N16-C15-N12	3.48	123.09	116.52
3	I	1007	U5U	C9-N11-N12	3.41	128.87	121.18
3	A	1007	U5U	C10-C11-C1	3.33	123.64	120.36
3	A	1007	U5U	C2-C14-N13	-3.04	119.11	124.08
3	A	1007	U5U	C11-C1-C4	-3.04	114.70	118.57
3	A	1007	U5U	N16-C15-N12	2.69	121.59	116.52
3	I	1007	U5U	C2-C14-C9	2.43	132.48	125.78
2	I	1002	PLM	O2-C1-C2	-2.30	115.81	123.09

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1007	U5U	S17-C15-N16-C13
3	A	1007	U5U	C4-C1-C9-N11
3	A	1007	U5U	C11-C1-C9-N11
3	I	1007	U5U	C4-C1-C9-N11
3	I	1007	U5U	C11-C1-C9-N11
3	I	1007	U5U	C4-C1-C9-C14
3	I	1007	U5U	C11-C1-C9-C14
3	A	1007	U5U	N12-C15-N16-C13
3	A	1007	U5U	C4-C1-C9-C14
3	A	1007	U5U	C11-C1-C9-C14
2	A	1006	PLM	CC-CD-CE-CF
2	I	1006	PLM	C1-C2-C3-C4
3	A	1007	U5U	N12-C15-N16-C12
2	A	1004	PLM	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1006	PLM	C5-C6-C7-C8
2	I	1003	PLM	CA-CB-CC-CD
2	A	1002	PLM	CB-CC-CD-CE
2	A	1006	PLM	C2-C3-C4-C5
2	I	1005	PLM	C1-C2-C3-C4
2	A	1006	PLM	CA-CB-CC-CD
2	I	1004	PLM	C4-C5-C6-C7
2	I	1004	PLM	C8-C9-CA-CB
2	I	1006	PLM	CC-CD-CE-CF
2	A	1005	PLM	C9-CA-CB-CC
2	I	1001	PLM	C6-C7-C8-C9
2	A	1005	PLM	C1-C2-C3-C4
2	A	1002	PLM	C2-C3-C4-C5
2	A	1004	PLM	C4-C5-C6-C7
2	I	1003	PLM	C5-C6-C7-C8
2	I	1003	PLM	C3-C4-C5-C6
2	I	1002	PLM	C3-C4-C5-C6
2	A	1004	PLM	C1-C2-C3-C4
2	A	1003	PLM	CB-CC-CD-CE
2	A	1004	PLM	C8-C9-CA-CB
2	I	1001	PLM	C3-C4-C5-C6
2	I	1006	PLM	C6-C7-C8-C9
2	A	1003	PLM	C3-C4-C5-C6
2	I	1005	PLM	C9-CA-CB-CC
2	A	1001	PLM	C3-C4-C5-C6
2	A	1003	PLM	C6-C7-C8-C9
2	I	1004	PLM	C9-CA-CB-CC
2	A	1002	PLM	C3-C4-C5-C6
2	I	1001	PLM	C4-C5-C6-C7
2	I	1003	PLM	CB-CC-CD-CE
2	I	1006	PLM	CA-CB-CC-CD
2	A	1006	PLM	C1-C2-C3-C4
2	A	1003	PLM	C2-C3-C4-C5
2	A	1003	PLM	C9-CA-CB-CC
2	I	1002	PLM	C9-CA-CB-CC
2	I	1003	PLM	C2-C3-C4-C5
2	I	1005	PLM	CA-CB-CC-CD
2	I	1004	PLM	C6-C7-C8-C9
2	A	1001	PLM	C2-C3-C4-C5
2	I	1002	PLM	C2-C3-C4-C5
2	A	1003	PLM	C4-C5-C6-C7
2	I	1003	PLM	CC-CD-CE-CF

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1002	PLM	C9-CA-CB-CC
2	A	1005	PLM	CA-CB-CC-CD
2	I	1002	PLM	C6-C7-C8-C9
2	I	1006	PLM	C5-C6-C7-C8
2	A	1002	PLM	CA-CB-CC-CD
2	A	1002	PLM	CD-CE-CF-CG
2	I	1005	PLM	C5-C6-C7-C8
2	A	1002	PLM	C8-C9-CA-CB
2	A	1003	PLM	CC-CD-CE-CF
2	A	1004	PLM	CA-CB-CC-CD
2	I	1002	PLM	C7-C8-C9-CA
3	A	1007	U5U	S17-C15-N16-C12
2	I	1004	PLM	C3-C4-C5-C6
2	A	1001	PLM	C4-C5-C6-C7
2	A	1001	PLM	C1-C2-C3-C4
2	A	1006	PLM	C9-CA-CB-CC
2	I	1004	PLM	C1-C2-C3-C4
2	I	1003	PLM	C1-C2-C3-C4
2	I	1006	PLM	C2-C3-C4-C5
2	I	1002	PLM	C8-C9-CA-CB
2	I	1002	PLM	CA-CB-CC-CD
2	A	1006	PLM	C8-C9-CA-CB
2	A	1001	PLM	O2-C1-C2-C3
2	A	1002	PLM	O2-C1-C2-C3
2	I	1003	PLM	C8-C9-CA-CB
2	A	1005	PLM	O2-C1-C2-C3
2	I	1006	PLM	O2-C1-C2-C3
2	A	1002	PLM	O1-C1-C2-C3
2	A	1005	PLM	O1-C1-C2-C3
2	I	1003	PLM	O2-C1-C2-C3
2	A	1001	PLM	O1-C1-C2-C3
2	I	1006	PLM	O1-C1-C2-C3
2	I	1002	PLM	CB-CC-CD-CE
2	I	1003	PLM	O1-C1-C2-C3
2	A	1006	PLM	O1-C1-C2-C3
2	A	1005	PLM	C3-C4-C5-C6
2	I	1003	PLM	C4-C5-C6-C7
2	A	1004	PLM	O1-C1-C2-C3
2	A	1006	PLM	O2-C1-C2-C3
2	A	1004	PLM	O2-C1-C2-C3
2	I	1004	PLM	O1-C1-C2-C3
2	I	1005	PLM	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

