



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:45 AM UTC

PDB ID : 8B1K / pdb_00008b1k
Title : DtpB-Nb132-NV
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Deposited on : 2022-09-09
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

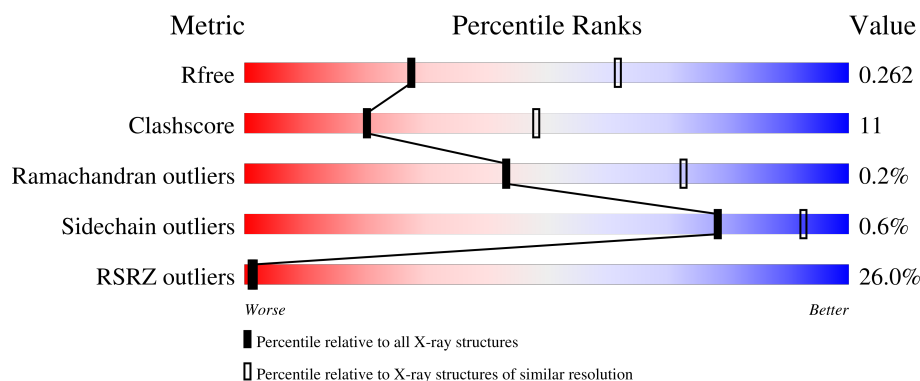
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
2	B	127	
3	C	2	

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 4789 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			

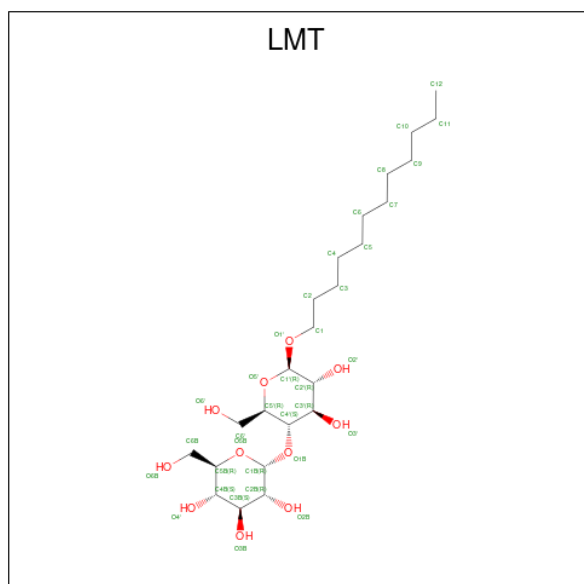
- Molecule 2 is a protein called Nanobody 132.

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 ASN-VAL.

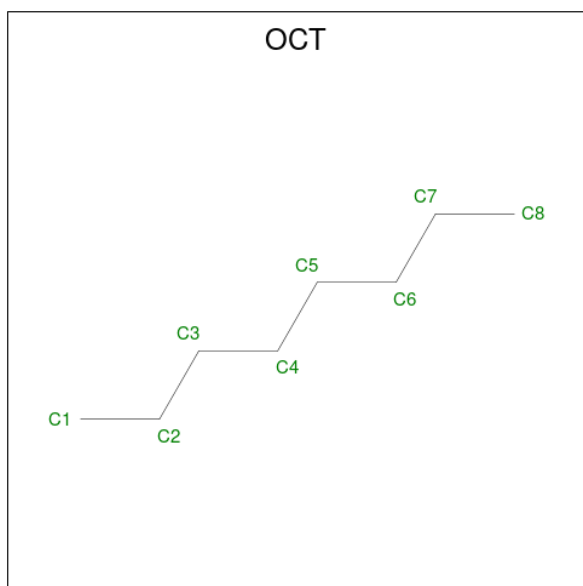
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			16	9	3	4			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



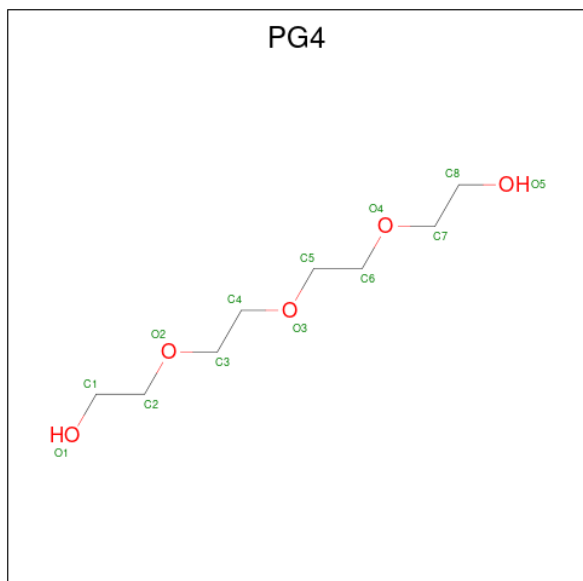
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

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



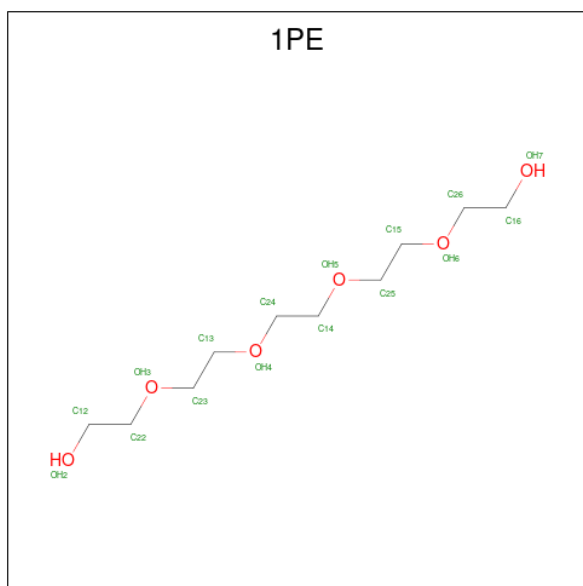
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			8	8		

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



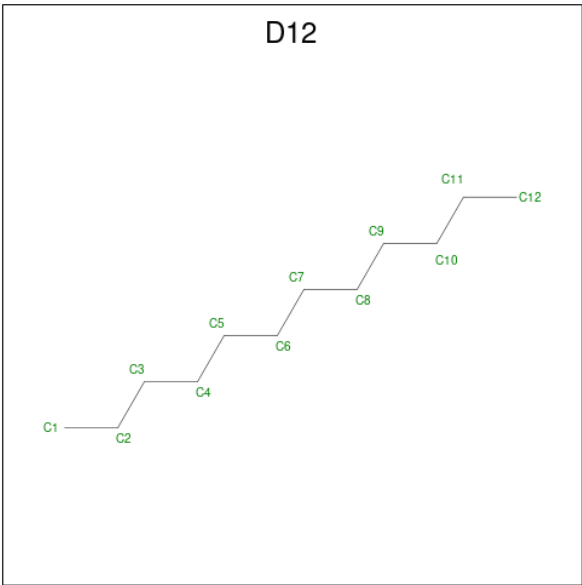
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

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



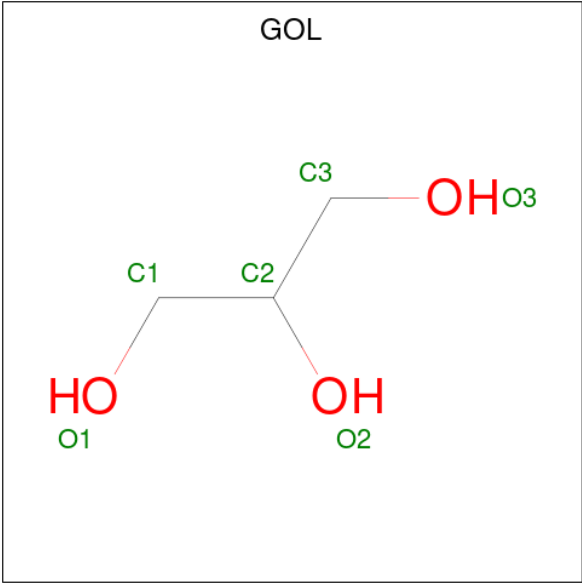
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

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



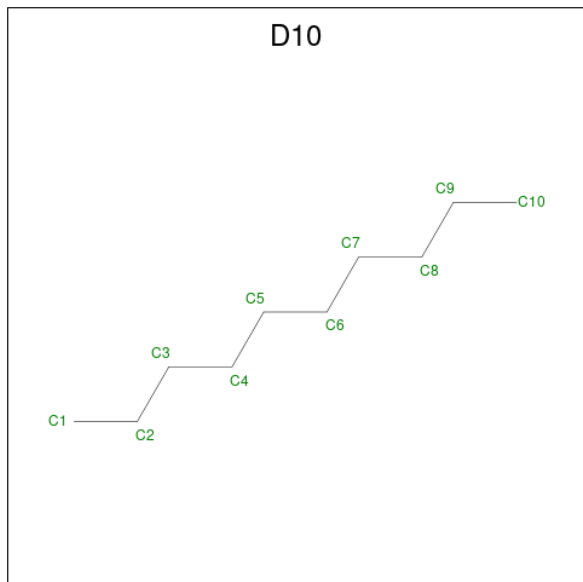
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			12	12		

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



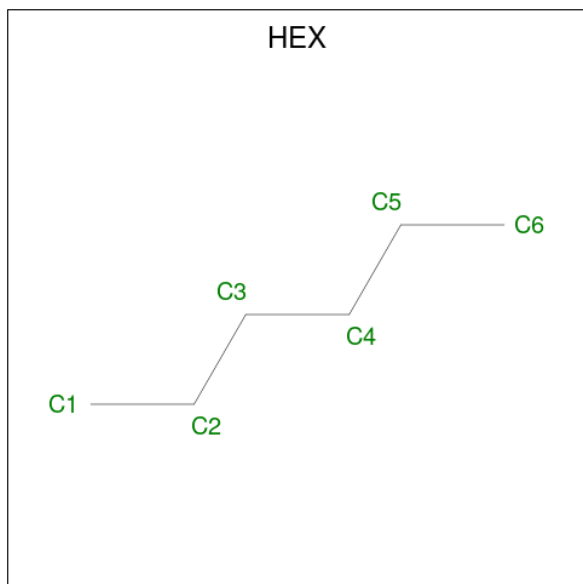
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- 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

