



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:08 AM UTC

PDB ID : 5YB1 / pdb_00005yb1
Title : Structure and function of human serum albumin-metal agent complex
Authors : Yang, F.; Wang, T.; Wang, J.; Gou, Y.; Zhang, Z.L.
Deposited on : 2017-09-02
Resolution : 2.62 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

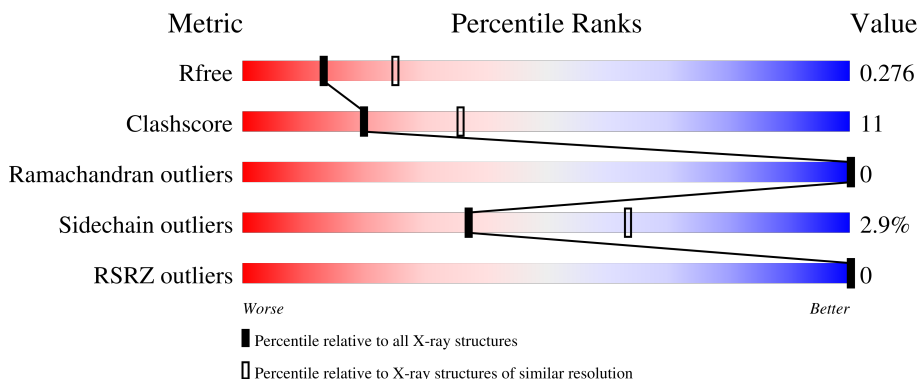
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	581	 77% 21% .
1	B	581	 77% 22% .

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
2	PLM	A	604	-	-	X	-
2	PLM	A	607	-	-	X	-
2	PLM	B	604	-	-	X	-
2	PLM	B	607	-	-	X	-

2 Entry composition [i](#)

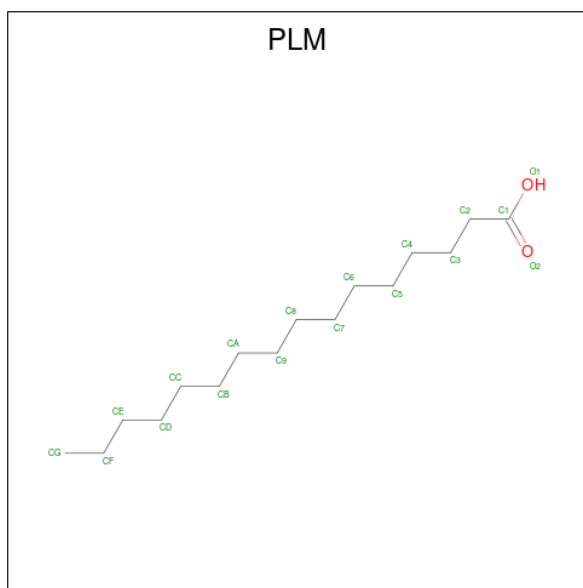
There are 4 unique types of molecules in this entry. The entry contains 9581 atoms, of which 26 are hydrogens and 0 are deuteriums.

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
			4623	2920	780	882	41			
1	B	581	Total	C	N	O	S	0	0	0
			4626	2921	782	882	41			

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



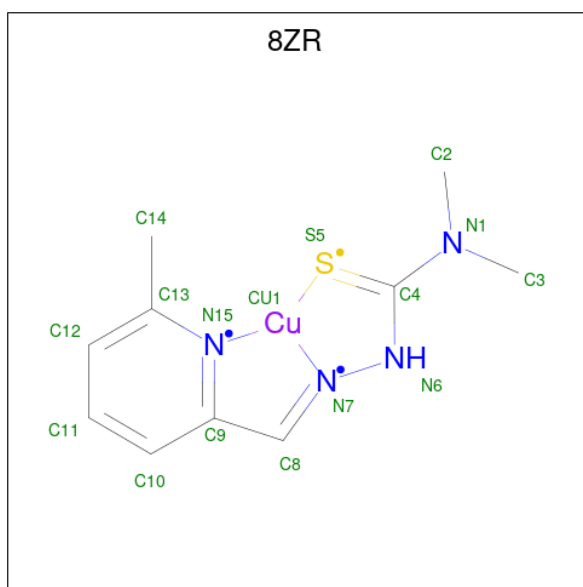
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			18	16	2		
2	A	1	Total	C	O	0	0
			17	15	2		
2	A	1	Total	C	O	0	0
			18	16	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is {N}, {N},12-trimethyl-3 λ^3 -thia-1 λ^4 ,5,6 λ^4 -triaz-2 λ^3 -cupratricyclo[6.4.0.0 $\wedge$ {2,6}]dodeca-1(8),3,6,9,11-pentaen-4-amine (CCD ID: 8ZR) (formula: C₁₀H₁₄CuN₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 29	C 10	Cu 1	H 13	N 4	S 1	0	0
3	B	1	Total 29	C 10	Cu 1	H 13	N 4	S 1	0	0

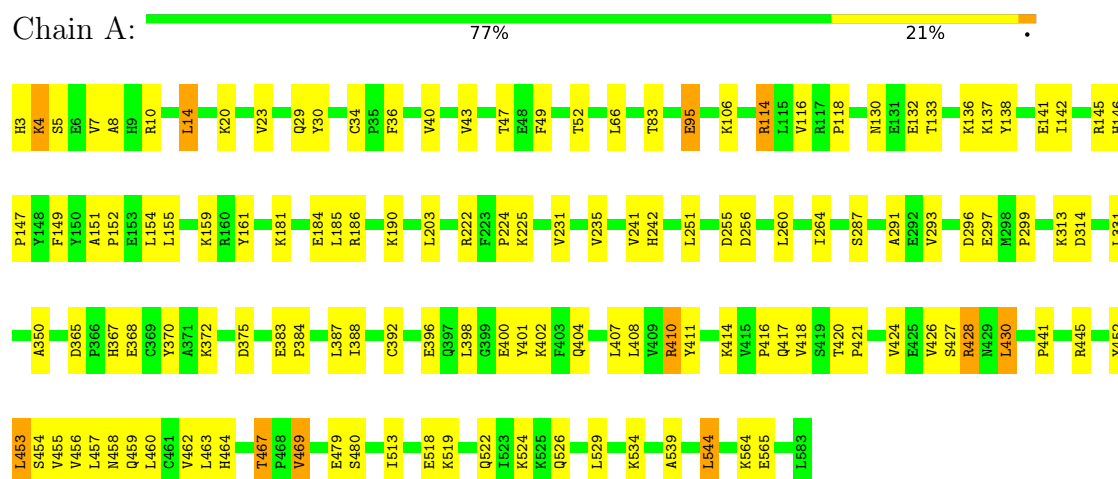
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	B	16	Total 16	O 16	0	0

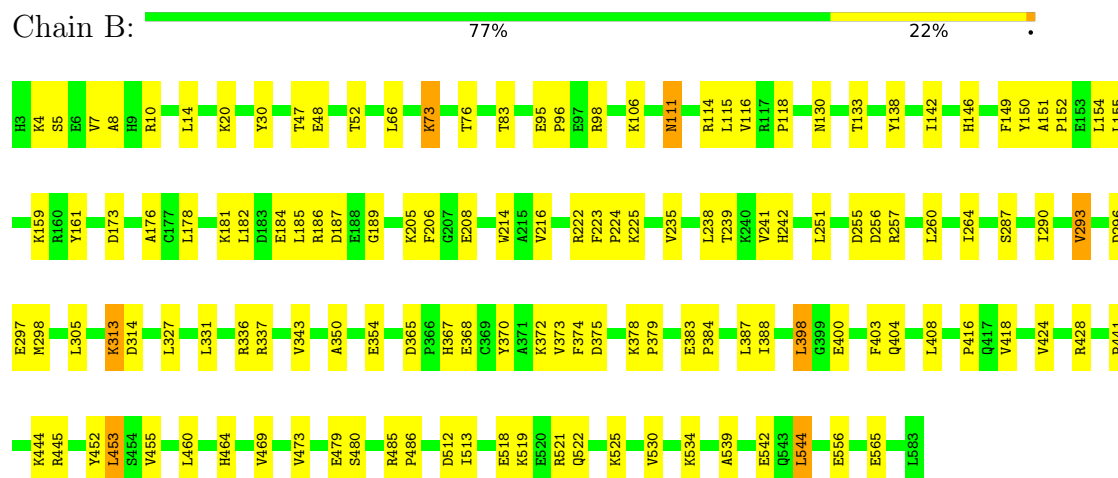
3 Residue-property plots

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	38.49Å 95.65Å 96.64Å 104.67° 101.43° 89.97°	Depositor
Resolution (Å)	33.00 – 2.62 33.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.00-2.62) 98.0 (33.00-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.24 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.278 0.220 , 0.276	Depositor DCC
R_{free} test set	1948 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.470 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9581	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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, 8ZR

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	0.26	0/4713	0.43	1/6357 (0.0%)
1	B	0.23	0/4716	0.42	0/6361
All	All	0.25	0/9429	0.42	1/12718 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	LYS	N-CA-C	7.69	119.66	111.28

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	4623	0	4544	104	0
1	B	4626	0	4549	103	0
2	A	119	0	194	32	0
2	B	119	0	194	28	0
3	A	16	13	0	1	0
3	B	16	13	0	1	0
4	A	20	0	0	1	0
4	B	16	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9555	26	9481	217	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 11.