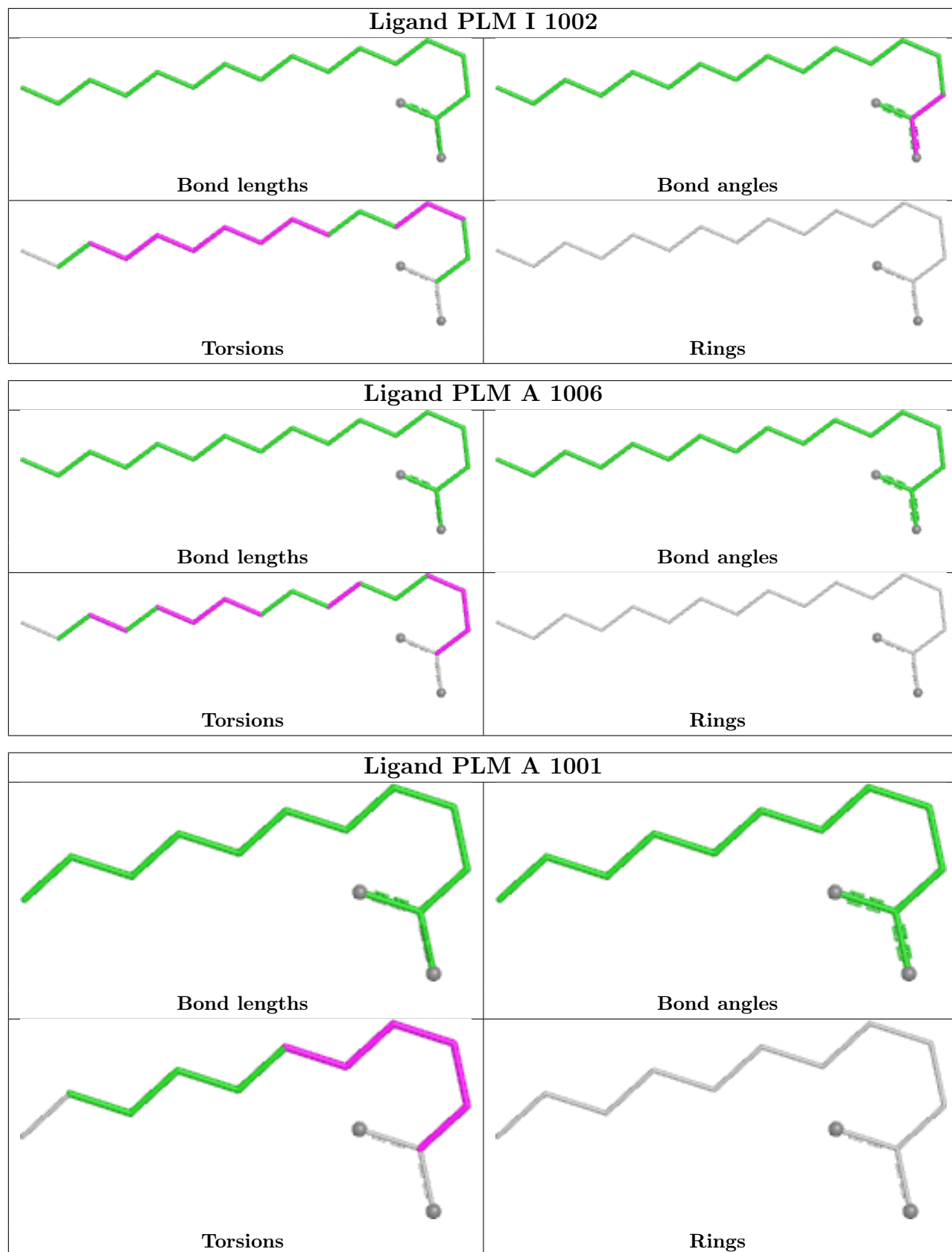
Mol	Chain	Res	Type	Atoms
2	I	1004	PLM	O2-C1-C2-C3
2	I	1004	PLM	CA-CB-CC-CD
2	I	1002	PLM	CC-CD-CE-CF
2	I	1004	PLM	C5-C6-C7-C8
2	A	1003	PLM	C1-C2-C3-C4
2	I	1005	PLM	C3-C4-C5-C6