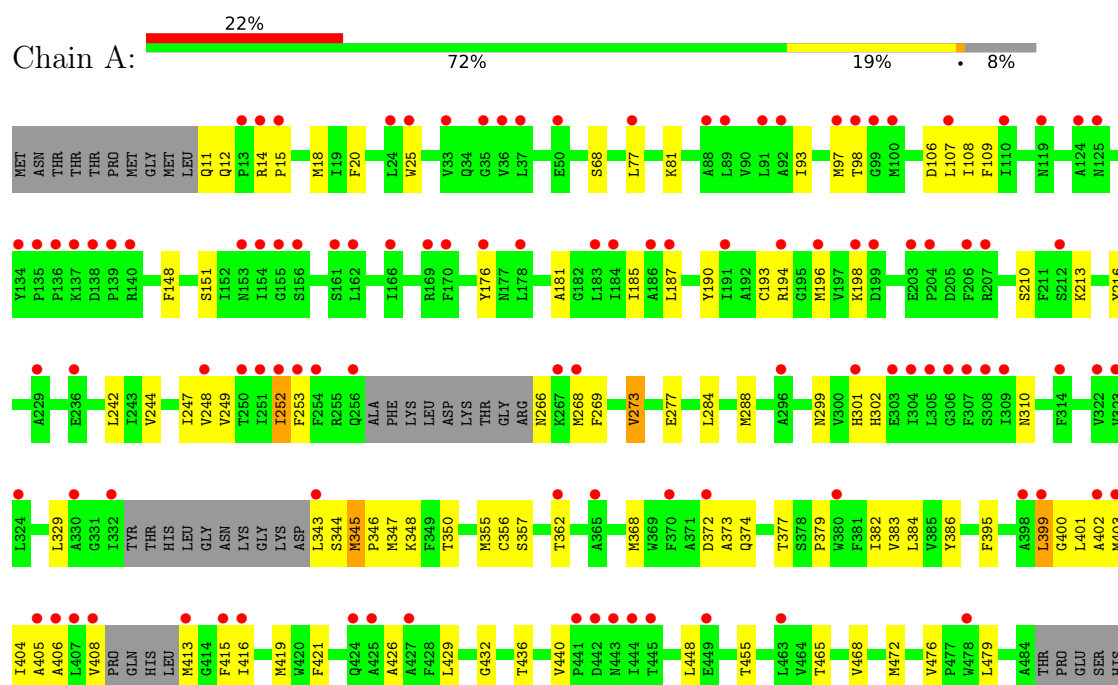
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	72	Total O 72 72	0	0
12	B	57	Total O 57 57	0	0
12	C	2	Total O 2 2	0	0

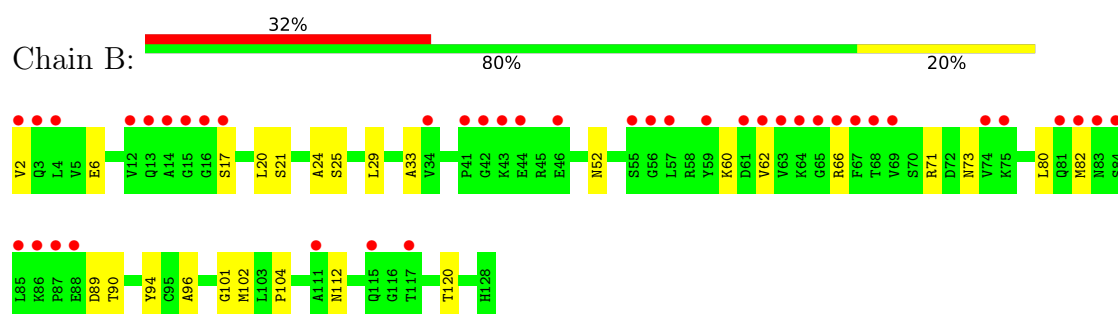
3 Residue-property plots [i](#)

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: ASN-VAL



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	54.14Å 124.92Å 165.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.14 – 2.80 54.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (54.14-2.80) 87.1 (54.14-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.226 , 0.250 (Not available) , 0.262	Depositor DCC
R_{free} test set	1384 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 40.2	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	0.80	EDS
Total number of atoms	4789	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, OCT, D10, 1PE, PG4, LMT, D12, GOL

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	0.55	1/3572 (0.0%)	0.79	3/4859 (0.1%)
2	B	0.50	0/1004	0.78	0/1361
3	C	0.55	0/15	1.20	0/18
All	All	0.54	1/4591 (0.0%)	0.79	3/6238 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	MET	CB-CG	-8.46	1.27	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	MET	CG-SD-CE	-9.39	80.25	100.90
1	A	345	MET	CB-CG-SD	-5.52	96.15	112.70
1	A	399	LEU	CA-CB-CG	5.35	135.03	116.30

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	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	976	0	939	16	0
3	C	16	0	17	0	0
4	A	35	0	46	2	0
5	A	8	0	18	0	0
6	A	65	0	90	2	0
7	A	32	0	44	0	0
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	0	0
12	A	72	0	0	3	0
12	B	57	0	0	1	0
12	C	2	0	0	0	0
All	All	4789	0	4851	107	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 (107) 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:249:VAL:HG12	1:A:419:MET:CE	1.51	1.38
1:A:249:VAL:CG1	1:A:419:MET:CE	2.27	1.13
1:A:249:VAL:CG1	1:A:419:MET:HE2	1.82	1.09
1:A:249:VAL:CG1	1:A:419:MET:HE3	1.97	0.94
1:A:348:LYS:HD2	1:A:399:LEU:HD21	1.51	0.92
2:B:90:THR:HG23	2:B:120:THR:HA	1.53	0.88
1:A:368:MET:HG3	1:A:455:THR:HG21	1.53	0.88
1:A:249:VAL:HG12	1:A:419:MET:HE2	0.87	0.86
1:A:403:MET:HG2	1:A:406:ALA:CB	2.08	0.83
1:A:301:HIS:NE2	1:A:372:ASP:OD2	2.11	0.80
1:A:346:PRO:HG3	1:A:479:LEU:HD22	1.66	0.77
1:A:194:ARG:HH21	1:A:198:LYS:HZ2	1.30	0.76
1:A:403:MET:HG2	1:A:406:ALA:HB2	1.66	0.76
1:A:345:MET:HB2	1:A:346:PRO:HD3	1.66	0.76
1:A:350:THR:HA	1:A:472:MET:HE2	1.67	0.76
1:A:368:MET:HG3	1:A:455:THR:CG2	2.23	0.68
1:A:253:PHE:HB2	1:A:419:MET:HE1	1.75	0.68
1:A:194:ARG:NH2	1:A:198:LYS:HZ2	1.91	0.68
1:A:401:LEU:HA	1:A:404:ILE:HB	1.77	0.66
1:A:266:ASN:OD1	1:A:269:PHE:CE2	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TYR:HB3	6:A:807:PG4:H42	1.81	0.63
1:A:266:ASN:HA	1:A:269:PHE:HD2	1.65	0.62
1:A:346:PRO:CG	1:A:479:LEU:HD22	2.29	0.61
1:A:249:VAL:HG13	1:A:419:MET:HE3	1.83	0.61
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.34	0.61
1:A:268:MET:HE1	1:A:408:VAL:HG13	1.84	0.60
1:A:181:ALA:O	1:A:185:ILE:HG23	2.02	0.60
1:A:273:VAL:O	1:A:277:GLU:HG3	2.03	0.59
1:A:347:MET:HE2	1:A:476:VAL:HG11	1.84	0.59
1:A:288:MET:HG2	1:A:386:TYR:CE1	2.37	0.59
1:A:284:LEU:HD12	1:A:356:CYS:HB3	1.85	0.58
1:A:194:ARG:HE	1:A:198:LYS:HZ1	1.50	0.58
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.86	0.58
1:A:194:ARG:HE	1:A:198:LYS:NZ	2.00	0.58
1:A:468:VAL:O	1:A:472:MET:HG3	2.04	0.58
1:A:403:MET:HG2	1:A:406:ALA:HB3	1.84	0.57
1:A:14:ARG:HB3	1:A:196:MET:CE	2.33	0.57
2:B:33:ALA:HA	2:B:52:ASN:HA	1.87	0.56
1:A:302:HIS:HD2	12:B:217:HOH:O	1.89	0.55
1:A:350:THR:HA	1:A:472:MET:CE	2.36	0.55
1:A:344:SER:O	1:A:348:LYS:HE2	2.07	0.55
1:A:344:SER:OG	1:A:345:MET:N	2.41	0.54
2:B:2:VAL:HA	2:B:112:ASN:ND2	2.21	0.54
1:A:93:ILE:HG22	1:A:97:MET:HE2	1.90	0.53
1:A:400:GLY:O	1:A:404:ILE:HG12	2.08	0.53
1:A:248:VAL:O	1:A:252:ILE:HG23	2.09	0.53
1:A:346:PRO:HB3	1:A:479:LEU:HD13	1.91	0.53
2:B:71:ARG:HD3	2:B:73:ASN:OD1	2.09	0.52
1:A:266:ASN:HA	1:A:269:PHE:CD2	2.44	0.52
2:B:20:LEU:HD12	2:B:80:LEU:HD23	1.92	0.52
2:B:6:GLU:OE2	2:B:94:TYR:HA	2.11	0.50
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.94	0.50
1:A:20:PHE:CE2	1:A:151:SER:HB2	2.47	0.50
1:A:81:LYS:HB3	1:A:190:TYR:OH	2.11	0.49
2:B:24:ALA:HB2	2:B:29:LEU:HD13	1.94	0.48
1:A:429:LEU:HD12	12:A:931:HOH:O	2.14	0.48
1:A:11:GLN:HG3	1:A:12:GLN:HG2	1.97	0.47
1:A:402:ALA:O	1:A:405:ALA:HB3	2.14	0.47
1:A:198:LYS:HA	1:A:198:LYS:HD3	1.62	0.47
1:A:210:SER:OG	1:A:213:LYS:HG2	2.14	0.47
1:A:413:MET:O	1:A:416:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:THR:HG22	1:A:176:TYR:CD2	2.50	0.47
2:B:62:VAL:O	2:B:66:ARG:NH1	2.48	0.46
1:A:242:LEU:HD23	1:A:426:ALA:HA	1.97	0.46
1:A:14:ARG:HB3	1:A:196:MET:HE3	1.97	0.46
1:A:355:MET:HA	1:A:355:MET:HE2	1.97	0.46
1:A:25:TRP:CE3	1:A:185:ILE:HD11	2.51	0.45
1:A:213:LYS:HD3	6:A:807:PG4:H12	1.98	0.45
1:A:329:LEU:HD21	1:A:395:PHE:CE1	2.52	0.45
1:A:343:LEU:HA	1:A:347:MET:HB3	1.98	0.45
1:A:299:ASN:O	1:A:377:THR:HG22	2.16	0.45
1:A:379:PRO:O	1:A:382:ILE:HG22	2.15	0.45
4:A:801:LMT:H12	4:A:801:LMT:H41	1.58	0.45
1:A:432:GLY:O	1:A:436:THR:HG23	2.16	0.45
2:B:96:ALA:HA	2:B:112:ASN:O	2.17	0.45
1:A:266:ASN:OD1	1:A:269:PHE:HE2	1.97	0.45
2:B:101:GLY:C	2:B:102:MET:HE2	2.41	0.45
1:A:357:SER:HB2	1:A:465:THR:HG22	1.99	0.45
2:B:2:VAL:HA	2:B:112:ASN:HD22	1.82	0.44
1:A:14:ARG:N	1:A:15:PRO:HD2	2.32	0.43
2:B:6:GLU:HA	2:B:21:SER:O	2.17	0.43
1:A:14:ARG:HB3	1:A:196:MET:HE2	2.00	0.43
1:A:401:LEU:HD12	1:A:404:ILE:HB	2.00	0.43
1:A:25:TRP:CZ3	1:A:185:ILE:HD11	2.54	0.43
1:A:107:LEU:HD13	10:A:812:D10:H72	2.00	0.43
1:A:362:THR:HG21	1:A:384:LEU:HD23	2.01	0.43
1:A:14:ARG:C	1:A:196:MET:HE2	2.43	0.43
1:A:148:PHE:O	1:A:151:SER:HB3	2.17	0.43
1:A:244:VAL:HA	1:A:247:ILE:HG13	2.00	0.43
1:A:415:PHE:CZ	1:A:419:MET:HE3	2.54	0.43
1:A:20:PHE:CD2	1:A:151:SER:HB2	2.54	0.42
1:A:247:ILE:HD12	1:A:248:VAL:N	2.33	0.42
1:A:68:SER:HB3	1:A:421:PHE:CD2	2.55	0.42
1:A:288:MET:HG2	1:A:386:TYR:HE1	1.81	0.42
1:A:379:PRO:O	1:A:383:VAL:HG23	2.19	0.42
1:A:344:SER:OG	12:A:902:HOH:O	2.21	0.42
1:A:310:ASN:HD22	4:A:801:LMT:H6'1	1.85	0.42
1:A:106:ASP:HB2	10:A:812:D10:H41	2.02	0.41
1:A:345:MET:CB	1:A:346:PRO:HD3	2.42	0.41
1:A:440:VAL:O	12:A:901:HOH:O	2.21	0.41
1:A:374:GLN:OE1	2:B:104:PRO:HB2	2.20	0.41
1:A:77:LEU:HD22	1:A:213:LYS:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:CYS:HB3	1:A:196:MET:SD	2.60	0.41
2:B:17:SER:HA	2:B:82:MET:O	2.20	0.41
1:A:344:SER:C	1:A:348:LYS:HE2	2.46	0.40
1:A:108:ILE:HG23	1:A:109:PHE:N	2.37	0.40
1:A:373:ALA:O	1:A:448:LEU:HD11	2.21	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%)	434 (98%)	9 (2%)	0	100	100
2	B	126/127 (99%)	123 (98%)	2 (2%)	1 (1%)	16	44
All	All	569/616 (92%)	557 (98%)	11 (2%)	1 (0%)	43	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/401 (92%)	365 (99%)	3 (1%)	73	90
2	B	102/101 (101%)	102 (100%)	0	100	100
3	C	2/2 (100%)	2 (100%)	0	100	100
All	All	472/504 (94%)	469 (99%)	3 (1%)	78	92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LEU
1	A	252	ILE
1	A	273	VAL