All (217) 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:B:73:LYS:O	1:B:76:THR:HG22	1.67	0.94
1:B:460:LEU:HD11	2:B:604:PLM:HC2	1.58	0.84
1:A:242:HIS:HE2	2:A:607:PLM:C1	2.00	0.75
1:B:138:TYR:O	1:B:142:ILE:HG12	1.87	0.75
1:A:138:TYR:O	1:A:142:ILE:HG12	1.88	0.74
2:A:607:PLM:HG1	2:A:607:PLM:O1	1.87	0.74
1:A:424:VAL:O	1:A:428:ARG:HG3	1.90	0.71
1:B:181:LYS:O	1:B:184:GLU:HG2	1.91	0.71
1:B:205:LYS:HE3	1:B:206:PHE:CZ	2.26	0.70
1:B:222:ARG:NH2	1:B:290:ILE:O	2.25	0.70
1:A:181:LYS:O	1:A:184:GLU:HG2	1.92	0.70
1:A:34:CYS:SG	4:A:712:HOH:O	2.51	0.69
2:B:607:PLM:HG1	2:B:607:PLM:O2	1.93	0.68
1:B:222:ARG:HH22	1:B:293:VAL:N	1.92	0.68
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.77	0.67
1:B:331:LEU:HG	1:B:350:ALA:HB2	1.76	0.67
1:B:114:ARG:NH1	1:B:116:VAL:HG12	2.09	0.67
1:A:331:LEU:HG	1:A:350:ALA:HB2	1.75	0.67
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.76	0.67
1:A:418:VAL:HG21	2:A:604:PLM:HD2	1.76	0.66
1:B:452:TYR:O	1:B:455:VAL:HG22	1.95	0.66
1:B:222:ARG:HH22	1:B:293:VAL:H	1.43	0.66
1:A:287:SER:HB2	2:A:607:PLM:HD2	1.79	0.65
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.79	0.65
1:A:66:LEU:HD22	2:A:602:PLM:HF2	1.79	0.64
1:B:155:LEU:HG	1:B:159:LYS:HE2	1.79	0.63
1:A:138:TYR:HB3	2:A:601:PLM:H81	1.80	0.63
1:B:205:LYS:HE3	1:B:206:PHE:CE2	2.33	0.63
1:A:287:SER:HB2	2:A:607:PLM:CD	2.29	0.63
1:B:222:ARG:NH2	1:B:293:VAL:H	1.97	0.63
1:A:400:GLU:O	1:A:404:GLN:HG3	1.99	0.63
1:B:287:SER:OG	2:B:602:PLM:O1	2.16	0.63
1:B:398:LEU:HD12	1:B:403:PHE:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:NH2	1:A:255:ASP:OD1	2.28	0.62
1:B:400:GLU:O	1:B:404:GLN:HG3	2.00	0.61
1:B:138:TYR:HB3	2:B:601:PLM:HA1	1.82	0.61
1:B:518:GLU:O	1:B:522:GLN:HG3	2.01	0.61
1:B:372:LYS:HB3	1:B:375:ASP:OD2	2.01	0.61
1:B:257:ARG:HE	2:B:607:PLM:HE1	1.66	0.61
1:A:426:VAL:HG22	1:A:460:LEU:HD11	1.83	0.60
1:A:242:HIS:NE2	2:A:607:PLM:O1	2.27	0.60
1:B:418:VAL:HG22	2:B:604:PLM:HF2	1.84	0.59
1:A:66:LEU:HB3	1:A:251:LEU:HD11	1.84	0.59
1:A:114:ARG:NH1	1:A:116:VAL:HG12	2.18	0.59
1:A:155:LEU:HG	1:A:159:LYS:HE2	1.84	0.58
1:A:222:ARG:HH11	1:A:293:VAL:N	2.02	0.58
1:B:424:VAL:O	1:B:428:ARG:HG3	2.04	0.58
1:B:287:SER:HB2	2:B:607:PLM:HD2	1.85	0.57
1:B:224:PRO:HB3	1:B:336:ARG:HB2	1.87	0.57
2:A:603:PLM:H91	2:A:603:PLM:HD1	1.86	0.57
1:B:542:GLU:OE1	1:B:542:GLU:HA	2.04	0.57
1:A:565:GLU:OE1	1:A:565:GLU:HA	2.03	0.57
1:B:460:LEU:HG	2:B:604:PLM:HE2	1.87	0.57
1:A:401:TYR:HA	1:A:404:GLN:HE21	1.69	0.57
1:A:518:GLU:O	1:A:522:GLN:HG3	2.05	0.56
1:A:14:LEU:HD21	2:A:602:PLM:H61	1.87	0.56
1:B:20:LYS:HE3	1:B:47:THR:HG21	1.88	0.56
1:A:264:ILE:CD1	2:A:607:PLM:H91	2.36	0.56
1:A:392:CYS:O	1:A:396:GLU:HG3	2.06	0.55
1:B:416:PRO:O	1:B:534:LYS:HE2	2.05	0.55
1:A:372:LYS:HB3	1:A:375:ASP:OD2	2.07	0.55
1:B:116:VAL:O	1:B:118:PRO:HD3	2.05	0.55
1:B:378:LYS:HB3	1:B:379:PRO:HD3	1.88	0.55
1:A:138:TYR:CB	2:A:601:PLM:H81	2.37	0.55
1:B:257:ARG:NH1	2:B:602:PLM:O1	2.40	0.55
1:A:411:TYR:HE2	1:A:430:LEU:HD23	1.71	0.54
1:A:146:HIS:HB3	1:A:149:PHE:HB2	1.88	0.54
1:A:430:LEU:HD13	1:A:456:VAL:HG11	1.89	0.54
1:A:452:TYR:O	1:A:455:VAL:HG22	2.07	0.54
1:B:66:LEU:HB3	1:B:251:LEU:HD11	1.90	0.54
1:B:184:GLU:HG3	1:B:185:LEU:N	2.21	0.54
1:B:222:ARG:NH2	1:B:293:VAL:N	2.53	0.54
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.90	0.53
1:A:116:VAL:O	1:A:118:PRO:HD3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:HIS:HD2	2:B:604:PLM:HG1	1.73	0.53
1:A:410:ARG:HG2	1:A:411:TYR:N	2.25	0.52
1:A:464:HIS:HB2	2:A:604:PLM:HG3	1.92	0.52
1:B:186:ARG:NH2	1:B:187:ASP:OD1	2.43	0.52
1:B:10:ARG:NH2	1:B:255:ASP:OD1	2.36	0.52
1:A:20:LYS:HE3	1:A:47:THR:HG21	1.92	0.52
1:A:416:PRO:O	1:A:534:LYS:HE2	2.10	0.52
1:A:441:PRO:O	1:A:445:ARG:HG3	2.11	0.51
1:A:410:ARG:O	1:A:414:LYS:HG3	2.10	0.51
1:B:418:VAL:CG2	2:B:604:PLM:HF2	2.40	0.51
1:B:521:ARG:HG2	1:B:525:LYS:HE3	1.93	0.51
1:A:479:GLU:HG3	1:A:480:SER:H	1.76	0.50
1:A:184:GLU:HG3	1:A:185:LEU:N	2.24	0.50
1:A:384:PRO:O	1:A:388:ILE:HG13	2.12	0.50
1:B:146:HIS:HB3	1:B:149:PHE:HB2	1.92	0.50
1:A:428:ARG:HD2	1:A:526:GLN:OE1	2.11	0.50
1:A:260:LEU:HD23	2:A:607:PLM:HC2	1.94	0.50
1:A:161:TYR:CD1	2:A:601:PLM:H71	2.46	0.50
1:A:367:HIS:HA	1:A:370:TYR:CZ	2.46	0.50
1:B:460:LEU:CD2	2:B:604:PLM:HE2	2.42	0.49
1:B:5:SER:HB3	1:B:8:ALA:HB3	1.94	0.49
1:B:208:GLU:HG2	1:B:239:THR:HG21	1.94	0.49
1:B:257:ARG:NE	2:B:607:PLM:HE1	2.28	0.49
1:B:473:VAL:HG11	2:B:604:PLM:HF1	1.94	0.48
1:A:137:LYS:O	1:A:141:GLU:HG2	2.14	0.48
1:B:216:VAL:HG22	1:B:235:VAL:HG21	1.95	0.48
1:A:453:LEU:HD21	2:A:603:PLM:H92	1.96	0.48
1:B:365:ASP:OD2	1:B:368:GLU:HG2	2.12	0.48
1:A:464:HIS:HB2	2:A:604:PLM:CG	2.43	0.48
1:B:48:GLU:O	1:B:52:THR:HG23	2.14	0.48
2:B:607:PLM:H61	2:B:607:PLM:H22	1.94	0.48
2:A:603:PLM:H81	2:A:604:PLM:H21	1.95	0.48
1:B:241:VAL:HG22	1:B:256:ASP:HB3	1.96	0.48
1:B:264:ILE:CD1	2:B:607:PLM:H91	2.44	0.48
1:A:411:TYR:CE2	1:A:430:LEU:HD23	2.49	0.48
1:A:30:TYR:CZ	1:A:106:LYS:HE3	2.50	0.47
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.44	0.47
1:A:407:LEU:HD13	1:A:430:LEU:HB3	1.95	0.47
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.49	0.47
1:B:464:HIS:CD2	2:B:604:PLM:HG1	2.49	0.47
1:B:565:GLU:OE1	1:B:565:GLU:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:CE1	2:A:601:PLM:H42	2.50	0.47
1:B:384:PRO:O	1:B:388:ILE:HG13	2.14	0.47
1:B:479:GLU:HG3	1:B:480:SER:H	1.80	0.47
1:A:467:THR:O	1:A:467:THR:OG1	2.26	0.47
1:B:30:TYR:CZ	1:B:106:LYS:HE3	2.49	0.47
1:B:331:LEU:HG	1:B:350:ALA:CB	2.45	0.47
1:A:203:LEU:HD23	1:A:203:LEU:O	2.14	0.47
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.97	0.47
1:A:460:LEU:HD23	2:A:604:PLM:HC2	1.96	0.47
1:B:313:LYS:O	1:B:314:ASP:HB2	2.15	0.47
1:A:313:LYS:O	1:A:314:ASP:HB2	2.15	0.46
1:B:460:LEU:HD11	2:B:604:PLM:H91	1.97	0.46
2:A:607:PLM:CB	2:A:607:PLM:HF1	2.45	0.46
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.72	0.46
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.98	0.46
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.97	0.46
1:B:556:GLU:O	1:B:556:GLU:HG2	2.16	0.46
1:A:225:LYS:HE3	1:A:297:GLU:O	2.15	0.46
1:B:225:LYS:HE3	1:B:297:GLU:O	2.15	0.46
1:B:287:SER:HB2	2:B:607:PLM:CD	2.46	0.46
1:A:95:GLU:O	1:A:95:GLU:OE1	2.34	0.46
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.51	0.46
1:B:460:LEU:CG	2:B:604:PLM:HE2	2.45	0.45
1:B:149:PHE:CD2	1:B:154:LEU:HD13	2.50	0.45
1:A:203:LEU:HD23	1:A:203:LEU:C	2.42	0.45
1:B:460:LEU:HD21	2:B:604:PLM:HE2	1.98	0.45
1:A:242:HIS:NE2	2:A:607:PLM:C1	2.76	0.45
1:B:111:ASN:O	1:B:111:ASN:ND2	2.42	0.45
1:B:161:TYR:CG	2:B:601:PLM:H91	2.51	0.45
1:B:189:GLY:HA3	3:B:608:8ZR:C11	2.47	0.45
1:B:327:LEU:HD11	1:B:354:GLU:HG3	1.98	0.45
1:A:49:PHE:O	1:A:52:THR:HB	2.16	0.45
1:B:539:ALA:CB	1:B:544:LEU:HD13	2.47	0.45
1:A:4:LYS:HA	1:A:4:LYS:HD3	1.60	0.45
1:B:10:ARG:HG3	1:B:66:LEU:HD11	1.98	0.45
1:A:222:ARG:NH1	1:A:291:ALA:O	2.51	0.44
1:B:264:ILE:HD13	2:B:607:PLM:H91	2.00	0.44
1:B:441:PRO:O	1:B:445:ARG:HG3	2.18	0.44
1:B:539:ALA:HB1	1:B:544:LEU:HD13	1.99	0.44
1:A:529:LEU:HB2	2:A:605:PLM:H61	2.00	0.43
1:B:441:PRO:HG2	1:B:444:LYS:HE3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:O	1:A:235:VAL:HG23	2.18	0.43
1:A:264:ILE:HD13	2:A:607:PLM:H91	1.99	0.43
2:A:603:PLM:HA1	2:A:604:PLM:H21	2.00	0.43
1:A:5:SER:HB3	1:A:8:ALA:HB3	2.01	0.43
1:A:149:PHE:CD2	1:A:154:LEU:HD13	2.53	0.43
1:B:178:LEU:HG	1:B:182:LEU:HG	2.00	0.43
1:A:222:ARG:NH1	1:A:293:VAL:O	2.51	0.43
1:A:132:GLU:O	1:A:136:LYS:HG2	2.18	0.43
1:A:242:HIS:NE2	2:A:607:PLM:O2	2.52	0.43
2:A:603:PLM:HD1	2:A:603:PLM:C9	2.49	0.43
1:B:485:ARG:HB3	1:B:486:PRO:HD3	2.00	0.43
1:B:512:ASP:OD1	1:B:513:ILE:N	2.52	0.43
1:A:519:LYS:HE3	1:A:519:LYS:HB2	1.90	0.42
1:A:36:PHE:CE2	1:A:40:VAL:HG21	2.54	0.42
1:A:454:SER:O	1:A:458:ASN:HB2	2.19	0.42
1:B:305:LEU:HD11	1:B:337:ARG:HD2	2.01	0.42
1:B:383:GLU:HB3	1:B:384:PRO:HD3	2.00	0.42
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.78	0.42
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.85	0.42
1:A:479:GLU:HG3	1:A:480:SER:N	2.34	0.42
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.49	0.42
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.80	0.42
1:A:145:ARG:HD3	3:A:608:8ZR:C3	2.49	0.42
1:A:186:ARG:HG2	1:A:190:LYS:NZ	2.35	0.42
1:B:130:ASN:OD1	1:B:133:THR:HG23	2.20	0.42
1:A:459:GLN:O	1:A:462:VAL:HG22	2.20	0.42
1:A:23:VAL:HG12	1:A:43:VAL:HG22	2.01	0.42
1:A:411:TYR:OH	2:A:604:PLM:O1	2.26	0.42
1:A:539:ALA:CB	1:A:544:LEU:HD13	2.50	0.42
1:B:114:ARG:HH12	1:B:116:VAL:HG12	1.82	0.42
1:B:260:LEU:HD23	2:B:607:PLM:HC2	2.02	0.42
1:A:130:ASN:OD1	1:A:133:THR:HG23	2.20	0.41
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.94	0.41
2:B:603:PLM:H81	2:B:604:PLM:H22	2.02	0.41
1:A:365:ASP:OD2	1:A:368:GLU:HG2	2.20	0.41
1:A:513:ILE:HD12	1:A:524:LYS:HD2	2.03	0.41
1:B:519:LYS:HE3	1:B:519:LYS:HB2	1.84	0.41
1:A:457:LEU:HD21	2:A:604:PLM:H51	2.03	0.41
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.86	0.41
1:B:408:LEU:HG	1:B:530:VAL:HG22	2.02	0.41
1:B:95:GLU:N	1:B:96:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASP:OD2	1:B:176:ALA:HB2	2.19	0.41
1:B:161:TYR:CD1	2:B:601:PLM:H72	2.56	0.41
1:B:222:ARG:HD3	1:B:223:PHE:CZ	2.56	0.41
1:B:418:VAL:HG21	2:B:604:PLM:HD2	2.02	0.41
1:A:287:SER:HB2	2:A:607:PLM:HD1	2.03	0.41
1:B:513:ILE:HG12	1:B:521:ARG:HG3	2.03	0.41
1:B:66:LEU:HD22	2:B:602:PLM:HF2	2.03	0.41
1:A:10:ARG:HG3	1:A:66:LEU:HD11	2.02	0.41
1:A:185:LEU:HA	1:A:185:LEU:HD23	1.78	0.40
1:A:398:LEU:HB3	1:A:402:LYS:HB2	2.03	0.40
1:A:426:VAL:CG2	1:A:460:LEU:HD11	2.51	0.40
1:A:462:VAL:HG23	1:A:463:LEU:N	2.36	0.40
1:A:417:GLN:CB	1:A:469:VAL:HG13	2.51	0.40
1:B:95:GLU:OE1	1:B:98:ARG:NH2	2.52	0.40
2:A:603:PLM:H81	2:A:604:PLM:C2	2.51	0.40
1:B:150:TYR:CE2	1:B:152:PRO:HD2	2.56	0.40
1:A:29:GLN:HG2	1:A:147:PRO:HA	2.04	0.40
1:A:420:THR:N	1:A:421:PRO:HD2	2.36	0.40
1:A:408:LEU:HD13	1:A:427:SER:HB2	2.04	0.40
1:A:460:LEU:CD2	2:A:604:PLM:HC2	2.52	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	579/581 (100%)	564 (97%)	15 (3%)	0	100	100
1	B	579/581 (100%)	562 (97%)	17 (3%)	0	100	100
All	All	1158/1162 (100%)	1126 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	508/509 (100%)	494 (97%)	14 (3%)	38	64
1	B	509/509 (100%)	494 (97%)	15 (3%)	37	63
All	All	1017/1018 (100%)	988 (97%)	29 (3%)	37	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	LYS
1	A	7	VAL
1	A	14	LEU
1	A	83	THR
1	A	95	GLU
1	A	114	ARG
1	A	410	ARG
1	A	428	ARG
1	A	430	LEU
1	A	453	LEU
1	A	467	THR
1	A	469	VAL
1	A	544	LEU
1	B	4	LYS
1	B	7	VAL
1	B	14	LEU
1	B	73	LYS
1	B	83	THR
1	B	111	ASN
1	B	238	LEU
1	B	242	HIS
1	B	293	VAL
1	B	298	MET
1	B	313	LYS
1	B	398	LEU
1	B	453	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	469	VAL
1	B	544	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	404	GLN
1	A	458	ASN
1	A	503	ASN
1	B	39	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	8ZR	B	608	1	13,18,18	3.68	7 (53%)	12,27,27	4.13	3 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLM	B	603	-	16,16,17	0.59	0	16,16,17	0.83	0
2	PLM	B	607	-	17,17,17	0.61	0	17,17,17	0.81	0
2	PLM	A	605	-	16,16,17	0.61	0	16,16,17	0.88	1 (6%)
2	PLM	A	602	-	17,17,17	0.58	0	17,17,17	0.85	1 (5%)
2	PLM	B	602	-	17,17,17	0.57	0	17,17,17	0.87	1 (5%)
3	8ZR	A	608	1	13,18,18	3.68	7 (53%)	12,27,27	4.12	3 (25%)
2	PLM	A	604	-	17,17,17	0.57	0	17,17,17	0.80	1 (5%)
2	PLM	A	601	-	12,12,17	0.70	0	12,12,17	0.83	0
2	PLM	B	601	-	12,12,17	0.67	0	12,12,17	0.78	0
2	PLM	A	603	-	16,16,17	0.56	0	16,16,17	0.86	1 (6%)
2	PLM	B	604	-	17,17,17	0.60	0	17,17,17	0.72	0
2	PLM	A	606	-	17,17,17	0.65	0	17,17,17	0.70	0
2	PLM	B	606	-	17,17,17	0.66	0	17,17,17	0.66	0
2	PLM	B	605	-	16,16,17	0.68	0	16,16,17	0.72	0
2	PLM	A	607	-	17,17,17	0.63	0	17,17,17	0.84	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
3	8ZR	B	608	1	-	4/4/38/38	0/3/3/3
2	PLM	B	603	-	-	8/14/14/15	-
2	PLM	B	607	-	-	12/15/15/15	-
2	PLM	A	605	-	-	9/14/14/15	-
2	PLM	A	602	-	-	7/15/15/15	-
2	PLM	B	602	-	-	6/15/15/15	-
3	8ZR	A	608	1	-	4/4/38/38	0/3/3/3
2	PLM	A	604	-	-	7/15/15/15	-
2	PLM	A	601	-	-	4/10/10/15	-
2	PLM	B	601	-	-	8/10/10/15	-
2	PLM	A	603	-	-	7/14/14/15	-
2	PLM	B	604	-	-	7/15/15/15	-
2	PLM	A	606	-	-	8/15/15/15	-
2	PLM	B	606	-	-	4/15/15/15	-
2	PLM	B	605	-	-	7/14/14/15	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLM	A	607	-	-	11/15/15/15	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	608	8ZR	C4-N1	8.93	1.47	1.33
3	B	608	8ZR	C4-N1	8.60	1.47	1.33
3	B	608	8ZR	C4-S5	-5.47	1.65	1.70
3	B	608	8ZR	N6-N7	5.03	1.39	1.36
3	A	608	8ZR	N6-N7	5.02	1.39	1.36
3	B	608	8ZR	C4-N6	-4.94	1.26	1.35
3	A	608	8ZR	C4-N6	-4.92	1.26	1.35
3	A	608	8ZR	C4-S5	-4.84	1.66	1.70
3	A	608	8ZR	C9-N15	2.61	1.36	1.34
3	B	608	8ZR	C9-N15	2.31	1.36	1.34
3	B	608	8ZR	C14-C13	2.27	1.54	1.50
3	A	608	8ZR	C14-C13	2.07	1.54	1.50
3	B	608	8ZR	C11-C12	-2.06	1.35	1.41
3	A	608	8ZR	C11-C12	-2.04	1.35	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	608	8ZR	S5-C4-N6	-11.68	106.58	121.06
3	B	608	8ZR	S5-C4-N6	-11.21	107.17	121.06
3	B	608	8ZR	N6-C4-N1	7.51	126.81	116.76
3	A	608	8ZR	N6-C4-N1	6.78	125.84	116.76
3	A	608	8ZR	C8-C9-C10	-3.45	116.25	125.24
3	B	608	8ZR	C8-C9-C10	-3.37	116.44	125.24
2	A	605	PLM	O1-C1-C2	2.29	121.24	114.00
2	A	602	PLM	O1-C1-C2	2.20	120.97	114.00
2	A	607	PLM	O1-C1-C2	2.12	120.71	114.00
2	B	602	PLM	O1-C1-C2	2.09	120.61	114.00
2	A	603	PLM	O1-C1-C2	2.05	120.49	114.00
2	A	604	PLM	O1-C1-C2	2.00	120.32	114.00