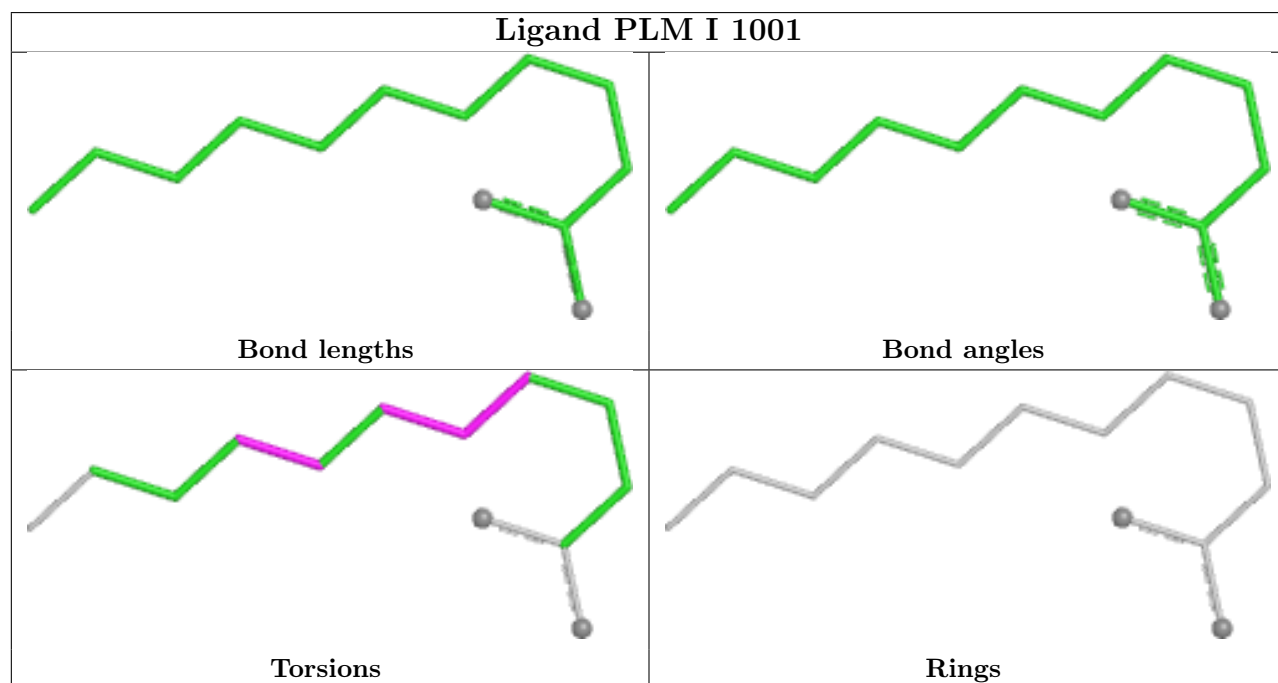
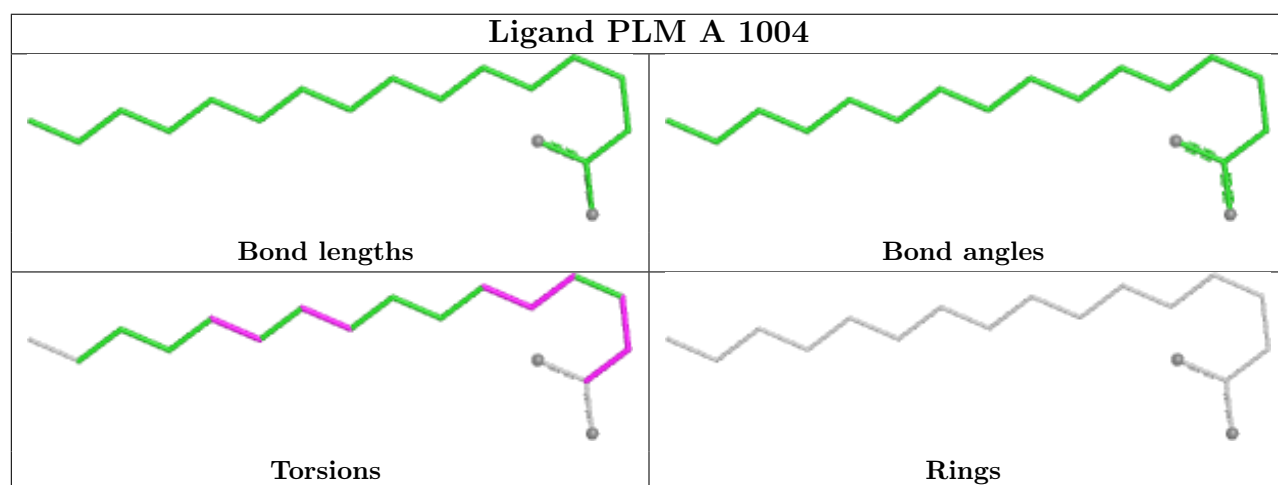
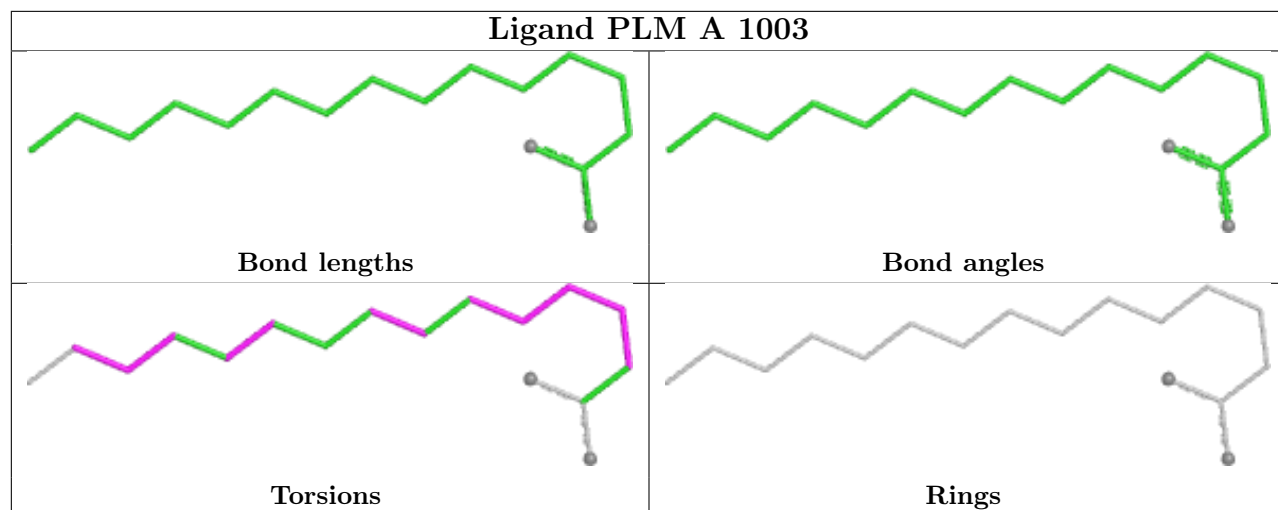
There are no ring outliers.

7 monomers are involved in 8 short contacts:

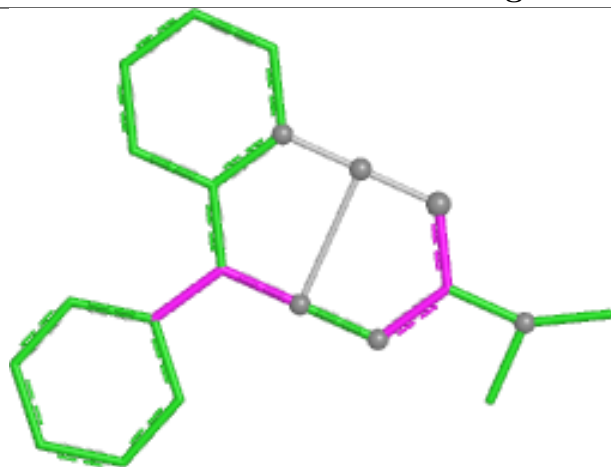
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1002	PLM	1	0
2	A	1003	PLM	1	0
2	A	1004	PLM	1	0
3	A	1007	U5U	2	0
3	I	1007	U5U	1	0
2	I	1003	PLM	1	0
2	I	1004	PLM	1	0

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.

