



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:40 PM UTC

PDB ID : 8B1G / pdb_00008b1g
Title : DtpB-Nb132-AW
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Deposited on : 2022-09-09
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

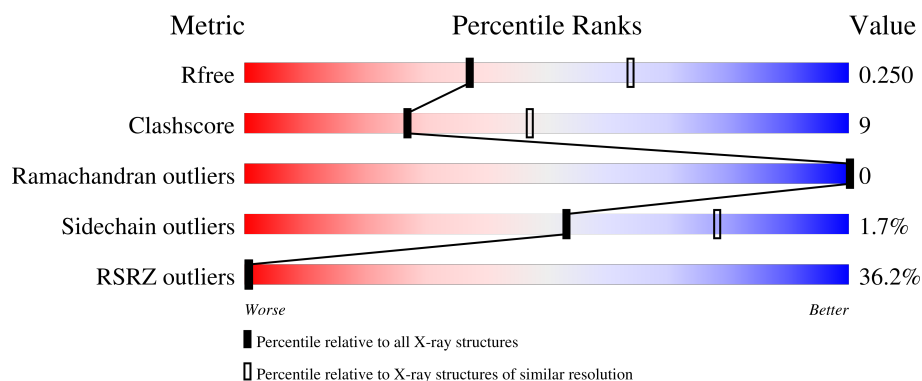
1 Overall quality at a glance

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	489	35% 75% 17% 8%
2	B	127	31% 80% 20%
3	C	2	50% 50%

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
8	D12	A	809	-	-	-	X

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 4786 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			

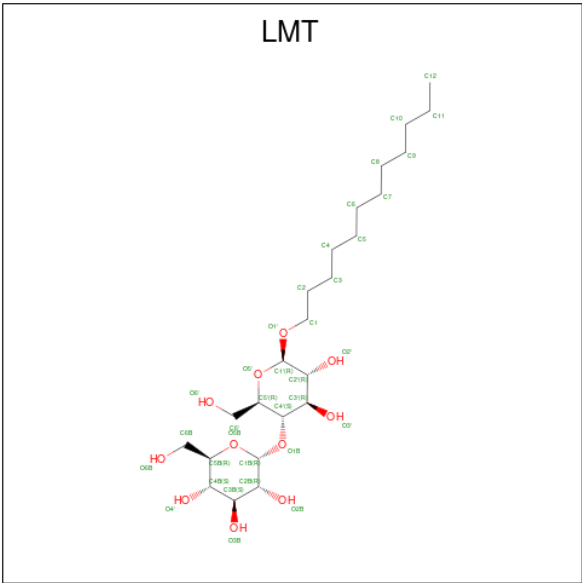
- Molecule 2 is a protein called Nanobody 132.

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-TRP.

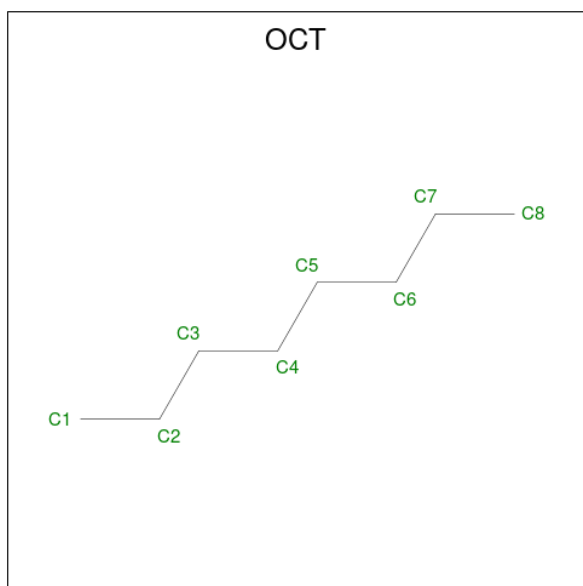
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			20	14	3	3			

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



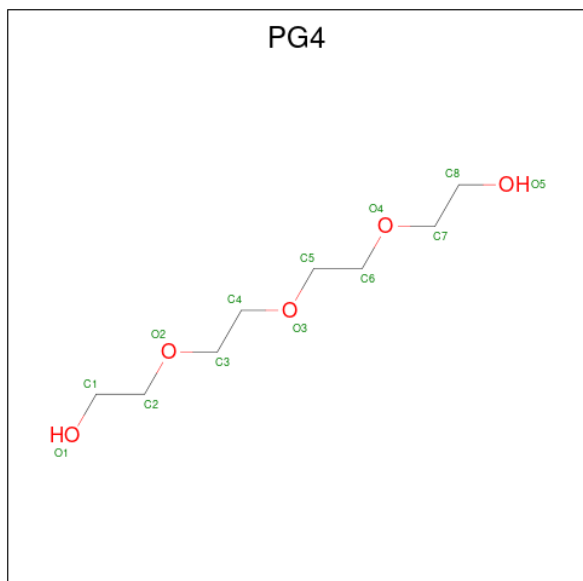
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

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



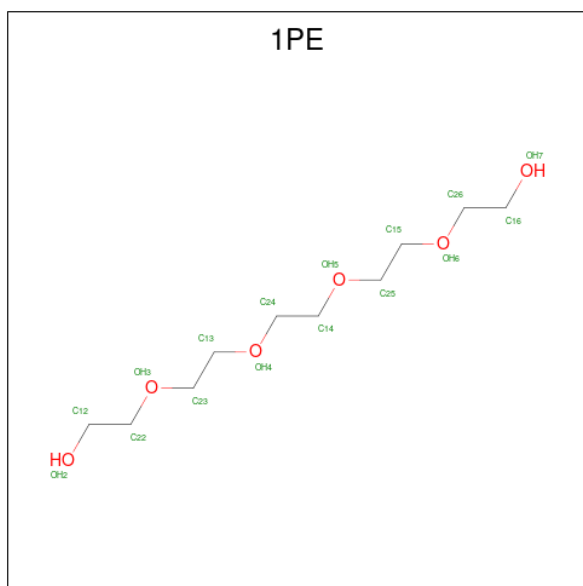
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			8	8		

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



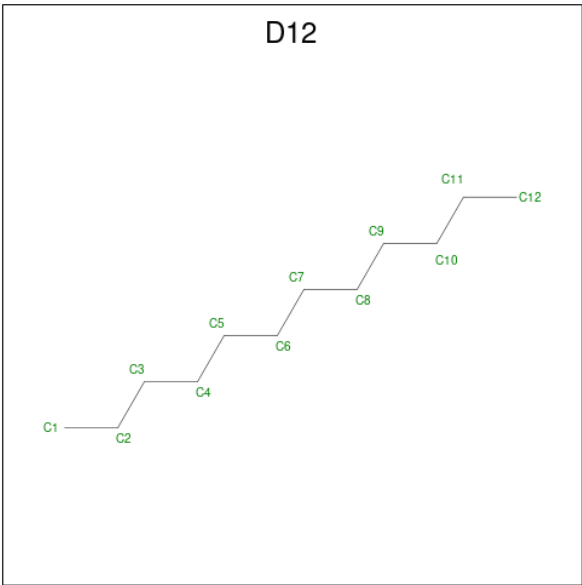
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

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



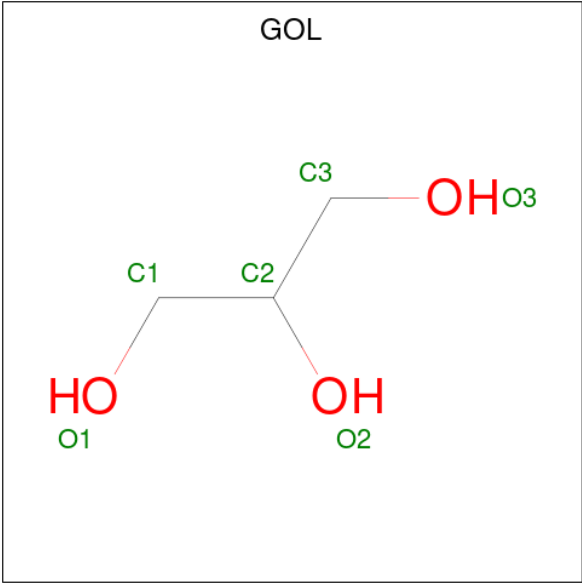
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

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



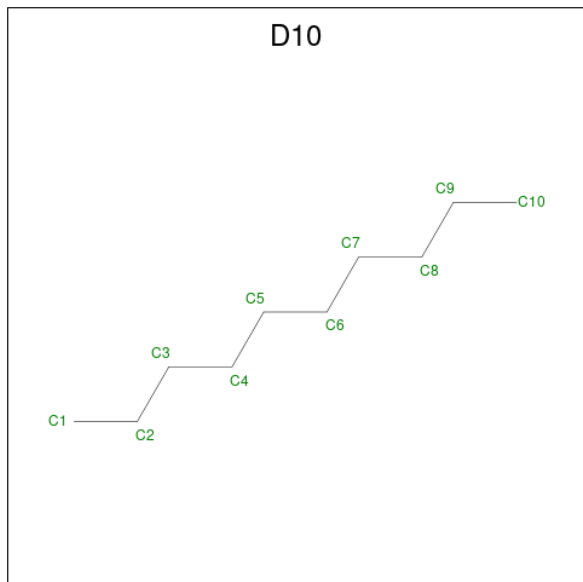
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			12	12		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



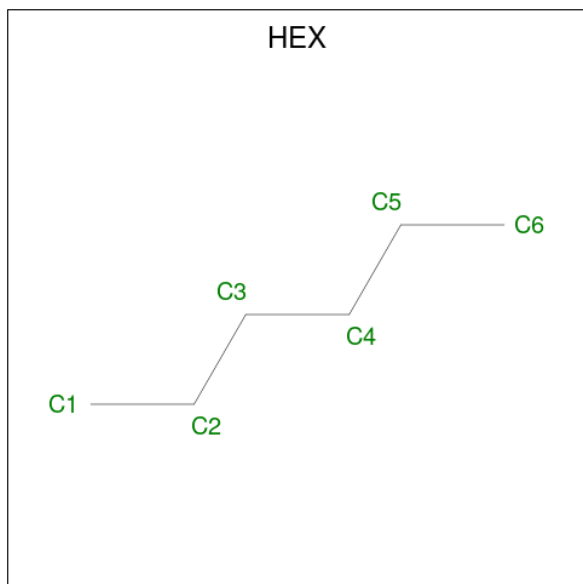
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- 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