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	608	8ZR	N6-C4-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	608	8ZR	N6-C4-N1-C3
3	A	608	8ZR	S5-C4-N1-C2
3	A	608	8ZR	S5-C4-N1-C3
3	B	608	8ZR	N6-C4-N1-C2
3	B	608	8ZR	N6-C4-N1-C3
3	B	608	8ZR	S5-C4-N1-C2
3	B	608	8ZR	S5-C4-N1-C3
2	B	604	PLM	C1-C2-C3-C4
2	A	602	PLM	CC-CD-CE-CF
2	A	602	PLM	C1-C2-C3-C4
2	B	602	PLM	C1-C2-C3-C4
2	B	605	PLM	C1-C2-C3-C4
2	A	601	PLM	C1-C2-C3-C4
2	A	602	PLM	C6-C7-C8-C9
2	A	602	PLM	C9-CA-CB-CC
2	A	607	PLM	C6-C7-C8-C9
2	A	607	PLM	C7-C8-C9-CA
2	B	607	PLM	C7-C8-C9-CA
2	B	604	PLM	C2-C3-C4-C5
2	B	605	PLM	CB-CC-CD-CE
2	A	602	PLM	C7-C8-C9-CA
2	A	605	PLM	C6-C7-C8-C9
2	A	607	PLM	CA-CB-CC-CD
2	B	601	PLM	C4-C5-C6-C7
2	B	602	PLM	CA-CB-CC-CD
2	A	606	PLM	C2-C3-C4-C5
2	A	604	PLM	C4-C5-C6-C7
2	B	607	PLM	CA-CB-CC-CD
2	B	601	PLM	C1-C2-C3-C4
2	B	607	PLM	C6-C7-C8-C9
2	B	603	PLM	CA-CB-CC-CD
2	A	606	PLM	C6-C7-C8-C9
2	B	606	PLM	CC-CD-CE-CF
2	B	601	PLM	C3-C4-C5-C6
2	B	605	PLM	C6-C7-C8-C9
2	A	605	PLM	CA-CB-CC-CD
2	A	605	PLM	C9-CA-CB-CC
2	A	606	PLM	CC-CD-CE-CF
2	B	601	PLM	C5-C6-C7-C8
2	A	601	PLM	C2-C3-C4-C5
2	A	605	PLM	C2-C3-C4-C5
2	A	605	PLM	C8-C9-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	602	PLM	C9-CA-CB-CC
2	B	603	PLM	CB-CC-CD-CE
2	B	606	PLM	C5-C6-C7-C8
2	A	602	PLM	CA-CB-CC-CD
2	B	607	PLM	C9-CA-CB-CC
2	B	607	PLM	CB-CC-CD-CE
2	A	607	PLM	C9-CA-CB-CC
2	A	606	PLM	C1-C2-C3-C4
2	B	604	PLM	C3-C4-C5-C6
2	B	604	PLM	C7-C8-C9-CA
2	A	607	PLM	CB-CC-CD-CE
2	B	604	PLM	CA-CB-CC-CD
2	B	607	PLM	C5-C6-C7-C8
2	A	606	PLM	C5-C6-C7-C8
2	B	603	PLM	C4-C5-C6-C7
2	A	607	PLM	C2-C3-C4-C5
2	A	603	PLM	C3-C4-C5-C6
2	B	603	PLM	C6-C7-C8-C9
2	B	607	PLM	C2-C3-C4-C5
2	A	607	PLM	C5-C6-C7-C8
2	B	602	PLM	CC-CD-CE-CF
2	B	606	PLM	C9-CA-CB-CC
2	A	605	PLM	C5-C6-C7-C8
2	B	607	PLM	C3-C4-C5-C6
2	A	603	PLM	C4-C5-C6-C7
2	A	607	PLM	C8-C9-CA-CB
2	B	602	PLM	C2-C3-C4-C5
2	A	604	PLM	C7-C8-C9-CA
2	A	603	PLM	CB-CC-CD-CE
2	B	601	PLM	C2-C3-C4-C5
2	B	606	PLM	C6-C7-C8-C9
2	B	603	PLM	C3-C4-C5-C6
2	B	605	PLM	CC-CD-CE-CF
2	A	601	PLM	C8-C9-CA-CB
2	A	606	PLM	C3-C4-C5-C6
2	A	607	PLM	C3-C4-C5-C6
2	A	605	PLM	CB-CC-CD-CE
2	B	603	PLM	CC-CD-CE-CF
2	A	604	PLM	CA-CB-CC-CD
2	A	603	PLM	CA-CB-CC-CD
2	A	604	PLM	O1-C1-C2-C3
2	A	605	PLM	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	604	PLM	O2-C1-C2-C3
2	B	605	PLM	O2-C1-C2-C3
2	A	607	PLM	O1-C1-C2-C3
2	A	605	PLM	O1-C1-C2-C3
2	A	604	PLM	C9-CA-CB-CC
2	B	602	PLM	C7-C8-C9-CA
2	A	606	PLM	O1-C1-C2-C3
2	A	606	PLM	O2-C1-C2-C3
2	B	604	PLM	O1-C1-C2-C3
2	A	604	PLM	C8-C9-CA-CB
2	A	604	PLM	O2-C1-C2-C3
2	B	605	PLM	O1-C1-C2-C3
2	B	607	PLM	O1-C1-C2-C3
2	A	607	PLM	O2-C1-C2-C3
2	B	603	PLM	O1-C1-C2-C3
2	B	607	PLM	O2-C1-C2-C3
2	A	602	PLM	C4-C5-C6-C7
2	B	603	PLM	O2-C1-C2-C3
2	B	601	PLM	O1-C1-C2-C3
2	A	603	PLM	O1-C1-C2-C3
2	A	603	PLM	O2-C1-C2-C3
2	B	601	PLM	O2-C1-C2-C3
2	B	607	PLM	C1-C2-C3-C4
2	B	607	PLM	C8-C9-CA-CB
2	B	605	PLM	CA-CB-CC-CD
2	A	601	PLM	C4-C5-C6-C7
2	B	601	PLM	C6-C7-C8-C9
2	A	603	PLM	C5-C6-C7-C8

