



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:43 PM UTC

PDB ID : 8B18 / pdb_00008b18
Title : DtpB-Nb132-AF
Authors : Killer, M.; Finocchio, G.; Lei, J.; Jungnickel, K.; Kotov, V.; Steinke, J.; Bartels, K.; Strauss, J.; Dupeux, F.; Humm, A.S.; Cornaciu, I.; Marquez, J.; Pardon, E.; Steyeart, J.; Loew, C.
Deposited on : 2022-09-09
Resolution : 2.30 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

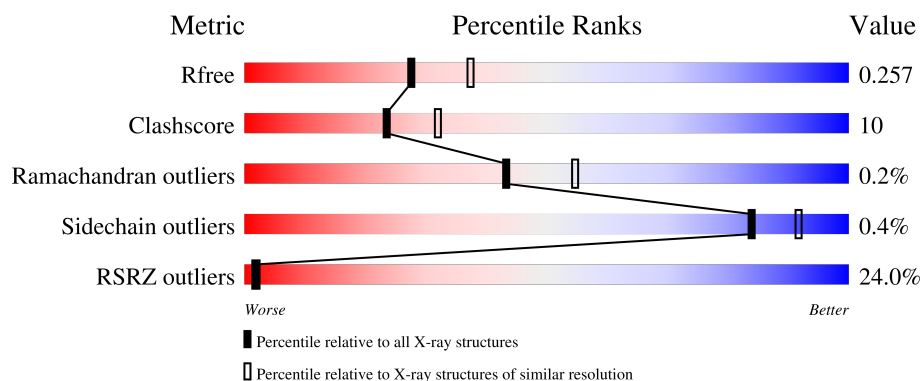
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	489	21% 77% 15% 8%
2	B	127	27% 80% 20%
3	C	2	100%

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
10	D10	A	812	-	-	-	X

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4718 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 Dipeptide and tripeptide permease B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	4	0	0
			3480	2349	531	573	27			

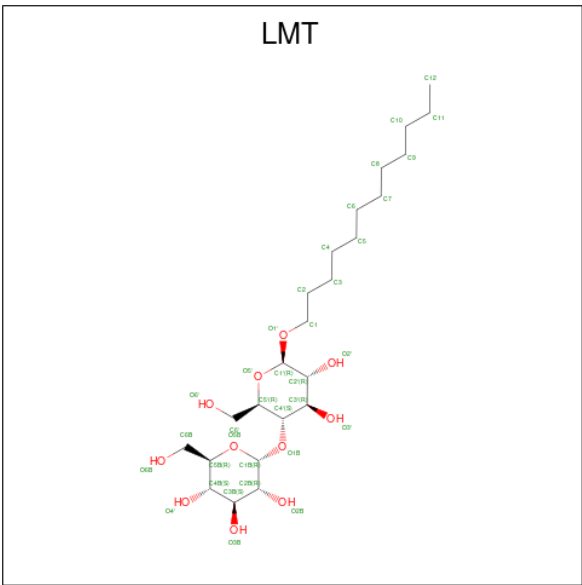
- Molecule 2 is a protein called Nanobody 132.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	5	1	0
			976	613	178	181	4			

- Molecule 3 is a protein called ALA-PHE.

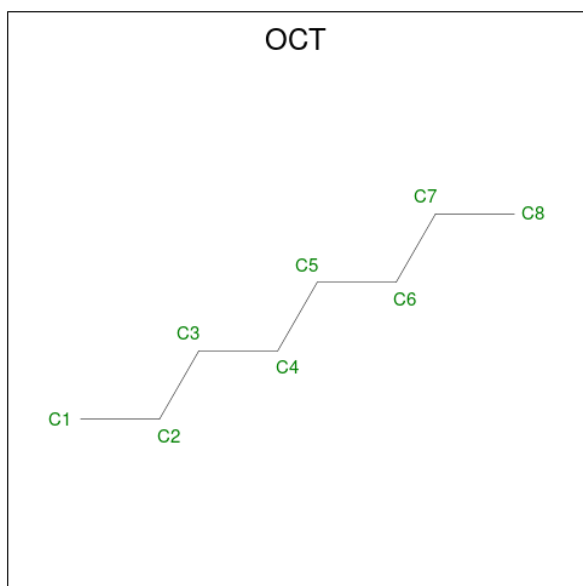
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			17	12	2	3			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



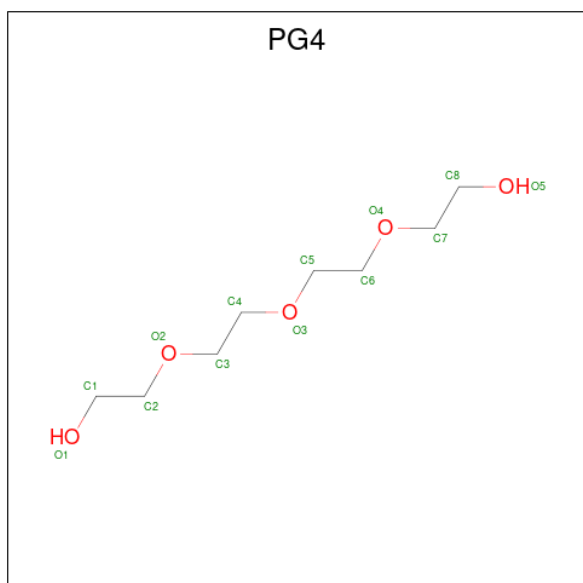
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}) (labeled as "Ligand of Interest" by depositor).



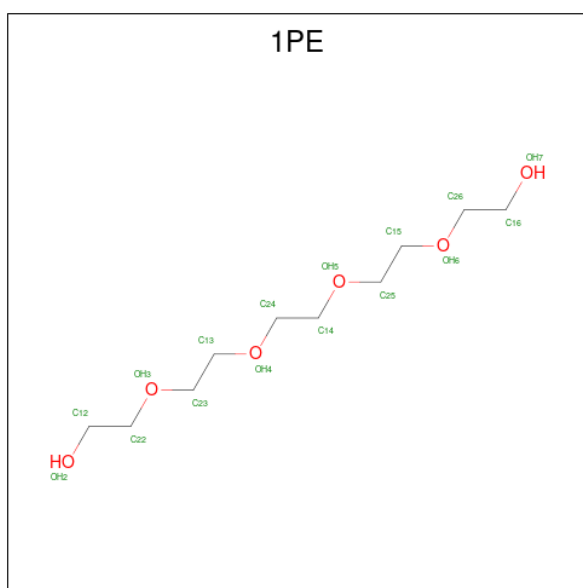
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			8	8		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



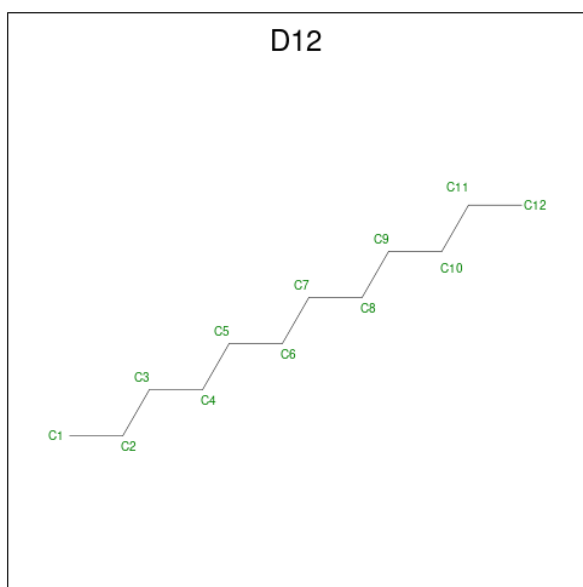
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



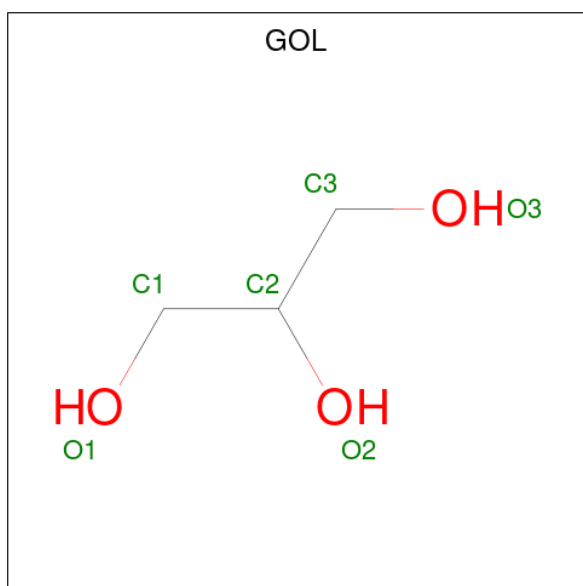
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$) (labeled as "Ligand of Interest" by depositor).



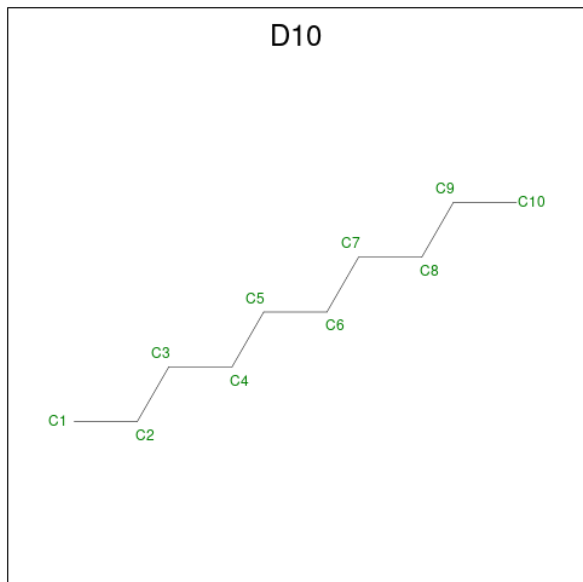
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			12	12		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



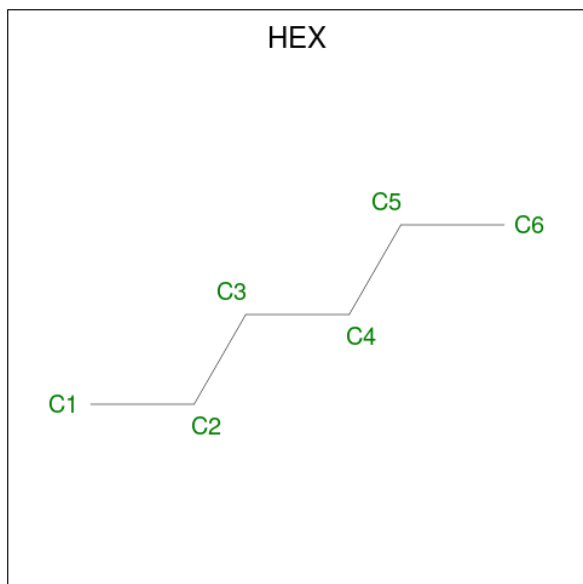
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	C	0	0
			10	10		

- Molecule 11 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}) (labeled as "Ligand of Interest" by depositor).