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	299	ASN
1	A	389	GLN

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
9	GOL	A	810	-	5,5,5	1.22	1 (20%)	5,5,5	0.85	0
6	PG4	A	803	-	12,12,12	0.56	0	11,11,11	0.40	0
6	PG4	A	805	-	12,12,12	0.62	0	11,11,11	0.82	0
6	PG4	A	807	-	12,12,12	0.57	0	11,11,11	0.60	0
7	1PE	A	811	-	15,15,15	0.53	0	14,14,14	0.39	0
10	D10	A	812	-	9,9,9	0.52	0	8,8,8	0.47	0
6	PG4	A	806	-	12,12,12	0.57	0	11,11,11	0.61	0
11	HEX	A	814	-	5,5,5	0.46	0	4,4,4	0.50	0
4	LMT	A	801	-	36,36,36	1.32	4 (11%)	47,47,47	1.73	13 (27%)
7	1PE	A	804	-	15,15,15	0.57	0	14,14,14	0.64	0
11	HEX	A	815	-	5,5,5	0.52	0	4,4,4	0.28	0
6	PG4	A	808	-	12,12,12	0.54	0	11,11,11	0.60	0
5	OCT	A	802	-	7,7,7	0.60	0	6,6,6	0.36	0
9	GOL	A	813	-	5,5,5	0.94	0	5,5,5	1.09	0
8	D12	A	809	-	11,11,11	0.55	0	10,10,10	0.56	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
9	GOL	A	810	-	-	1/4/4/4	-
6	PG4	A	803	-	-	4/10/10/10	-
6	PG4	A	805	-	-	5/10/10/10	-
6	PG4	A	807	-	-	4/10/10/10	-
7	1PE	A	811	-	-	6/13/13/13	-
10	D10	A	812	-	-	1/7/7/7	-
6	PG4	A	806	-	-	6/10/10/10	-
11	HEX	A	814	-	-	0/3/3/3	-
4	LMT	A	801	-	-	17/21/61/61	0/2/2/2
7	1PE	A	804	-	-	4/13/13/13	-
11	HEX	A	815	-	-	0/3/3/3	-
6	PG4	A	808	-	-	4/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OCT	A	802	-	-	2/5/5/5	-
9	GOL	A	813	-	-	0/4/4/4	-
8	D12	A	809	-	-	3/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O5'-C1'	3.82	1.51	1.41
4	A	801	LMT	O5B-C1B	3.70	1.51	1.41
9	A	810	GOL	C1-C2	2.12	1.59	1.51
4	A	801	LMT	O1B-C4'	2.11	1.49	1.43
4	A	801	LMT	O3'-C3'	2.01	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	C1'-C2'-C3'	4.13	118.69	110.01
4	A	801	LMT	C3'-C4'-C5'	3.61	118.94	110.93
4	A	801	LMT	O5'-C1'-C2'	3.16	116.87	110.37
4	A	801	LMT	O3B-C3B-C2B	2.92	117.26	110.38
4	A	801	LMT	O5'-C5'-C4'	2.92	115.75	109.72
4	A	801	LMT	O1B-C4'-C3'	2.77	114.28	107.23
4	A	801	LMT	O4'-C4B-C3B	-2.77	103.84	110.38
4	A	801	LMT	C2'-C3'-C4'	2.63	115.66	109.68
4	A	801	LMT	C1B-O1B-C4'	2.58	124.10	117.98
4	A	801	LMT	C1-O1'-C1'	2.57	118.07	113.68
4	A	801	LMT	O5B-C5B-C4B	2.47	114.15	109.70
4	A	801	LMT	O1'-C1'-C2'	2.32	111.80	108.27
4	A	801	LMT	C1B-O5B-C5B	2.25	118.12	113.72

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C2'-C1'-O1'-C1
4	A	801	LMT	O5B-C5B-C6B-O6B
4	A	801	LMT	C4B-C5B-C6B-O6B
6	A	803	PG4	O3-C5-C6-O4
6	A	806	PG4	O2-C3-C4-O3
6	A	807	PG4	O3-C5-C6-O4
7	A	811	1PE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C4'-C5'-C6'-O6'
6	A	806	PG4	O3-C5-C6-O4
4	A	801	LMT	C3'-C4'-O1B-C1B
4	A	801	LMT	O5'-C5'-C6'-O6'
4	A	801	LMT	O5'-C1'-O1'-C1
7	A	811	1PE	OH4-C13-C23-OH3
4	A	801	LMT	C3-C4-C5-C6
7	A	811	1PE	OH6-C15-C25-OH5
6	A	805	PG4	O3-C5-C6-O4
4	A	801	LMT	C7-C8-C9-C10
4	A	801	LMT	C5-C6-C7-C8
4	A	801	LMT	C1-C2-C3-C4
7	A	804	1PE	OH7-C16-C26-OH6
5	A	802	OCT	C4-C5-C6-C7
4	A	801	LMT	C6-C7-C8-C9
5	A	802	OCT	C3-C4-C5-C6
8	A	809	D12	C9-C10-C11-C12
4	A	801	LMT	C11-C10-C9-C8
6	A	805	PG4	O4-C7-C8-O5
4	A	801	LMT	C5'-C4'-O1B-C1B
9	A	810	GOL	O2-C2-C3-O3
6	A	807	PG4	C8-C7-O4-C6
8	A	809	D12	C3-C4-C5-C6
7	A	811	1PE	C25-C15-OH6-C26
4	A	801	LMT	C4-C5-C6-C7
6	A	806	PG4	C1-C2-O2-C3
7	A	804	1PE	OH2-C12-C22-OH3
6	A	805	PG4	C3-C4-O3-C5
6	A	806	PG4	C4-C3-O2-C2
6	A	803	PG4	C1-C2-O2-C3
6	A	806	PG4	C6-C5-O3-C4
6	A	808	PG4	O2-C3-C4-O3
6	A	808	PG4	O3-C5-C6-O4
4	A	801	LMT	C2B-C1B-O1B-C4'
4	A	801	LMT	O5B-C1B-O1B-C4'
6	A	803	PG4	O2-C3-C4-O3
6	A	806	PG4	C5-C6-O4-C7
6	A	803	PG4	C4-C3-O2-C2
7	A	811	1PE	C12-C22-OH3-C23
6	A	808	PG4	C3-C4-O3-C5
6	A	808	PG4	C6-C5-O3-C4
6	A	805	PG4	O2-C3-C4-O3