There are no ring outliers.

13 monomers are involved in 62 short contacts:

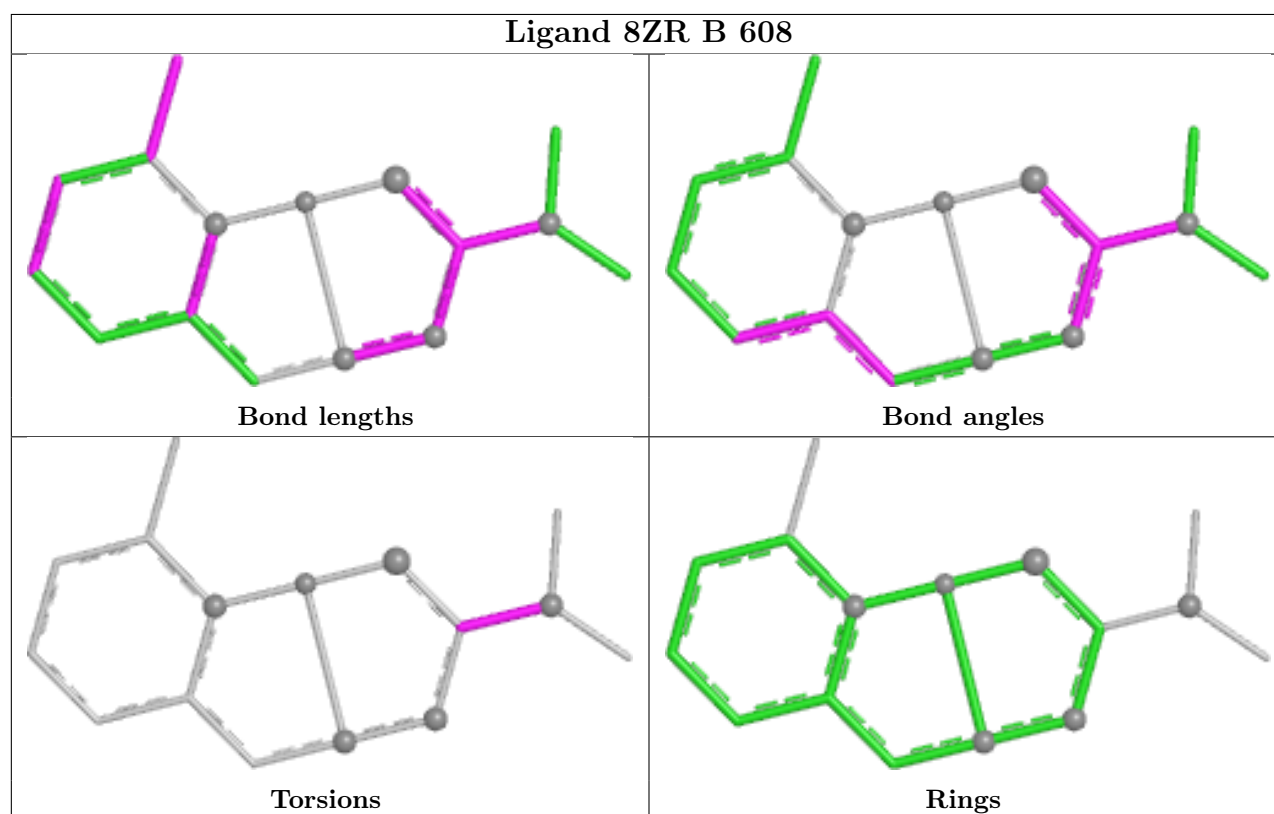
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	608	8ZR	1	0
2	B	603	PLM	1	0
2	B	607	PLM	9	0
2	A	605	PLM	1	0
2	A	602	PLM	2	0
2	B	602	PLM	3	0
3	A	608	8ZR	1	0
2	A	604	PLM	10	0
2	A	601	PLM	4	0