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

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

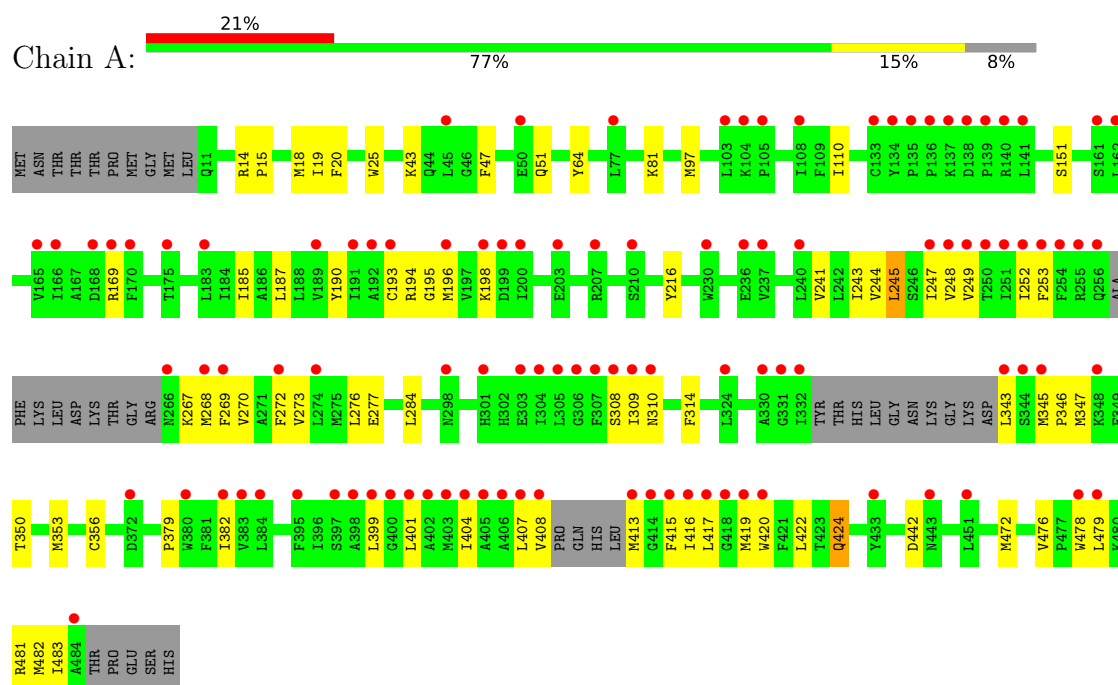
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	40	Total O 40 40	0	0
12	B	19	Total O 19 19	0	0

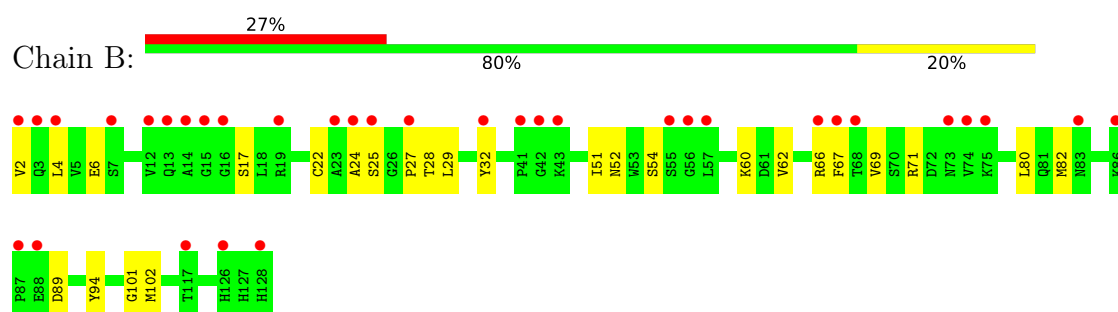
3 Residue-property plots [i](#)

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: Dipeptide and tripeptide permease B



• Molecule 2: Nanobody 132



• Molecule 3: ALA-PHE



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	54.41Å 125.07Å 168.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 2.30 49.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.90-2.30) 92.6 (49.90-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.227 , 0.254 (Not available) , 0.257	Depositor DCC
R_{free} test set	2590 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4718	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: HEX, GOL, OCT, 1PE, D12, PG4, LMT, D10

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	0.46	0/3572	0.70	0/4859
2	B	0.42	0/1004	0.68	0/1361
3	C	0.49	0/17	0.29	0/20
All	All	0.45	0/4593	0.69	0/6240

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3480	0	3605	77	0
2	B	976	0	939	17	0
3	C	17	0	16	0	0
4	A	35	0	46	8	0
5	A	8	0	18	0	0
6	A	65	0	90	2	0
7	A	32	0	44	1	0
8	A	12	0	26	0	0
9	A	12	0	16	1	0
10	A	10	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	12	0	28	1	0
12	A	40	0	0	1	0
12	B	19	0	0	0	0
All	All	4718	0	4850	97	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 10.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:O	1:A:198:LYS:NZ	1.92	1.00
1:A:399:LEU:HD23	1:A:399:LEU:O	1.80	0.82
1:A:194:ARG:C	1:A:198:LYS:HZ1	1.87	0.81
4:A:801:LMT:O4'	12:A:901:HOH:O	1.98	0.81
1:A:345:MET:SD	1:A:399:LEU:HD21	2.24	0.77
1:A:193:CYS:HB3	1:A:196:MET:HE2	1.71	0.70
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.74	0.69
1:A:25:TRP:CD2	1:A:185:ILE:HD11	2.28	0.68
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.75	0.67
1:A:249:VAL:HG13	1:A:415:PHE:HE1	1.60	0.65
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.26	0.65
1:A:284:LEU:HD12	1:A:356:CYS:HB3	1.79	0.65
1:A:345:MET:HB3	1:A:346:PRO:HD3	1.81	0.62
1:A:249:VAL:HG13	1:A:415:PHE:CE1	2.35	0.61
1:A:25:TRP:CG	1:A:185:ILE:HD11	2.36	0.61
1:A:245:LEU:HD22	1:A:422:LEU:HD22	1.83	0.60
1:A:413:MET:SD	1:A:417:LEU:HD21	2.42	0.60
1:A:267:LYS:HG2	1:A:407:LEU:O	2.04	0.56
1:A:243:ILE:HG13	7:A:811:1PE:H151	1.88	0.56
1:A:97:MET:HE1	1:A:110:ILE:HG22	1.88	0.56
1:A:481:ARG:HG3	1:A:481:ARG:HH11	1.71	0.55
1:A:401:LEU:HA	1:A:404:ILE:HB	1.88	0.55
1:A:25:TRP:CE2	1:A:185:ILE:HD11	2.42	0.54
1:A:401:LEU:HD21	1:A:417:LEU:HD12	1.90	0.54
1:A:81:LYS:HB3	1:A:190:TYR:OH	2.09	0.53
1:A:413:MET:O	1:A:416:ILE:HG13	2.08	0.53
4:A:801:LMT:H4B	2:B:32:TYR:OH	2.09	0.53
2:B:60:LYS:HD3	2:B:62:VAL:CG2	2.38	0.52
1:A:248:VAL:O	1:A:252:ILE:HG23	2.09	0.52
1:A:343:LEU:HA	1:A:347:MET:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:MET:HE2	1:A:345:MET:HA	1.92	0.52
6:A:806:PG4:H82	11:A:815:HEX:H22	1.92	0.51
1:A:14:ARG:HE	9:A:810:GOL:H12	1.74	0.51
1:A:190:TYR:OH	1:A:194:ARG:NH1	2.45	0.50
1:A:401:LEU:HD22	1:A:420:TRP:CD1	2.47	0.50
2:B:52:ASN:O	2:B:71:ARG:NH2	2.37	0.50
1:A:247:ILE:HD12	1:A:248:VAL:N	2.27	0.49
1:A:270:VAL:HG13	1:A:479:LEU:HD12	1.93	0.49
2:B:17:SER:HA	2:B:82:MET:O	2.11	0.49
2:B:67:PHE:CZ	2:B:82:MET:HG2	2.48	0.49
1:A:269:PHE:CD1	1:A:269:PHE:N	2.80	0.49
1:A:347:MET:HE2	1:A:476:VAL:HG21	1.95	0.48
2:B:24:ALA:HB2	2:B:29:LEU:HD13	1.96	0.47
1:A:18:MET:HE2	1:A:19:ILE:HG13	1.95	0.47
1:A:195:GLY:HA2	1:A:198:LYS:HE2	1.96	0.47
1:A:216:TYR:HB3	6:A:807:PG4:H42	1.97	0.47
1:A:268:MET:HE1	1:A:408:VAL:HA	1.96	0.46
1:A:308:SER:O	4:A:801:LMT:H4'	2.16	0.46
2:B:2:VAL:N	2:B:27:PRO:HG2	2.30	0.46
4:A:801:LMT:H41	4:A:801:LMT:H2'	1.97	0.46
1:A:267:LYS:HE2	1:A:267:LYS:HB2	1.74	0.46
1:A:478:TRP:HE1	1:A:482:MET:HE2	1.80	0.46
1:A:18:MET:HB2	1:A:196:MET:CE	2.46	0.45
1:A:481:ARG:HG3	1:A:481:ARG:NH1	2.30	0.45
1:A:64:TYR:HB3	1:A:424:GLN:HE21	1.83	0.44
4:A:801:LMT:H41	4:A:801:LMT:H12	1.48	0.44
1:A:169:ARG:NH1	4:A:801:LMT:O6B	2.50	0.44
1:A:350:THR:HA	1:A:472:MET:HE2	1.99	0.44
1:A:273:VAL:O	1:A:277:GLU:HG3	2.17	0.44
1:A:404:ILE:HA	1:A:407:LEU:HD12	2.00	0.44
1:A:195:GLY:HA2	1:A:198:LYS:CE	2.47	0.44
1:A:417:LEU:HD22	1:A:417:LEU:N	2.33	0.44
2:B:67:PHE:CE2	2:B:82:MET:HG2	2.53	0.43
1:A:15:PRO:HA	1:A:196:MET:HE3	2.00	0.43
1:A:14:ARG:N	1:A:15:PRO:HD2	2.33	0.43
1:A:47:PHE:HB3	1:A:51:GLN:HB2	2.01	0.43
1:A:267:LYS:HD2	1:A:407:LEU:HA	1.99	0.43
1:A:401:LEU:HD21	1:A:417:LEU:CD1	2.47	0.43
1:A:343:LEU:HA	1:A:347:MET:CB	2.49	0.43
1:A:345:MET:HE2	1:A:345:MET:CA	2.49	0.43
2:B:101:GLY:C	2:B:102:MET:HE2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TRP:O	1:A:478:TRP:HD1	2.01	0.43
1:A:43:LYS:HA	1:A:43:LYS:HD2	1.84	0.43
1:A:244:VAL:HA	1:A:247:ILE:HG13	2.01	0.43
1:A:309:ILE:HD11	1:A:314:PHE:CZ	2.54	0.43
1:A:379:PRO:O	1:A:382:ILE:HG22	2.19	0.42
1:A:195:GLY:HA2	1:A:198:LYS:NZ	2.34	0.42
1:A:479:LEU:O	1:A:483:ILE:HG13	2.18	0.42
1:A:353:MET:HE2	1:A:353:MET:HB2	1.84	0.42
1:A:478:TRP:CD1	1:A:478:TRP:C	2.96	0.42
2:B:28:THR:H	2:B:28:THR:HG23	1.60	0.42
1:A:198:LYS:HD3	1:A:198:LYS:HA	1.35	0.42
1:A:241:VAL:O	1:A:245:LEU:HB2	2.20	0.42
1:A:247:ILE:HD12	1:A:248:VAL:HG23	2.02	0.42
1:A:97:MET:CE	1:A:110:ILE:HG22	2.48	0.41
1:A:169:ARG:NH1	4:A:801:LMT:O2'	2.53	0.41
1:A:310:ASN:HB2	4:A:801:LMT:H6'1	2.03	0.41
2:B:51:ILE:HD13	2:B:71:ARG:HB2	2.02	0.41
2:B:6:GLU:OE1	2:B:94:TYR:HA	2.20	0.41
1:A:20:PHE:CE2	1:A:151:SER:HB2	2.56	0.41
1:A:253:PHE:CD2	1:A:419:MET:HE1	2.56	0.41
1:A:442:ASP:HB3	2:B:54:SER:OG	2.21	0.41
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.60	0.41
1:A:249:VAL:HA	1:A:252:ILE:HG12	2.03	0.40
2:B:69:VAL:HG22	2:B:80:LEU:HD13	2.03	0.40
1:A:272:PHE:CZ	1:A:276:LEU:HD21	2.56	0.40
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.87	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	443/489 (91%)	435 (98%)	8 (2%)	0	100	100
2	B	126/127 (99%)	125 (99%)	0	1 (1%)	16	20
All	All	569/616 (92%)	560 (98%)	8 (1%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	SER

