



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:21 AM UTC

PDB ID : 8B1A / pdb_00008b1a
Title : DtpB-Nb132-AI
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 : 2.15 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

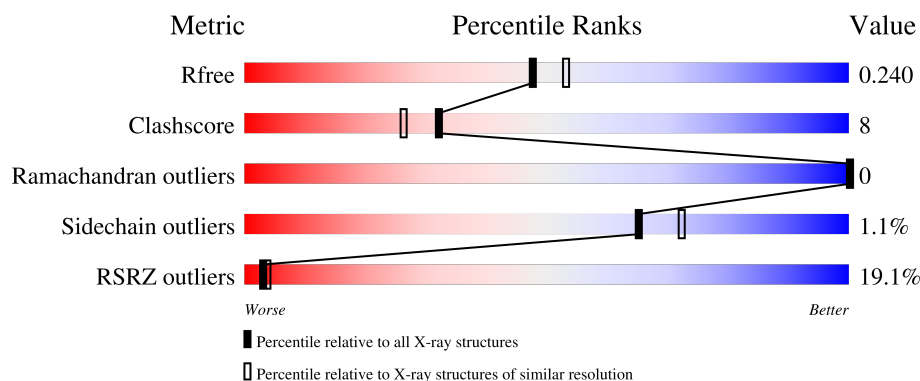
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	19% 79% 13% 8%
2	B	127	13% 91% 9%
3	C	2	50% 100%

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 4787 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			

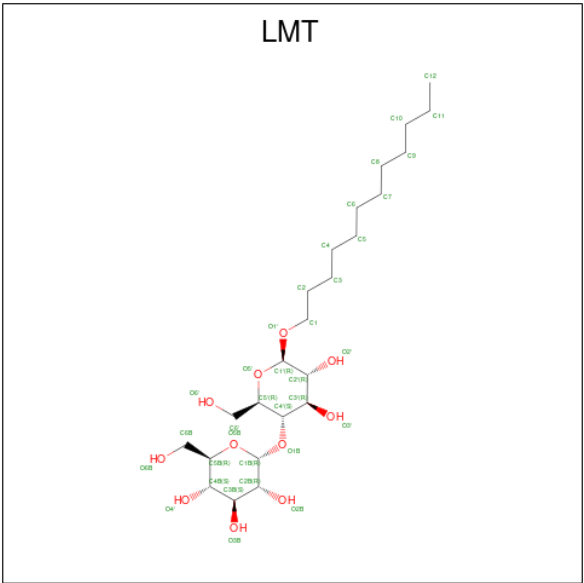
- Molecule 2 is a protein called Nanobody 132.

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-ILE.

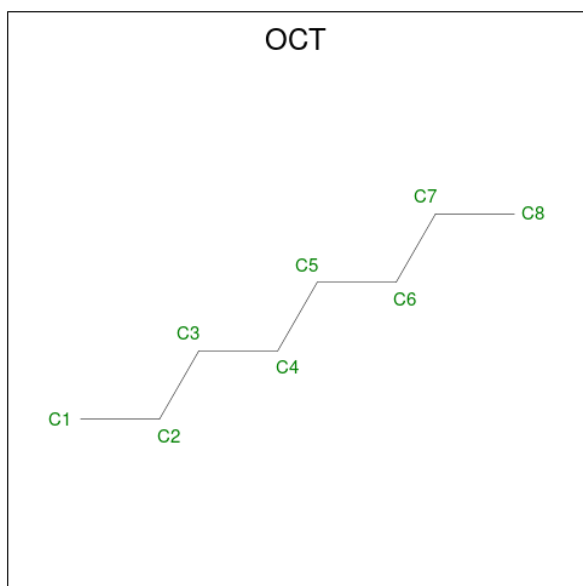
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			14	9	2	3			