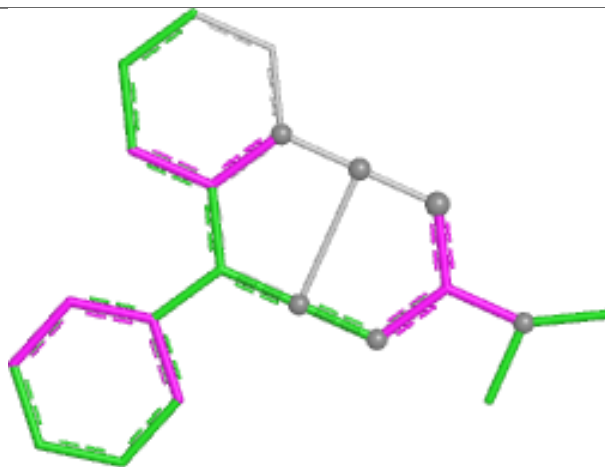




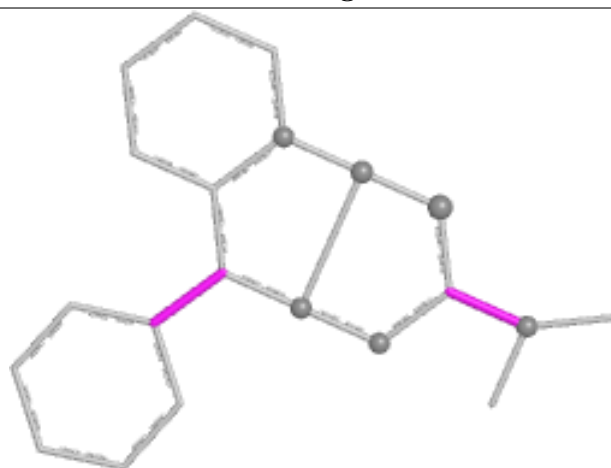
Ligand U5U A 1007



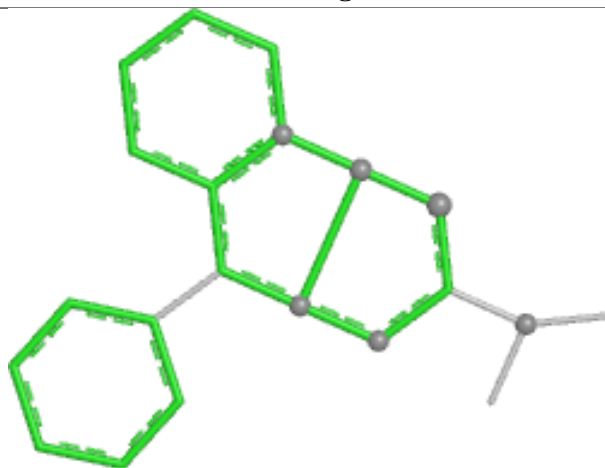
Bond lengths



Bond angles

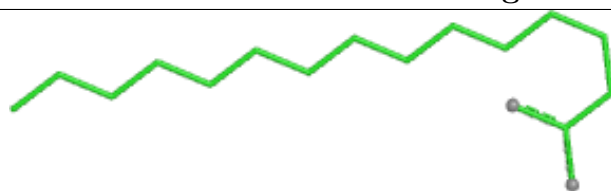


Torsions

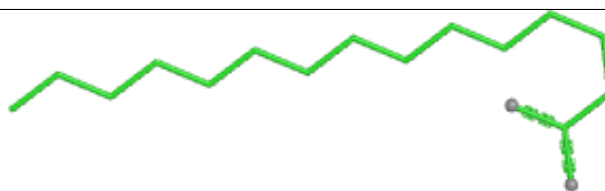


Rings

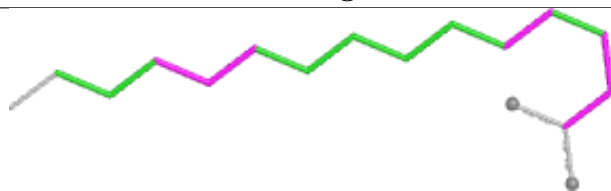
Ligand PLM A 1005



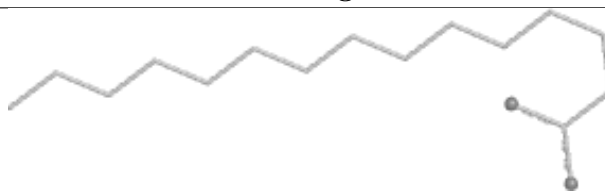
Bond lengths



Bond angles

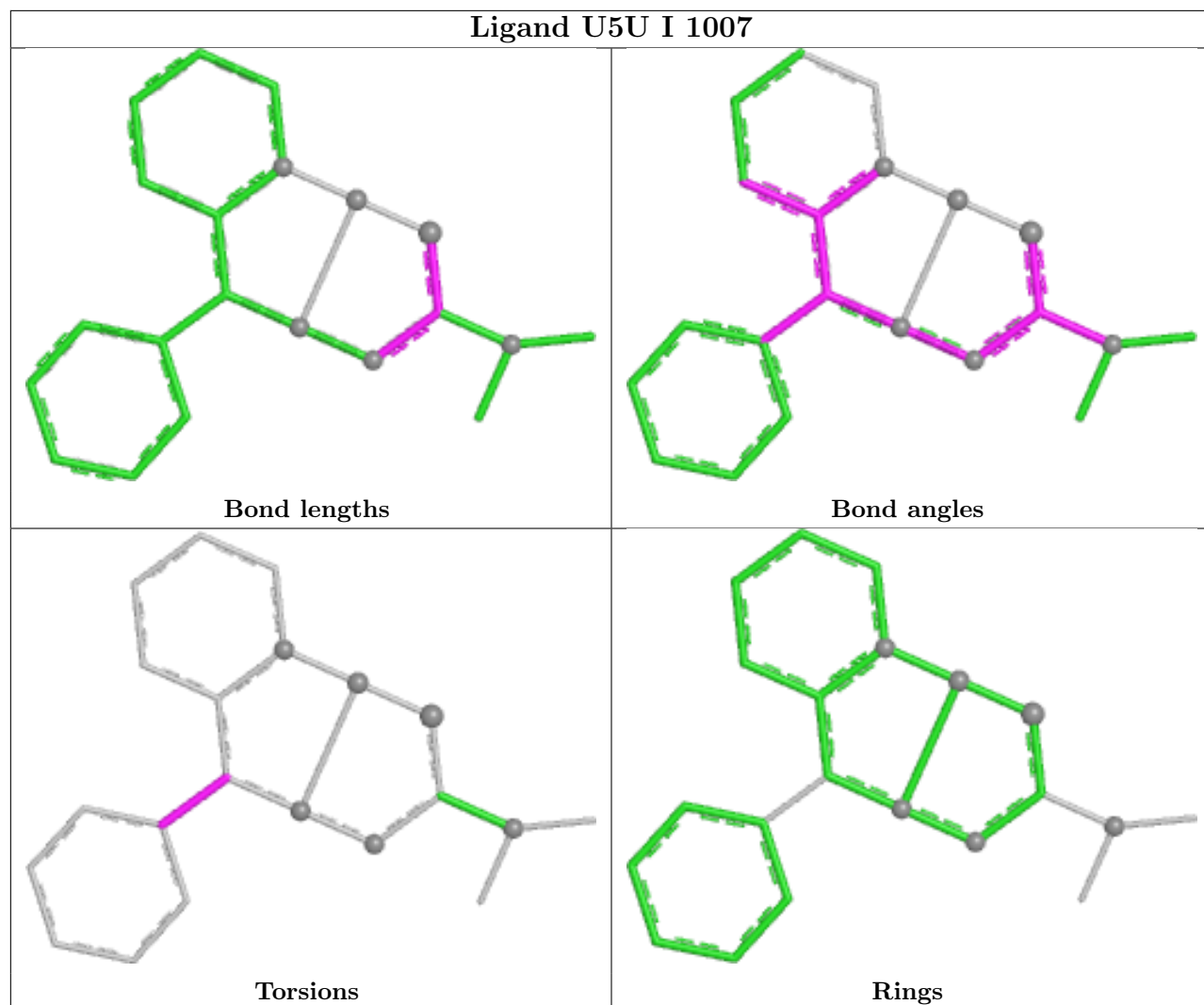


Torsions

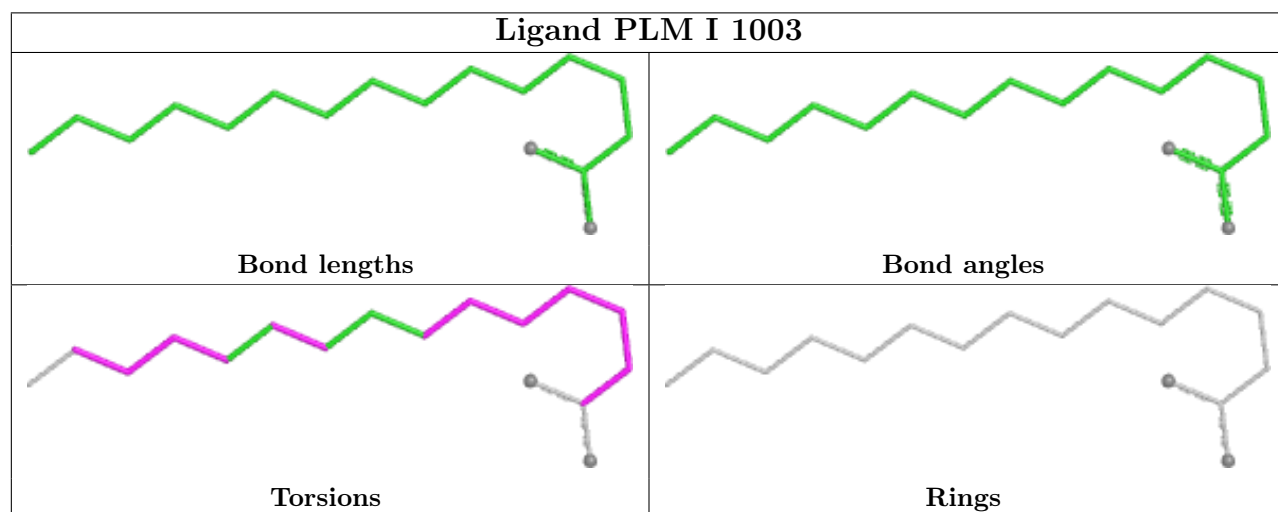


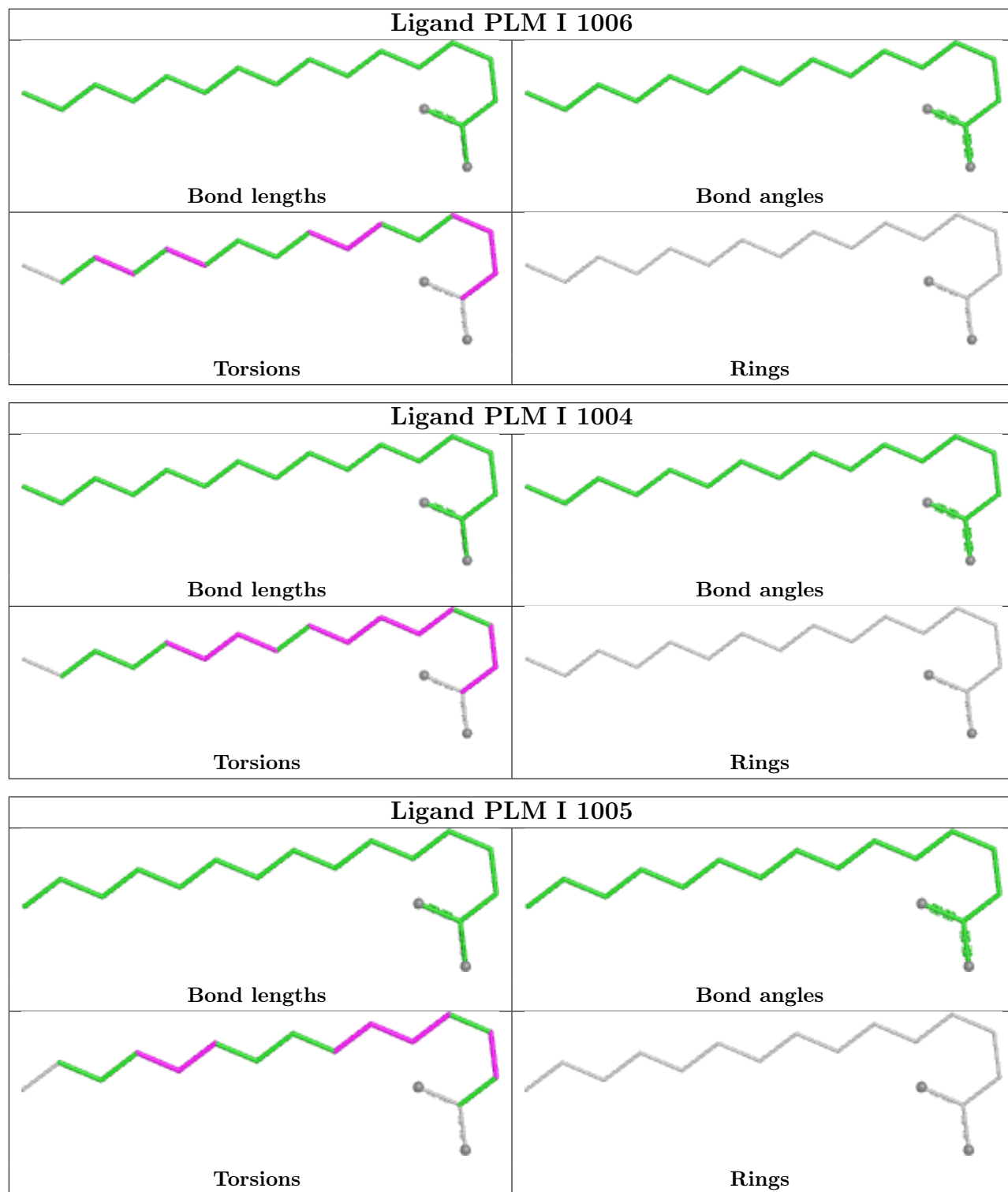
Rings

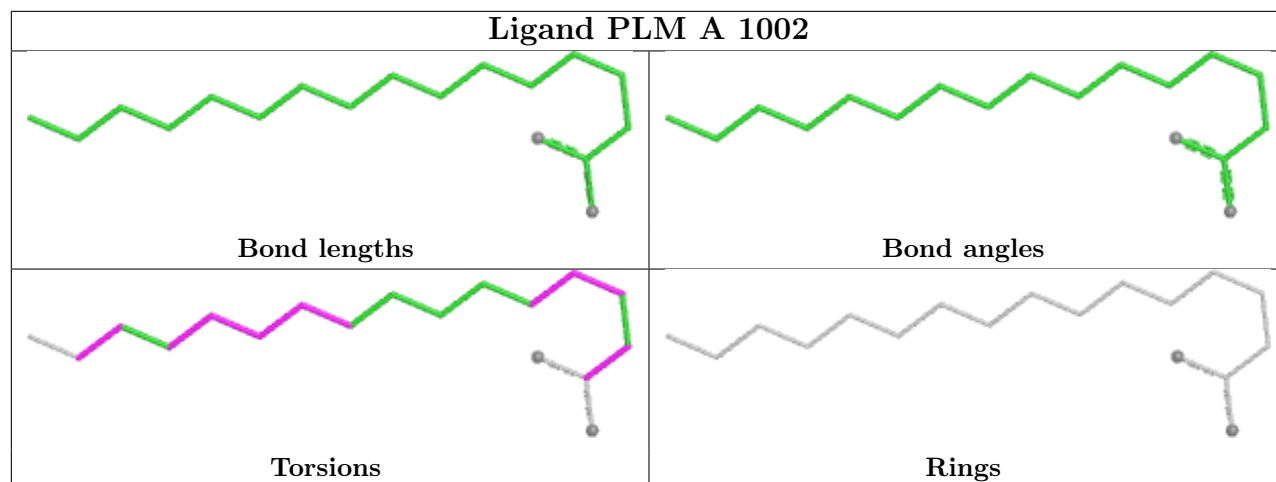
Ligand U5U I 1007



Ligand PLM I 1003







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, 95th 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 ²)	Q<0.9