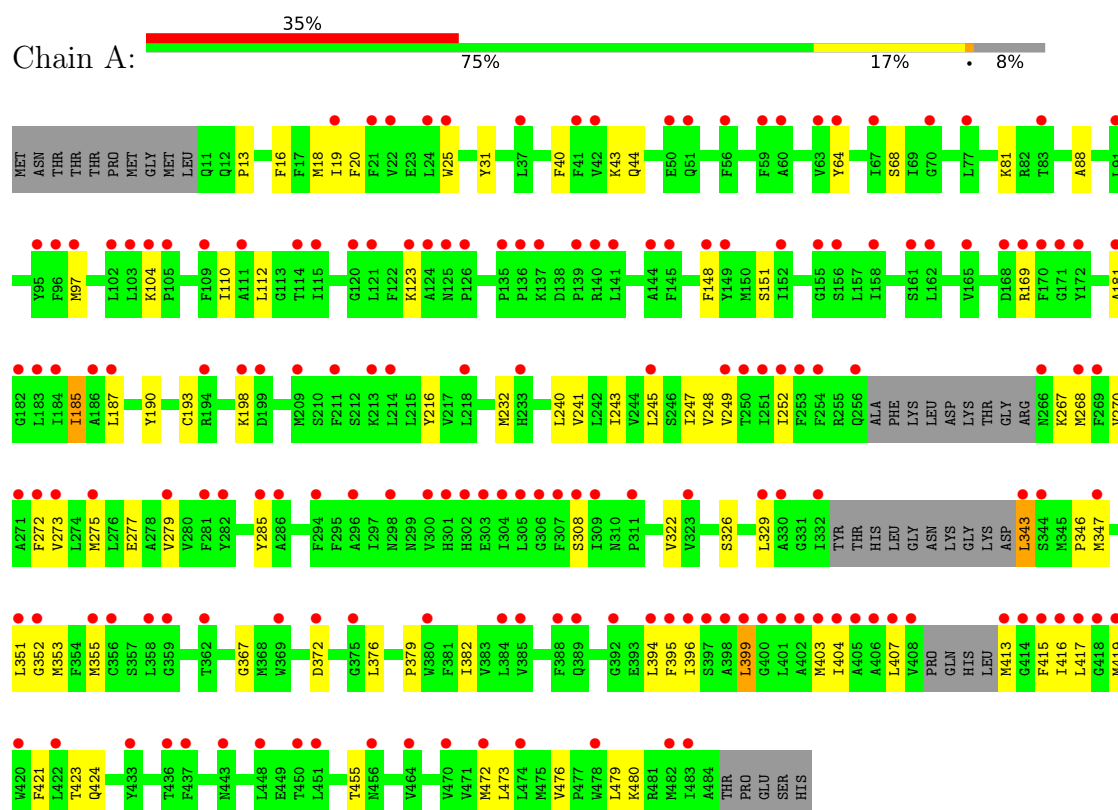
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	64	Total O 64 64	0	0
12	B	59	Total O 59 59	0	0
12	C	1	Total O 1 1	0	0

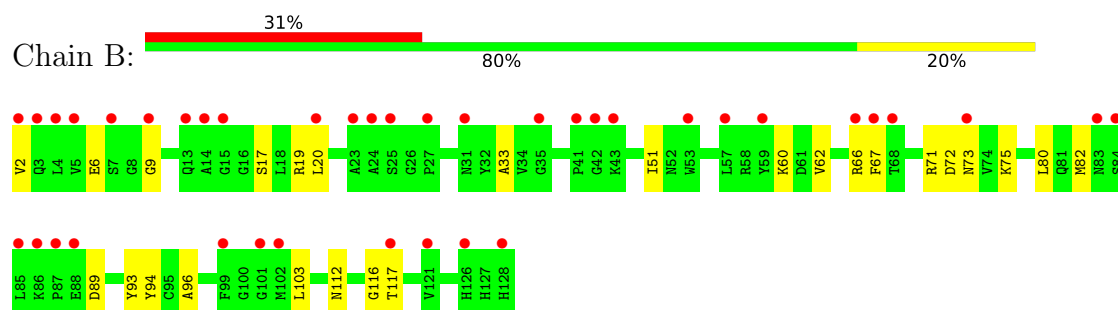
3 Residue-property plots [i](#)

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-TRP

Chain C:  50% 50% 50%



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	54.61Å 126.41Å 168.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.97 – 2.50 69.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (69.97-2.50) 91.0 (69.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.225 , 0.249 0.225 , 0.250	Depositor DCC
R_{free} test set	2018 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4786	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: OCT, D12, PG4, GOL, HEX, D10, LMT, 1PE

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	0.49	0/3572	0.73	1/4859 (0.0%)
2	B	0.49	0/1004	0.70	0/1361
3	C	0.51	0/21	0.61	0/27
All	All	0.49	0/4597	0.72	1/6247 (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	240	LEU	CB-CG-CD2	-5.02	95.64	110.70

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	67	0
2	B	976	0	939	18	0
3	C	20	0	17	2	0
4	A	35	0	45	3	0
5	A	8	0	18	0	0
6	A	65	0	90	1	0
7	A	32	0	44	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	26	0	0
9	A	12	0	16	0	0
10	A	10	0	22	2	0
11	A	12	0	28	1	0
12	A	64	0	0	0	0
12	B	59	0	0	1	0
12	C	1	0	0	0	0
All	All	4786	0	4850	87	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 9.

All (87) 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:346:PRO:HG3	1:A:479:LEU:HD22	1.52	0.89
1:A:25:TRP:CE2	1:A:185:ILE:HD11	2.20	0.77
1:A:64:TYR:CE2	1:A:424:GLN:HB2	2.26	0.70
2:B:19:ARG:NH1	12:B:201:HOH:O	2.18	0.69
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.74	0.68
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.26	0.65
1:A:346:PRO:HB3	1:A:479:LEU:HD13	1.79	0.64
1:A:472:MET:O	1:A:476:VAL:HG23	2.00	0.60
1:A:343:LEU:HA	1:A:347:MET:CB	2.33	0.59
1:A:248:VAL:O	1:A:252:ILE:HG23	2.03	0.58
1:A:241:VAL:O	1:A:245:LEU:HB2	2.02	0.58
1:A:249:VAL:HG12	1:A:419:MET:HG3	1.84	0.58
2:B:67:PHE:CZ	2:B:82:MET:HG2	2.38	0.58
1:A:64:TYR:HE2	1:A:424:GLN:HB2	1.69	0.58
1:A:343:LEU:N	1:A:480:LYS:HZ3	2.03	0.57
1:A:249:VAL:CG1	1:A:419:MET:HG3	2.35	0.56
1:A:181:ALA:O	1:A:185:ILE:HG23	2.06	0.56
1:A:413:MET:O	1:A:416:ILE:HG13	2.06	0.55
1:A:249:VAL:HA	1:A:252:ILE:HG12	1.88	0.54
1:A:268:MET:HE1	1:A:407:LEU:O	2.08	0.54
1:A:20:PHE:CE2	1:A:151:SER:HB2	2.42	0.54
1:A:81:LYS:HB3	1:A:190:TYR:OH	2.07	0.54
1:A:272:PHE:O	1:A:275:MET:HG2	2.08	0.54
2:B:20:LEU:HD12	2:B:80:LEU:HD23	1.90	0.54
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.90	0.53
1:A:343:LEU:HA	1:A:347:MET:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:CD1	1:A:232:MET:HE1	2.39	0.53
1:A:343:LEU:N	1:A:343:LEU:HD23	2.24	0.53
1:A:169:ARG:NH2	4:A:801:LMT:O2'	2.40	0.53
1:A:285:TYR:OH	3:C:1:ALA:HA	2.08	0.52
1:A:346:PRO:CG	1:A:479:LEU:HD22	2.35	0.52
1:A:18:MET:HE2	1:A:19:ILE:HG13	1.92	0.51
1:A:352:GLY:HA3	1:A:396:ILE:HG13	1.92	0.51
2:B:17:SER:HA	2:B:82:MET:O	2.10	0.51
1:A:267:LYS:C	1:A:268:MET:HE2	2.36	0.51
1:A:20:PHE:CD2	1:A:151:SER:HB2	2.46	0.51
1:A:273:VAL:O	1:A:277:GLU:HG3	2.11	0.50
1:A:279:VAL:HG23	1:A:424:GLN:HE22	1.76	0.50
1:A:347:MET:HE2	1:A:476:VAL:HG21	1.94	0.50
1:A:353:MET:HE3	1:A:472:MET:HE1	1.95	0.49
1:A:88:ALA:HB3	1:A:187:LEU:HD23	1.94	0.49
1:A:347:MET:HE2	1:A:347:MET:HA	1.94	0.48
2:B:2:VAL:HA	2:B:112:ASN:ND2	2.28	0.48
1:A:97:MET:CE	1:A:110:ILE:HG22	2.43	0.48
1:A:343:LEU:HD22	1:A:347:MET:HG2	1.94	0.48
1:A:322:VAL:HG13	1:A:394:LEU:HD21	1.96	0.47
2:B:9:GLY:H	2:B:117:THR:HG21	1.78	0.47
1:A:473:LEU:HA	1:A:476:VAL:HG23	1.97	0.47
2:B:72:ASP:OD2	2:B:75:LYS:HB2	2.15	0.47
1:A:31:TYR:CZ	3:C:1:ALA:HB1	2.50	0.46
1:A:247:ILE:HD12	1:A:248:VAL:N	2.30	0.46
1:A:308:SER:O	4:A:801:LMT:H4'	2.16	0.45
1:A:372:ASP:HB2	1:A:376:LEU:H	1.81	0.45
2:B:82:MET:HE3	2:B:82:MET:HB2	1.64	0.45
1:A:112:LEU:HD13	1:A:232:MET:HE1	1.99	0.45
2:B:51:ILE:HD13	2:B:71:ARG:HB2	1.99	0.45
2:B:6:GLU:OE2	2:B:94:TYR:HA	2.17	0.44
1:A:104:LYS:HB3	10:A:812:D10:H42	1.99	0.44
2:B:93:TYR:O	2:B:116:GLY:HA2	2.17	0.44
1:A:198:LYS:HD3	1:A:198:LYS:HA	1.79	0.44
1:A:395:PHE:O	1:A:399:LEU:HB2	2.17	0.44
4:A:801:LMT:H41	4:A:801:LMT:H12	1.64	0.44
1:A:423:THR:OG1	1:A:424:GLN:OE1	2.21	0.44
1:A:216:TYR:HB3	6:A:807:PG4:H42	1.99	0.44
1:A:18:MET:HG3	1:A:193:CYS:CB	2.47	0.44
1:A:347:MET:HE3	1:A:476:VAL:HG11	1.99	0.44
1:A:379:PRO:O	1:A:382:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:CG2	1:A:424:GLN:HE22	2.32	0.43
1:A:43:LYS:HD2	1:A:43:LYS:HA	1.86	0.42
1:A:252:ILE:HD11	1:A:415:PHE:HE1	1.84	0.42
1:A:270:VAL:HG13	1:A:479:LEU:HD21	2.01	0.42
2:B:71:ARG:HD3	2:B:73:ASN:OD1	2.20	0.42
1:A:25:TRP:CD2	1:A:185:ILE:HD11	2.53	0.42
1:A:404:ILE:HD13	1:A:404:ILE:HA	1.88	0.42
1:A:40:PHE:CE1	1:A:44:GLN:HG2	2.55	0.42
2:B:67:PHE:CE1	2:B:82:MET:HG2	2.55	0.42
1:A:243:ILE:HG13	7:A:811:1PE:H151	2.02	0.41
1:A:351:LEU:O	1:A:355:MET:HG2	2.19	0.41
1:A:68:SER:HB3	1:A:421:PHE:CD2	2.55	0.41
2:B:96:ALA:HA	2:B:112:ASN:O	2.21	0.41
1:A:104:LYS:HB3	10:A:812:D10:C4	2.51	0.41
7:A:811:1PE:H261	11:A:814:HEX:H32	2.03	0.41
2:B:33:ALA:HB1	2:B:103:LEU:CD2	2.51	0.41
1:A:367:GLY:HA3	1:A:455:THR:CG2	2.51	0.41
2:B:67:PHE:CE2	2:B:82:MET:HG2	2.56	0.41
1:A:148:PHE:O	1:A:151:SER:HB3	2.21	0.40
1:A:13:PRO:O	1:A:16:PHE:HB3	2.22	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	443/489 (91%)	436 (98%)	7 (2%)	0	100	100
2	B	126/127 (99%)	122 (97%)	4 (3%)	0	100	100
All	All	569/616 (92%)	558 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/401 (92%)	360 (98%)	8 (2%)	45	73
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%)	463 (98%)	8 (2%)	53	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	LYS
1	A	185	ILE
1	A	326	SER
1	A	329	LEU
1	A	343	LEU
1	A	399	LEU
1	A	403	MET
1	A	417	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	GLN
2	B	106	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](#)