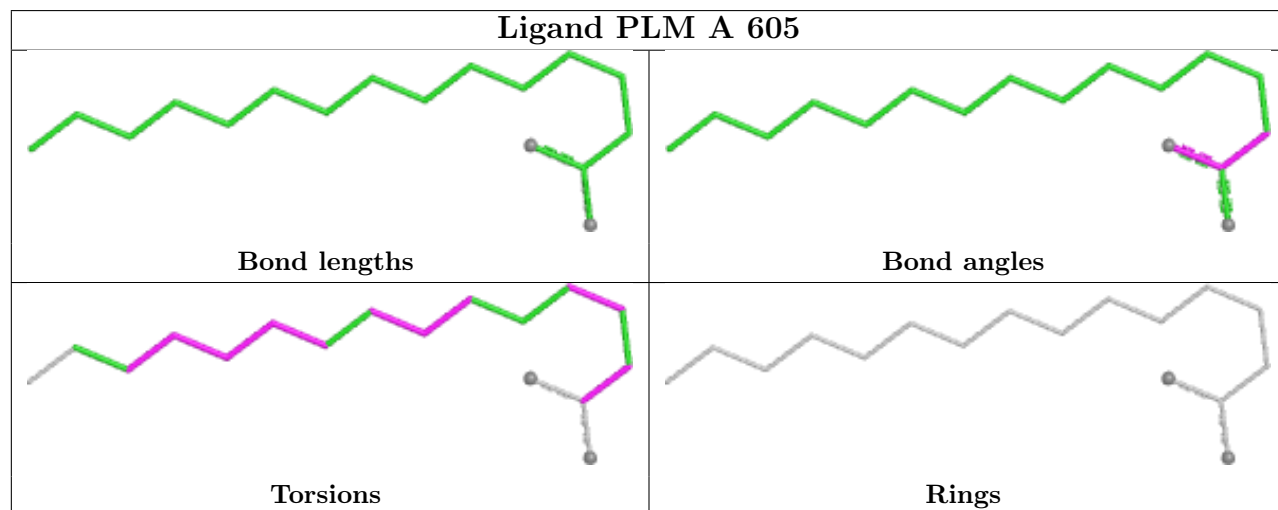
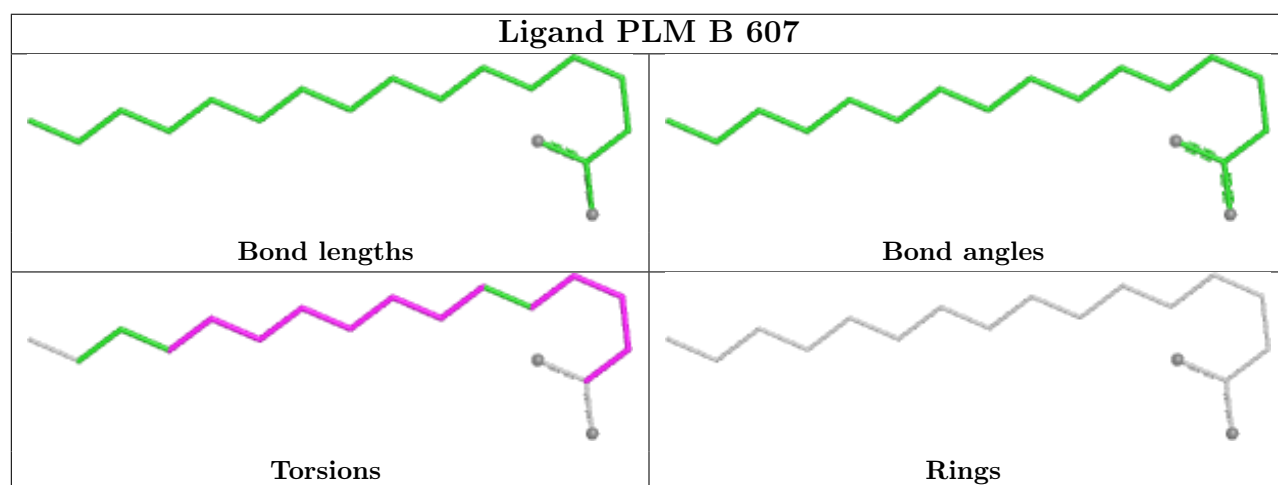
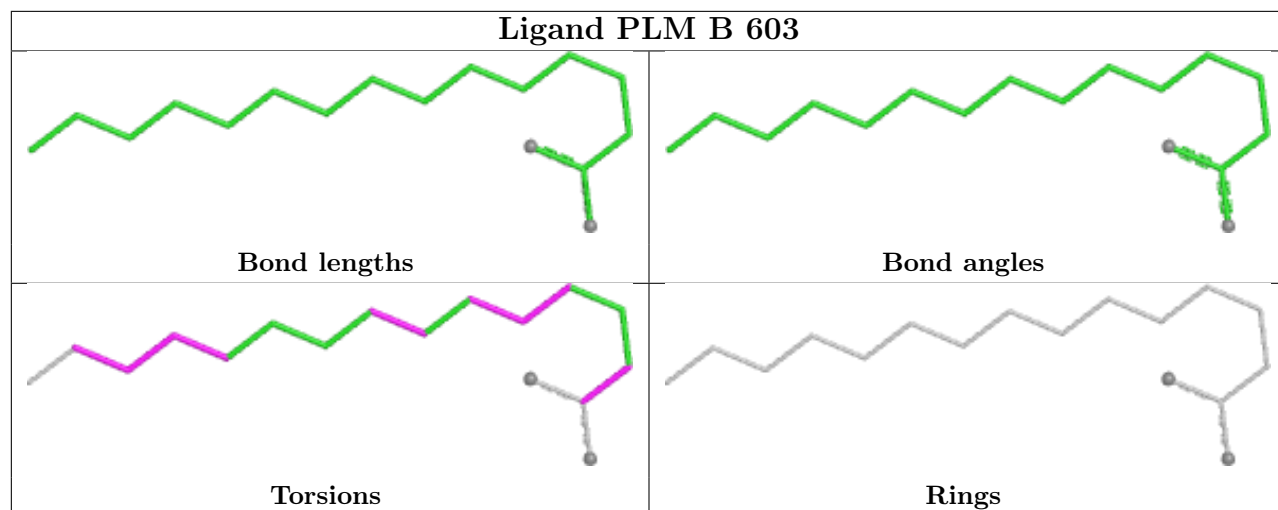
Continued on next page...

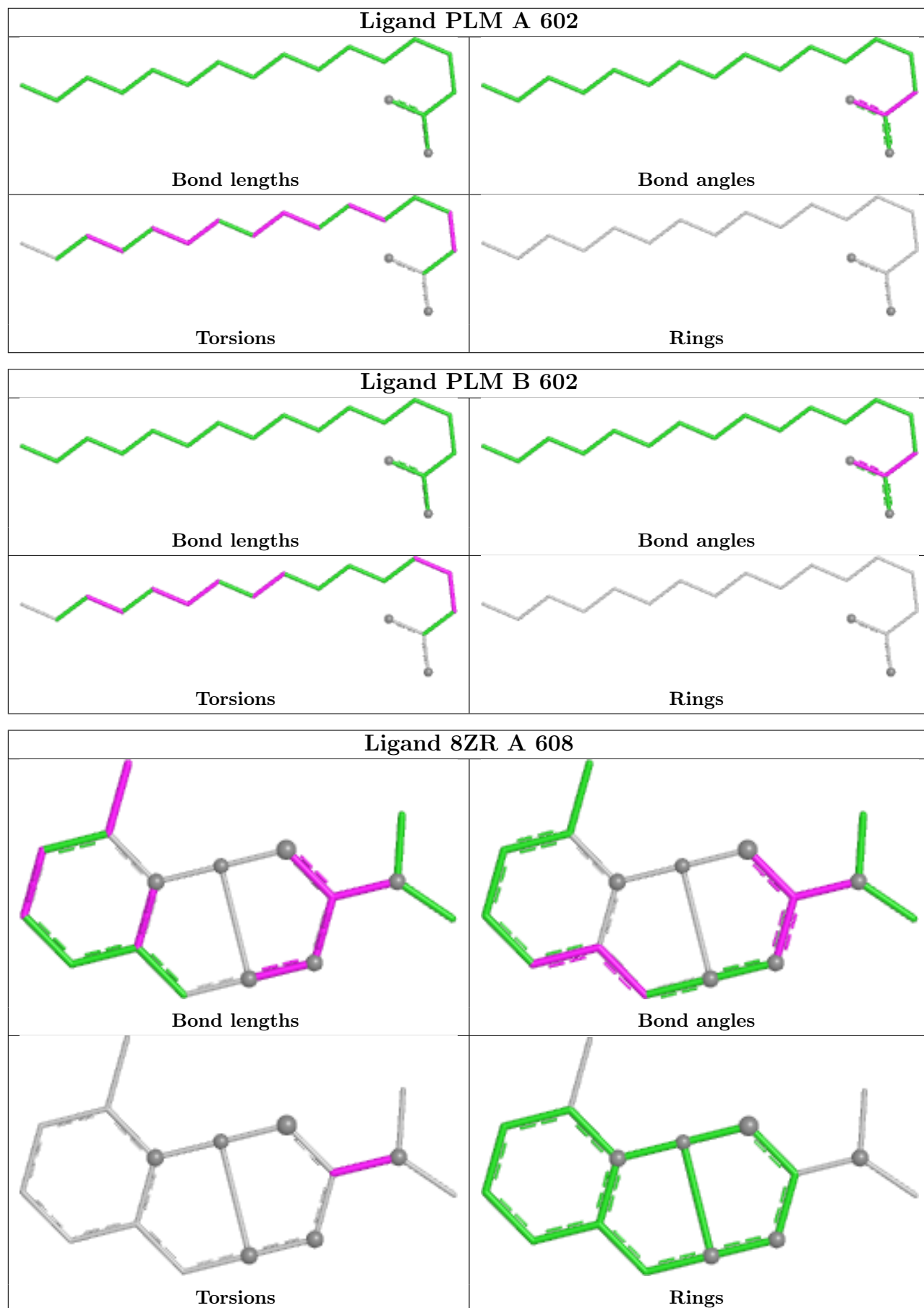
Continued from previous page...

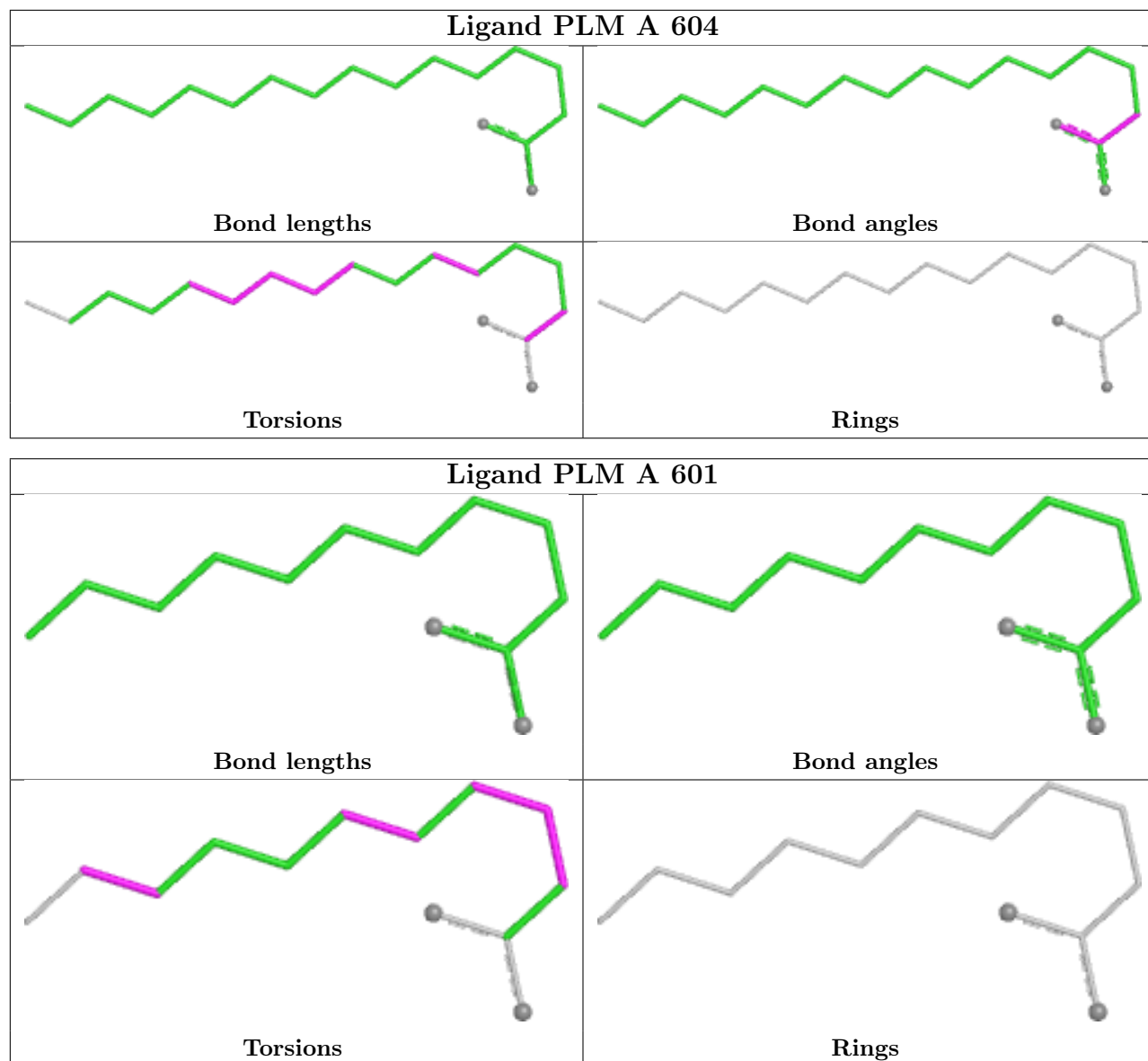
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	PLM	3	0
2	A	603	PLM	6	0
2	B	604	PLM	13	0
2	A	607	PLM	12	0