1	A	581/585 (99%)	-1.10	0 100 100	23, 46, 77, 100	0
1	I	581/585 (99%)	-1.14	0 100 100	22, 45, 83, 115	0
All	All	1162/1170 (99%)	-1.12	0 100 100	22, 45, 81, 115	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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, 95th 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 ²)	Q<0.9
2	PLM	A	1006	18/18	0.97	0.11	56,64,89,90	0
2	PLM	I	1001	13/18	0.97	0.07	42,54,66,68	0
2	PLM	A	1003	17/18	0.98	0.08	45,48,53,54	0
2	PLM	A	1005	17/18	0.98	0.09	60,64,66,66	0
2	PLM	A	1001	13/18	0.98	0.10	64,76,86,89	0
2	PLM	A	1002	18/18	0.98	0.07	54,64,71,72	0
2	PLM	I	1002	18/18	0.98	0.07	41,46,50,50	0

Continued on next page...

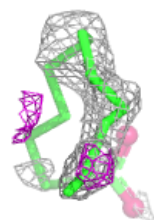
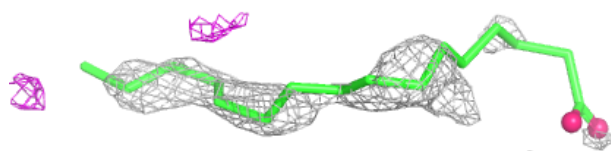