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	$\# Z > 2$
8	D12	A	809	-	11,11,11	0.50	0	10,10,10	0.66	0
9	GOL	A	810	-	5,5,5	1.12	0	5,5,5	0.93	0
11	HEX	A	814	-	5,5,5	0.39	0	4,4,4	0.69	0
6	PG4	A	808	-	12,12,12	0.27	0	11,11,11	0.49	0
7	1PE	A	804	-	15,15,15	0.22	0	14,14,14	0.26	0
4	LMT	A	801	-	36,36,36	1.14	2 (5%)	47,47,47	1.66	9 (19%)
6	PG4	A	807	-	12,12,12	0.27	0	11,11,11	0.44	0
5	OCT	A	802	-	7,7,7	0.40	0	6,6,6	0.67	0
10	D10	A	812	-	9,9,9	0.41	0	8,8,8	1.00	1 (12%)
6	PG4	A	806	-	12,12,12	0.28	0	11,11,11	0.47	0
11	HEX	A	815	-	5,5,5	0.42	0	4,4,4	0.48	0
7	1PE	A	811	-	15,15,15	0.13	0	14,14,14	0.22	0
6	PG4	A	803	-	12,12,12	0.18	0	11,11,11	0.59	0
9	GOL	A	813	-	5,5,5	1.33	1 (20%)	5,5,5	0.91	0
6	PG4	A	805	-	12,12,12	0.16	0	11,11,11	0.64	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
8	D12	A	809	-	-	3/9/9/9	-
9	GOL	A	810	-	-	1/4/4/4	-
11	HEX	A	814	-	-	0/3/3/3	-
6	PG4	A	808	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	A	804	-	-	6/13/13/13	-
4	LMT	A	801	-	-	16/21/61/61	0/2/2/2
6	PG4	A	807	-	-	5/10/10/10	-
5	OCT	A	802	-	-	2/5/5/5	-
10	D10	A	812	-	-	1/7/7/7	-
6	PG4	A	806	-	-	6/10/10/10	-
11	HEX	A	815	-	-	0/3/3/3	-
7	1PE	A	811	-	-	6/13/13/13	-
6	PG4	A	803	-	-	4/10/10/10	-
9	GOL	A	813	-	-	0/4/4/4	-
6	PG4	A	805	-	-	4/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O2B-C2B	-3.35	1.34	1.43
4	A	801	LMT	O3B-C3B	-2.20	1.37	1.43
9	A	813	GOL	C3-C2	2.02	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	C1B-O1B-C4'	4.21	127.97	117.98
4	A	801	LMT	O5B-C5B-C4B	4.09	117.06	109.70
4	A	801	LMT	C1'-O5'-C5'	-3.19	107.50	113.72
4	A	801	LMT	O1B-C4'-C3'	2.97	114.79	107.23
4	A	801	LMT	O1'-C1'-C2'	2.57	112.17	108.27
10	A	812	D10	C6-C5-C4	-2.32	102.62	114.37
4	A	801	LMT	C1'-C2'-C3'	2.23	114.71	110.01
4	A	801	LMT	C3B-C4B-C5B	-2.23	106.19	110.23
4	A	801	LMT	C1B-O5B-C5B	2.13	117.87	113.72
4	A	801	LMT	C2'-C3'-C4'	2.06	114.36	109.68

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	LMT	O5'-C1'-O1'-C1
4	A	801	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
6	A	803	PG4	O3-C5-C6-O4
6	A	806	PG4	O2-C3-C4-O3
4	A	801	LMT	C3'-C4'-O1B-C1B
4	A	801	LMT	C4'-C5'-C6'-O6'
4	A	801	LMT	C2'-C1'-O1'-C1
6	A	807	PG4	O3-C5-C6-O4
7	A	811	1PE	OH5-C14-C24-OH4
6	A	806	PG4	O3-C5-C6-O4
7	A	811	1PE	OH4-C13-C23-OH3
4	A	801	LMT	C3-C4-C5-C6
4	A	801	LMT	C1-C2-C3-C4
4	A	801	LMT	C5-C6-C7-C8
7	A	811	1PE	OH6-C15-C25-OH5
4	A	801	LMT	C7-C8-C9-C10
6	A	805	PG4	O3-C5-C6-O4
5	A	802	OCT	C4-C5-C6-C7
4	A	801	LMT	C6-C7-C8-C9
4	A	801	LMT	C5'-C4'-O1B-C1B
7	A	804	1PE	OH7-C16-C26-OH6
9	A	810	GOL	O2-C2-C3-O3
8	A	809	D12	C9-C10-C11-C12
5	A	802	OCT	C3-C4-C5-C6
6	A	805	PG4	O4-C7-C8-O5
4	A	801	LMT	C11-C10-C9-C8
6	A	807	PG4	C8-C7-O4-C6
6	A	806	PG4	C5-C6-O4-C7
6	A	808	PG4	C3-C4-O3-C5
6	A	803	PG4	C1-C2-O2-C3
6	A	806	PG4	C1-C2-O2-C3
6	A	805	PG4	C5-C6-O4-C7
8	A	809	D12	C3-C4-C5-C6
6	A	807	PG4	C3-C4-O3-C5
7	A	811	1PE	C12-C22-OH3-C23
4	A	801	LMT	C4-C5-C6-C7
7	A	804	1PE	C25-C15-OH6-C26
6	A	808	PG4	O2-C3-C4-O3
6	A	806	PG4	C4-C3-O2-C2
7	A	804	1PE	OH2-C12-C22-OH3
7	A	804	1PE	C23-C13-OH4-C24
6	A	806	PG4	C6-C5-O3-C4
6	A	803	PG4	O2-C3-C4-O3
6	A	808	PG4	O3-C5-C6-O4