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



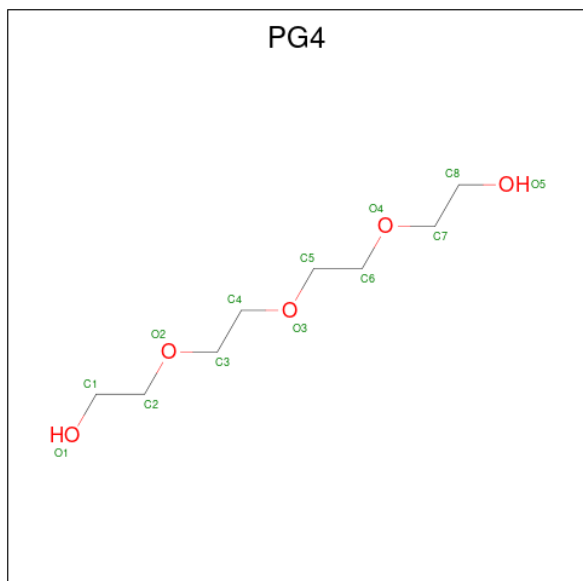
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

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



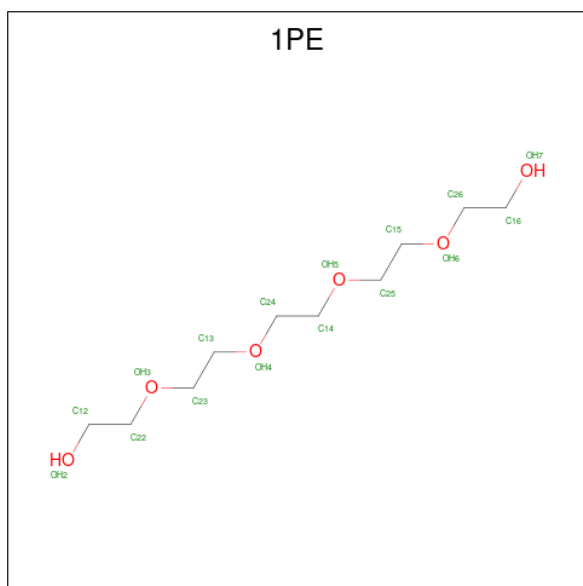
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			8	8		

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



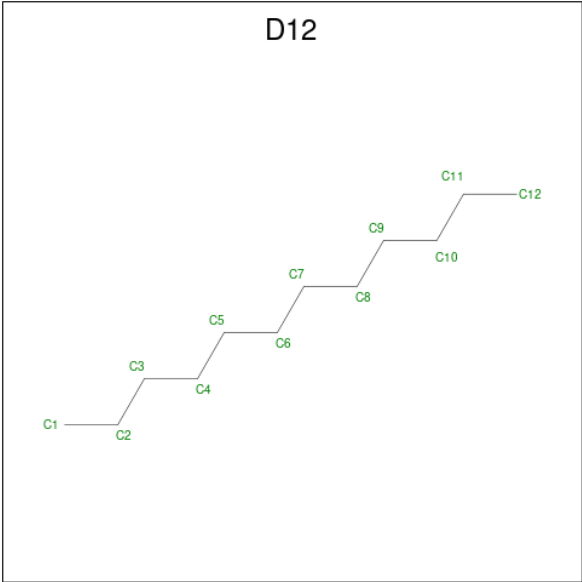
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

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



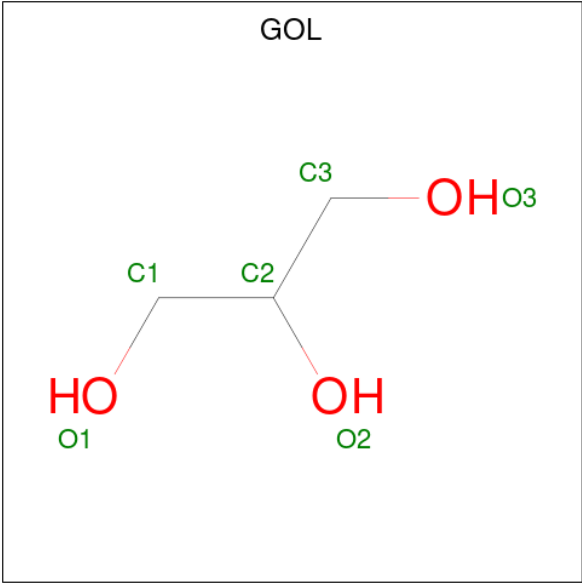
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