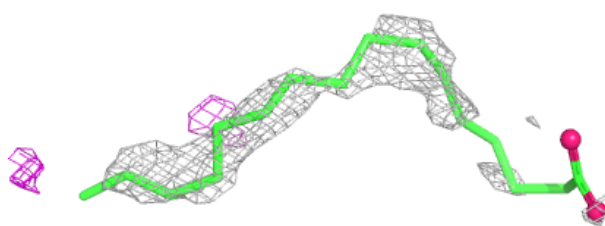
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLM	I	1003	17/18	0.98	0.06	44,48,56,57	0
2	PLM	I	1005	17/18	0.98	0.06	51,55,69,76	0
2	PLM	I	1004	18/18	0.99	0.08	64,70,73,76	0
2	PLM	A	1004	18/18	0.99	0.09	54,65,94,95	0
2	PLM	I	1006	18/18	0.99	0.07	45,55,63,64	0
3	U5U	I	1007	21/21	0.99	0.05	67,76,89,94	0
3	U5U	A	1007	21/21	1.00	0.04	52,64,71,71	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.

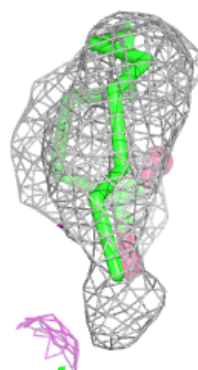
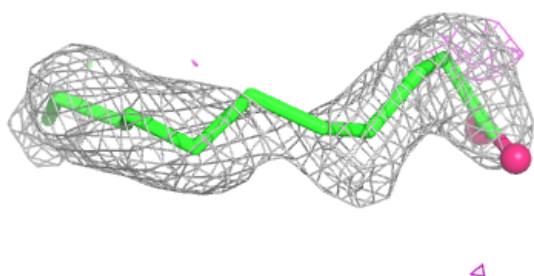
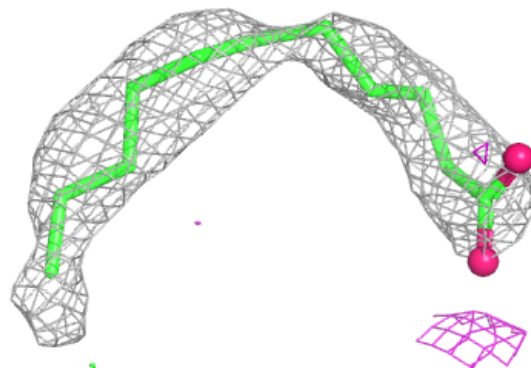
Electron density around PLM A 1006:

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

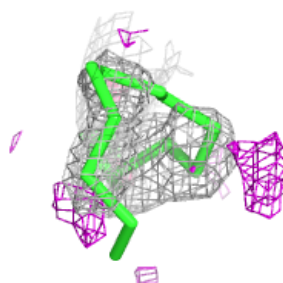
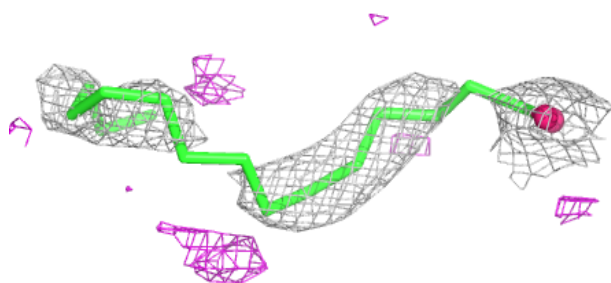
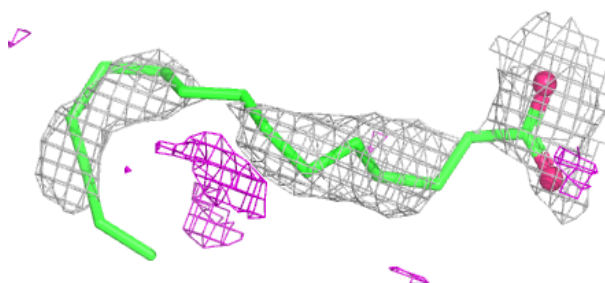