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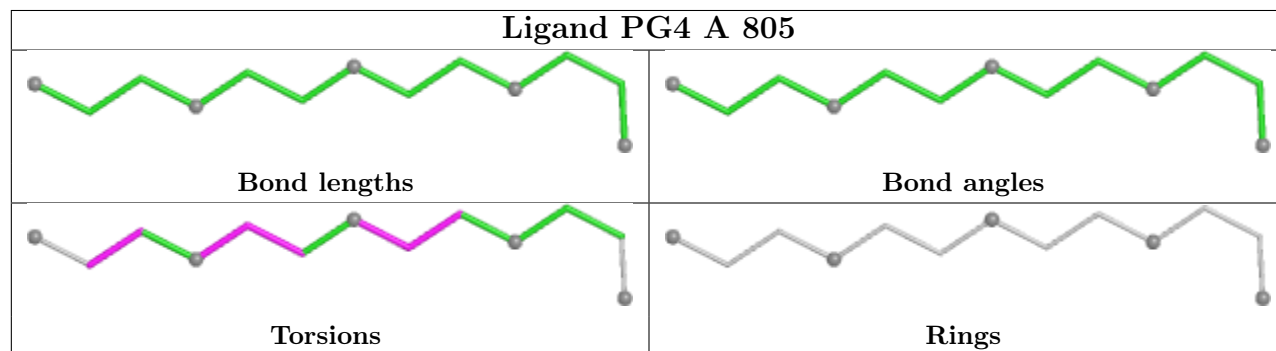
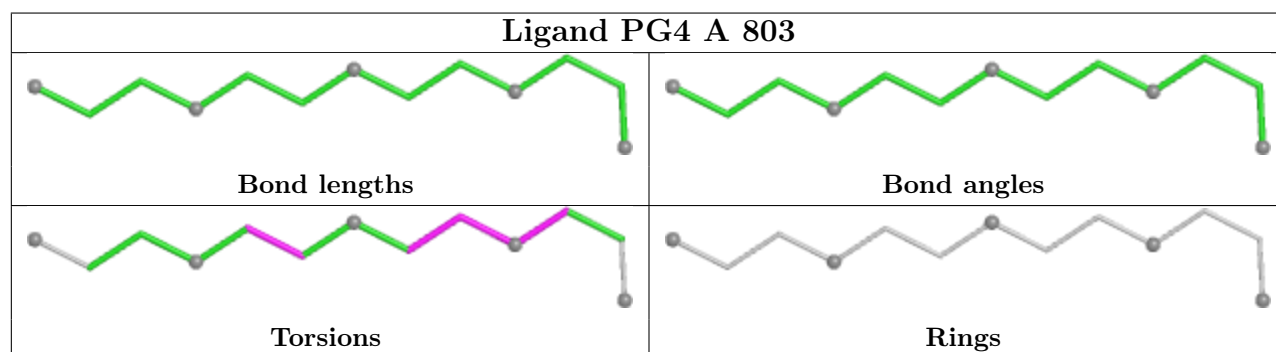
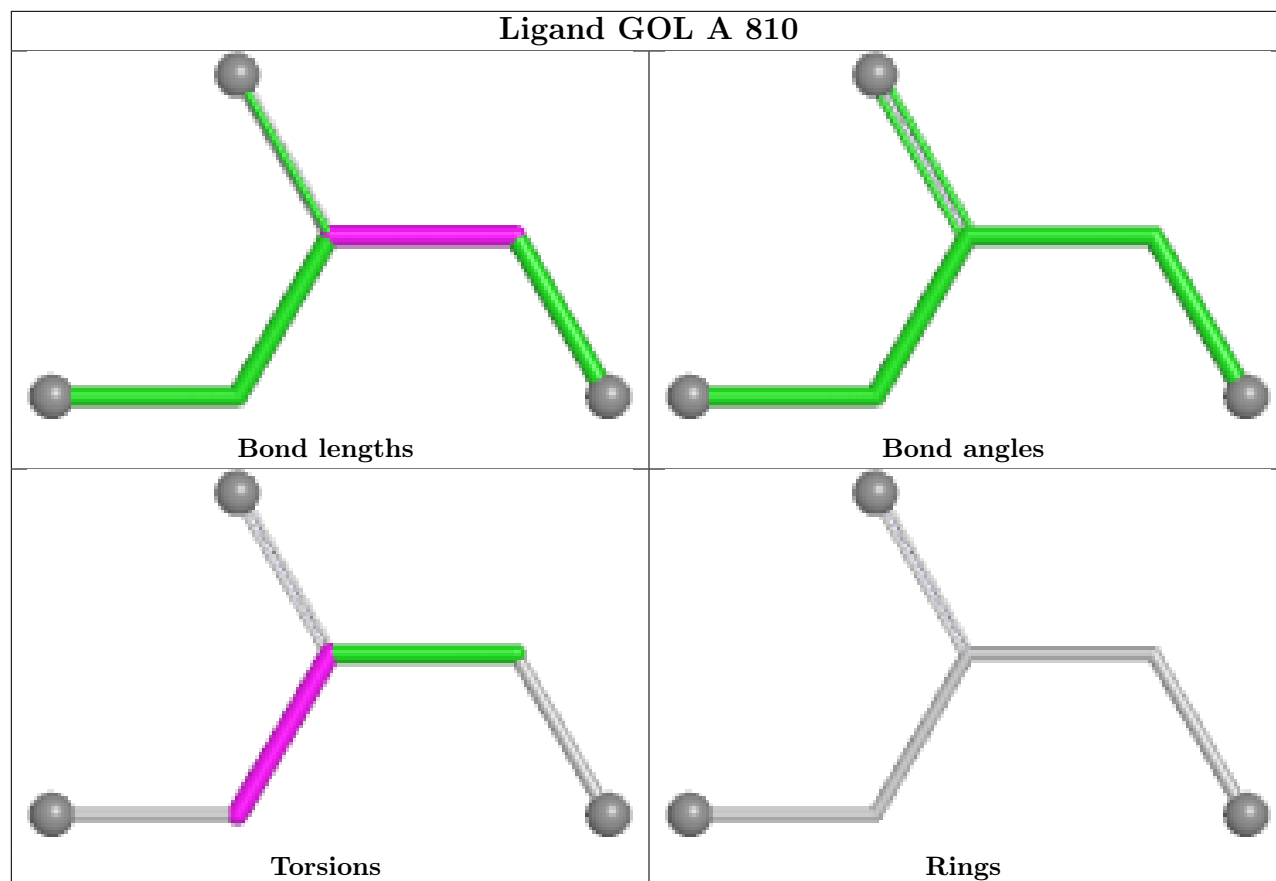
Mol	Chain	Res	Type	Atoms
8	A	809	D12	C1-C2-C3-C4
7	A	804	1PE	OH4-C13-C23-OH3
7	A	811	1PE	C15-C25-OH5-C14
6	A	807	PG4	O2-C3-C4-O3
10	A	812	D10	C5-C6-C7-C8
7	A	804	1PE	OH6-C15-C25-OH5
6	A	805	PG4	C5-C6-O4-C7
6	A	807	PG4	C1-C2-O2-C3