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



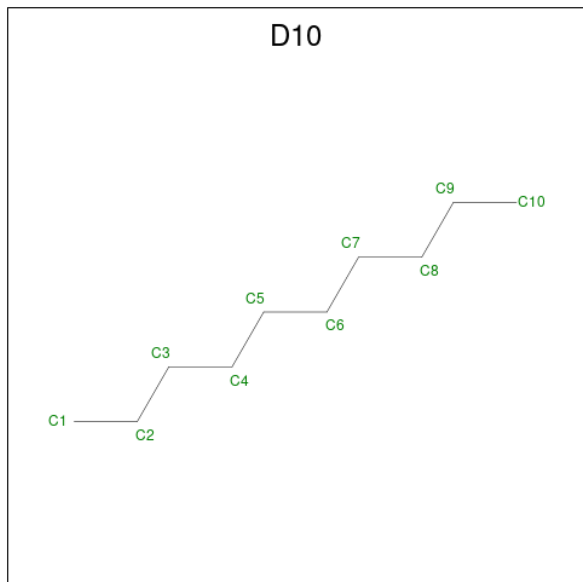
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	C	0	0
			12	12		

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



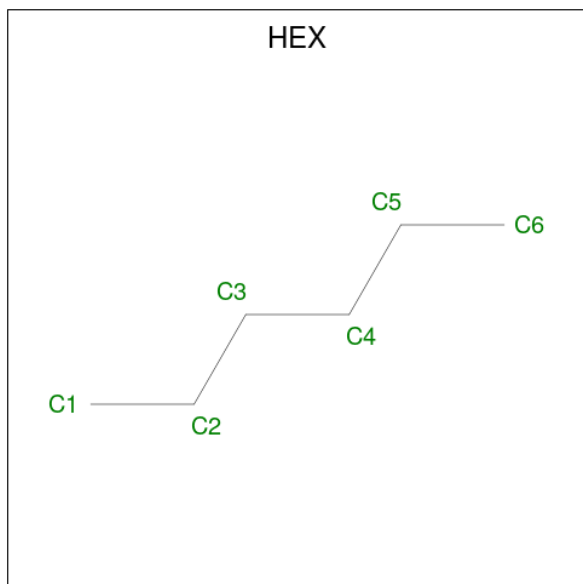
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- 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		

Continued on next page...

Continued from previous page...

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

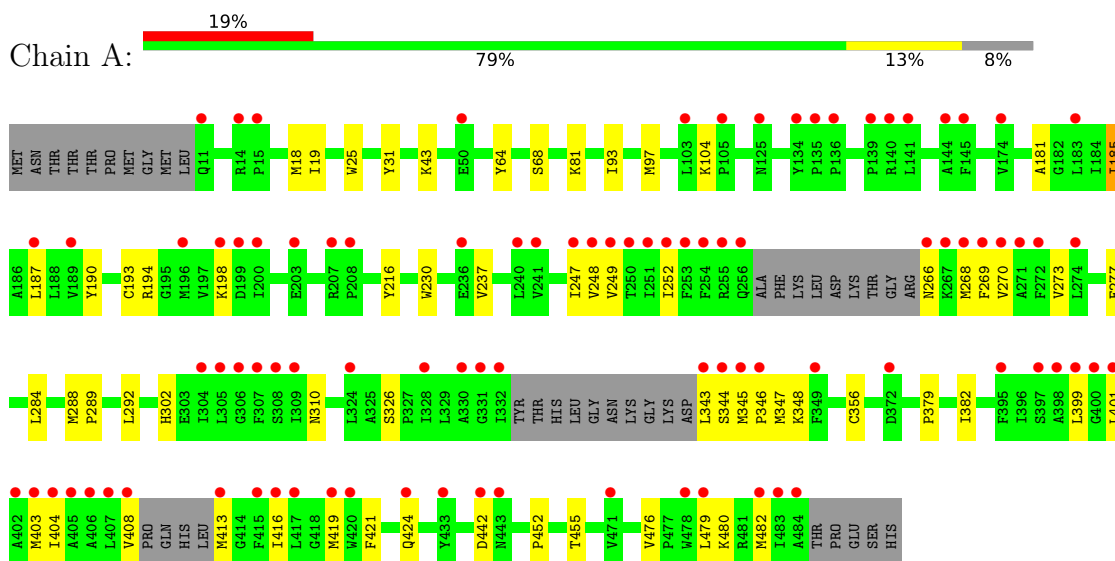
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	75	Total O 75 75	0	0
12	B	55	Total O 55 55	0	0
12	C	1	Total O 1 1	0	0