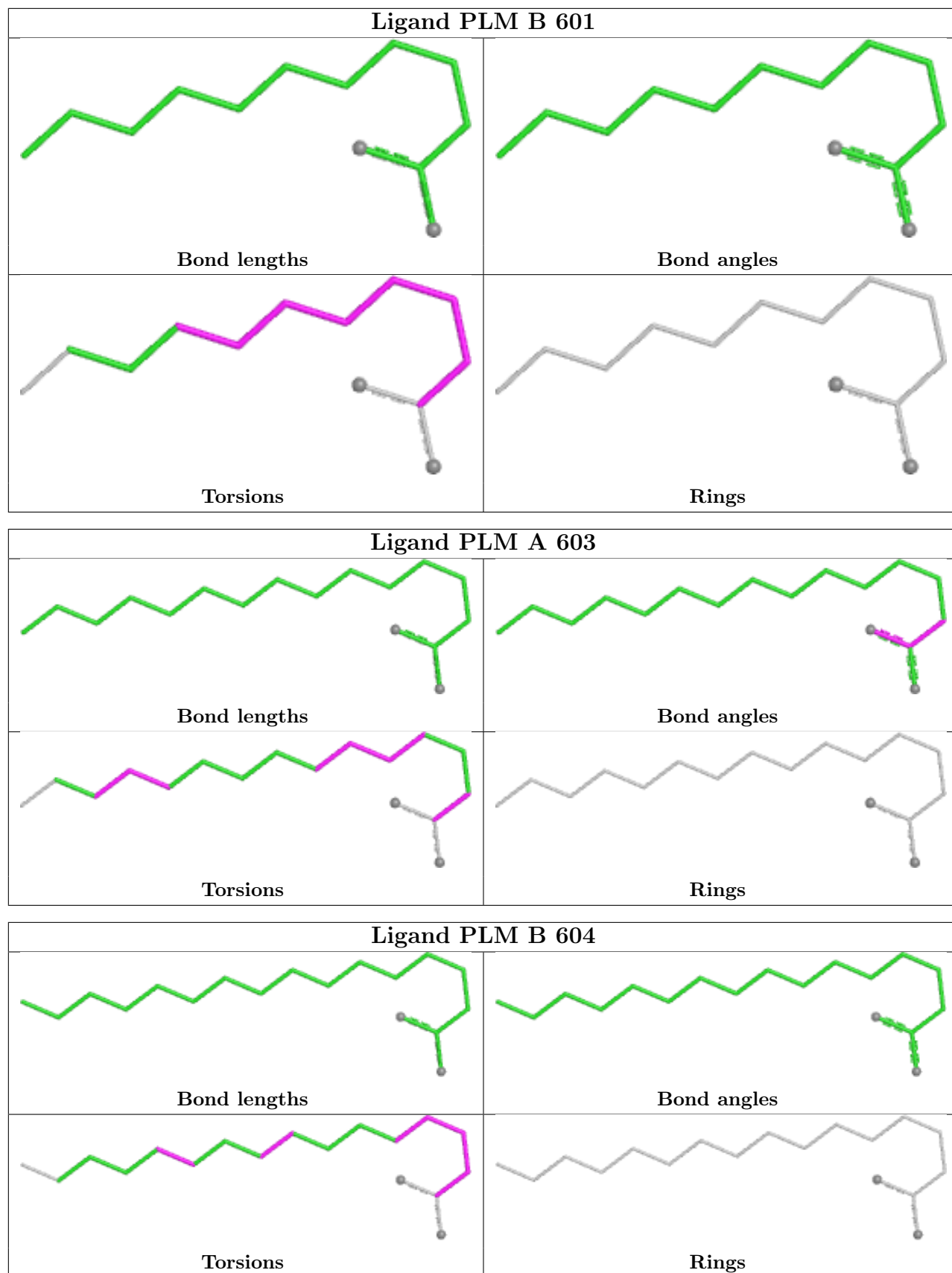
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

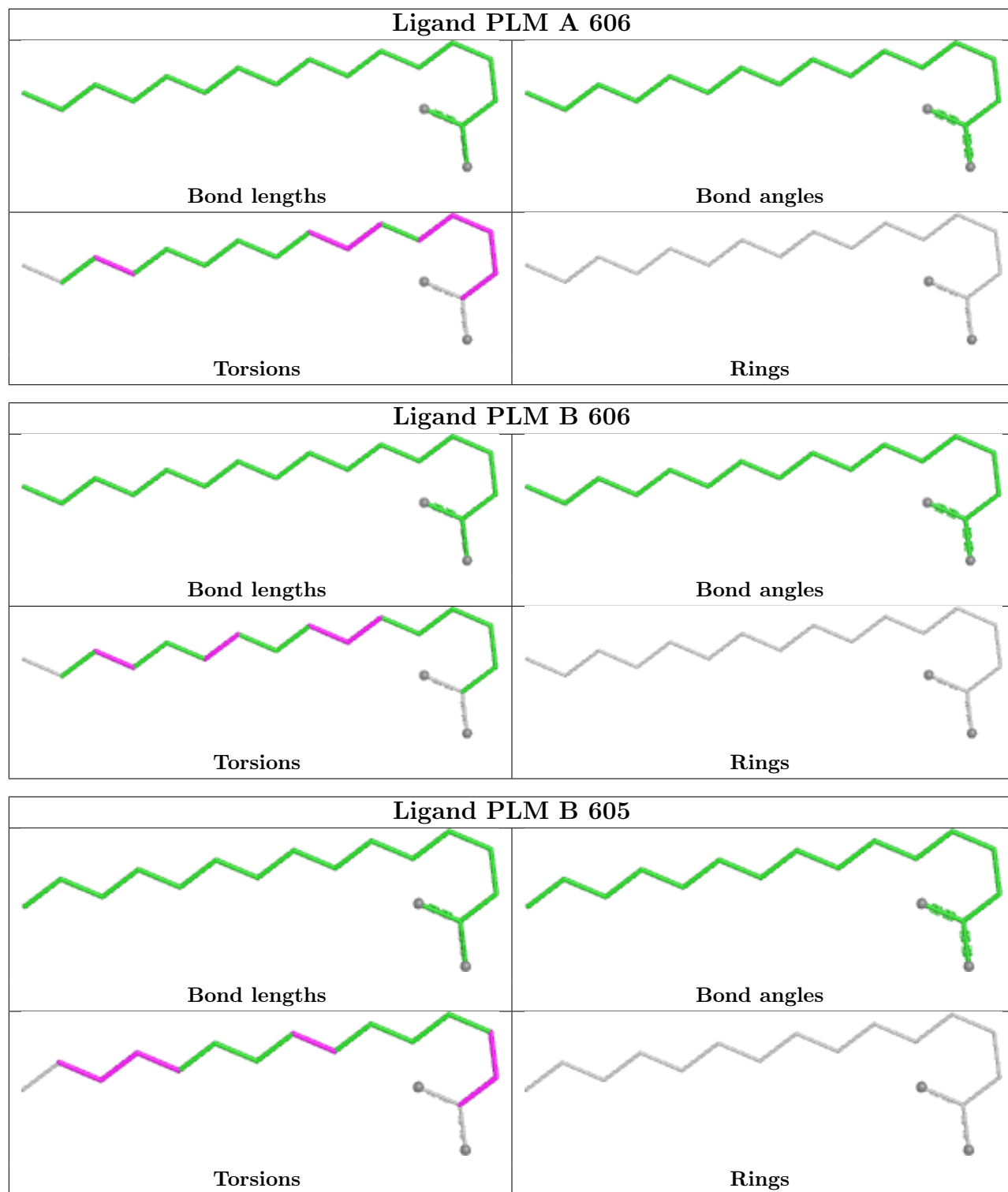


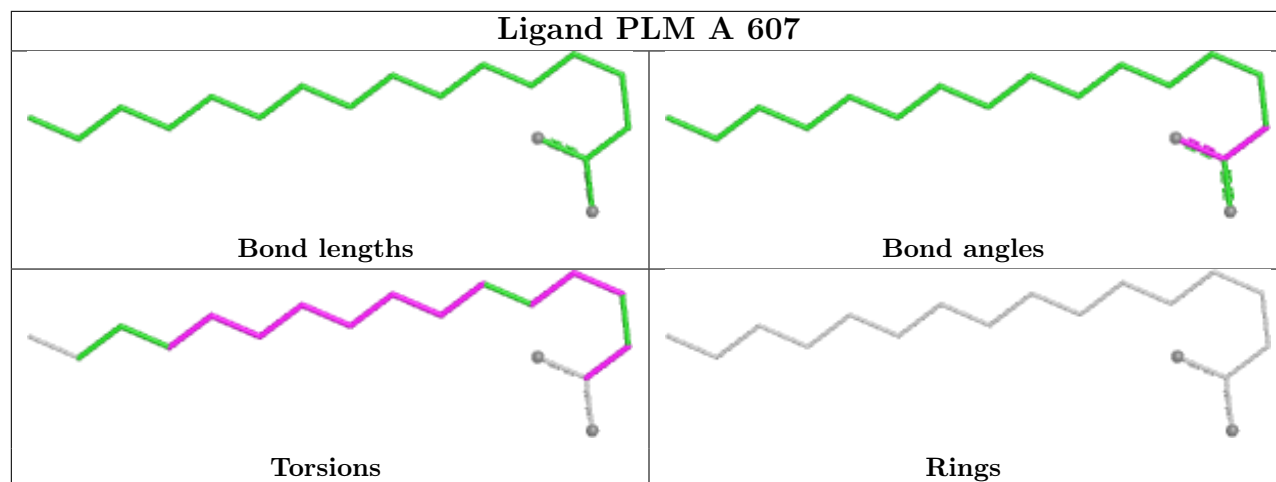












5.7 Other polymers [i](#)

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, 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	581/581 (100%)	-1.17	0 100 100	38, 59, 88, 122	0
1	B	581/581 (100%)	-1.13	0 100 100	37, 60, 90, 128	0
All	All	1162/1162 (100%)	-1.15	0 100 100	37, 60, 89, 128	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.