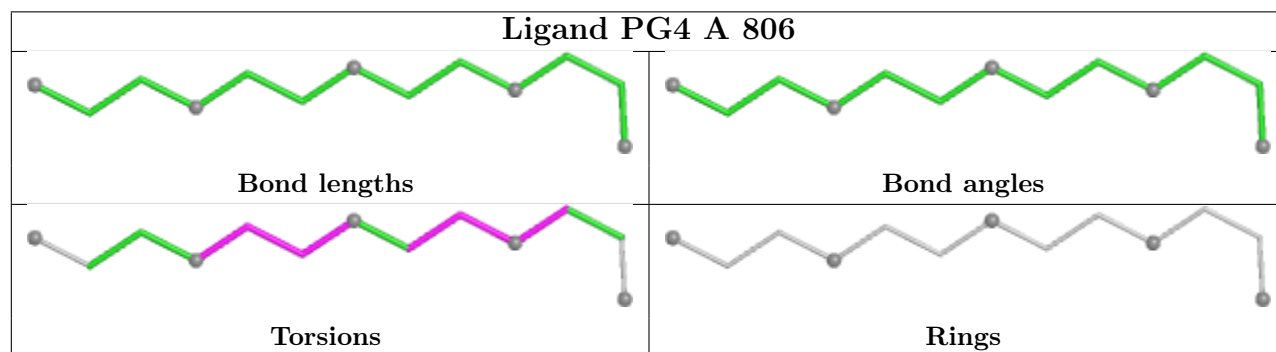
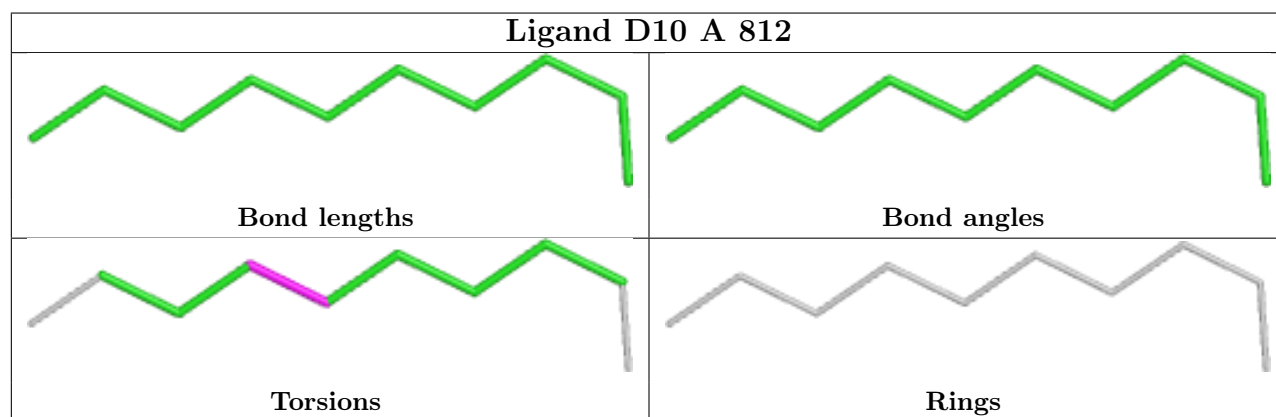
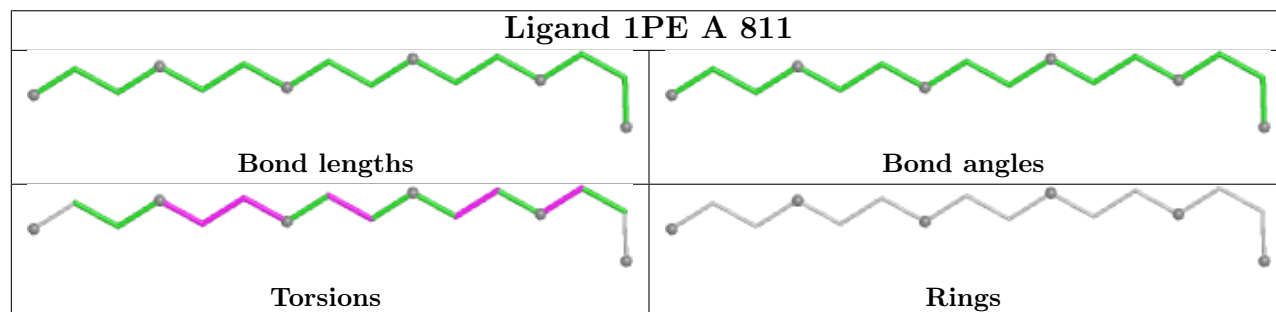
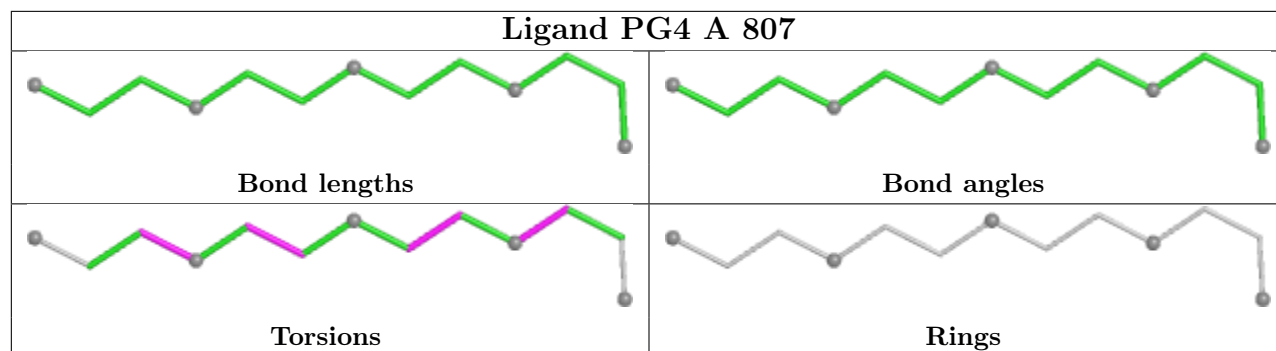
There are no ring outliers.

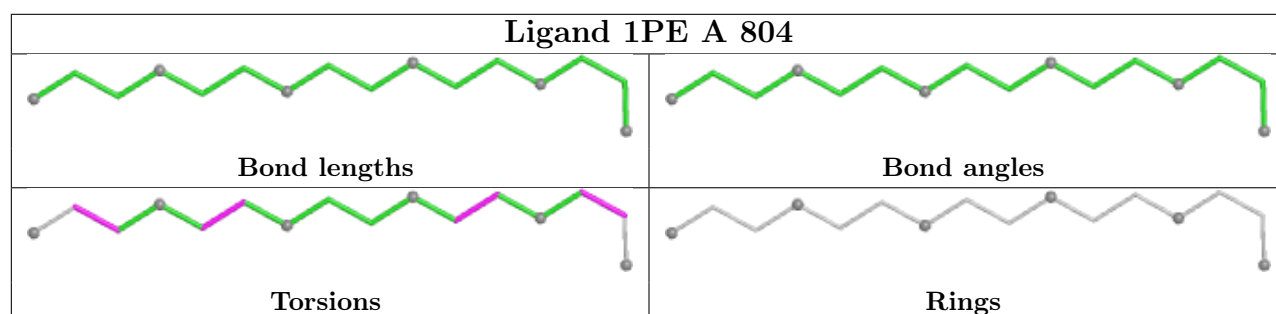
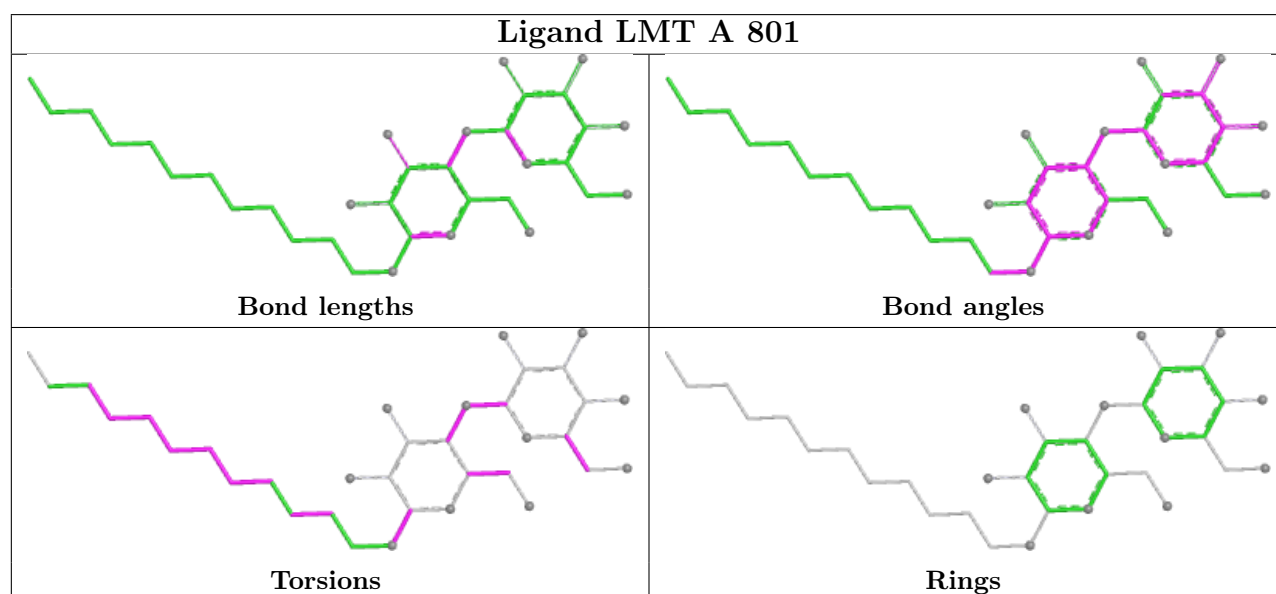
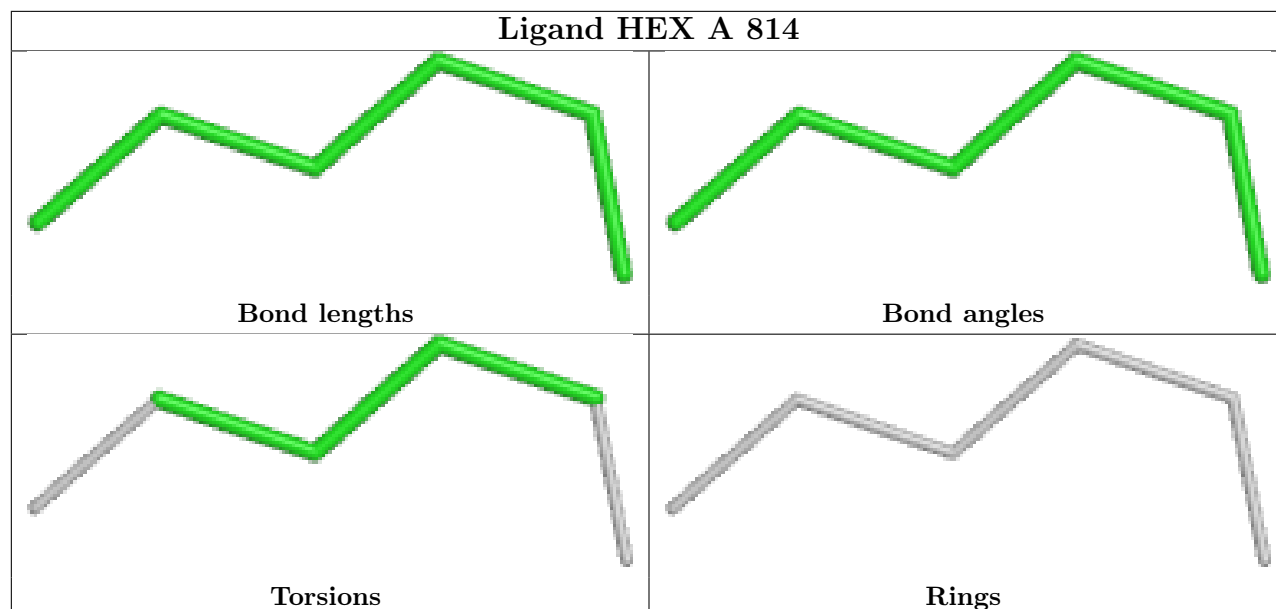
3 monomers are involved in 6 short contacts:

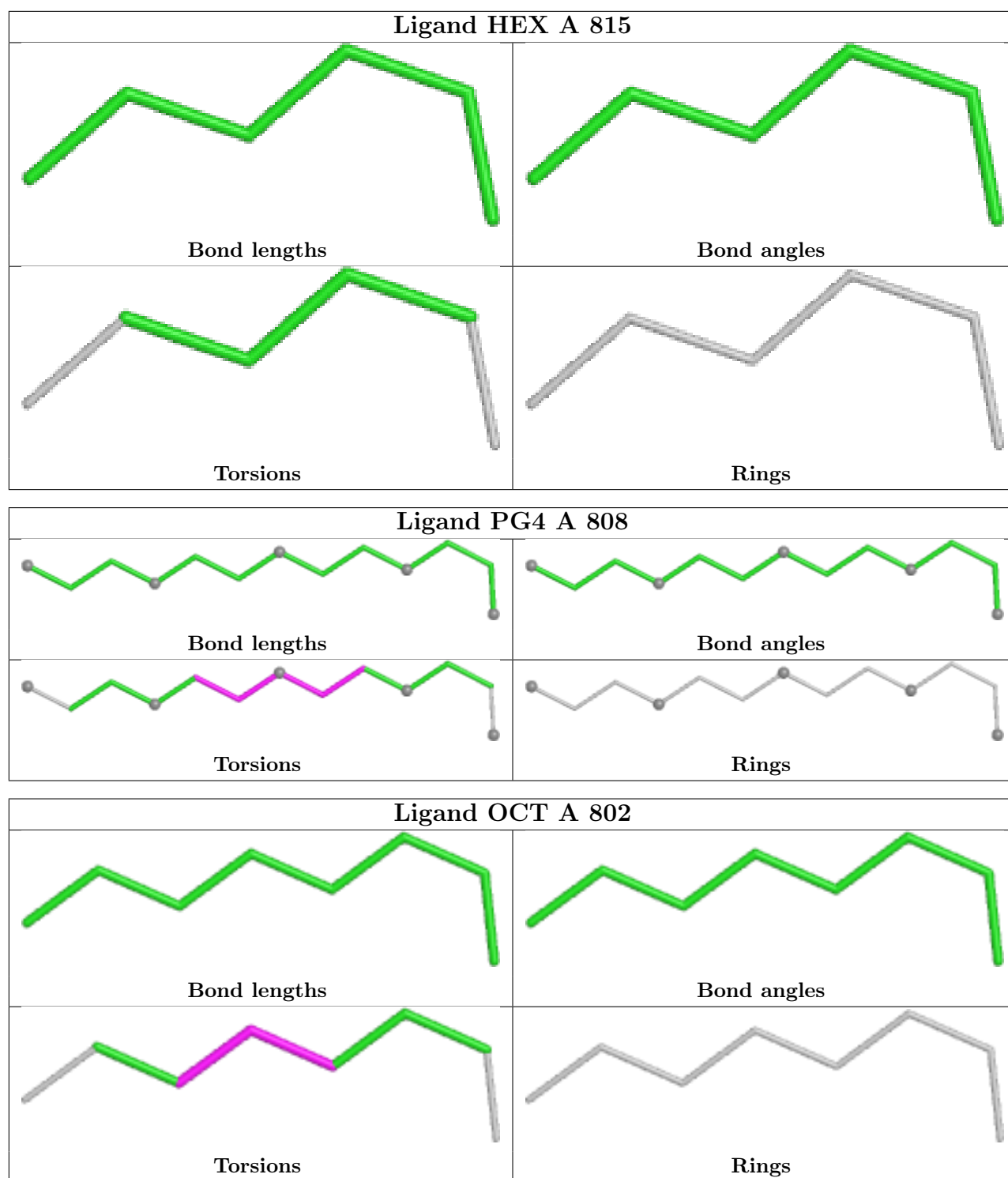
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	807	PG4	2	0
10	A	812	D10	2	0
4	A	801	LMT	2	0

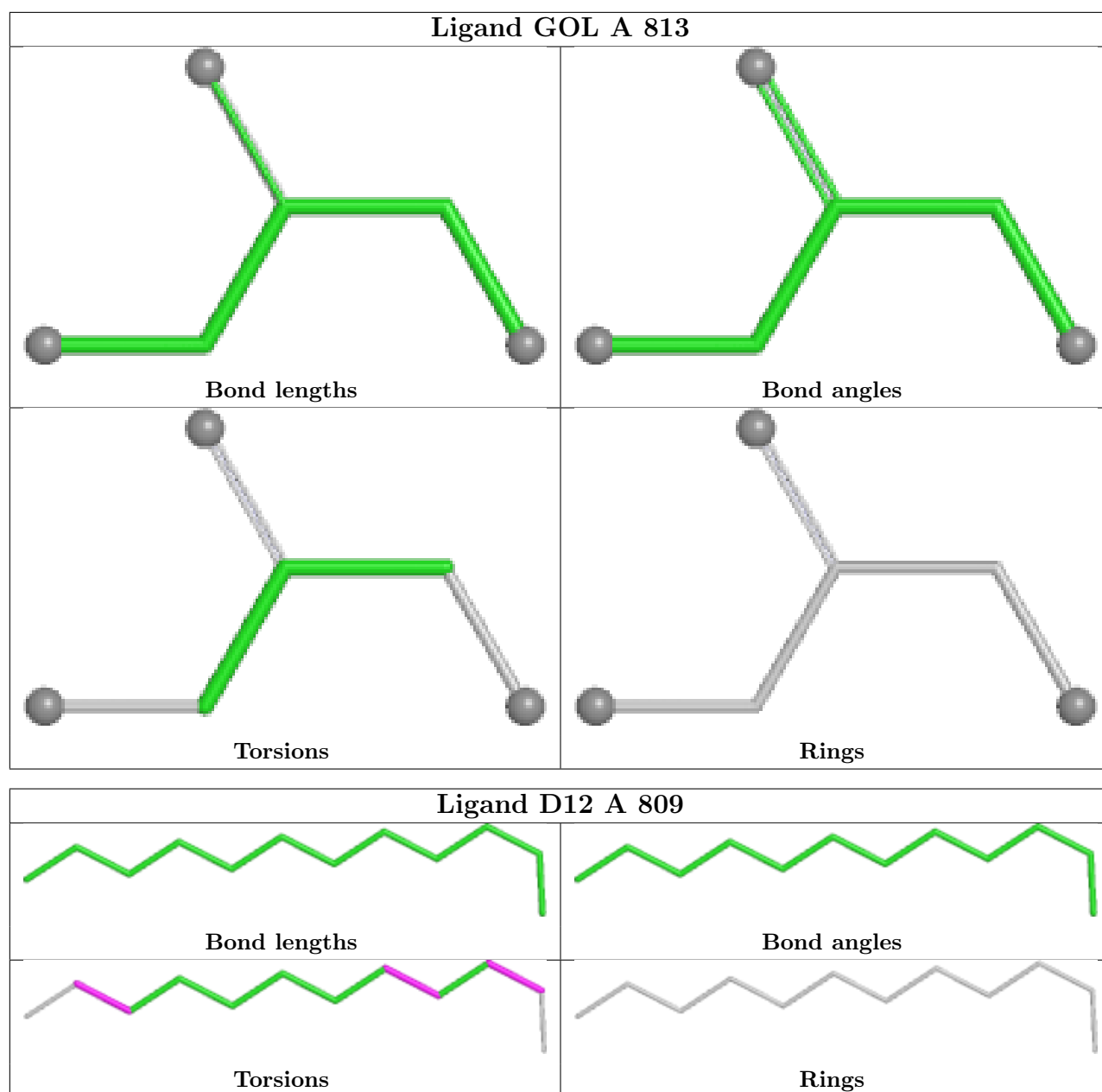
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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%)	1.49	110 (24%)  	48, 75, 122, 148	1 (0%)
2	B	127/127 (100%)	2.10	41 (32%)  	51, 77, 107, 120	2 (1%)
3	C	2/2 (100%)	0.28	0  	70, 70, 70, 77	0
All	All	580/618 (93%)	1.62	151 (26%)  	48, 76, 119, 148	3 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	PHE	16.4
2	B	83	ASN	14.4
2	B	84	SER	13.9
1	A	443	ASN	12.5
2	B	65	GLY	12.3
2	B	66	ARG	12.3
1	A	199	ASP	11.9
1	A	305	LEU	11.6
2	B	86	LYS	11.3
2	B	15	GLY	10.7
1	A	203	GLU	9.7
1	A	308	SER	9.1
1	A	304	ILE	8.4
2	B	14	ALA	8.3
2	B	57	LEU	7.8
1	A	140	ARG	7.7
1	A	162	LEU	7.6
2	B	64	LYS	7.6
2	B	16	GLY	7.4
1	A	136	PRO	7.0
2	B	68	THR	6.9
2	B	67	PHE	6.7
2	B	17	SER	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	6.1
2	B	85	LEU	6.1
2	B	59	TYR	6.0
1	A	183	LEU	5.9
1	A	161	SER	5.5
1	A	406	ALA	5.4
1	A	332	ILE	5.4
1	A	370	PHE	5.3
1	A	253	PHE	5.2
1	A	176	TYR	5.2
1	A	251	ILE	5.2
1	A	306	GLY	5.2
1	A	399	LEU	5.2
1	A	442	ASP	5.1
2	B	87	PRO	5.0
1	A	135	PRO	5.0
1	A	398	ALA	4.9
1	A	139	PRO	4.9
1	A	380	TRP	4.9
1	A	444	ILE	4.7
2	B	13	GLN	4.5
2	B	88	GLU	4.5
1	A	207	ARG	4.4
2	B	55	SER	4.4
1	A	138	ASP	4.3
1	A	296	ALA	4.2
2	B	63	VAL	4.2
1	A	134	TYR	4.1
1	A	166	ILE	4.0
1	A	303	GLU	4.0
1	A	309	ILE	4.0
2	B	41	PRO	3.8
1	A	322	VAL	3.7
2	B	75	LYS	3.6
1	A	187	LEU	3.6
2	B	81	GLN	3.5
2	B	44	GLU	3.5
1	A	323	VAL	3.5
2	B	115	GLN	3.4
2	B	62	VAL	3.4
2	B	61[A]	ASP	3.4
1	A	178	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	186	ALA	3.3
1	A	137	LYS	3.3
1	A	441	PRO	3.3
1	A	88	ALA	3.3
1	A	125	ASN	3.2
1	A	252	ILE	3.2
1	A	156	SER	3.2
1	A	449	GLU	3.2
1	A	100	MET	3.2
2	B	42	GLY	3.2
1	A	24	LEU	3.2
1	A	256	GLN	3.2
1	A	37	LEU	3.2
2	B	3	GLN	3.2
1	A	362	THR	3.2
1	A	110	ILE	3.2
1	A	206	PHE	3.1
1	A	14	ARG	3.1
1	A	155	GLY	3.1
2	B	43	LYS	3.1
1	A	15	PRO	3.0
1	A	170	PHE	3.0
1	A	402	ALA	3.0
1	A	36	VAL	3.0
1	A	99	GLY	2.9
1	A	184	ILE	2.9
1	A	236	GLU	2.9
1	A	405	ALA	2.9
1	A	254	PHE	2.9
1	A	169	ARG	2.9
2	B	74	VAL	2.9
1	A	403	MET	2.8
1	A	50	GLU	2.8
1	A	194	ARG	2.8
1	A	413	MET	2.8
1	A	98	THR	2.8
1	A	415	PHE	2.8
1	A	91	LEU	2.8
1	A	97	MET	2.8
1	A	107	LEU	2.7
1	A	154	ILE	2.7
1	A	229	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	478	TRP	2.6
1	A	198	LYS	2.6
2	B	12	VAL	2.6
1	A	196	MET	2.6
1	A	92	ALA	2.6
1	A	33	VAL	2.6
1	A	13	PRO	2.6
1	A	408	VAL	2.6
1	A	445	THR	2.5
1	A	372	ASP	2.5
1	A	314	PHE	2.5
2	B	117	THR	2.4
2	B	69	VAL	2.4
1	A	124	ALA	2.4
1	A	250	THR	2.4
1	A	268	MET	2.4
1	A	25	TRP	2.3
1	A	301	HIS	2.3
1	A	425	ALA	2.3
1	A	153	ASN	2.3
1	A	119	ASN	2.2
1	A	324	LEU	2.2
1	A	204	PRO	2.2
2	B	46	GLU	2.2
2	B	111	ALA	2.2
1	A	191	ILE	2.2
1	A	424	GLN	2.1
1	A	248	VAL	2.1
2	B	2	VAL	2.1
2	B	34	VAL	2.1
1	A	407	LEU	2.1
1	A	212	SER	2.1
2	B	56	GLY	2.1
1	A	35	GLY	2.1
1	A	427	ALA	2.1
1	A	267	LYS	2.1
1	A	77	LEU	2.1
1	A	365	ALA	2.1
1	A	416	ILE	2.1
2	B	82	MET	2.0
1	A	89	LEU	2.0
2	B	4	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	330	ALA	2.0
1	A	463	LEU	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](#)