Electron density around PLM I 1001:

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

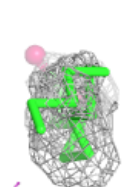
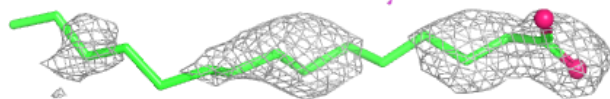
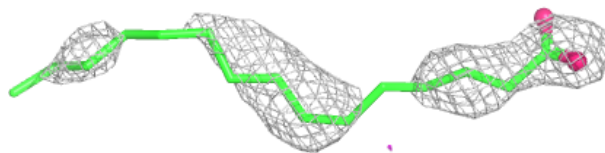
**Electron density around PLM A 1003:**

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

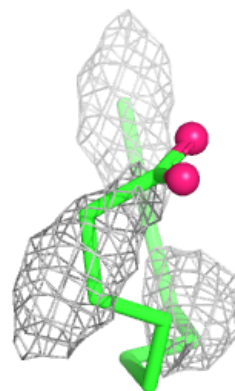
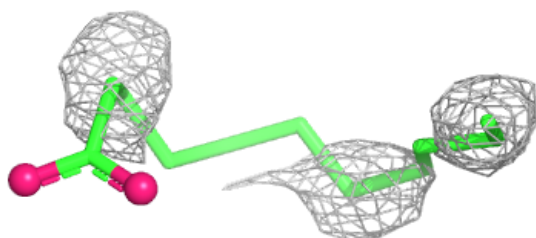
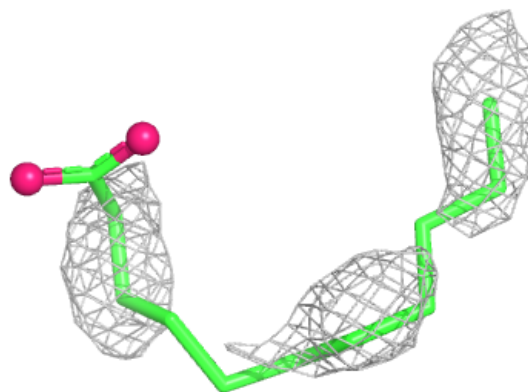


Electron density around PLM A 1005:

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

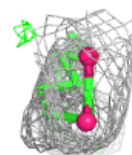
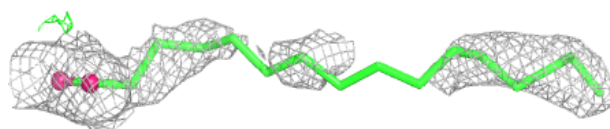
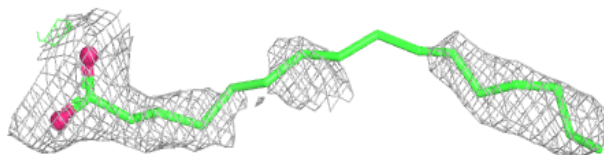
**Electron density around PLM A 1001:**

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

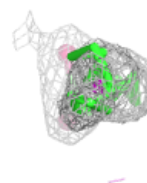
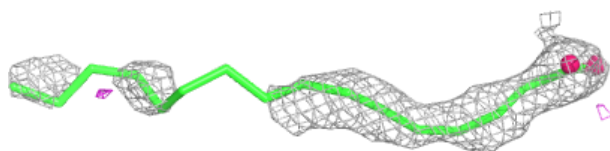
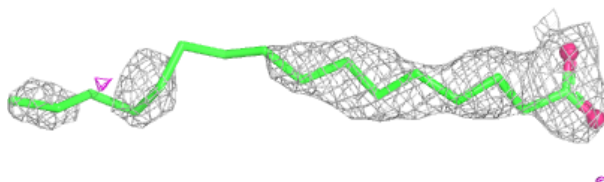


Electron density around PLM A 1002:

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

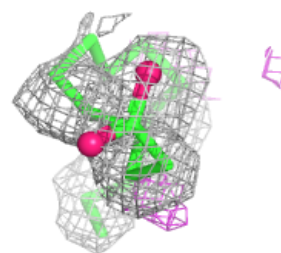
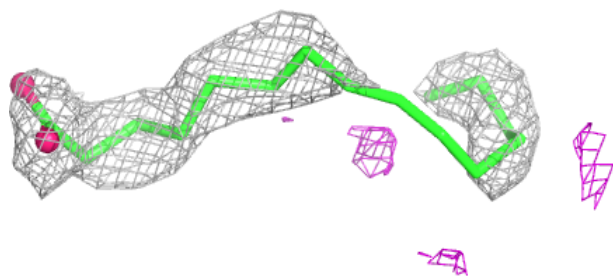
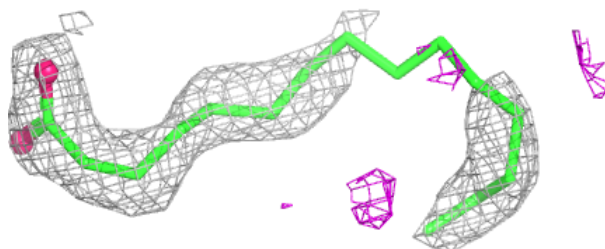
**Electron density around PLM I 1002:**

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

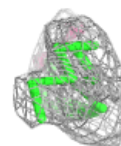
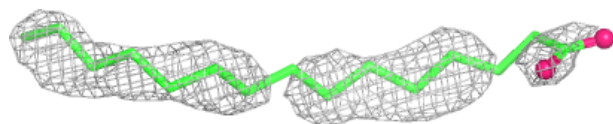
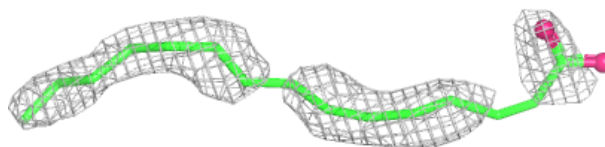


Electron density around PLM I 1003:

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

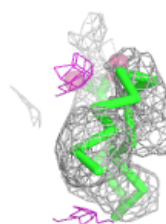
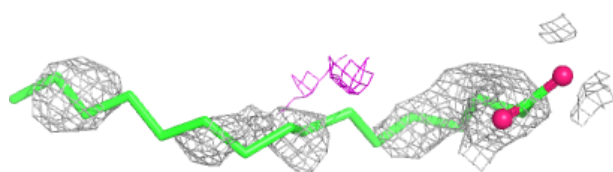
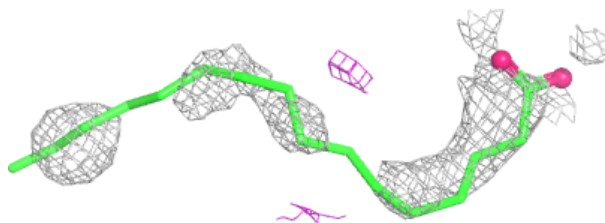
**Electron density around PLM I 1005:**