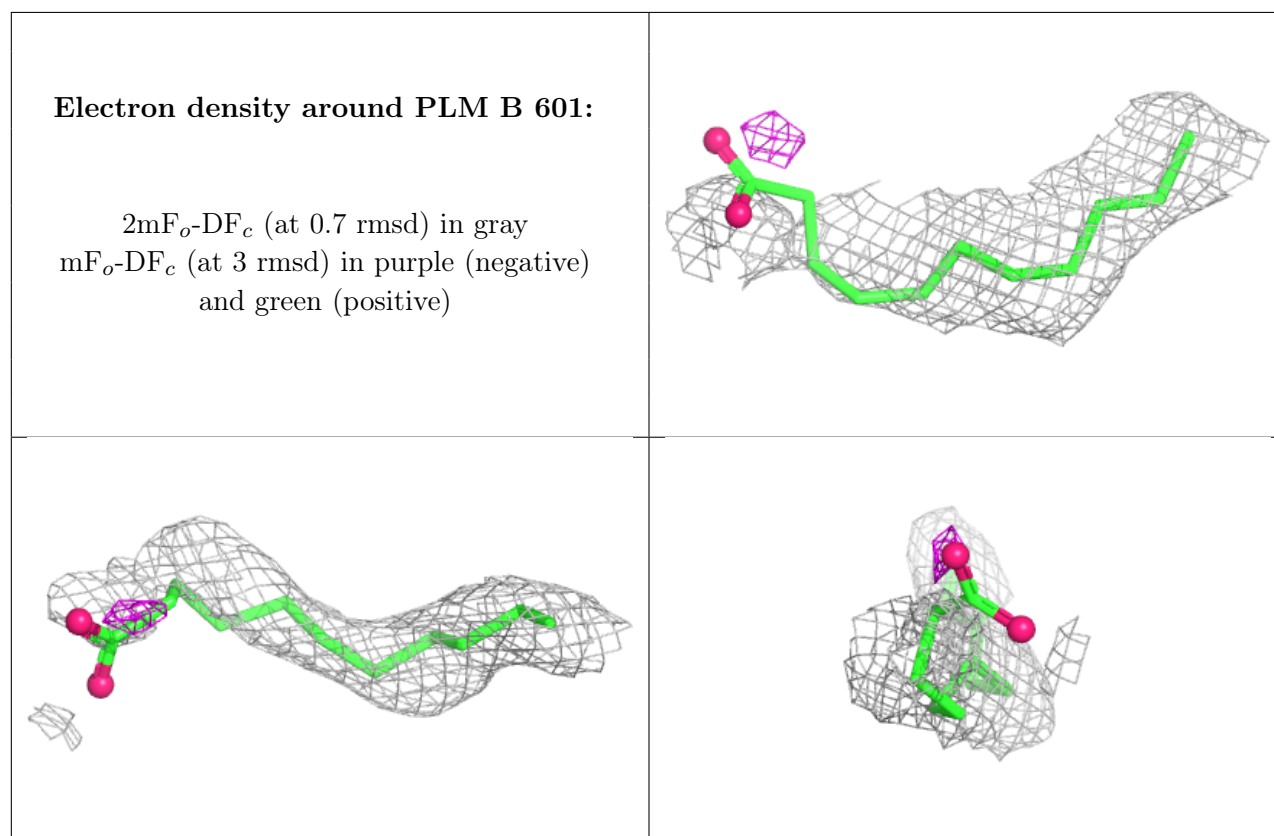
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLM	B	601	13/18	0.97	0.09	77,90,99,99	0
2	PLM	A	605	17/18	0.98	0.06	47,53,66,67	0
2	PLM	A	606	18/18	0.98	0.07	57,68,86,86	0
2	PLM	A	607	18/18	0.98	0.08	93,99,112,112	0
2	PLM	A	601	13/18	0.98	0.07	73,85,95,95	0
2	PLM	B	602	18/18	0.98	0.07	53,60,72,73	0
2	PLM	B	604	18/18	0.98	0.07	68,76,90,91	0

Continued on next page...

Continued from previous page...

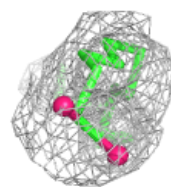
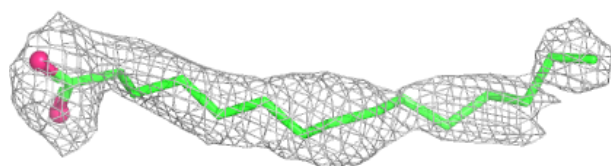
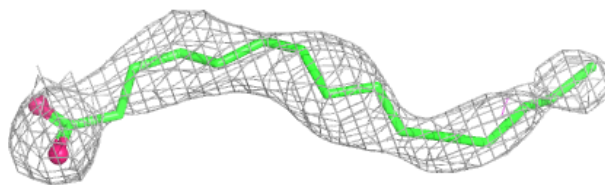
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLM	B	606	18/18	0.98	0.07	48,66,92,93	0
2	PLM	B	607	18/18	0.98	0.09	86,91,106,106	0
2	PLM	B	603	17/18	0.99	0.05	57,65,73,73	0
2	PLM	A	604	18/18	0.99	0.06	61,69,79,80	0
2	PLM	B	605	17/18	0.99	0.05	47,50,64,64	0
2	PLM	A	602	18/18	0.99	0.07	47,56,65,67	0
2	PLM	A	603	17/18	0.99	0.05	56,60,68,68	0
3	8ZR	A	608	16/16	0.99	0.06	110,113,136,136	0
3	8ZR	B	608	16/16	0.99	0.06	119,122,149,149	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.

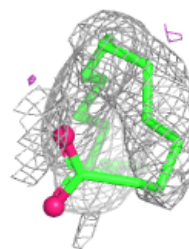
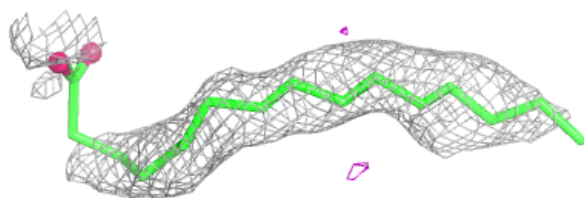
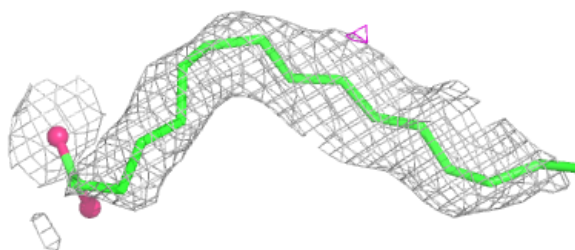


Electron density around PLM A 605:

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

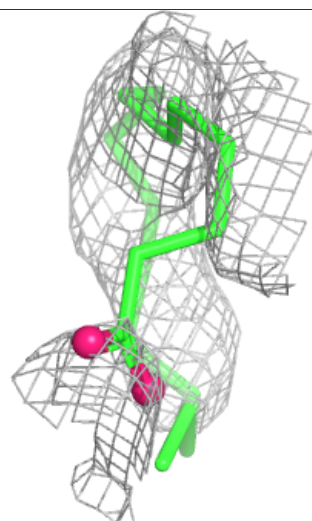
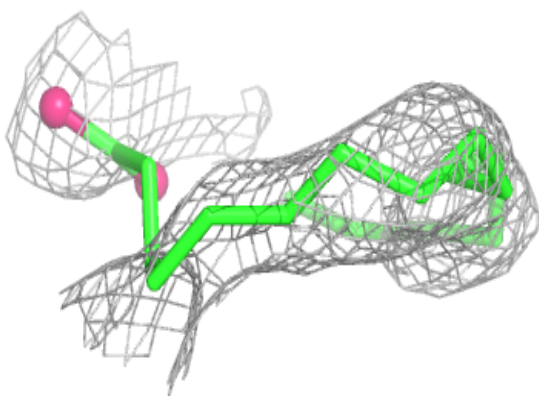
**Electron density around PLM A 606:**

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



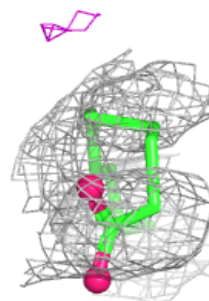
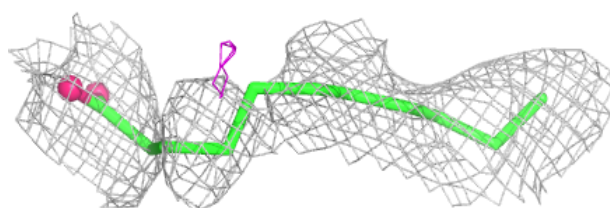
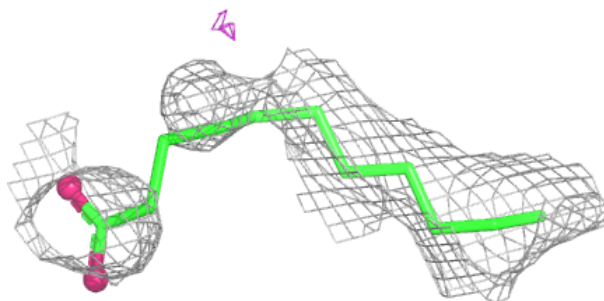
Electron density around PLM A 607:

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

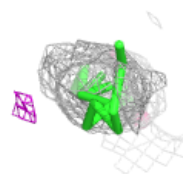
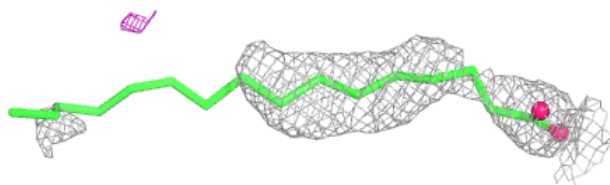
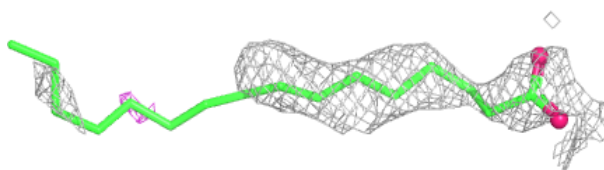


Electron density around PLM A 601:

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

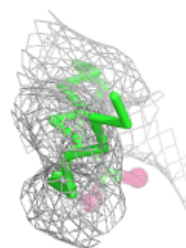
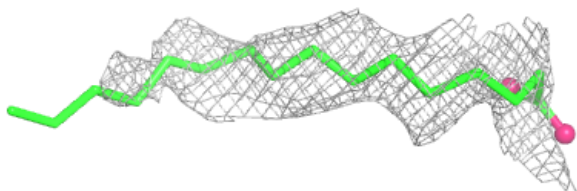
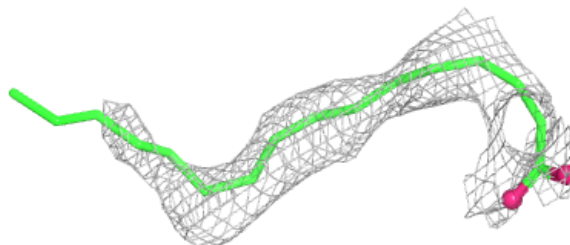
**Electron density around PLM B 602:**

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

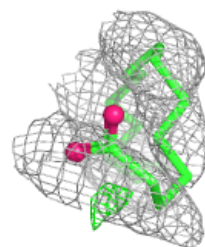
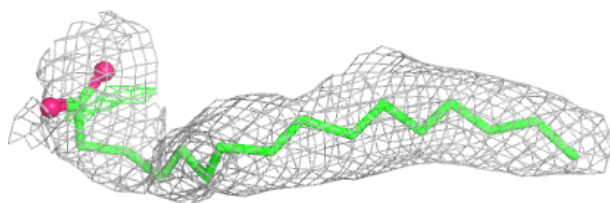
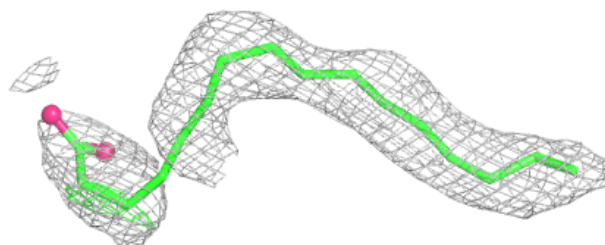