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	368/401 (92%)	366 (100%)	2 (0%)	81	90
2	B	102/101 (101%)	102 (100%)	0	100	100
3	C	1/1 (100%)	1 (100%)	0	100	100
All	All	471/503 (94%)	469 (100%)	2 (0%)	84	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LEU
1	A	424	GLN

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	293	ASN
1	A	299	ASN
1	A	301	HIS
2	B	13	GLN
2	B	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	$\# Z > 2$
4	LMT	A	801	-	36,36,36	1.21	2 (5%)	47,47,47	1.50	11 (23%)
5	OCT	A	802	-	7,7,7	0.39	0	6,6,6	0.79	0
7	1PE	A	811	-	15,15,15	0.54	0	14,14,14	0.48	0
6	PG4	A	808	-	12,12,12	0.54	0	11,11,11	0.44	0
11	HEX	A	815	-	5,5,5	0.38	0	4,4,4	0.60	0
9	GOL	A	810	-	5,5,5	1.04	0	5,5,5	0.91	0
7	1PE	A	804	-	15,15,15	0.48	0	14,14,14	0.45	0
6	PG4	A	805	-	12,12,12	0.52	0	11,11,11	0.53	0
11	HEX	A	814	-	5,5,5	0.37	0	4,4,4	0.60	0
9	GOL	A	813	-	5,5,5	0.88	0	5,5,5	0.94	0
6	PG4	A	806	-	12,12,12	0.58	0	11,11,11	0.52	0
6	PG4	A	803	-	12,12,12	0.51	0	11,11,11	0.26	0
8	D12	A	809	-	11,11,11	0.45	0	10,10,10	0.63	0
6	PG4	A	807	-	12,12,12	0.53	0	11,11,11	0.40	0
10	D10	A	812	-	9,9,9	0.30	0	8,8,8	1.13	1 (12%)

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
4	LMT	A	801	-	-	16/21/61/61	0/2/2/2
5	OCT	A	802	-	-	2/5/5/5	-
7	1PE	A	811	-	-	6/13/13/13	-
6	PG4	A	808	-	-	3/10/10/10	-
11	HEX	A	815	-	-	0/3/3/3	-
9	GOL	A	810	-	-	1/4/4/4	-
7	1PE	A	804	-	-	6/13/13/13	-
6	PG4	A	805	-	-	5/10/10/10	-
11	HEX	A	814	-	-	0/3/3/3	-
9	GOL	A	813	-	-	0/4/4/4	-
6	PG4	A	806	-	-	6/10/10/10	-
6	PG4	A	803	-	-	4/10/10/10	-
8	D12	A	809	-	-	3/9/9/9	-
6	PG4	A	807	-	-	5/10/10/10	-
10	D10	A	812	-	-	1/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O5B-C1B	3.79	1.51	1.41
4	A	801	LMT	O5'-C1'	3.06	1.49	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	C1'-C2'-C3'	3.26	116.87	110.01
4	A	801	LMT	C2'-C3'-C4'	3.20	116.95	109.68
4	A	801	LMT	C3'-C4'-C5'	2.50	116.46	110.93
4	A	801	LMT	O5B-C5B-C6B	2.44	112.48	106.44
4	A	801	LMT	C4B-C3B-C2B	-2.41	106.60	110.83
4	A	801	LMT	C3B-C4B-C5B	-2.36	105.96	110.23
4	A	801	LMT	O3B-C3B-C2B	2.34	115.89	110.38
4	A	801	LMT	C1B-O1B-C4'	2.29	123.40	117.98
10	A	812	D10	C6-C5-C4	-2.18	103.35	114.37
4	A	801	LMT	O1B-C4'-C5'	2.15	115.12	109.48
4	A	801	LMT	C1B-C2B-C3B	-2.15	105.49	110.01
4	A	801	LMT	C1'-O5'-C5'	-2.09	109.63	113.72

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C2'-C1'-O1'-C1
4	A	801	LMT	O5'-C1'-O1'-C1
4	A	801	LMT	O5B-C5B-C6B-O6B
4	A	801	LMT	O5'-C5'-C6'-O6'
6	A	803	PG4	O3-C5-C6-O4
6	A	806	PG4	O2-C3-C4-O3
4	A	801	LMT	C4B-C5B-C6B-O6B
4	A	801	LMT	C4'-C5'-C6'-O6'
6	A	807	PG4	O3-C5-C6-O4
7	A	811	1PE	OH5-C14-C24-OH4
6	A	806	PG4	O3-C5-C6-O4
4	A	801	LMT	C3'-C4'-O1B-C1B
7	A	811	1PE	OH4-C13-C23-OH3
4	A	801	LMT	C3-C4-C5-C6
6	A	805	PG4	O3-C5-C6-O4
4	A	801	LMT	C1-C2-C3-C4
7	A	811	1PE	OH6-C15-C25-OH5
4	A	801	LMT	C7-C8-C9-C10
4	A	801	LMT	C5-C6-C7-C8
5	A	802	OCT	C4-C5-C6-C7
4	A	801	LMT	C6-C7-C8-C9
7	A	804	1PE	OH7-C16-C26-OH6
4	A	801	LMT	C5'-C4'-O1B-C1B
9	A	810	GOL	O2-C2-C3-O3
5	A	802	OCT	C3-C4-C5-C6
8	A	809	D12	C9-C10-C11-C12
6	A	805	PG4	O4-C7-C8-O5
4	A	801	LMT	C11-C10-C9-C8
6	A	805	PG4	C5-C6-O4-C7
6	A	807	PG4	C8-C7-O4-C6
7	A	811	1PE	C12-C22-OH3-C23
7	A	811	1PE	C25-C15-OH6-C26
6	A	803	PG4	C1-C2-O2-C3
8	A	809	D12	C3-C4-C5-C6
4	A	801	LMT	C4-C5-C6-C7
6	A	806	PG4	C3-C4-O3-C5
7	A	804	1PE	C25-C15-OH6-C26
7	A	804	1PE	OH2-C12-C22-OH3
6	A	806	PG4	C4-C3-O2-C2
6	A	807	PG4	C1-C2-O2-C3