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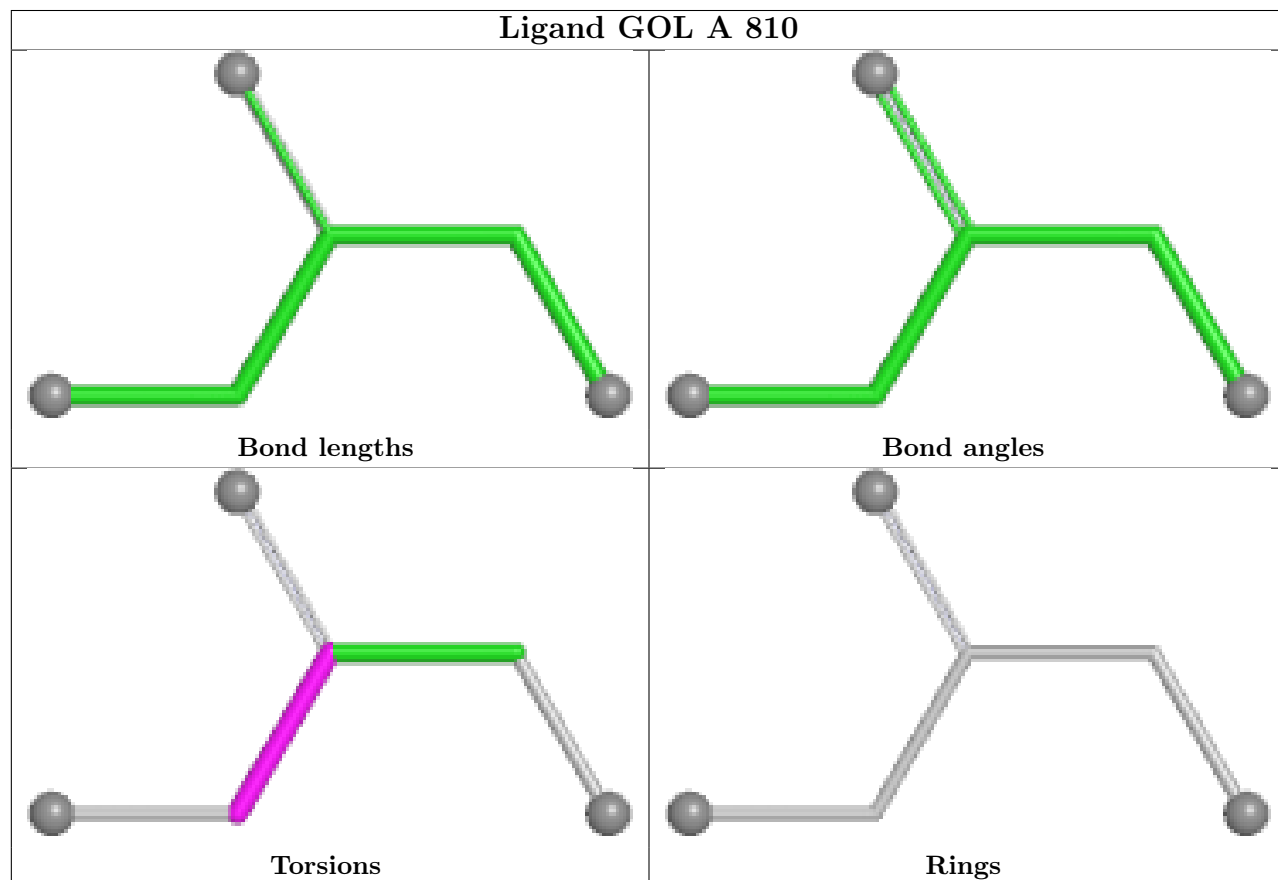
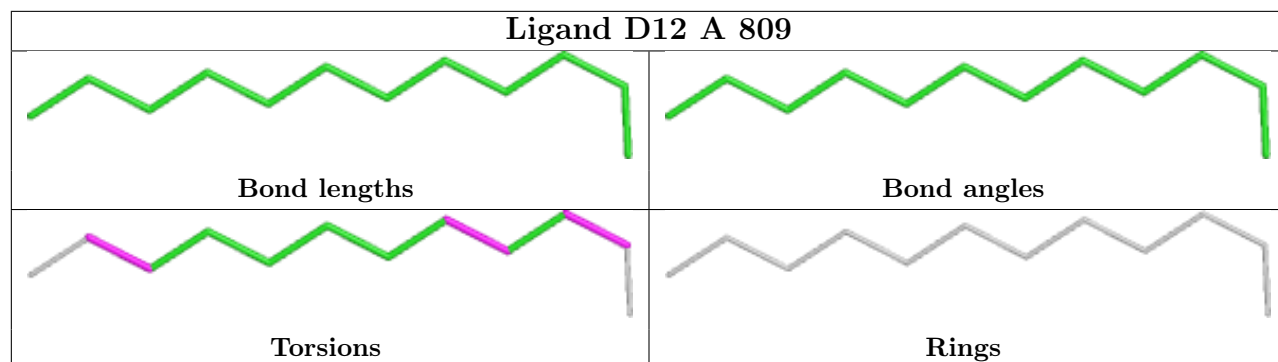
Mol	Chain	Res	Type	Atoms
6	A	803	PG4	C4-C3-O2-C2
6	A	807	PG4	C1-C2-O2-C3
6	A	808	PG4	C6-C5-O3-C4
6	A	805	PG4	O2-C3-C4-O3
7	A	811	1PE	C25-C15-OH6-C26
10	A	812	D10	C5-C6-C7-C8
4	A	801	LMT	O5B-C5B-C6B-O6B
7	A	804	1PE	OH4-C13-C23-OH3
8	A	809	D12	C1-C2-C3-C4
7	A	811	1PE	C15-C25-OH5-C14
6	A	807	PG4	O2-C3-C4-O3
4	A	801	LMT	C2B-C1B-O1B-C4'
7	A	804	1PE	OH6-C15-C25-OH5
4	A	801	LMT	O5B-C1B-O1B-C4'

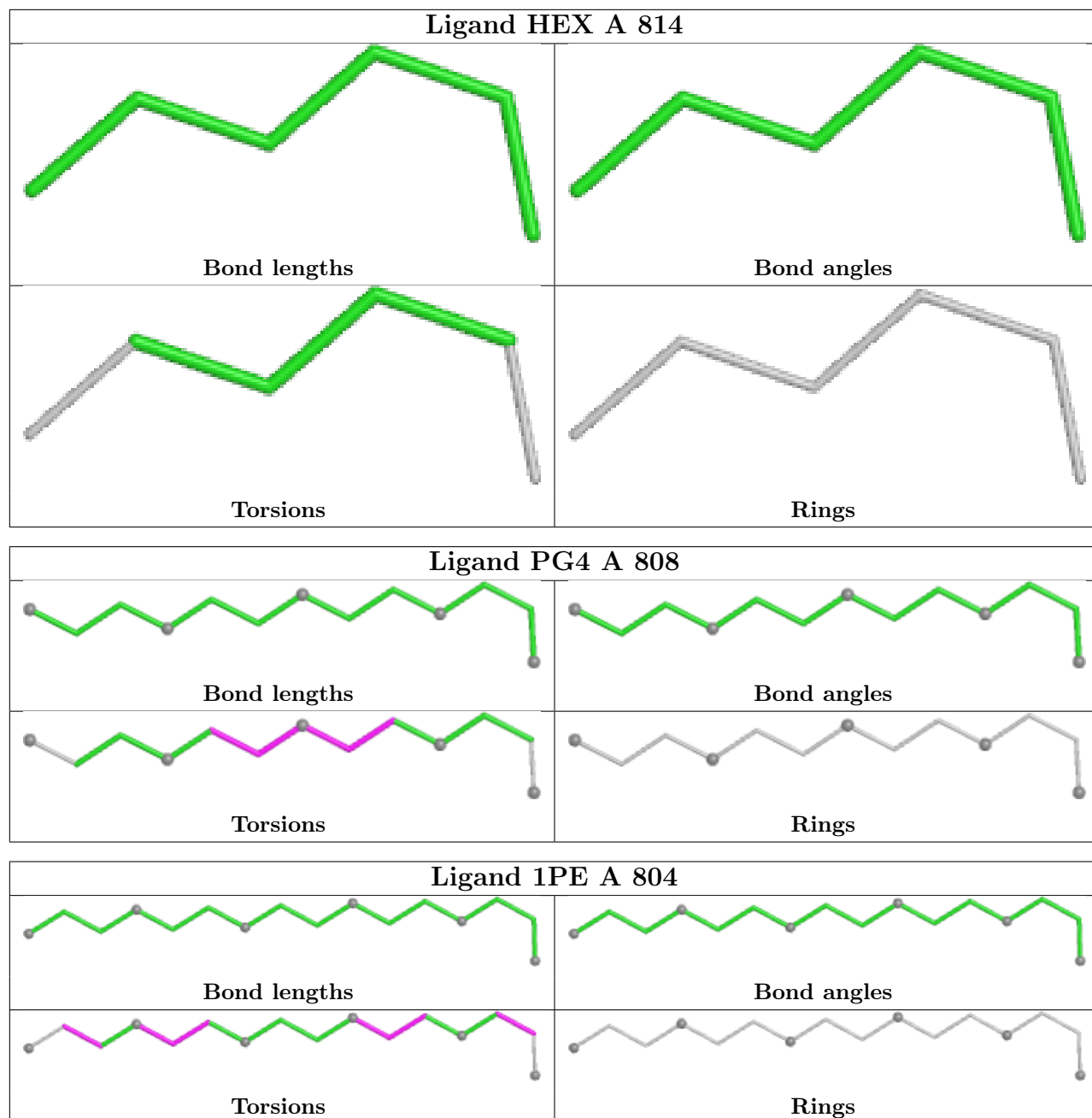
There are no ring outliers.