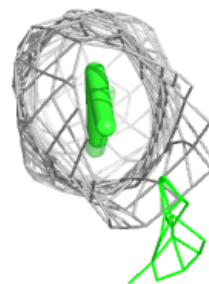
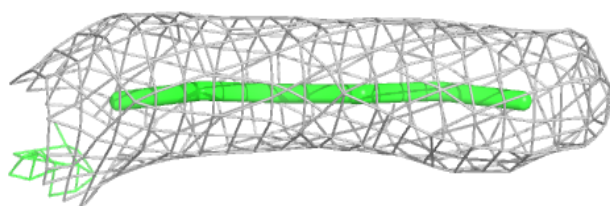
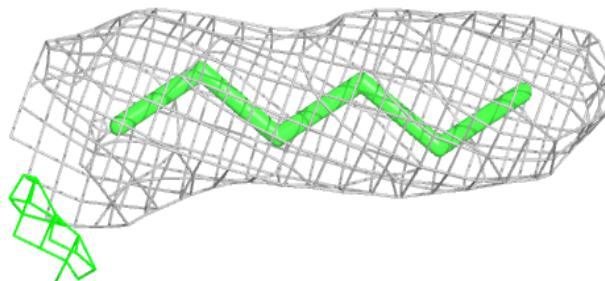
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	HEX	A	815	6/6	0.56	0.37	67,78,79,84	0
10	D10	A	812	10/10	0.59	0.58	83,92,98,99	0
9	GOL	A	810	6/6	0.59	0.23	100,106,115,115	0
6	PG4	A	806	13/13	0.61	0.28	89,97,110,111	0
8	D12	A	809	12/12	0.67	0.38	73,90,94,96	0
6	PG4	A	808	13/13	0.67	0.34	83,91,103,104	0
9	GOL	A	813	6/6	0.69	0.19	90,92,97,98	0
6	PG4	A	803	13/13	0.72	0.31	78,90,106,107	0
6	PG4	A	805	13/13	0.73	0.27	85,98,113,115	0
5	OCT	A	802	8/8	0.73	0.31	63,77,80,83	0
7	1PE	A	811	16/16	0.77	0.18	91,98,104,106	0
11	HEX	A	814	6/6	0.78	0.23	79,85,94,95	0
4	LMT	A	801	35/35	0.78	0.17	67,90,112,119	0
6	PG4	A	807	13/13	0.82	0.19	82,91,99,101	0
7	1PE	A	804	16/16	0.88	0.13	65,88,109,110	0

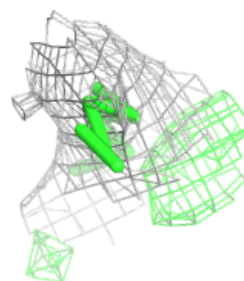
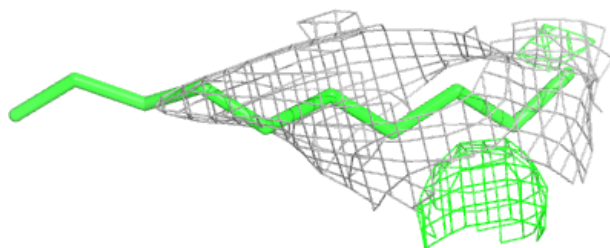
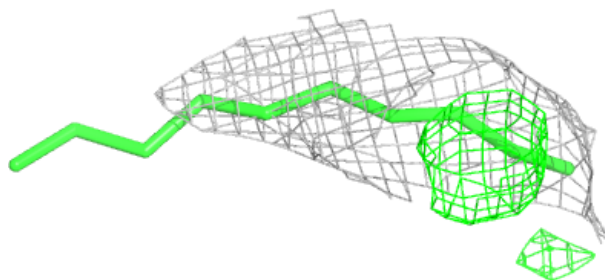
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

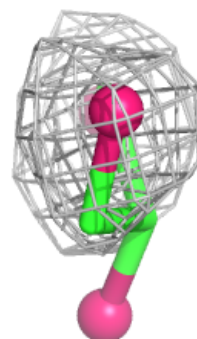
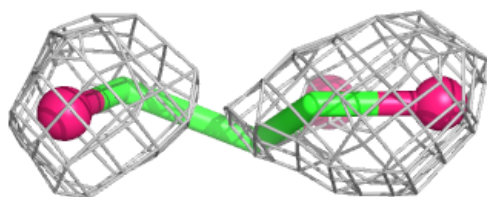
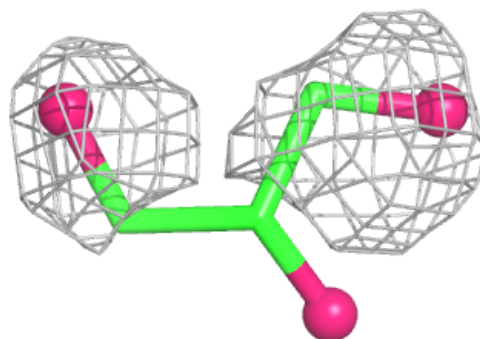
**Electron density around D10 A 812:**

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

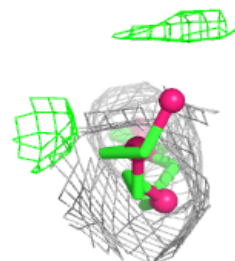
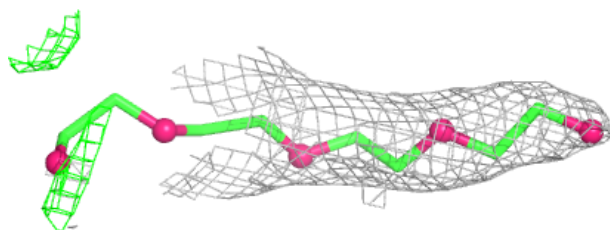
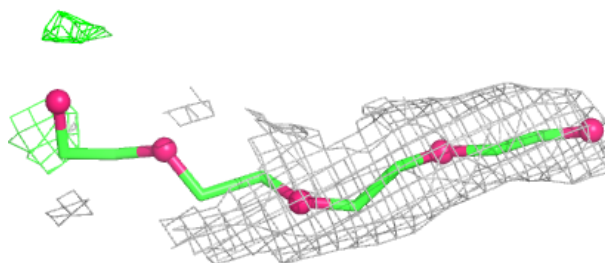


Electron density around GOL A 810:

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

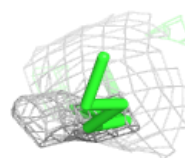
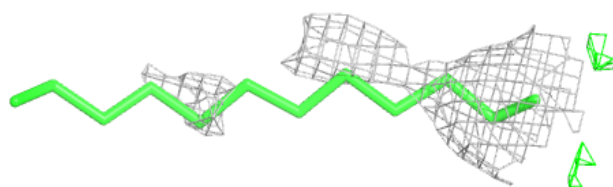
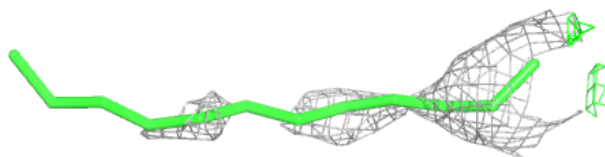
**Electron density around PG4 A 806:**

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

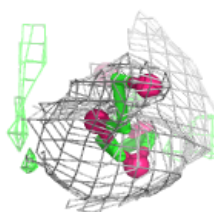
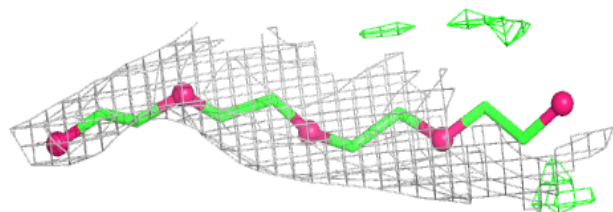
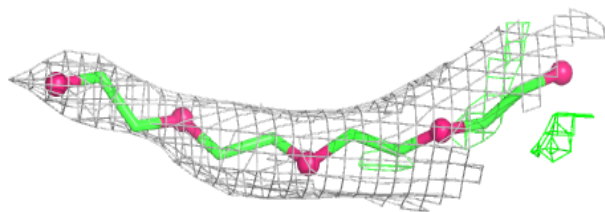