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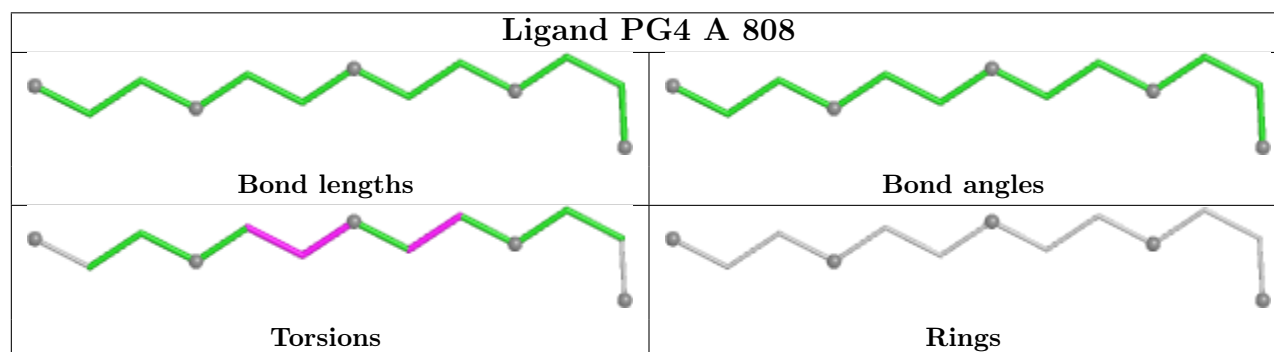
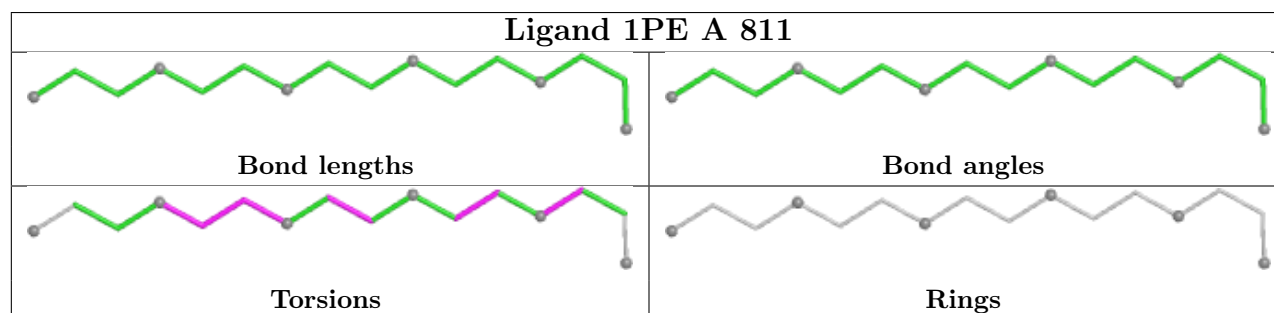
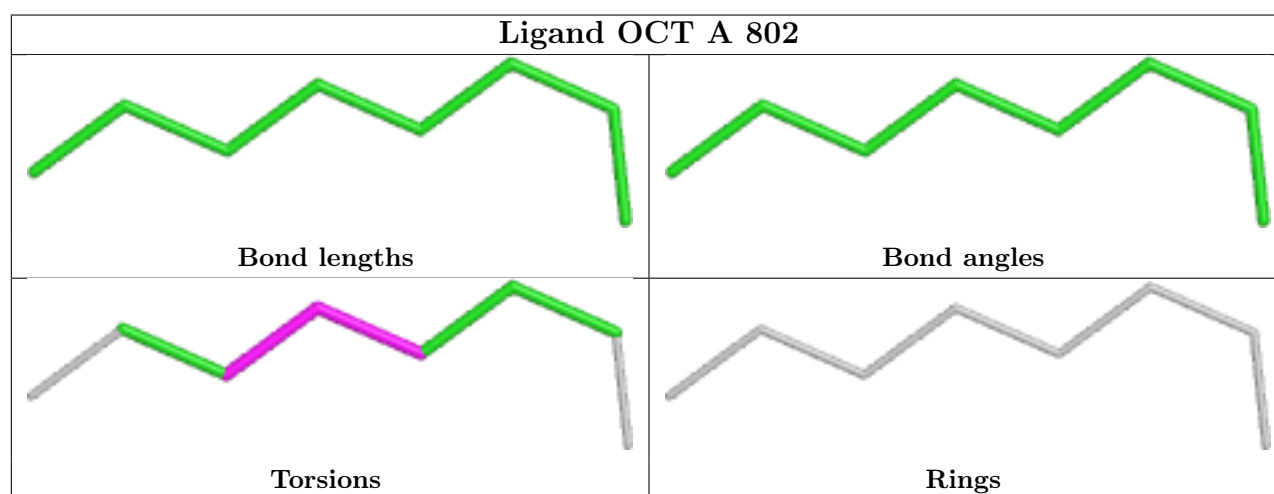
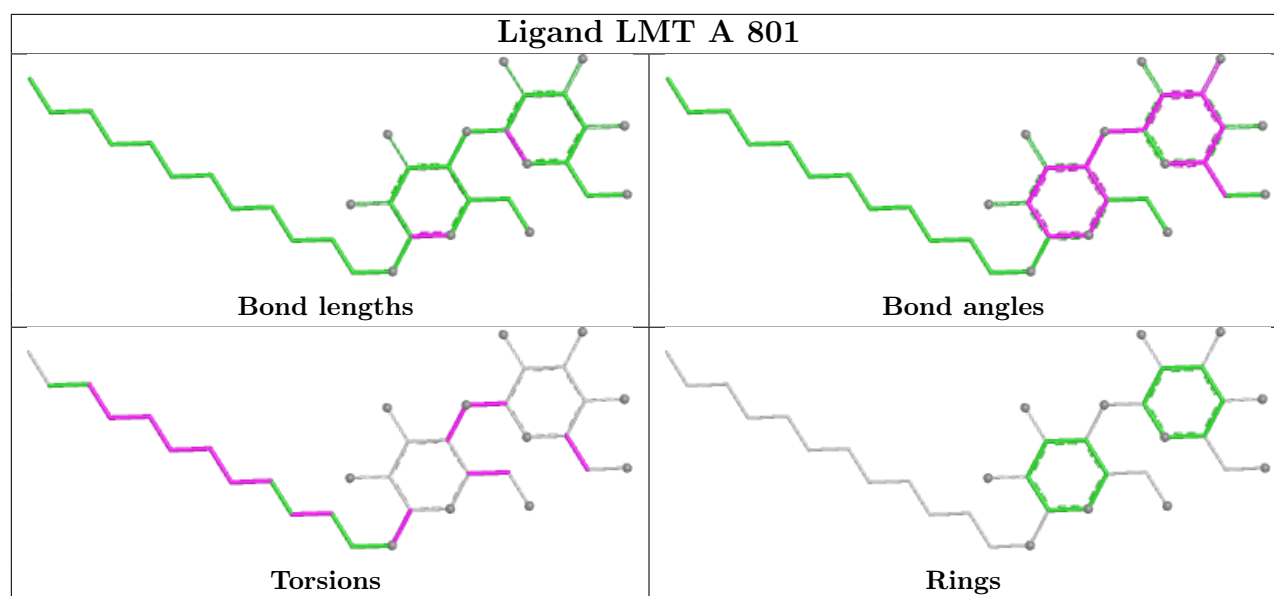
Mol	Chain	Res	Type	Atoms
6	A	806	PG4	C6-C5-O3-C4
7	A	804	1PE	C12-C22-OH3-C23
6	A	806	PG4	C1-C2-O2-C3
6	A	808	PG4	O3-C5-C6-O4
6	A	807	PG4	C3-C4-O3-C5
6	A	808	PG4	O2-C3-C4-O3
6	A	803	PG4	O2-C3-C4-O3
6	A	803	PG4	C4-C3-O2-C2
4	A	801	LMT	C2B-C1B-O1B-C4'
6	A	805	PG4	C1-C2-O2-C3
6	A	805	PG4	O2-C3-C4-O3
6	A	808	PG4	C6-C5-O3-C4
10	A	812	D10	C5-C6-C7-C8
7	A	811	1PE	C15-C25-OH5-C14
8	A	809	D12	C1-C2-C3-C4
6	A	807	PG4	O2-C3-C4-O3
7	A	804	1PE	OH4-C13-C23-OH3
7	A	804	1PE	OH6-C15-C25-OH5

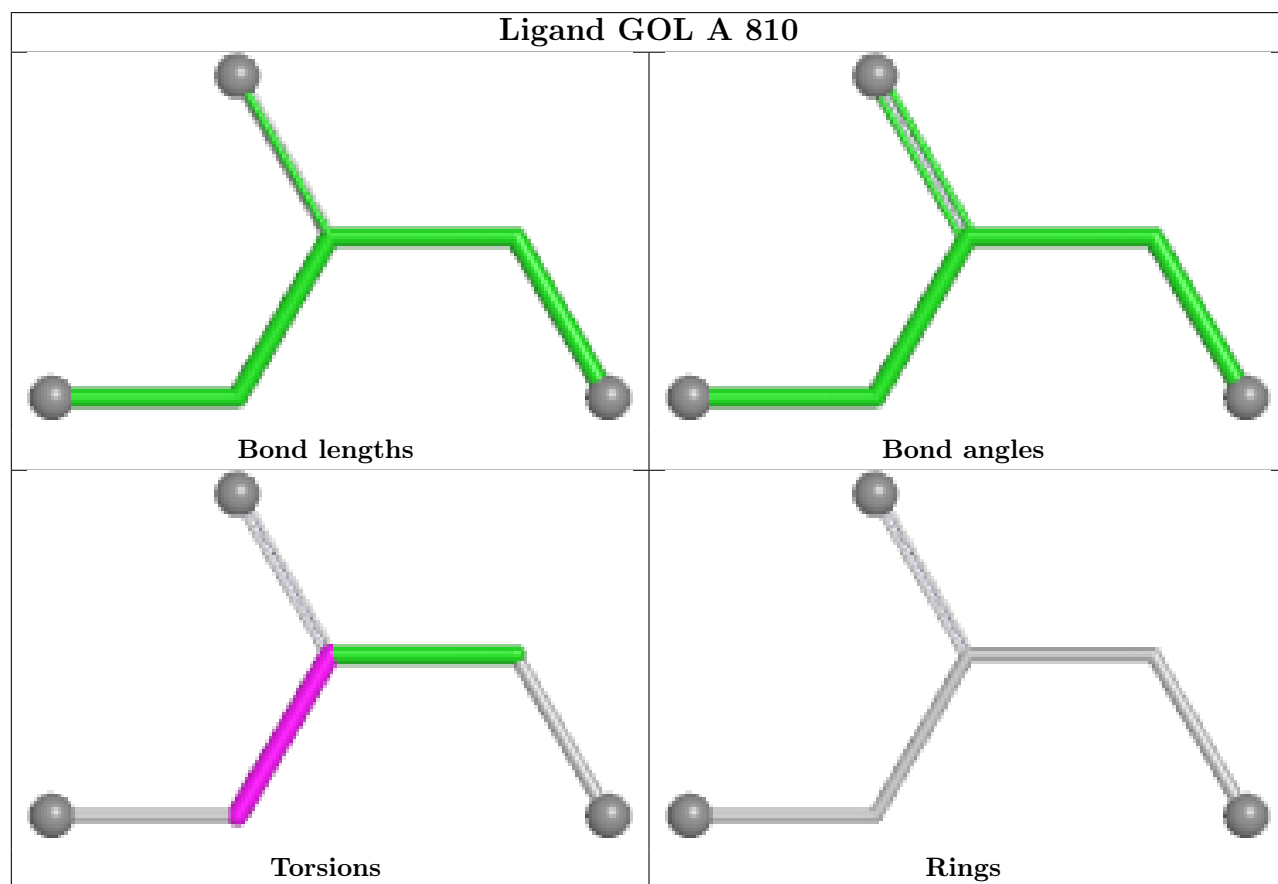
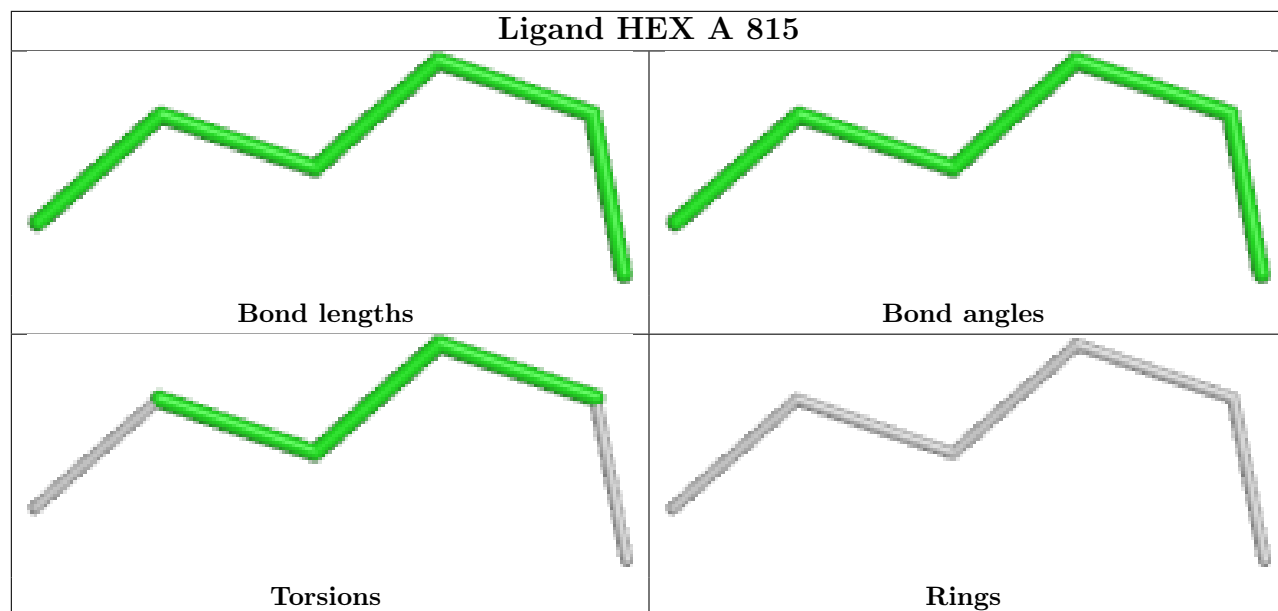
There are no ring outliers.