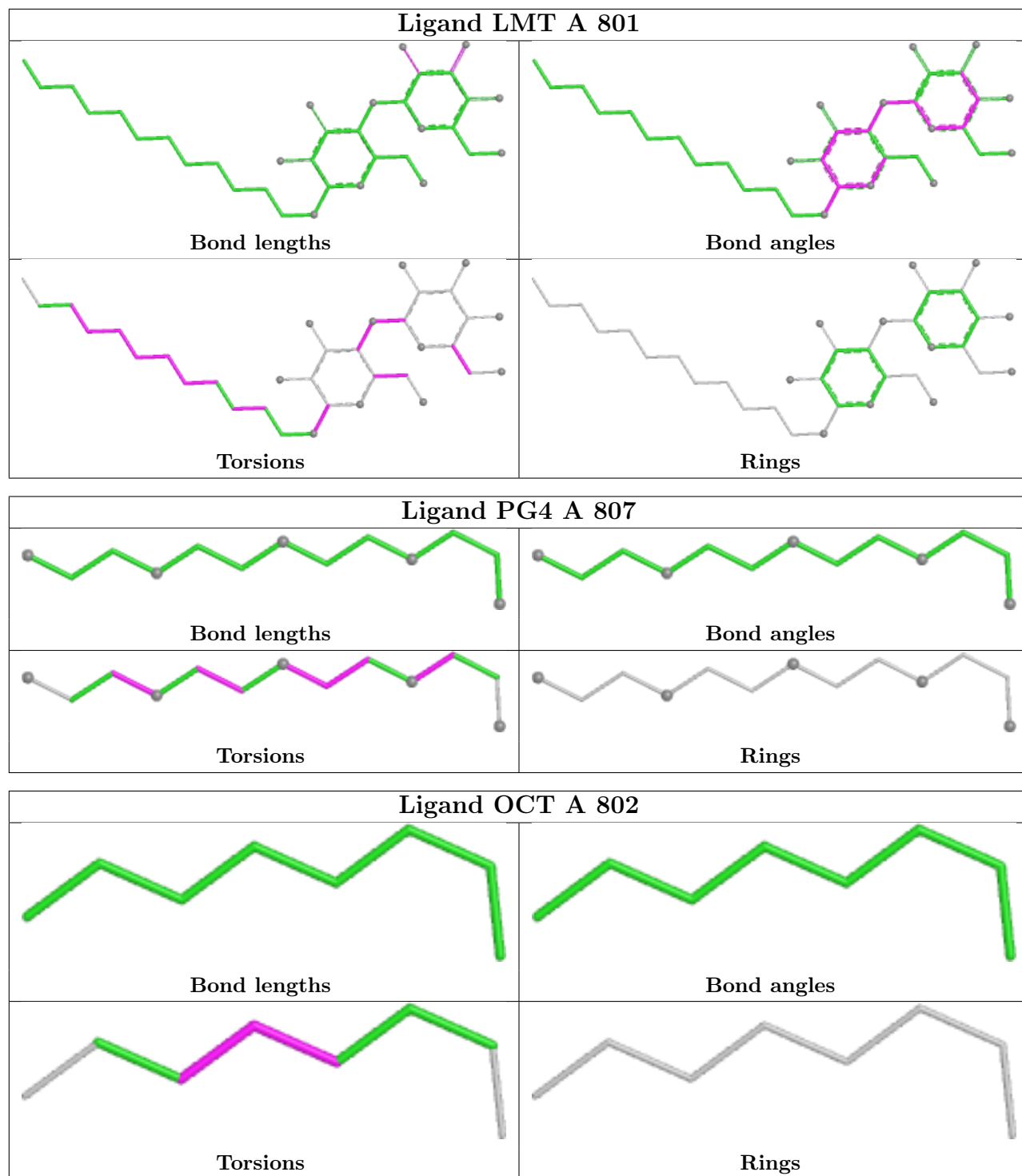
5 monomers are involved in 8 short contacts:

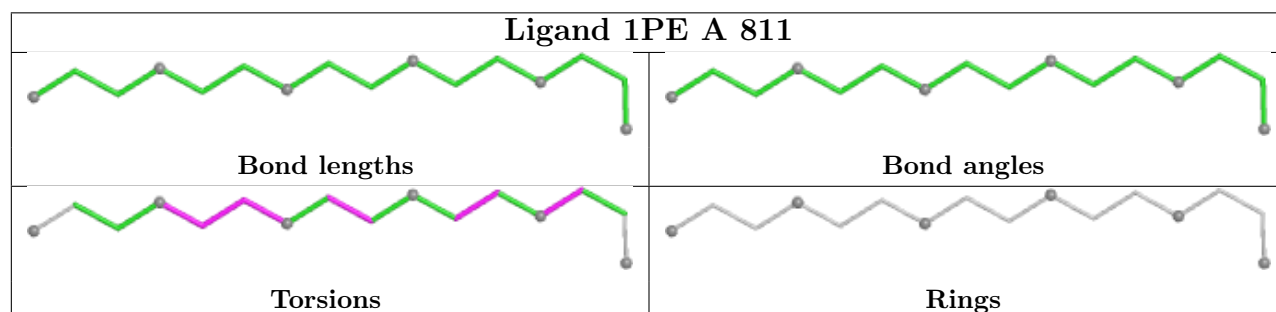
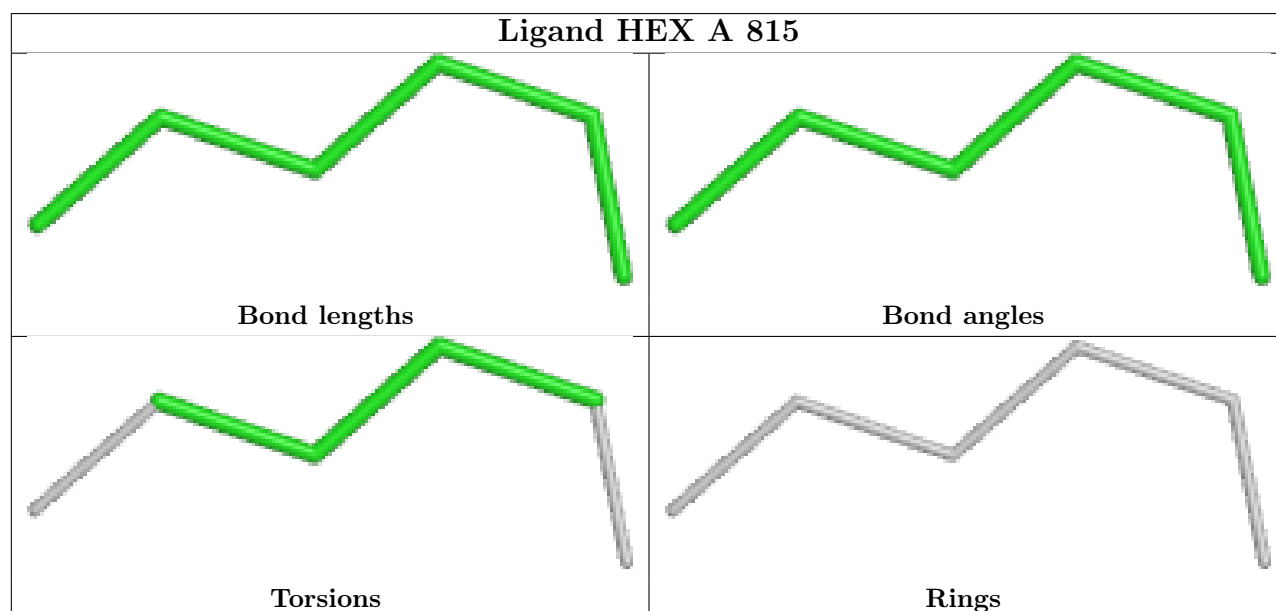
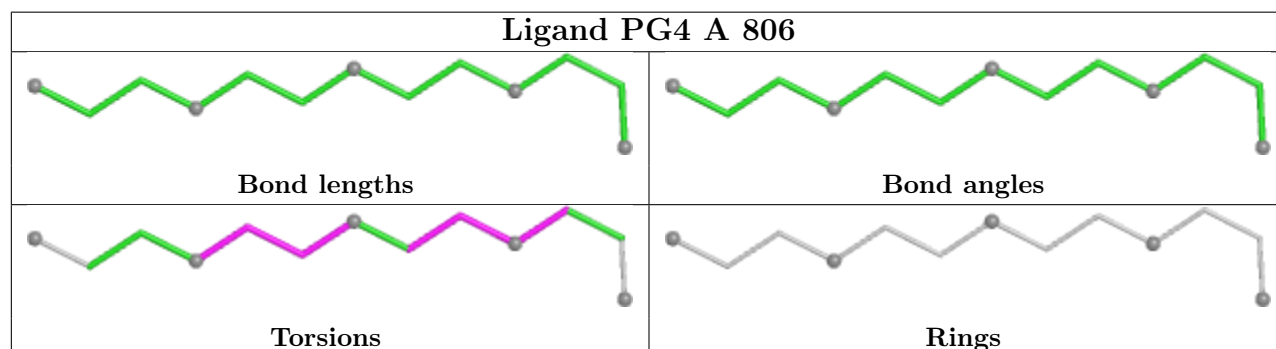
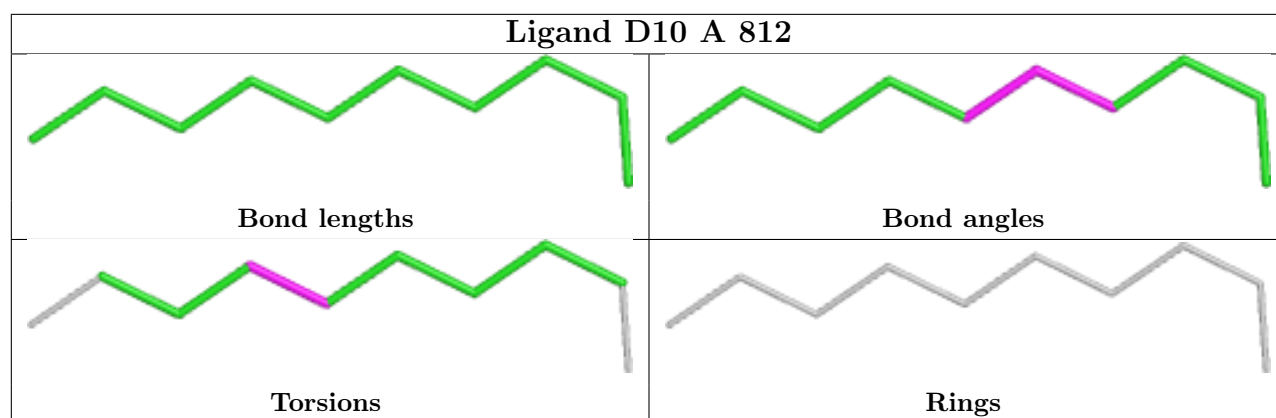
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	814	HEX	1	0
4	A	801	LMT	3	0
6	A	807	PG4	1	0
10	A	812	D10	2	0
7	A	811	1PE	2	0