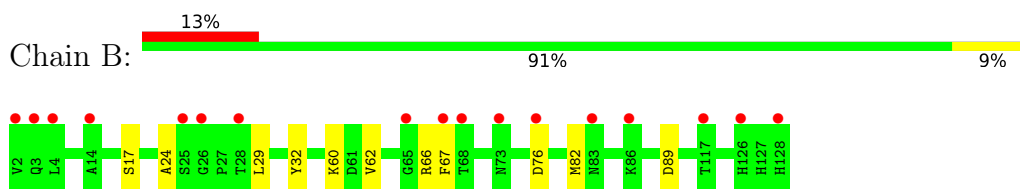
3 Residue-property plots [i](#)

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.

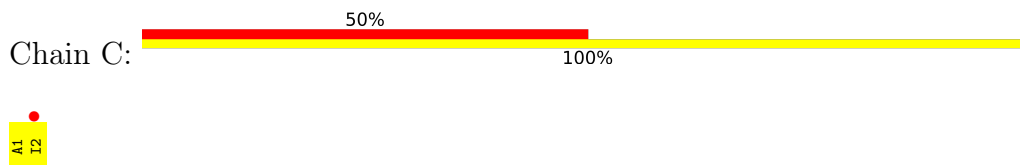
- Molecule 1: Dipeptide and tripeptide permease B



- Molecule 2: Nanobody 132



- Molecule 3: ALA-ILE



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	54.32Å 125.74Å 168.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.69 – 2.15 51.69 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.69-2.15) 93.3 (51.69-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.239 0.215 , 0.240	Depositor DCC
R_{free} test set	3115 reflections (4.15%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.6	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	0.92	EDS
Total number of atoms	4787	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, PG4, D12, 1PE, D10, GOL, OCT, LMT

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	0.37	0/3572	0.53	0/4859
2	B	0.43	0/1004	0.64	0/1361
3	C	0.47	0/13	0.54	0/15
All	All	0.38	0/4589	0.56	0/6235

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	63	0
2	B	976	0	939	10	0
3	C	14	0	18	1	0
4	A	35	0	46	5	0
5	A	8	0	18	0	0
6	A	65	0	90	1	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	12	0	28	0	0
12	A	75	0	0	2	0
12	B	55	0	0	1	0
12	C	1	0	0	0	0
All	All	4787	0	4852	76	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 8.