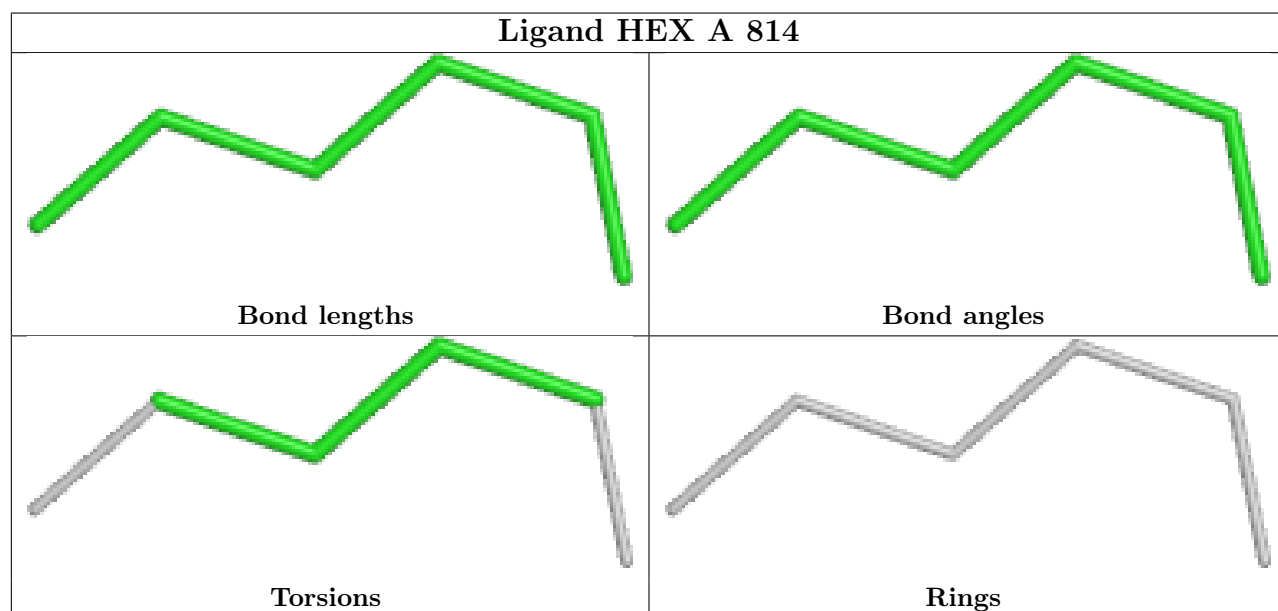
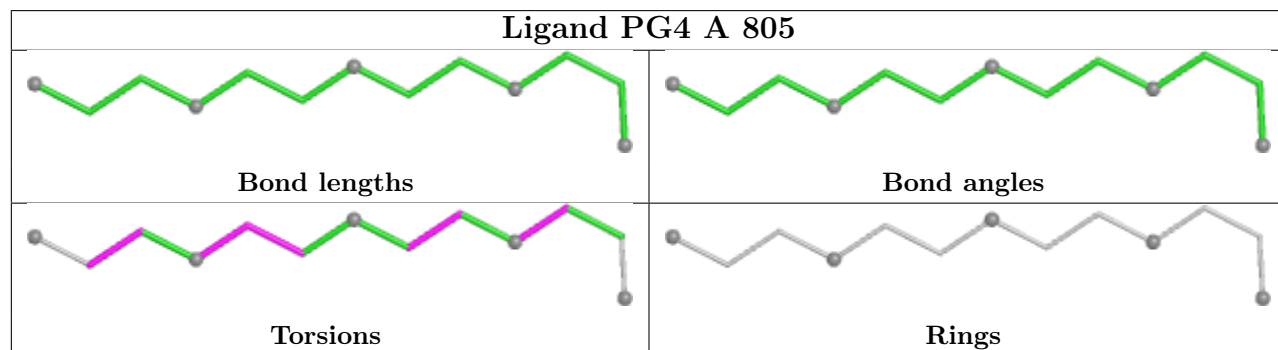
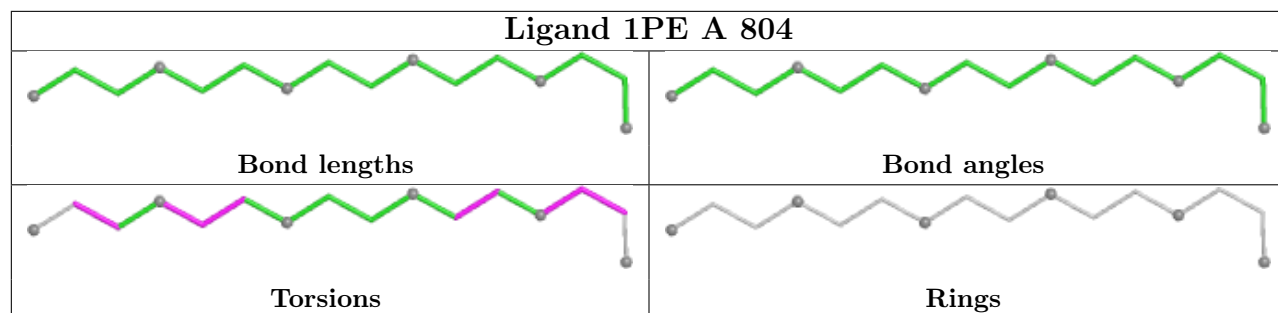
6 monomers are involved in 12 short contacts:

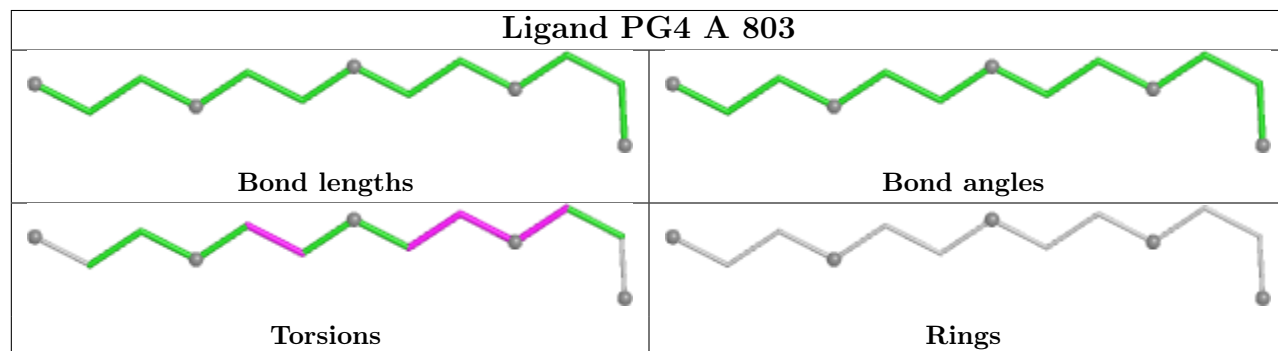
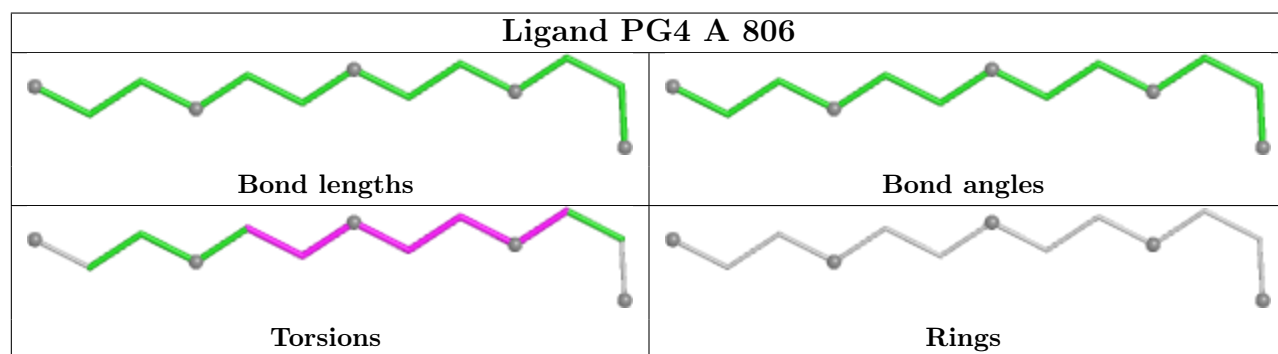
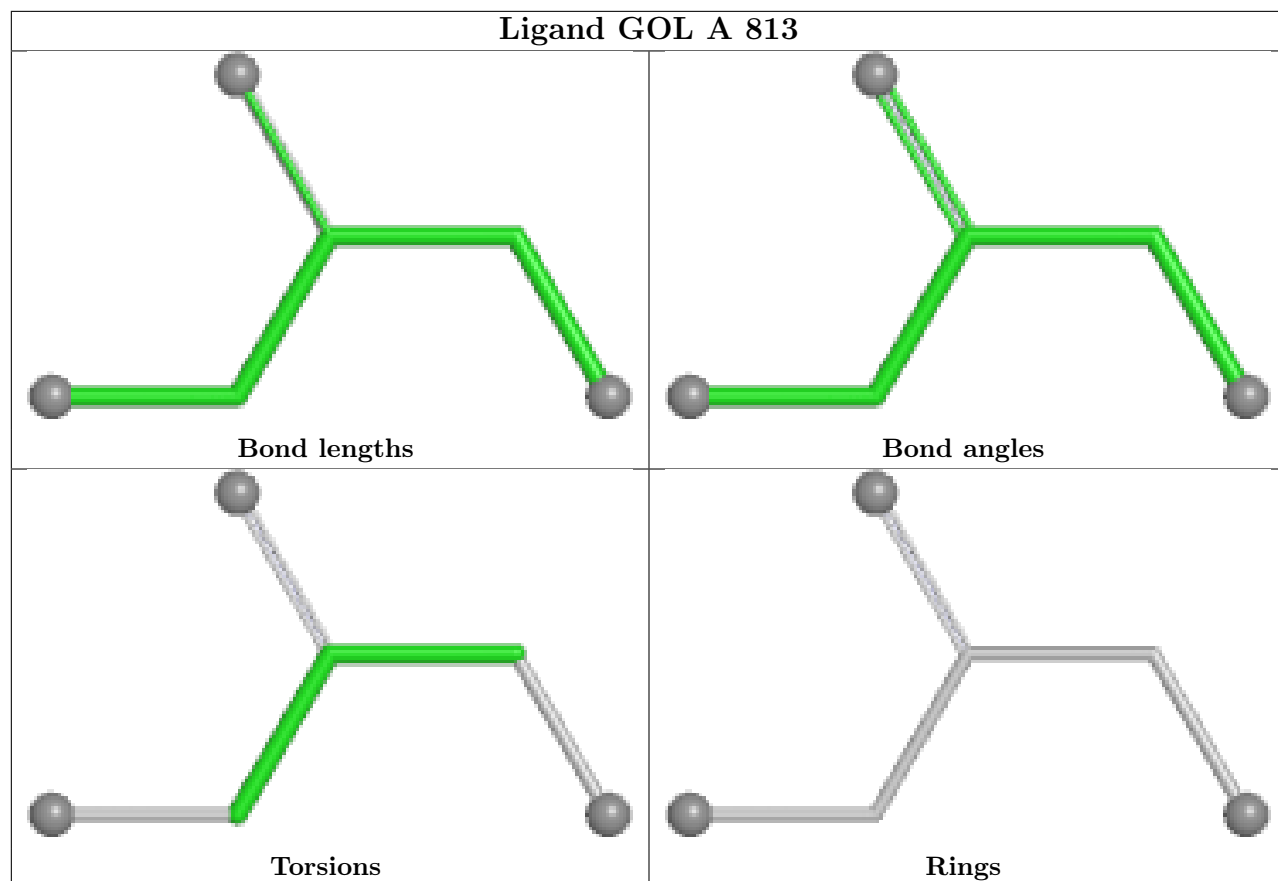
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	LMT	8	0
7	A	811	1PE	1	0
11	A	815	HEX	1	0
9	A	810	GOL	1	0
6	A	806	PG4	1	0
6	A	807	PG4	1	0