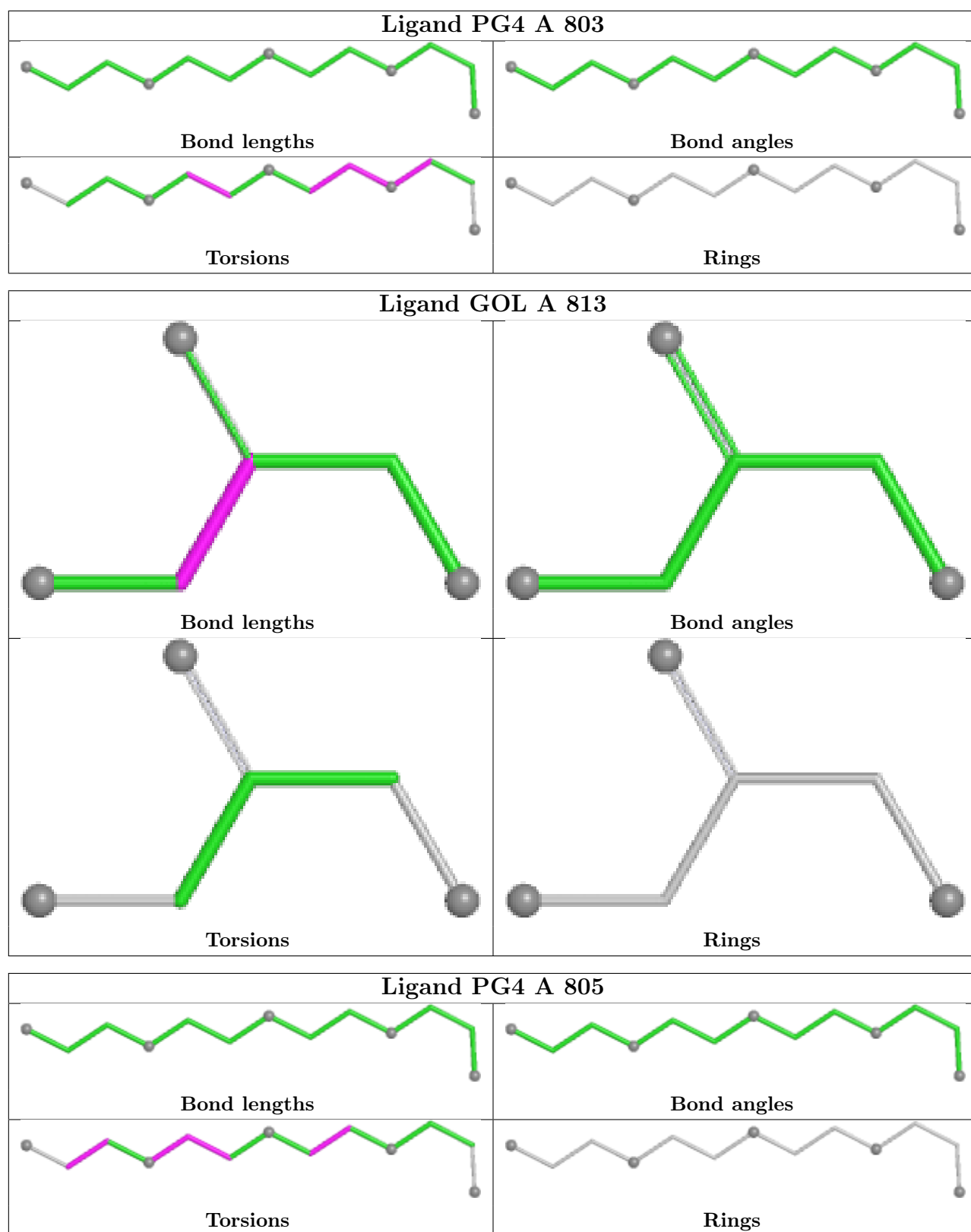
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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%)	2.02	170 (37%)	1 0	42, 70, 131, 160	1 (0%)
2	B	127/127 (100%)	1.69	39 (30%)	1 1	45, 66, 101, 110	2 (1%)
3	C	2/2 (100%)	2.12	1 (50%)	0 0	67, 67, 67, 80	0
All	All	580/618 (93%)	1.95	210 (36%)	1 1	42, 69, 124, 160	3 (0%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	PHE	15.5
1	A	305	LEU	12.7
1	A	304	ILE	10.8
1	A	199	ASP	9.1
1	A	50	GLU	8.9
1	A	399	LEU	8.9
1	A	397	SER	8.4
2	B	14	ALA	7.8
1	A	398	ALA	7.0
1	A	308	SER	7.0
2	B	2	VAL	6.9
1	A	404	ILE	6.8
1	A	303	GLU	6.8
1	A	443	ASN	6.8
1	A	309	ILE	6.5
1	A	395	PHE	6.5
1	A	402	ALA	6.3
1	A	124	ALA	6.3
1	A	306	GLY	6.1
1	A	301	HIS	6.0
2	B	15	GLY	5.9
1	A	394	LEU	5.7
1	A	70	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	5.4
2	B	87	PRO	5.3
1	A	351	LEU	5.1
2	B	117	THR	5.0
1	A	135	PRO	5.0
1	A	125	ASN	4.9
1	A	162	LEU	4.8
2	B	128	HIS	4.8
1	A	269	PHE	4.7
2	B	101	GLY	4.6
1	A	249	VAL	4.6
1	A	121	LEU	4.5
1	A	183	LEU	4.5
1	A	401	LEU	4.5
1	A	415	PHE	4.4
1	A	407	LEU	4.4
1	A	456	ASN	4.3
2	B	57	LEU	4.3
1	A	233	HIS	4.2
1	A	148	PHE	4.2
1	A	186	ALA	4.2
2	B	9	GLY	4.1
2	B	66	ARG	4.1
1	A	433	TYR	4.1
1	A	172	TYR	4.1
1	A	413	MET	4.1
1	A	414	GLY	4.1
1	A	149	TYR	4.1
1	A	355	MET	4.1
1	A	385	VAL	4.1
1	A	437	PHE	4.1
1	A	120	GLY	4.0
1	A	170	PHE	4.0
1	A	392	GLY	4.0
2	B	4	LEU	4.0
2	B	68	THR	3.9
1	A	273	VAL	3.9
1	A	285	TYR	3.9
1	A	218	LEU	3.9
1	A	56	PHE	3.8
2	B	23	ALA	3.8
2	B	13	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	ARG	3.8
1	A	396	ILE	3.8
1	A	266	ASN	3.8
1	A	405	ALA	3.7
1	A	64	TYR	3.7
2	B	59	TYR	3.7
1	A	161	SER	3.7
1	A	184	ILE	3.7
1	A	137	LYS	3.7
1	A	416	ILE	3.6
1	A	268	MET	3.6
2	B	41	PRO	3.6
1	A	253	PHE	3.5
1	A	352	GLY	3.5
1	A	408	VAL	3.5
1	A	103	LEU	3.5
1	A	380	TRP	3.5
1	A	67	ILE	3.4
1	A	252	ILE	3.4
2	B	67	PHE	3.4
1	A	389	GLN	3.4
1	A	25	TRP	3.4
1	A	420	TRP	3.4
1	A	144	ALA	3.3
1	A	356	CYS	3.3
1	A	372	ASP	3.3
1	A	194	ARG	3.2
1	A	24	LEU	3.2
1	A	323	VAL	3.2
1	A	139	PRO	3.2
1	A	358	LEU	3.2
1	A	271	ALA	3.1
1	A	478	TRP	3.1
2	B	86	LYS	3.1
1	A	474	LEU	3.1
1	A	298	ASN	3.1
2	B	24	ALA	3.1
1	A	403	MET	3.1
1	A	51	GLN	3.0
1	A	245	LEU	3.0
1	A	359	GLY	3.0
3	C	2	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	362	THR	3.0
1	A	136	PRO	3.0
1	A	83	THR	3.0
2	B	102	MET	3.0
1	A	211	PHE	3.0
1	A	272	PHE	3.0
1	A	400	GLY	3.0
1	A	187	LEU	2.9
2	B	84	SER	2.9
1	A	406	ALA	2.9
1	A	254	PHE	2.9
1	A	182	GLY	2.9
1	A	169	ARG	2.9
1	A	105	PRO	2.9
1	A	102	LEU	2.9
1	A	77	LEU	2.8
1	A	286	ALA	2.8
1	A	417	LEU	2.8
1	A	21	PHE	2.8
1	A	123	LYS	2.8
1	A	294	PHE	2.8
1	A	115	ILE	2.8
2	B	83	ASN	2.8
1	A	37	LEU	2.8
1	A	165	VAL	2.8
2	B	126	HIS	2.8
1	A	311	PRO	2.7
1	A	63	VAL	2.7
2	B	121	VAL	2.7
1	A	104	LYS	2.7
1	A	198	LYS	2.7
1	A	95	TYR	2.7
2	B	31	ASN	2.7
1	A	332	ILE	2.6
1	A	470	VAL	2.6
1	A	256	GLN	2.6
1	A	109	PHE	2.6
1	A	275	MET	2.6
1	A	329	LEU	2.6
1	A	41	PHE	2.6
1	A	59	PHE	2.6
1	A	155	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	171	GLY	2.6
1	A	300	VAL	2.5
1	A	302	HIS	2.5
1	A	251	ILE	2.5
1	A	419	MET	2.5
1	A	96	PHE	2.5
1	A	282	TYR	2.4
2	B	20	LEU	2.4
1	A	279	VAL	2.4
1	A	111	ALA	2.4
2	B	7	SER	2.4
1	A	60	ALA	2.4
1	A	156	SER	2.4
2	B	5	VAL	2.4
2	B	43	LYS	2.4
1	A	482	MET	2.4
1	A	448	LEU	2.3
1	A	483	ILE	2.3
1	A	126	PRO	2.3
2	B	53	TRP	2.3
1	A	436	THR	2.3
1	A	344	SER	2.3
1	A	422	LEU	2.3
1	A	451	LEU	2.3
2	B	99	PHE	2.3
1	A	181	ALA	2.3
1	A	114	THR	2.3
1	A	418	GLY	2.3
1	A	19	ILE	2.3
1	A	141	LEU	2.3
1	A	168	ASP	2.3
1	A	42	VAL	2.3
1	A	158	ILE	2.2
2	B	88	GLU	2.2
1	A	388	PHE	2.2
1	A	347	MET	2.2
1	A	472	MET	2.2
1	A	281	PHE	2.2
1	A	384	LEU	2.2
1	A	152	ILE	2.2
1	A	214	LEU	2.2
1	A	375	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	25	SER	2.2
1	A	22	VAL	2.1
1	A	330	ALA	2.1
1	A	250	THR	2.1
1	A	450	THR	2.1
1	A	97	MET	2.1
1	A	91	LEU	2.1
2	B	42	GLY	2.1
1	A	213	LYS	2.1
1	A	464	VAL	2.1
2	B	73	ASN	2.1
2	B	3	GLN	2.0
2	B	85	LEU	2.0
1	A	209	MET	2.0
1	A	145	PHE	2.0
1	A	296	ALA	2.0
2	B	35	GLY	2.0
1	A	369	TRP	2.0
2	B	27	PRO	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 [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.