All (76) 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:348:LYS:HD3	1:A:399:LEU:HD21	1.52	0.89
1:A:266:ASN:HA	1:A:269:PHE:HD2	1.41	0.85
1:A:270:VAL:CG1	1:A:479:LEU:HD21	2.07	0.84
1:A:266:ASN:OD1	1:A:269:PHE:CE2	2.31	0.83
1:A:348:LYS:HD3	1:A:399:LEU:CD2	2.11	0.81
1:A:266:ASN:HA	1:A:269:PHE:CD2	2.19	0.77
1:A:270:VAL:CG1	1:A:479:LEU:CD2	2.63	0.76
1:A:270:VAL:HG13	1:A:479:LEU:HD21	1.68	0.75
1:A:346:PRO:HG3	1:A:479:LEU:HD22	1.69	0.74
1:A:270:VAL:HG13	1:A:479:LEU:CD2	2.17	0.73
1:A:345:MET:HE3	1:A:403:MET:HB2	1.72	0.72
1:A:25:TRP:CE2	1:A:185:ILE:HD11	2.28	0.67
2:B:29:LEU:CB	2:B:76:ASP:OD1	2.44	0.66
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.79	0.65
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.78	0.65
2:B:29:LEU:HB2	2:B:76:ASP:OD1	1.97	0.64
1:A:266:ASN:OD1	1:A:269:PHE:HE2	1.82	0.62
1:A:270:VAL:HG11	1:A:479:LEU:CD2	2.30	0.61
1:A:266:ASN:CA	1:A:269:PHE:HD2	2.12	0.60
1:A:181:ALA:O	1:A:185:ILE:HG23	2.00	0.60
1:A:268:MET:HE1	1:A:408:VAL:HA	1.84	0.59
1:A:346:PRO:HB3	1:A:479:LEU:HD13	1.83	0.59
1:A:348:LYS:CD	1:A:399:LEU:HD21	2.28	0.59
1:A:194:ARG:HG2	1:A:198:LYS:HZ1	1.68	0.58
1:A:413:MET:O	1:A:416:ILE:HG13	2.04	0.57
1:A:273:VAL:O	1:A:277:GLU:HG3	2.05	0.56
1:A:270:VAL:HG21	1:A:482:MET:HB2	1.87	0.56
1:A:302:HIS:HD2	12:B:228:HOH:O	1.87	0.56
1:A:216:TYR:HB3	6:A:807:PG4:H42	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG11	1:A:479:LEU:HD23	1.86	0.55
1:A:401:LEU:HA	1:A:404:ILE:HB	1.88	0.54
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.35	0.54
1:A:379:PRO:O	1:A:382:ILE:HG22	2.06	0.54
1:A:292:LEU:HB3	12:A:915:HOH:O	2.08	0.54
1:A:345:MET:HE3	1:A:403:MET:CB	2.37	0.54
1:A:345:MET:HE3	1:A:403:MET:HG3	1.90	0.53
1:A:345:MET:HE1	1:A:399:LEU:HG	1.90	0.53
1:A:343:LEU:HA	1:A:347:MET:HB3	1.91	0.53
1:A:442:ASP:OD2	12:A:901:HOH:O	2.18	0.53
1:A:68:SER:HB3	1:A:421:PHE:CD2	2.44	0.52
2:B:29:LEU:HB3	2:B:76:ASP:OD1	2.10	0.52
1:A:343:LEU:N	1:A:480:LYS:HZ3	2.08	0.52
1:A:230:TRP:CH2	1:A:237:VAL:HG21	2.46	0.51
1:A:284:LEU:HD12	1:A:356:CYS:HB3	1.92	0.51
1:A:248:VAL:O	1:A:252:ILE:HG23	2.14	0.48
1:A:343:LEU:HA	1:A:347:MET:CB	2.43	0.48
1:A:346:PRO:CG	1:A:479:LEU:HD22	2.42	0.48
1:A:25:TRP:CD2	1:A:185:ILE:HD11	2.48	0.47
1:A:64:TYR:CE2	1:A:424:GLN:HB2	2.49	0.47
1:A:81:LYS:HB3	1:A:190:TYR:OH	2.13	0.47
1:A:345:MET:HB3	1:A:346:PRO:HD3	1.96	0.47
2:B:67:PHE:CZ	2:B:82:MET:HG2	2.50	0.47
1:A:18:MET:HE2	1:A:19:ILE:HG13	1.97	0.46
1:A:93:ILE:HG22	1:A:97:MET:HE2	1.95	0.46
4:A:801:LMT:H4B	2:B:32:TYR:OH	2.14	0.46
1:A:104:LYS:HB3	10:A:812:D10:H42	1.98	0.46
1:A:347:MET:HE2	1:A:476:VAL:HG11	1.98	0.45
2:B:24:ALA:HB2	2:B:29:LEU:HD13	2.00	0.44
1:A:452:PRO:HA	1:A:455:THR:OG1	2.18	0.44
1:A:43:LYS:HA	1:A:43:LYS:HD2	1.81	0.43
1:A:266:ASN:OD1	1:A:269:PHE:CD2	2.70	0.43
1:A:401:LEU:HD12	1:A:404:ILE:HB	2.01	0.43
1:A:270:VAL:HA	1:A:273:VAL:HG12	2.01	0.42
4:A:801:LMT:H41	4:A:801:LMT:H12	1.63	0.42
1:A:31:TYR:CZ	3:C:1:ALA:HB1	2.54	0.42
1:A:249:VAL:CG1	1:A:419:MET:HG3	2.49	0.42
1:A:413:MET:O	1:A:416:ILE:N	2.52	0.42
2:B:67:PHE:CE2	2:B:82:MET:HG2	2.55	0.42
2:B:17:SER:HA	2:B:82:MET:O	2.19	0.41
4:A:801:LMT:H3'	4:A:801:LMT:H5B	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TRP:CZ3	1:A:237:VAL:HG21	2.55	0.41
1:A:345:MET:HE3	1:A:403:MET:CG	2.50	0.41
1:A:247:ILE:HD12	1:A:248:VAL:N	2.36	0.41
1:A:288:MET:HB2	1:A:289:PRO:HD3	2.03	0.41
4:A:801:LMT:H41	4:A:801:LMT:H2'	2.03	0.41
1:A:310:ASN:HB2	4:A:801:LMT:H6'1	2.04	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%)	435 (98%)	8 (2%)	0	100	100
2	B	126/127 (99%)	123 (98%)	3 (2%)	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%)	364 (99%)	4 (1%)	65	72
2	B	102/101 (101%)	102 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	1/1 (100%)	0	1 (100%)	0	0
All	All	471/503 (94%)	466 (99%)	5 (1%)	65	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ILE
1	A	187	LEU
1	A	326	SER
1	A	344	SER
3	C	2	ILE