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

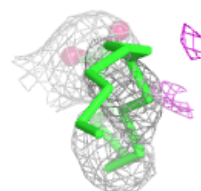
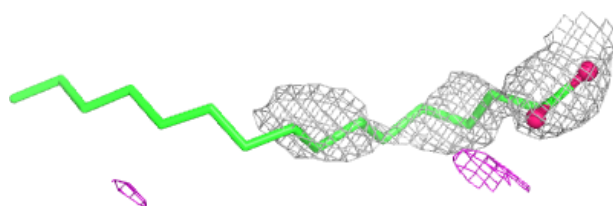
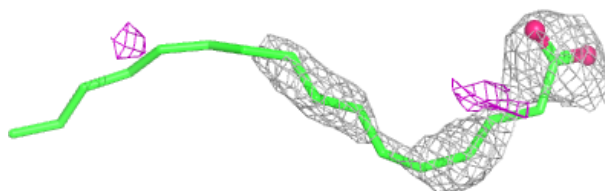


Electron density around PLM I 1004:

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

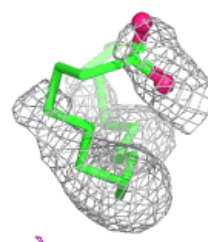
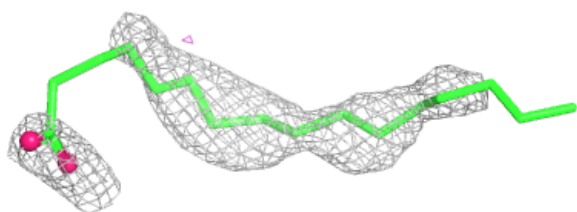
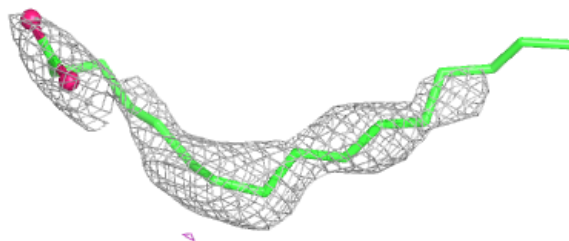
**Electron density around PLM A 1004:**

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



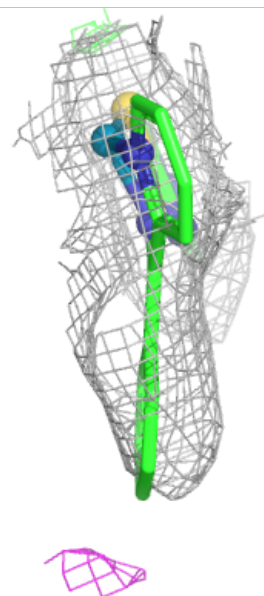
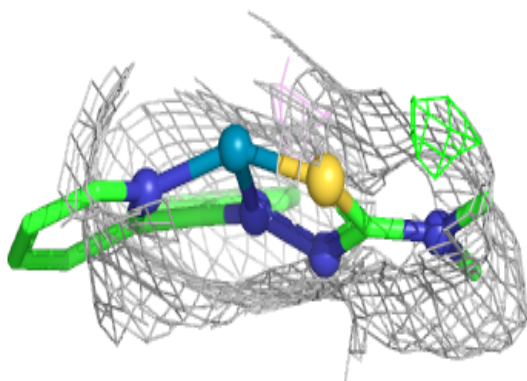
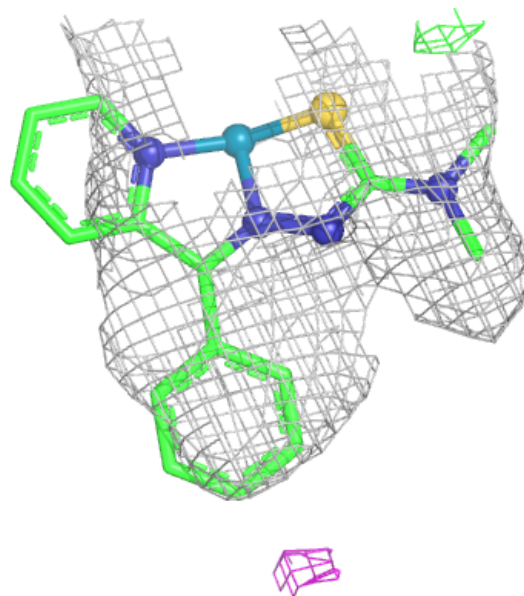
Electron density around PLM I 1006:

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



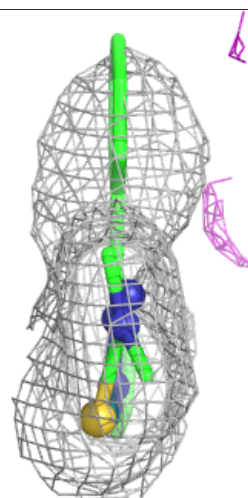
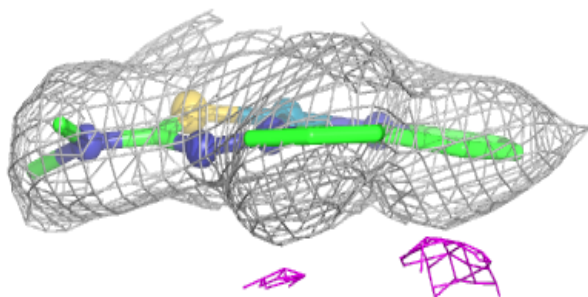
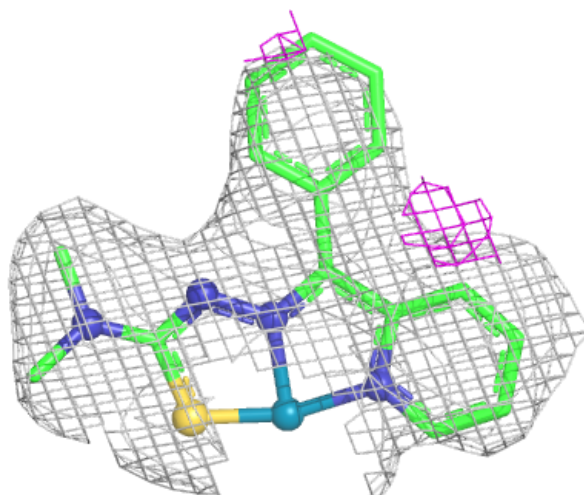
Electron density around U5U I 1007:

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



Electron density around U5U A 1007:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.