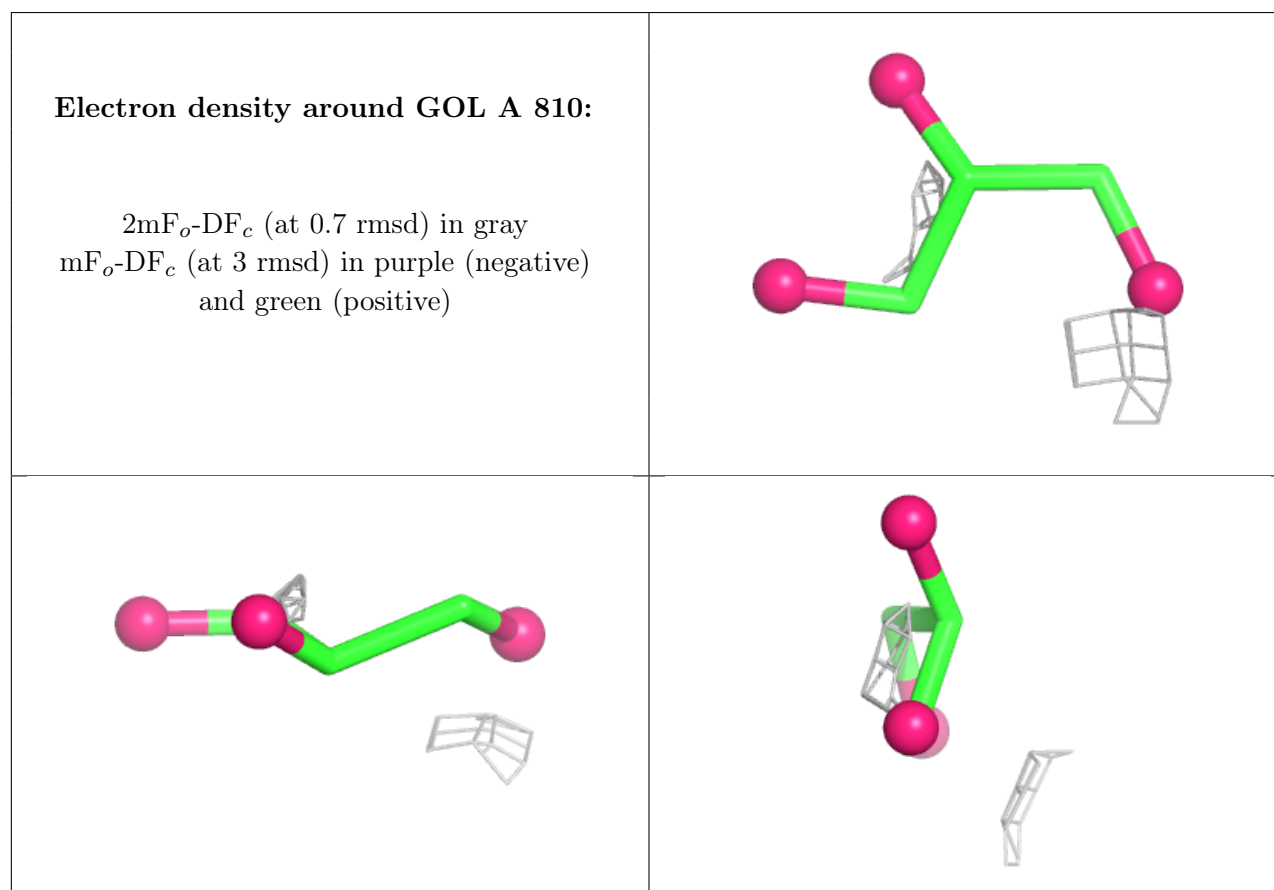
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	A	810	6/6	0.50	0.21	111,116,120,121	0
6	PG4	A	806	13/13	0.61	0.25	89,98,108,110	0
10	D10	A	812	10/10	0.63	0.49	74,81,93,101	0
8	D12	A	809	12/12	0.65	0.52	86,90,95,98	0

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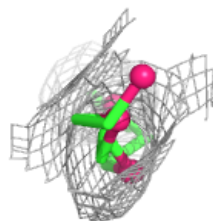
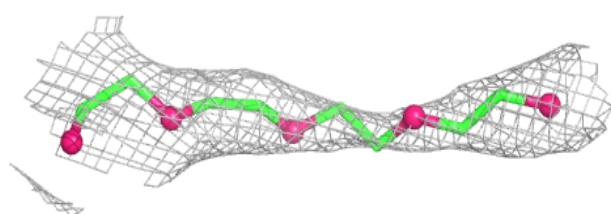
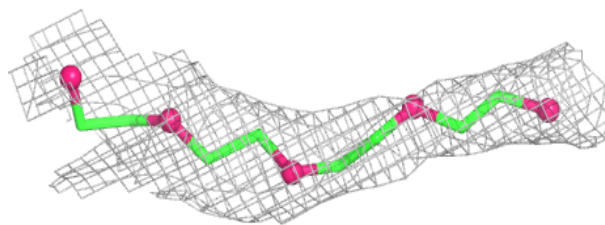
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	HEX	A	815	6/6	0.66	0.37	72,77,86,87	0
9	GOL	A	813	6/6	0.68	0.18	87,93,94,102	0
6	PG4	A	805	13/13	0.70	0.26	79,93,104,109	0
6	PG4	A	808	13/13	0.75	0.28	75,85,101,104	0
4	LMT	A	801	35/35	0.77	0.19	67,87,110,112	0
6	PG4	A	807	13/13	0.78	0.23	83,91,99,102	0
7	1PE	A	811	16/16	0.79	0.21	93,96,101,109	0
6	PG4	A	803	13/13	0.83	0.19	71,80,101,103	0
11	HEX	A	814	6/6	0.83	0.29	82,85,89,89	0
7	1PE	A	804	16/16	0.83	0.19	70,85,109,111	0
5	OCT	A	802	8/8	0.85	0.29	73,76,82,85	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.

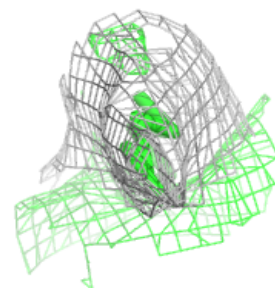
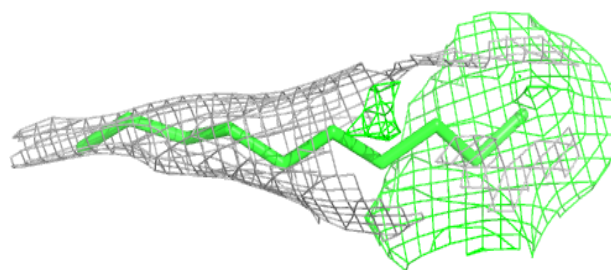
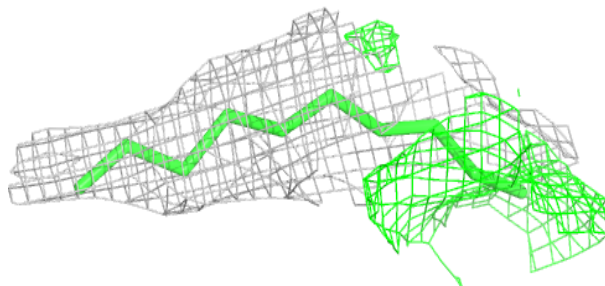


Electron density around PG4 A 806:

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

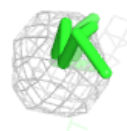
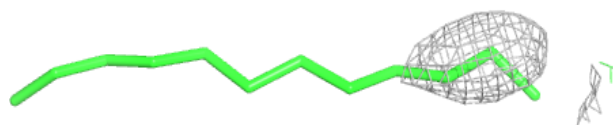
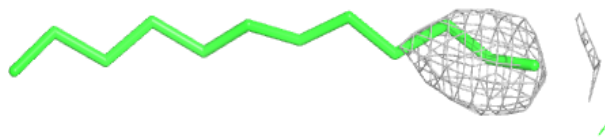
**Electron density around D10 A 812:**

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

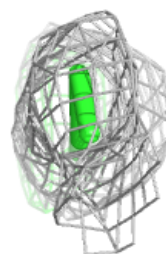
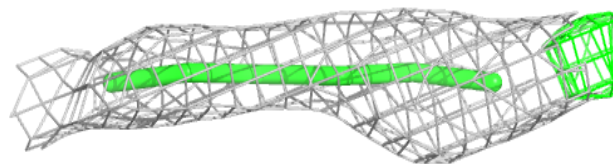
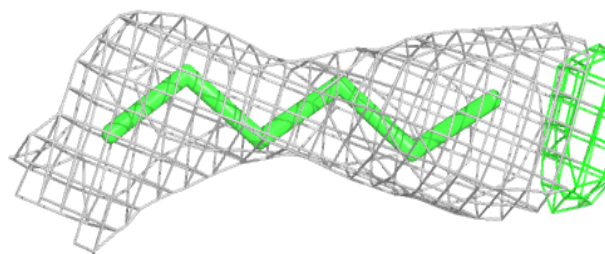


Electron density around D12 A 809:

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

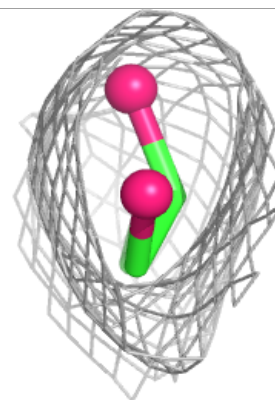
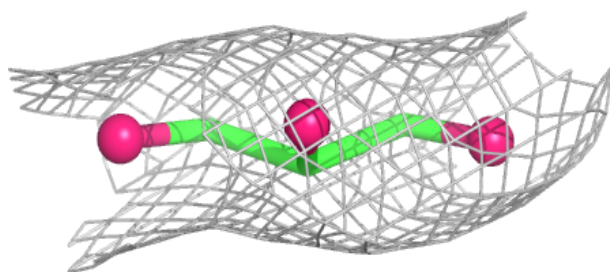
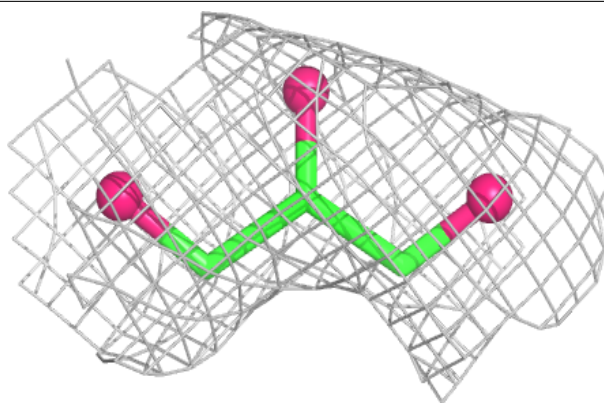
**Electron density around HEX A 815:**

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

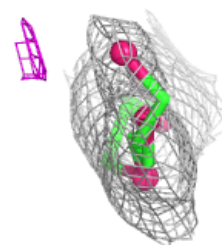
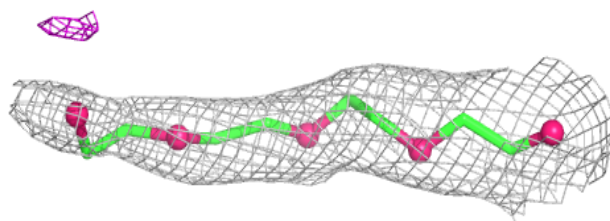
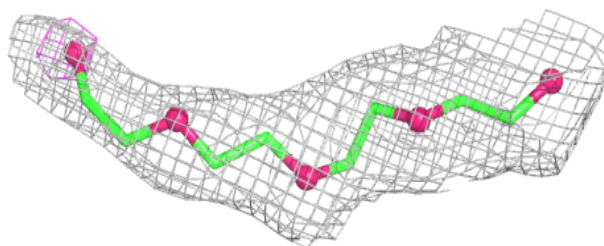


Electron density around GOL A 813:

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

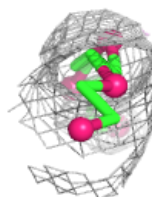
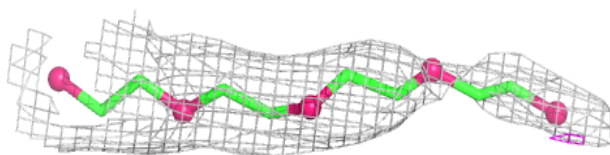
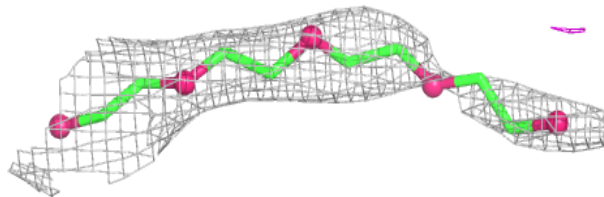
**Electron density around PG4 A 805:**

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

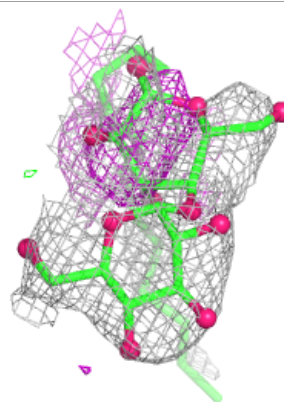
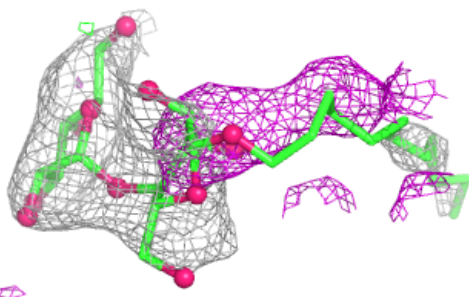
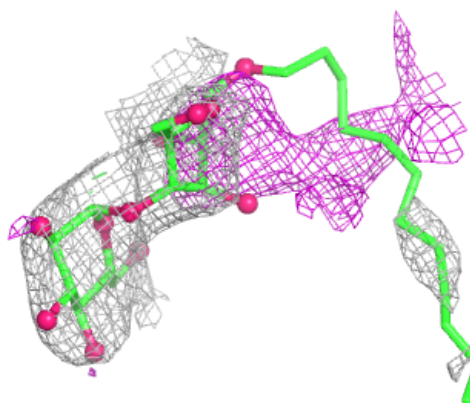


Electron density around PG4 A 808:

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

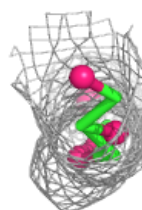
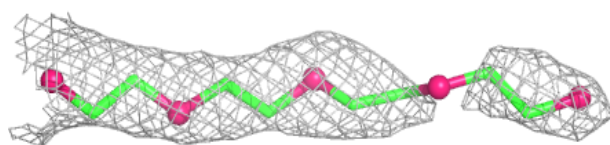
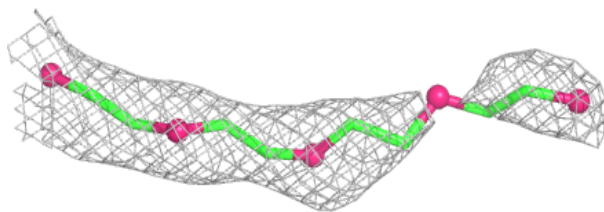
**Electron density around LMT A 801:**

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

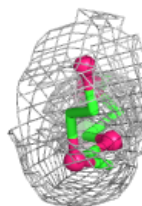
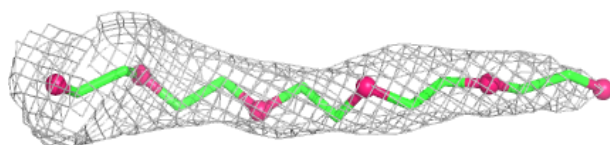
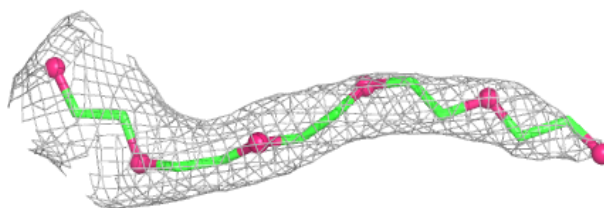


Electron density around PG4 A 807:

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

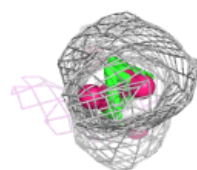
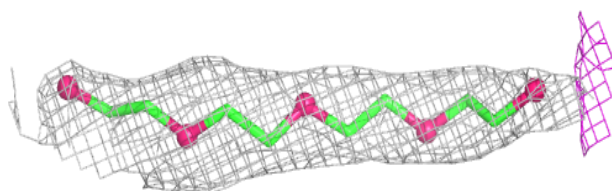
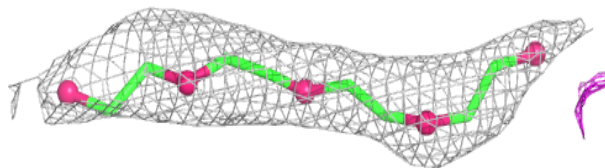
**Electron density around 1PE A 811:**

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

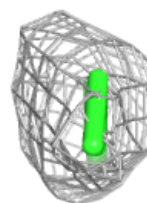
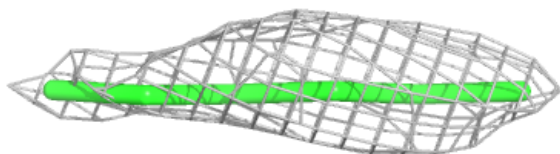
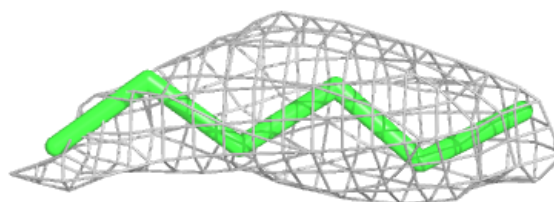


Electron density around PG4 A 803:

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

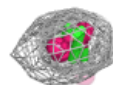
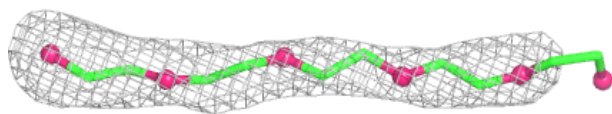
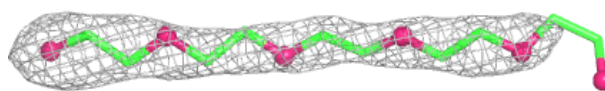
**Electron density around HEX A 814:**

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

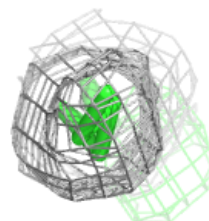
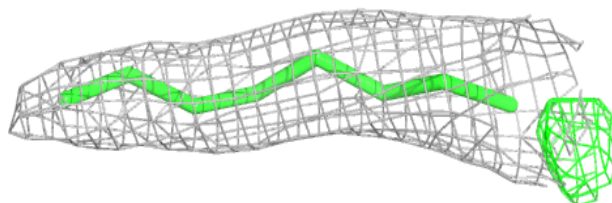
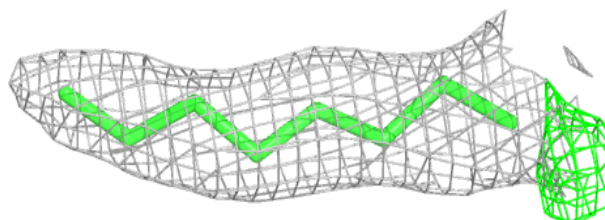


Electron density around 1PE A 804:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.