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	234	ASN
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
4	LMT	A	801	-	36,36,36	1.18	2 (5%)	47,47,47	1.34	5 (10%)
7	1PE	A	811	-	15,15,15	0.54	0	14,14,14	0.38	0
9	GOL	A	813	-	5,5,5	1.00	0	5,5,5	1.04	0
11	HEX	A	814	-	5,5,5	0.38	0	4,4,4	0.59	0
7	1PE	A	804	-	15,15,15	0.51	0	14,14,14	0.32	0
11	HEX	A	815	-	5,5,5	0.36	0	4,4,4	0.57	0
5	OCT	A	802	-	7,7,7	0.36	0	6,6,6	0.70	0
10	D10	A	812	-	9,9,9	0.34	0	8,8,8	0.82	0
6	PG4	A	805	-	12,12,12	0.51	0	11,11,11	0.32	0
6	PG4	A	807	-	12,12,12	0.52	0	11,11,11	0.28	0
9	GOL	A	810	-	5,5,5	0.96	0	5,5,5	1.03	0
6	PG4	A	803	-	12,12,12	0.53	0	11,11,11	0.25	0
8	D12	A	809	-	11,11,11	0.39	0	10,10,10	0.78	0
6	PG4	A	808	-	12,12,12	0.53	0	11,11,11	0.31	0
6	PG4	A	806	-	12,12,12	0.55	0	11,11,11	0.34	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
4	LMT	A	801	-	-	15/21/61/61	0/2/2/2
7	1PE	A	811	-	-	6/13/13/13	-
9	GOL	A	813	-	-	0/4/4/4	-
11	HEX	A	814	-	-	0/3/3/3	-
7	1PE	A	804	-	-	6/13/13/13	-
11	HEX	A	815	-	-	0/3/3/3	-
5	OCT	A	802	-	-	2/5/5/5	-
10	D10	A	812	-	-	1/7/7/7	-
6	PG4	A	805	-	-	5/10/10/10	-
6	PG4	A	807	-	-	4/10/10/10	-
9	GOL	A	810	-	-	1/4/4/4	-
6	PG4	A	803	-	-	4/10/10/10	-
8	D12	A	809	-	-	3/9/9/9	-
6	PG4	A	808	-	-	4/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	A	806	-	-	6/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O5B-C1B	3.60	1.51	1.41
4	A	801	LMT	O5'-C1'	3.28	1.50	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	C2'-C3'-C4'	3.68	118.03	109.68
4	A	801	LMT	C1'-C2'-C3'	3.21	116.76	110.01
4	A	801	LMT	C3'-C4'-C5'	2.63	116.76	110.93
4	A	801	LMT	C6'-C5'-C4'	-2.23	107.11	113.38
4	A	801	LMT	O5'-C5'-C4'	2.02	113.90	109.72

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	O5'-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
6	A	806	PG4	O3-C5-C6-O4
4	A	801	LMT	C5'-C4'-O1B-C1B
7	A	811	1PE	OH4-C13-C23-OH3
4	A	801	LMT	C3-C4-C5-C6
7	A	811	1PE	OH6-C15-C25-OH5
4	A	801	LMT	C7-C8-C9-C10
4	A	801	LMT	C5-C6-C7-C8
6	A	805	PG4	O3-C5-C6-O4
4	A	801	LMT	C1-C2-C3-C4
5	A	802	OCT	C4-C5-C6-C7
7	A	804	1PE	OH7-C16-C26-OH6
4	A	801	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