Electron density around D12 A 809:

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

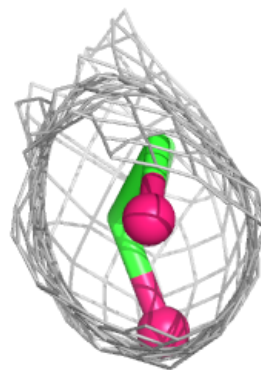
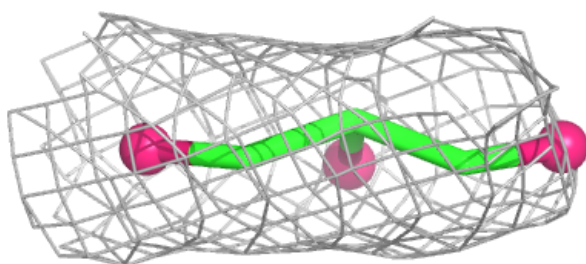
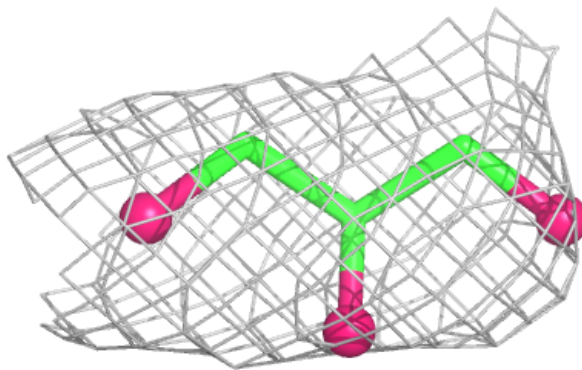
**Electron density around PG4 A 808:**

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

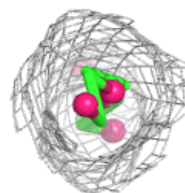
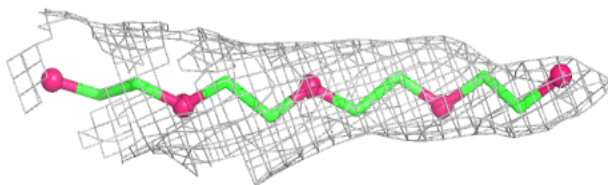
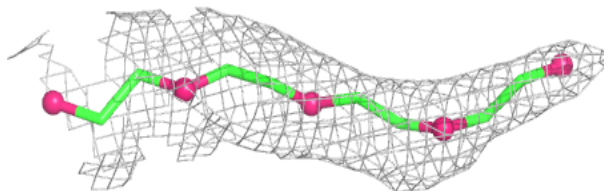


Electron density around GOL A 813:

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

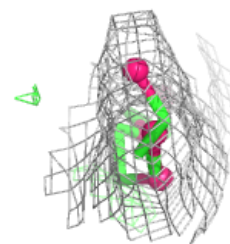
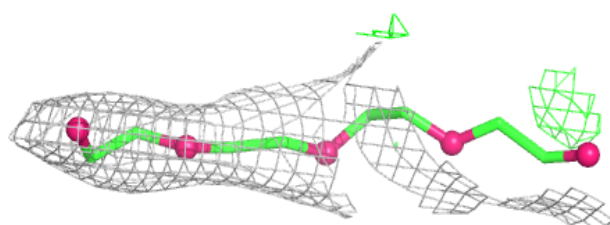
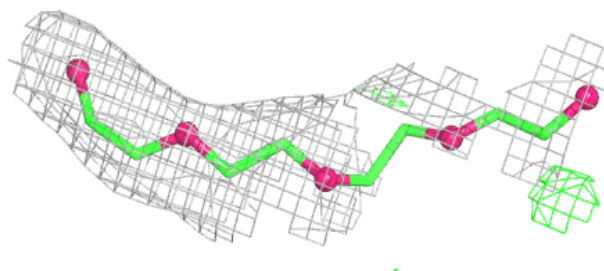
**Electron density around PG4 A 803:**

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

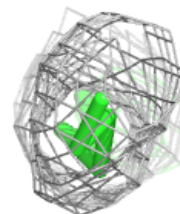
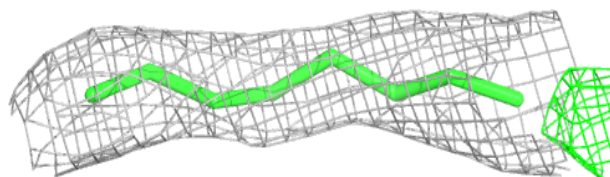
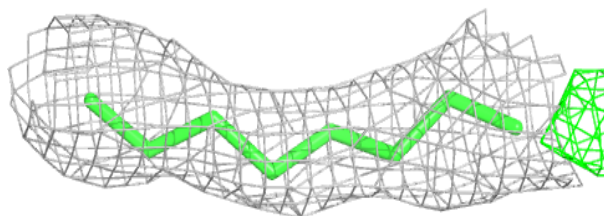


Electron density around PG4 A 805:

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

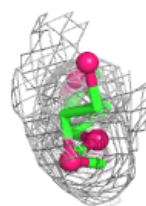
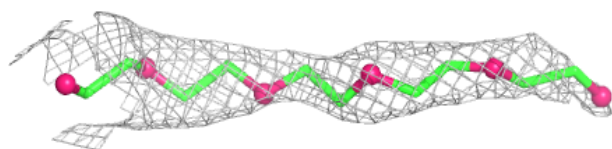
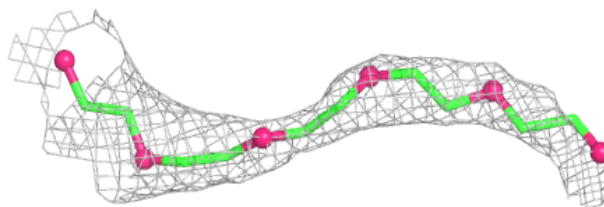
**Electron density around OCT A 802:**

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

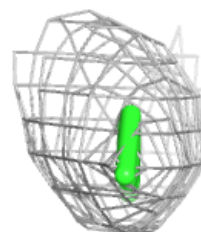
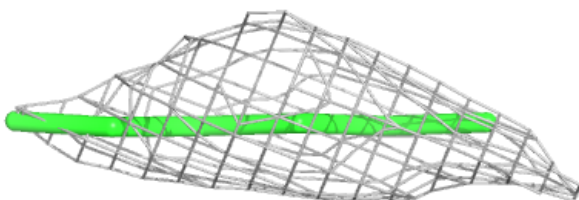
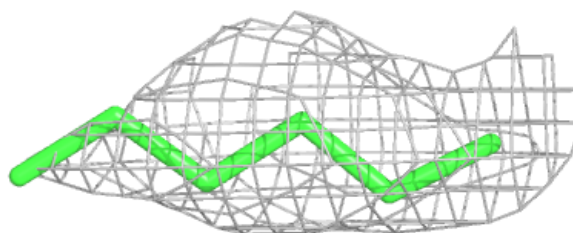


Electron density around 1PE A 811:

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

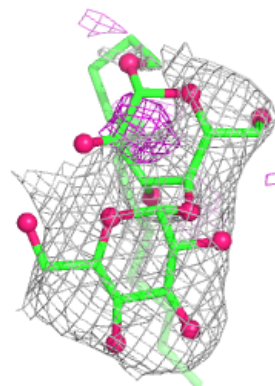
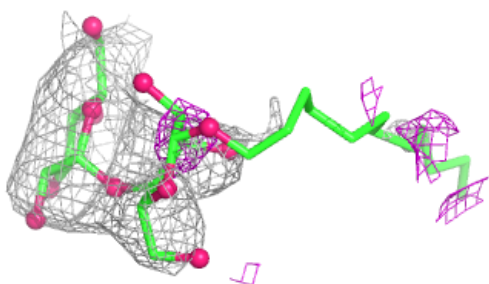
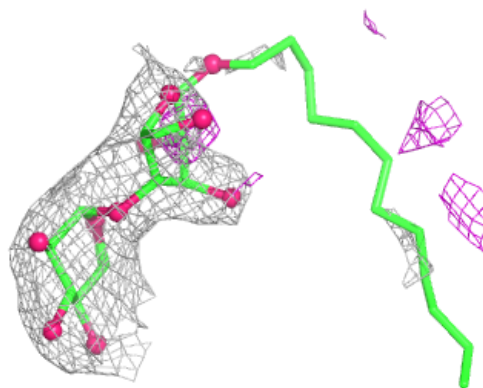
**Electron density around HEX A 814:**

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

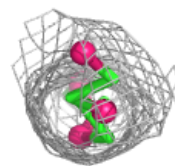
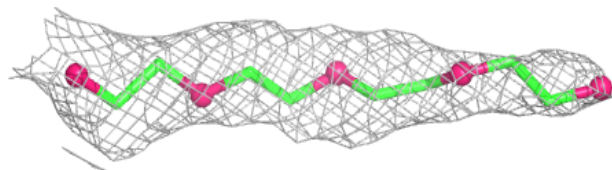
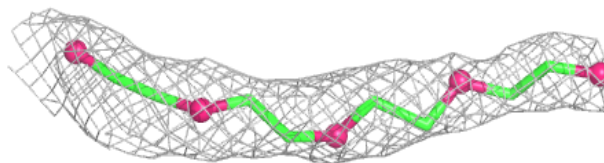


Electron density around LMT A 801:

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

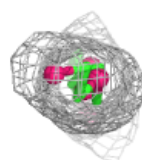
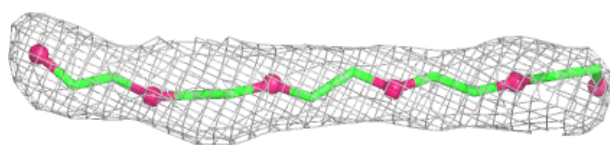
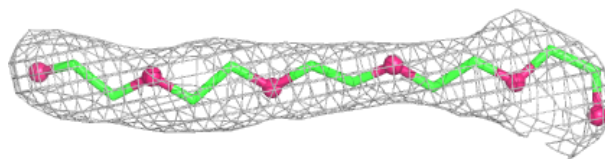
**Electron density around PG4 A 807:**

$2mF_o-DF_c$ (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.