Electron density around PLM B 604:

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

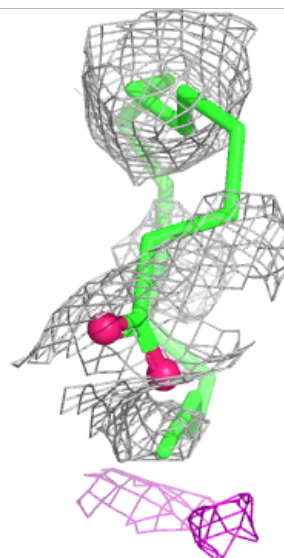
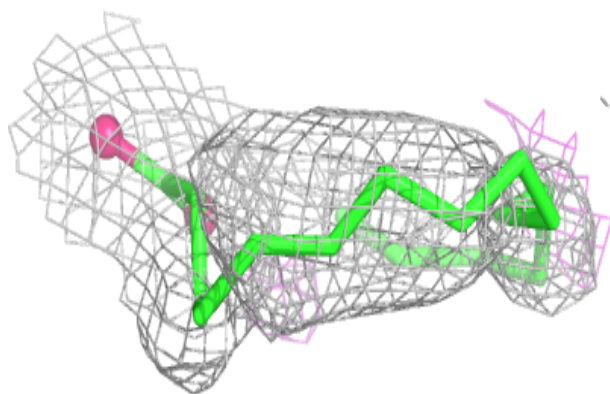
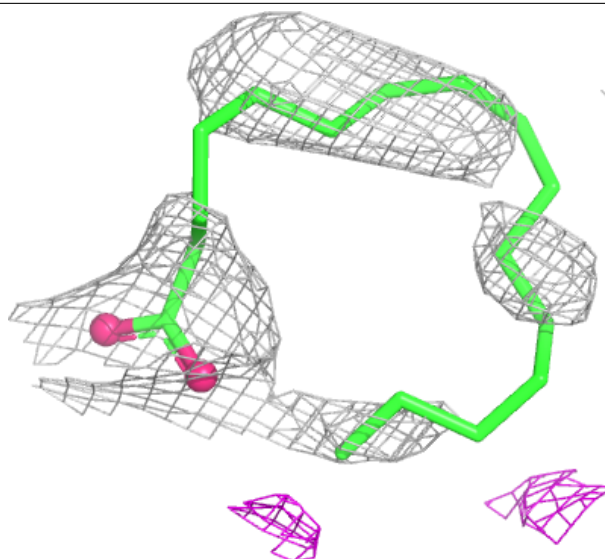
**Electron density around PLM B 606:**

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



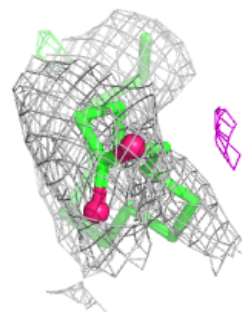
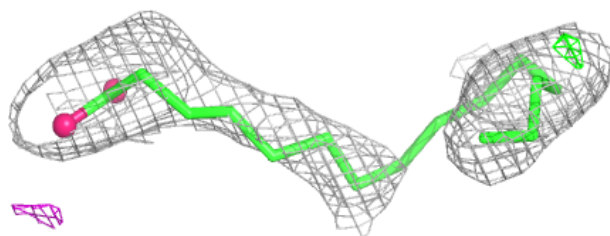
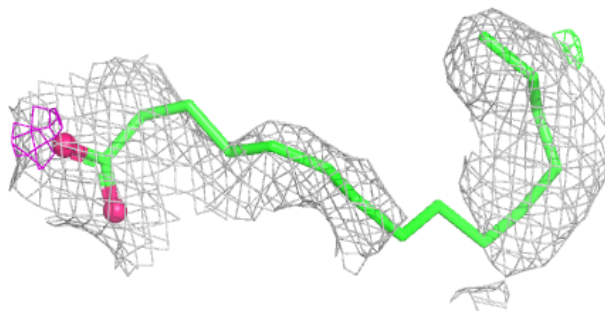
Electron density around PLM B 607:

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

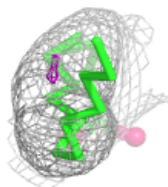
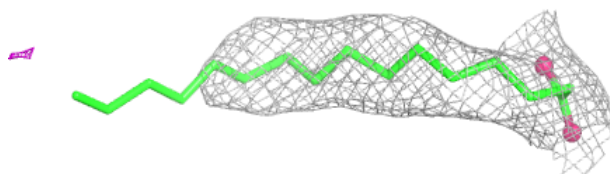
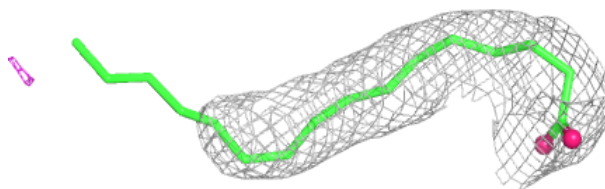


Electron density around PLM B 603:

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

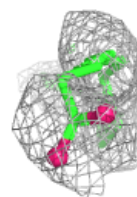
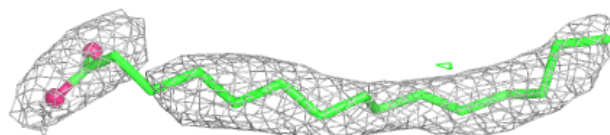
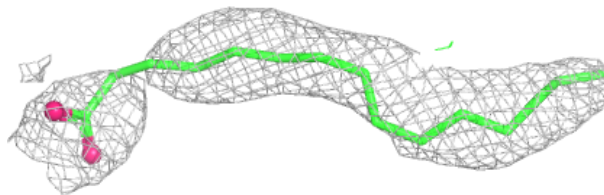
**Electron density around PLM A 604:**

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

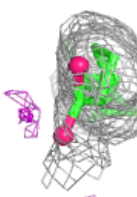
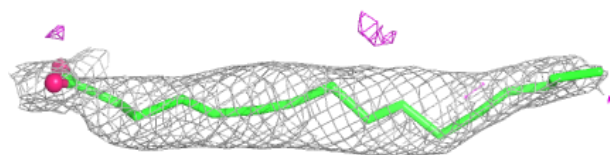
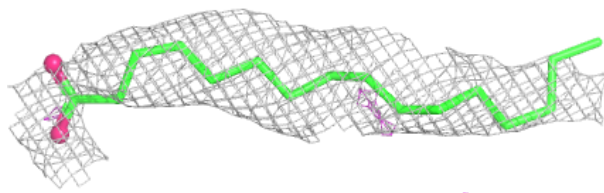


Electron density around PLM B 605:

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

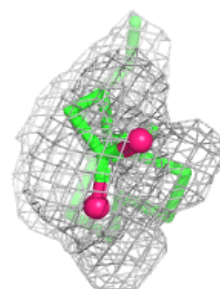
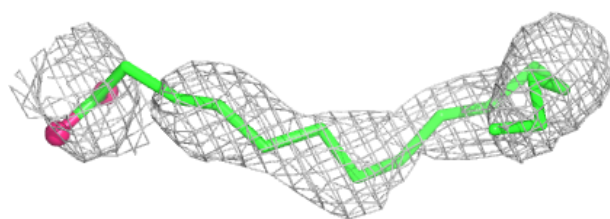
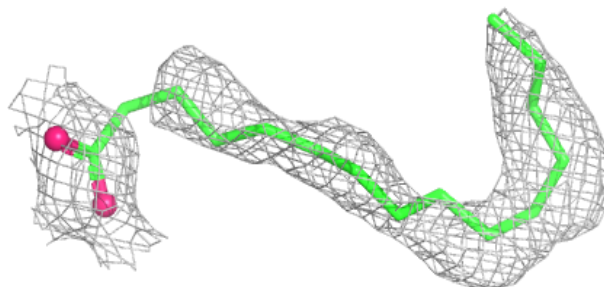
**Electron density around PLM A 602:**

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

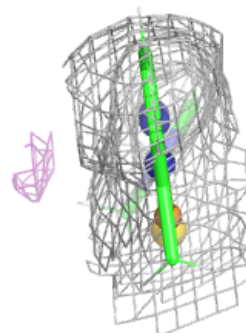
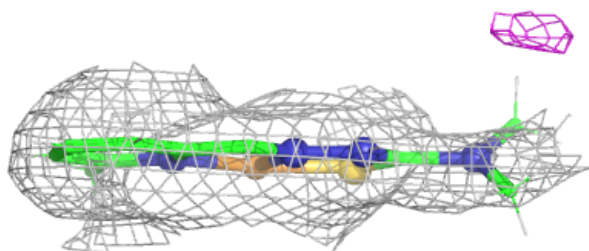
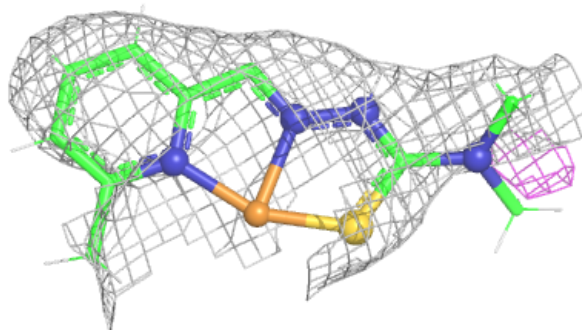


Electron density around PLM A 603:

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

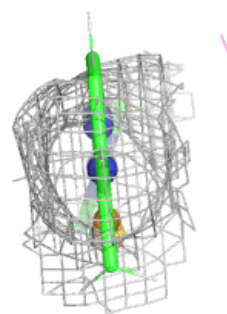
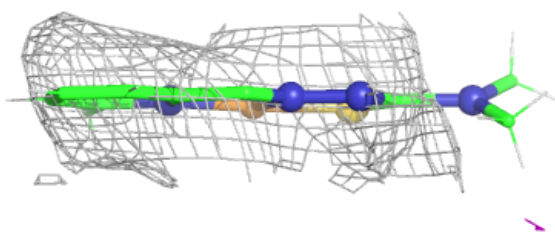
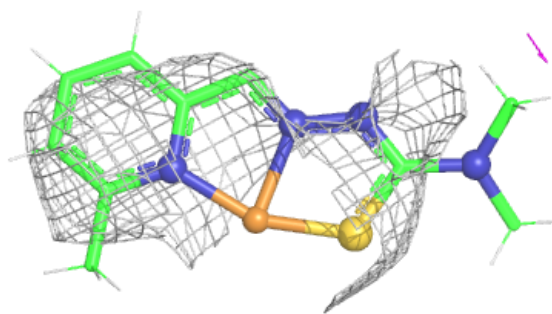
**Electron density around 8ZR A 608:**

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



Electron density around 8ZR B 608:

$2mF_o - DF_c$ (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.