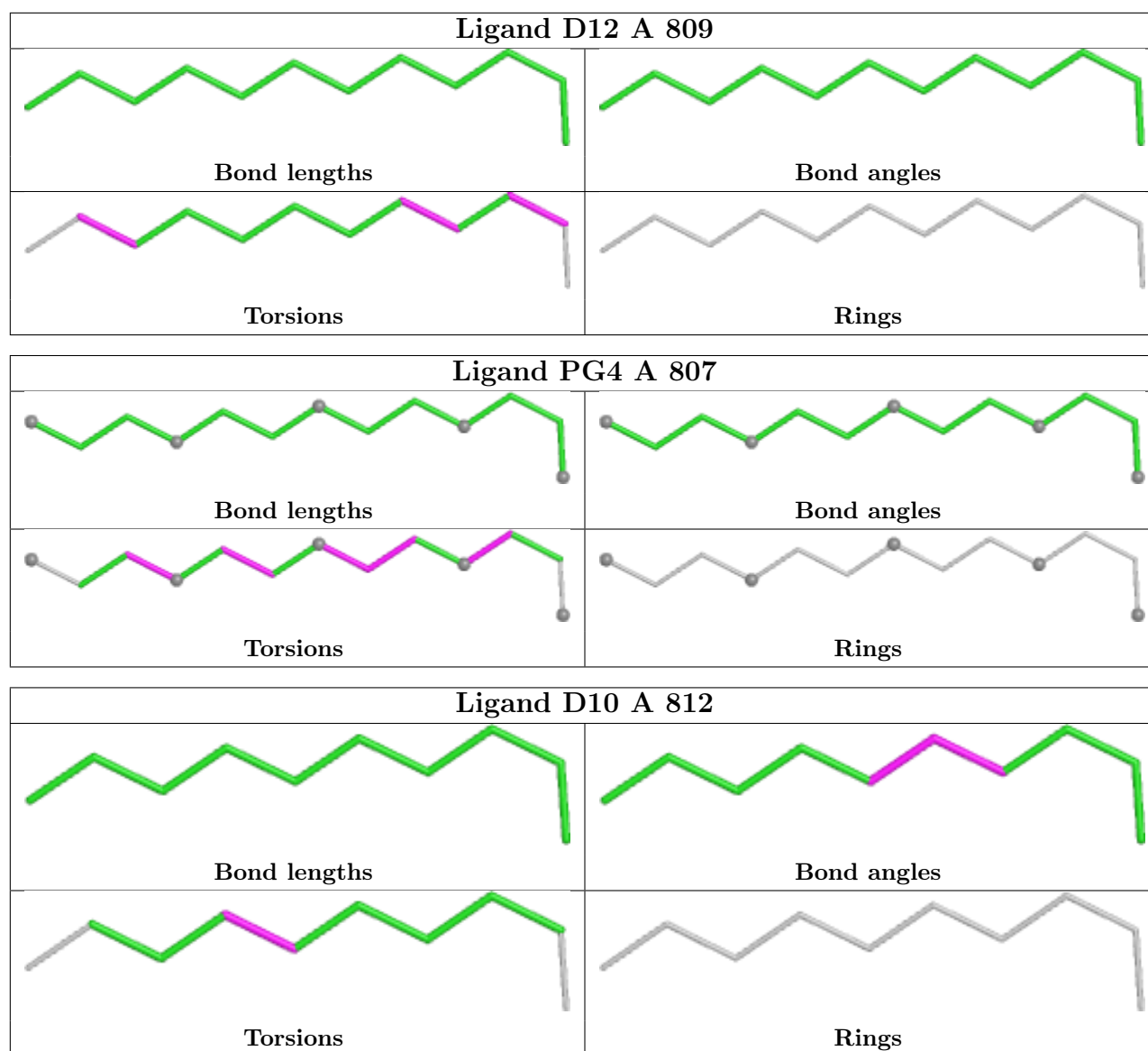
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	451/489 (92%)	1.41	105 (23%) 2 2	35, 60, 111, 140	1 (0%)
2	B	127/127 (100%)	1.48	34 (26%) 1 1	39, 62, 89, 98	2 (1%)
3	C	2/2 (100%)	1.28	0 100 100	58, 58, 58, 68	0
All	All	580/618 (93%)	1.42	139 (23%) 2 2	35, 61, 105, 140	3 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	PHE	11.0
1	A	305	LEU	9.9
1	A	199	ASP	9.7
1	A	308	SER	8.2
1	A	304	ILE	7.9
2	B	2	VAL	7.8
1	A	343	LEU	7.5
1	A	254	PHE	7.3
1	A	402	ALA	6.7
1	A	401	LEU	6.4
1	A	309	ILE	6.3
1	A	397	SER	6.1
1	A	192	ALA	6.0
1	A	251	ILE	5.9
2	B	14	ALA	5.9
1	A	332	ILE	5.5
2	B	128	HIS	5.3
1	A	303	GLU	4.9
1	A	413	MET	4.8
1	A	306	GLY	4.7
1	A	198	LYS	4.6
1	A	252	ILE	4.6
1	A	134	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	136	PRO	4.4
1	A	250	THR	4.4
1	A	406	ALA	4.4
1	A	133	CYS	4.4
1	A	137	LYS	4.3
1	A	417	LEU	4.3
1	A	408	VAL	4.2
1	A	253	PHE	4.2
1	A	344	SER	4.2
1	A	139	PRO	4.2
2	B	67	PHE	4.2
1	A	405	ALA	4.1
2	B	13	GLN	4.1
1	A	403	MET	4.0
1	A	399	LEU	4.0
1	A	200	ILE	4.0
1	A	404	ILE	3.9
1	A	135	PRO	3.9
1	A	331	GLY	3.9
1	A	380	TRP	3.9
2	B	42	GLY	3.8
1	A	301	HIS	3.7
1	A	443	ASN	3.7
2	B	117	THR	3.7
1	A	170	PHE	3.7
2	B	41	PRO	3.7
1	A	196	MET	3.7
1	A	433	TYR	3.6
1	A	169	ARG	3.6
1	A	330	ALA	3.4
1	A	398	ALA	3.4
1	A	256	GLN	3.4
1	A	255	ARG	3.4
1	A	189	VAL	3.3
1	A	384	LEU	3.3
1	A	105	PRO	3.3
1	A	249	VAL	3.3
2	B	68	THR	3.2
1	A	478	TRP	3.2
1	A	414	GLY	3.2
2	B	12	VAL	3.2
2	B	4	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	236	GLU	3.0
2	B	75	LYS	3.0
2	B	7	SER	3.0
1	A	50	GLU	3.0
1	A	162	LEU	3.0
1	A	415	PHE	3.0
1	A	240	LEU	3.0
1	A	45	LEU	2.9
1	A	407	LEU	2.9
2	B	55	SER	2.9
2	B	15	GLY	2.9
1	A	395	PHE	2.9
1	A	77	LEU	2.9
1	A	140	ARG	2.9
2	B	57	LEU	2.9
1	A	348	LYS	2.8
2	B	43	LYS	2.8
1	A	230	TRP	2.8
2	B	87	PRO	2.8
2	B	3	GLN	2.7
2	B	23	ALA	2.7
1	A	175	THR	2.7
1	A	372	ASP	2.7
1	A	268	MET	2.7
2	B	73	ASN	2.7
1	A	103	LEU	2.7
1	A	420	TRP	2.7
2	B	24	ALA	2.6
1	A	269	PHE	2.6
2	B	32	TYR	2.6
1	A	183	LEU	2.6
1	A	416	ILE	2.6
1	A	400	GLY	2.5
1	A	104	LYS	2.5
1	A	168	ASP	2.5
1	A	298	ASN	2.5
2	B	86	LYS	2.5
2	B	88	GLU	2.4
1	A	141	LEU	2.4
1	A	479	LEU	2.4
2	B	74	VAL	2.4
1	A	166	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	237	VAL	2.4
1	A	274	LEU	2.4
2	B	83	ASN	2.3
2	B	27	PRO	2.3
1	A	418	GLY	2.3
1	A	484	ALA	2.3
1	A	345	MET	2.3
1	A	207	ARG	2.3
2	B	56	GLY	2.3
1	A	191	ILE	2.3
1	A	382	ILE	2.3
1	A	248	VAL	2.3
2	B	16	GLY	2.3
1	A	138	ASP	2.2
1	A	247	ILE	2.2
1	A	419	MET	2.2
1	A	161	SER	2.2
2	B	66	ARG	2.1
1	A	193	CYS	2.1
1	A	108	ILE	2.1
1	A	266	ASN	2.1
1	A	165	VAL	2.1
2	B	126	HIS	2.1
1	A	272	PHE	2.1
2	B	19	ARG	2.1
2	B	25	SER	2.1
1	A	324	LEU	2.1
1	A	451	LEU	2.1
1	A	310	ASN	2.1
1	A	383	VAL	2.1
1	A	203	GLU	2.1
1	A	210	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

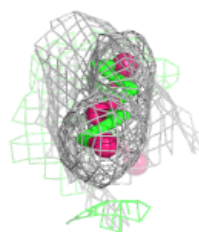
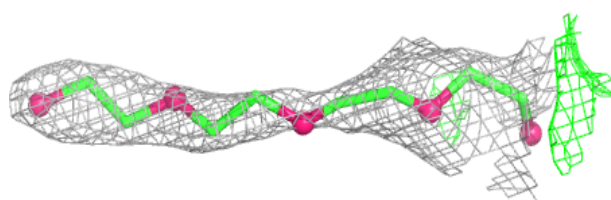
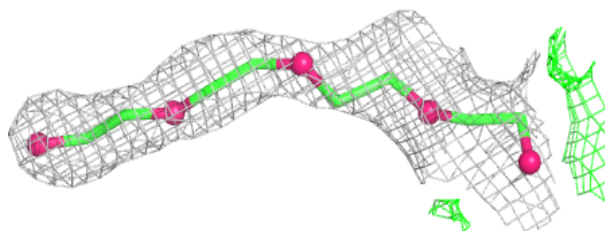
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PG4	A	806	13/13	0.54	0.32	74,84,110,112	0
10	D10	A	812	10/10	0.62	0.43	64,67,86,88	0
8	D12	A	809	12/12	0.68	0.36	67,76,81,82	0
7	1PE	A	811	16/16	0.71	0.27	83,86,91,93	0
6	PG4	A	805	13/13	0.74	0.27	74,86,98,101	0
6	PG4	A	808	13/13	0.76	0.27	74,79,92,97	0
9	GOL	A	810	6/6	0.77	0.20	97,102,103,106	0
5	OCT	A	802	8/8	0.78	0.30	61,68,73,73	0
11	HEX	A	815	6/6	0.79	0.32	73,80,81,85	0
9	GOL	A	813	6/6	0.80	0.18	81,83,85,87	0
11	HEX	A	814	6/6	0.81	0.31	83,83,87,89	0
4	LMT	A	801	35/35	0.81	0.19	57,84,100,101	0
6	PG4	A	807	13/13	0.83	0.19	67,77,85,89	0
7	1PE	A	804	16/16	0.86	0.17	58,75,96,100	0
6	PG4	A	803	13/13	0.87	0.18	66,74,91,97	0

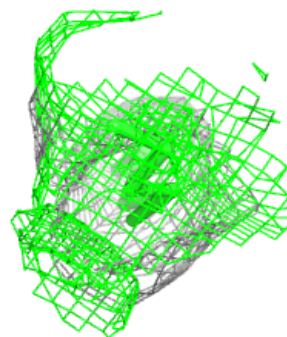
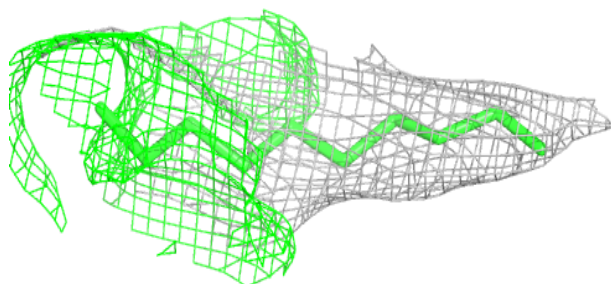
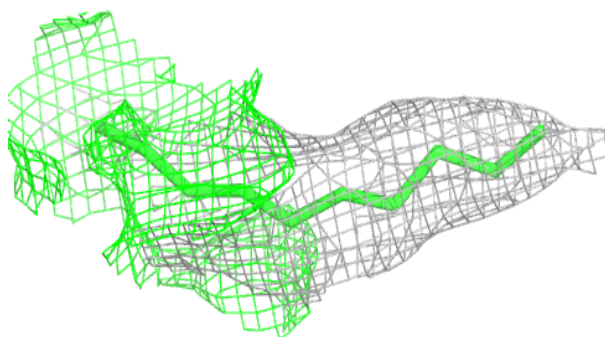
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PG4 A 806:

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

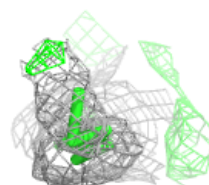
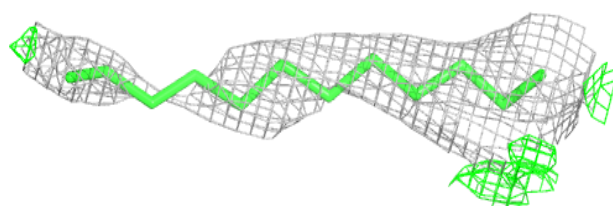
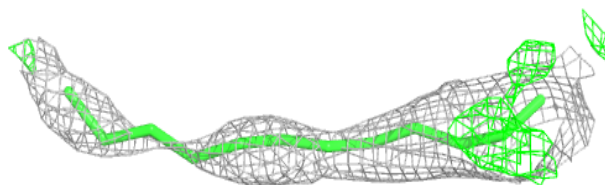
**Electron density around D10 A 812:**

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

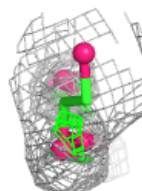
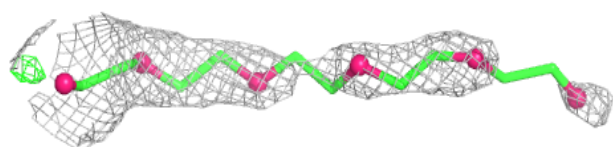
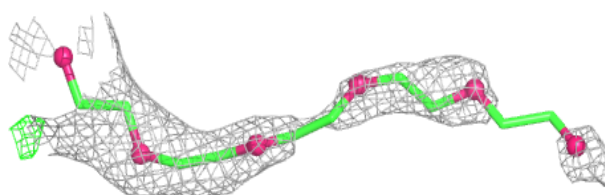


Electron density around D12 A 809:

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

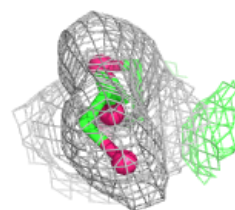
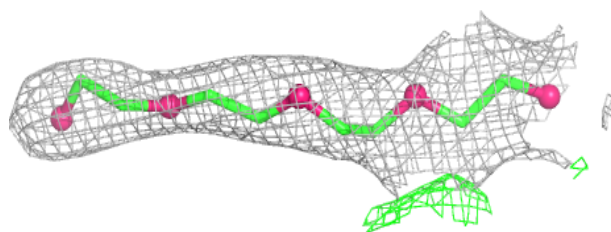
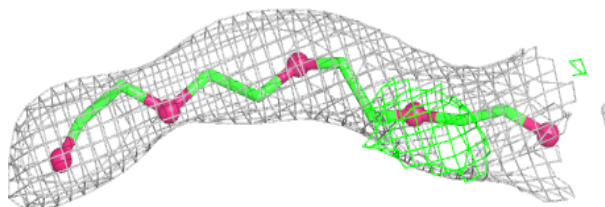
**Electron density around 1PE A 811:**

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

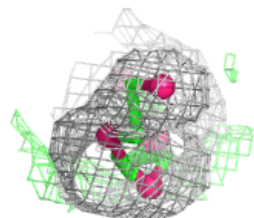
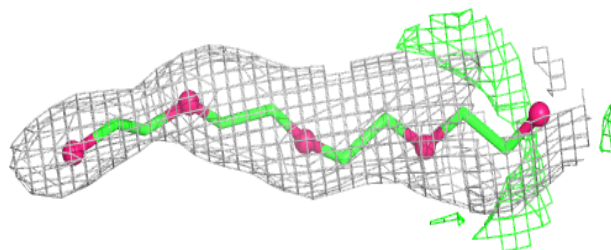
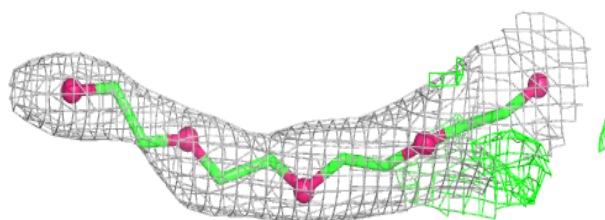


Electron density around PG4 A 805:

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

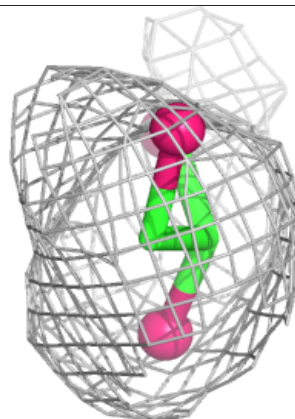
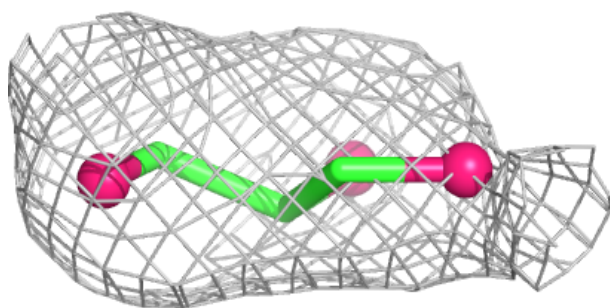
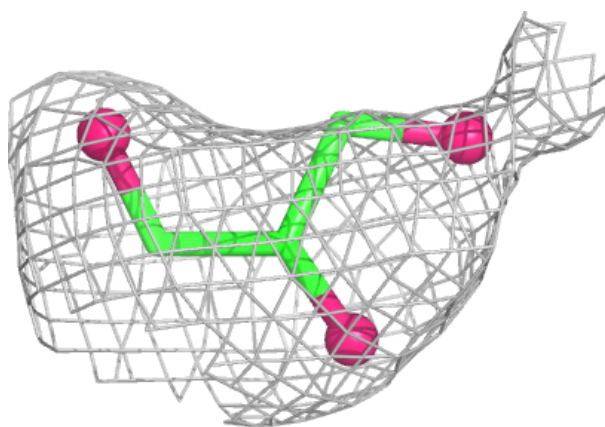
**Electron density around PG4 A 808:**

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

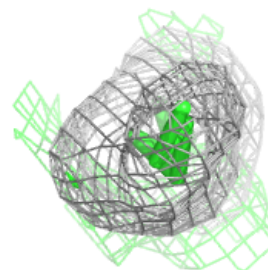
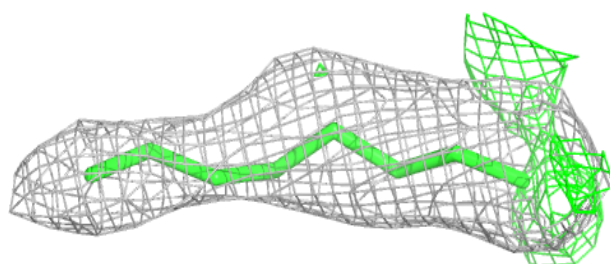
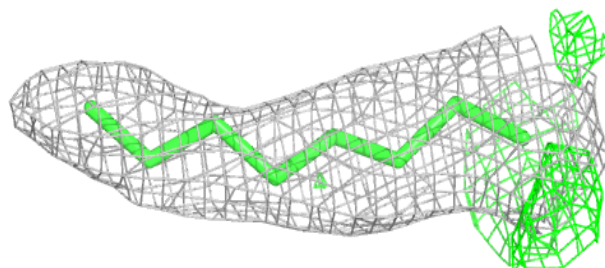


Electron density around GOL A 810:

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

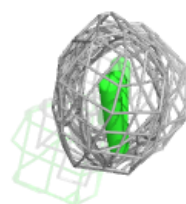
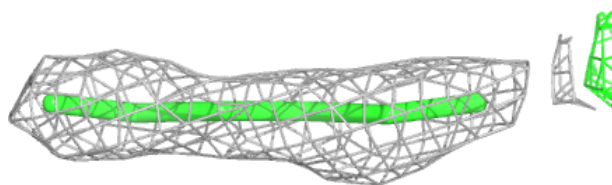
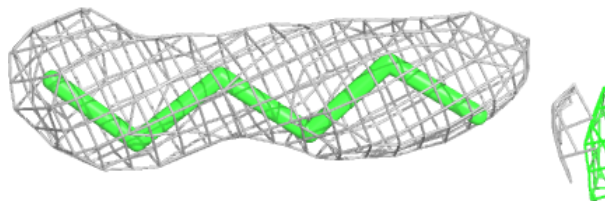
**Electron density around OCT A 802:**

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

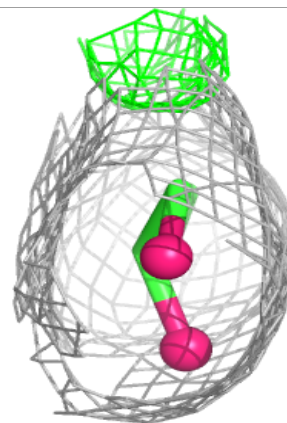
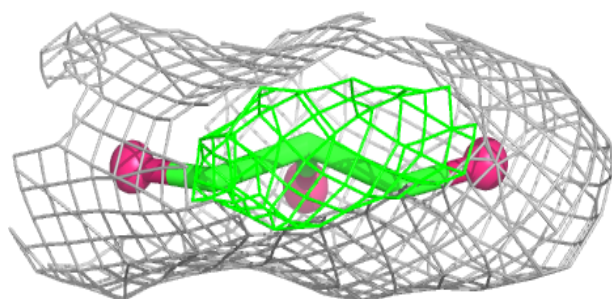
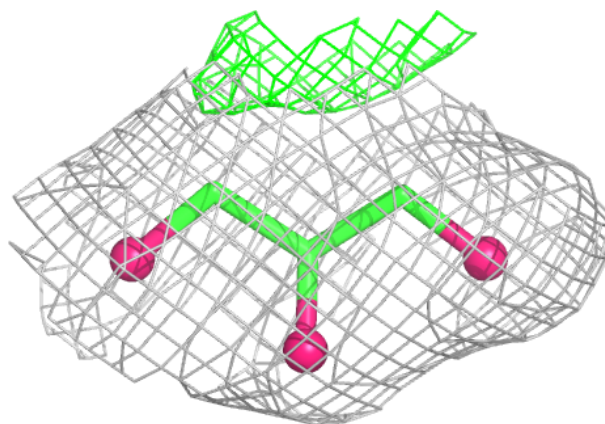


Electron density around HEX A 815:

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

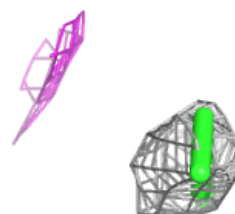
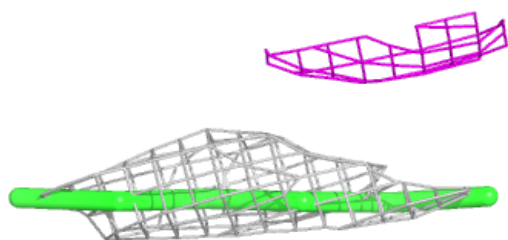
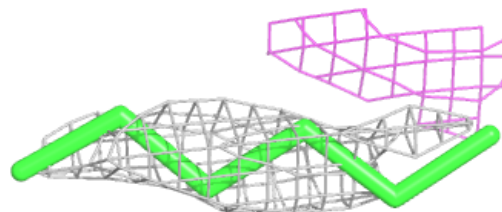
**Electron density around GOL A 813:**

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

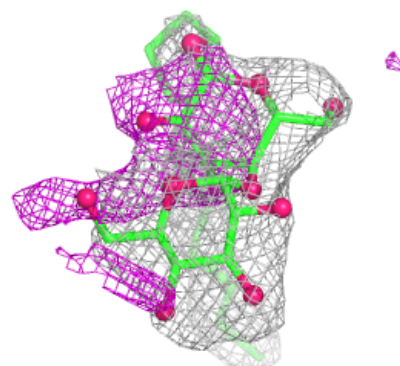
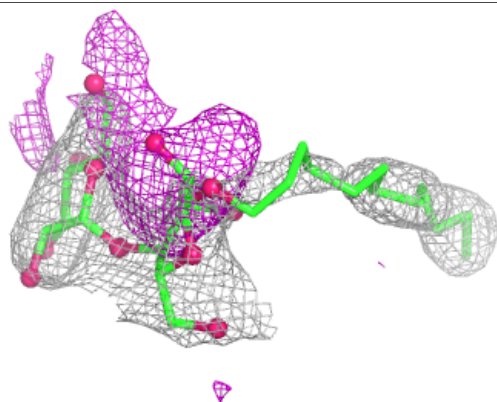
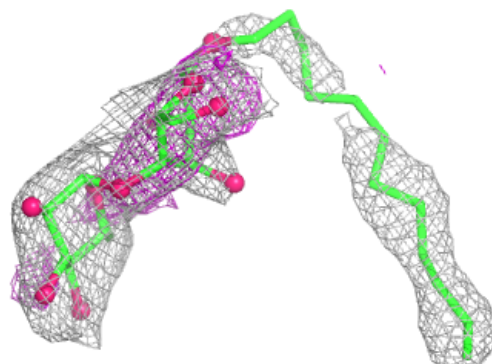


Electron density around HEX A 814:

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

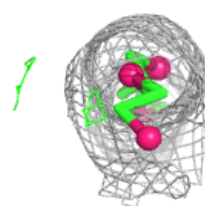
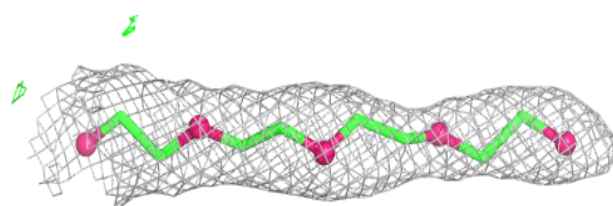
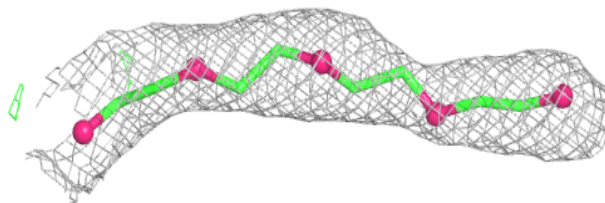
**Electron density around LMT A 801:**

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

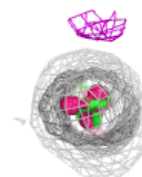
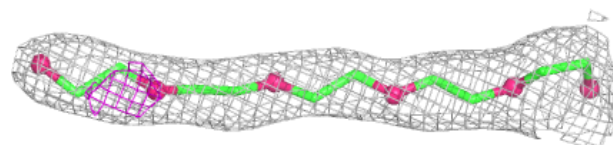
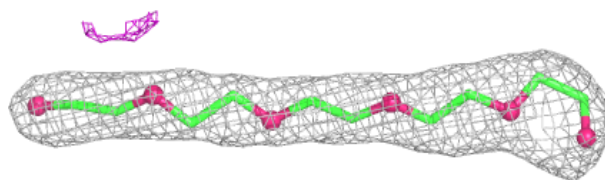


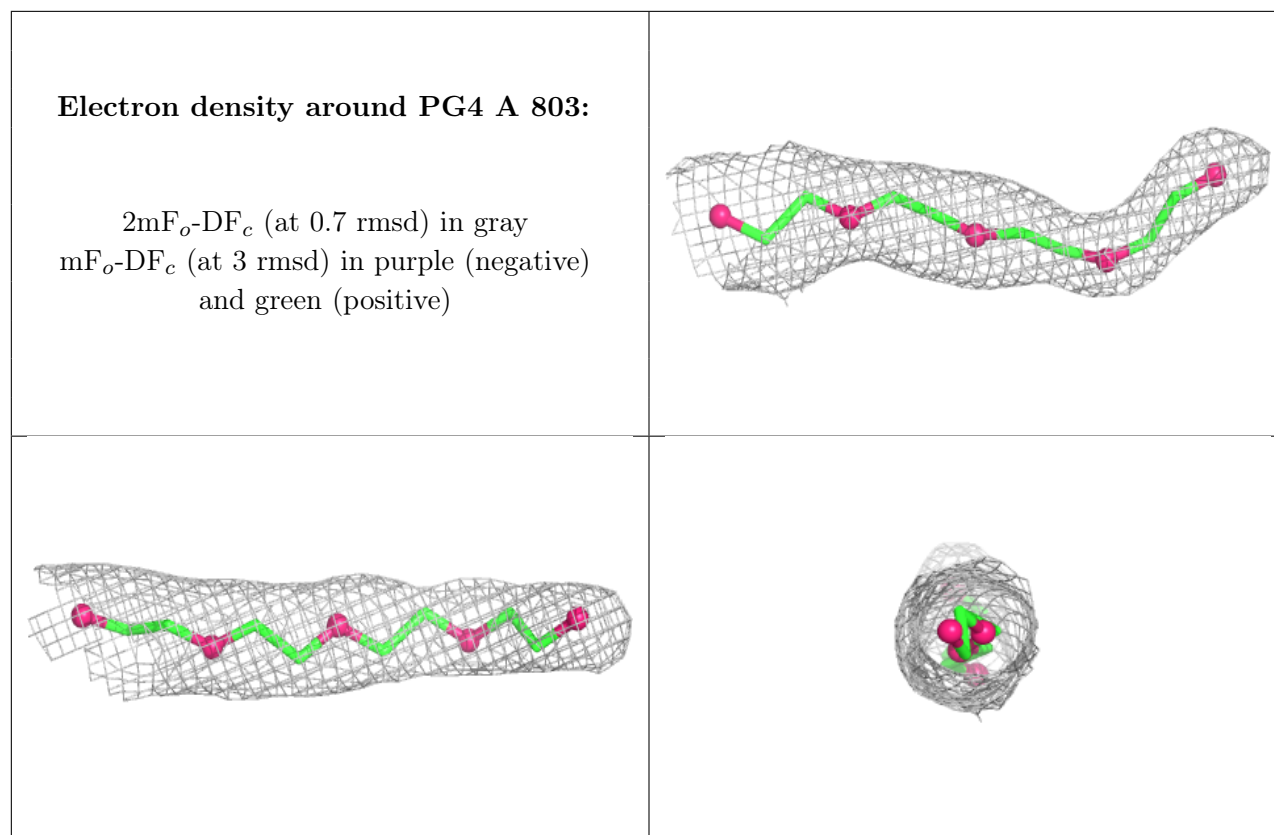
Electron density around PG4 A 807:

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

**Electron density around 1PE A 804:**

$2mF_o-DF_c$ (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.