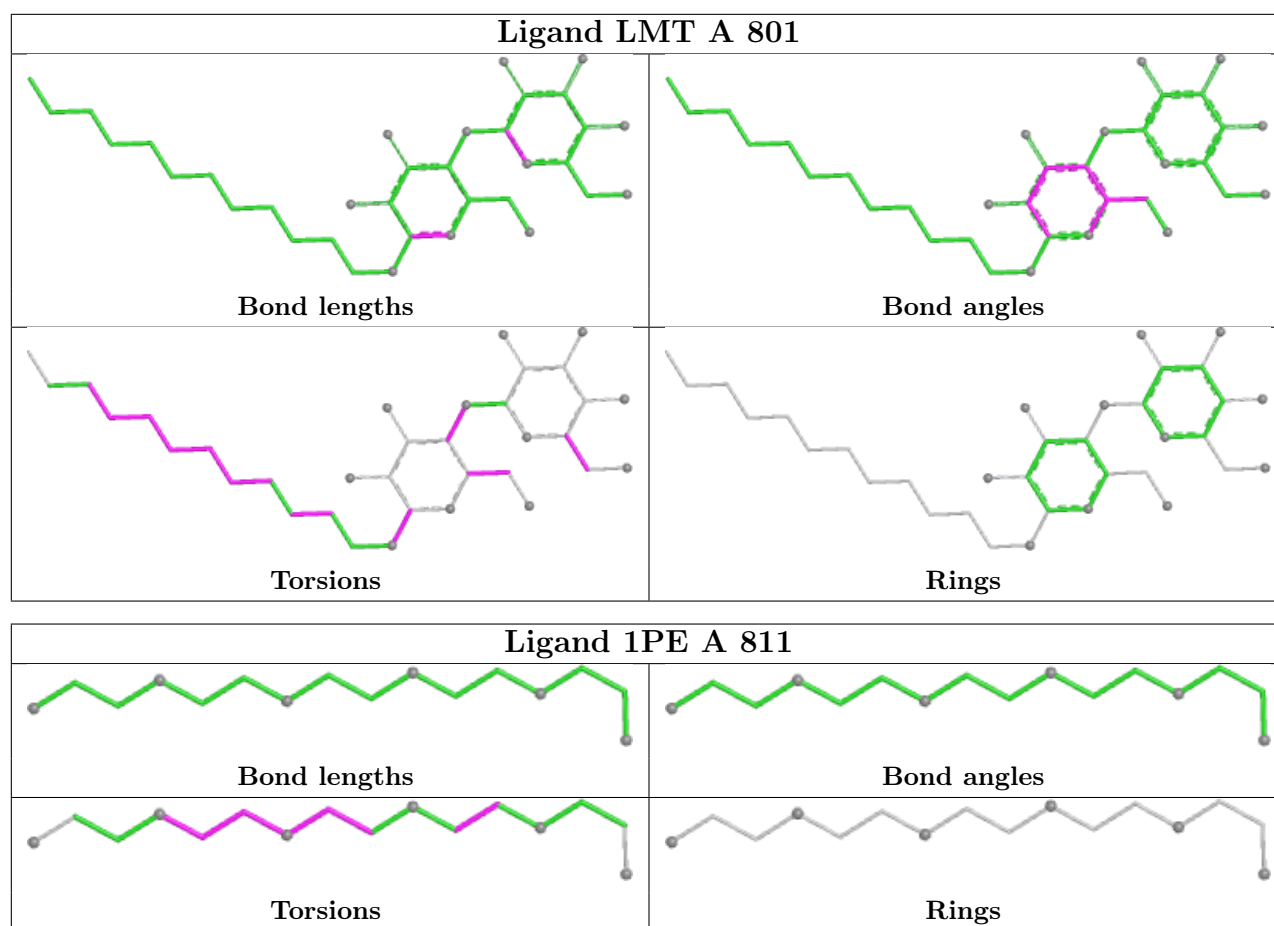
Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C4'-C5'-C6'-O6'
4	A	801	LMT	C3'-C4'-O1B-C1B
4	A	801	LMT	C6-C7-C8-C9
8	A	809	D12	C9-C10-C11-C12
5	A	802	OCT	C3-C4-C5-C6
4	A	801	LMT	C11-C10-C9-C8
6	A	805	PG4	O4-C7-C8-O5
9	A	810	GOL	O2-C2-C3-O3
6	A	805	PG4	C5-C6-O4-C7
6	A	807	PG4	C8-C7-O4-C6
8	A	809	D12	C3-C4-C5-C6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

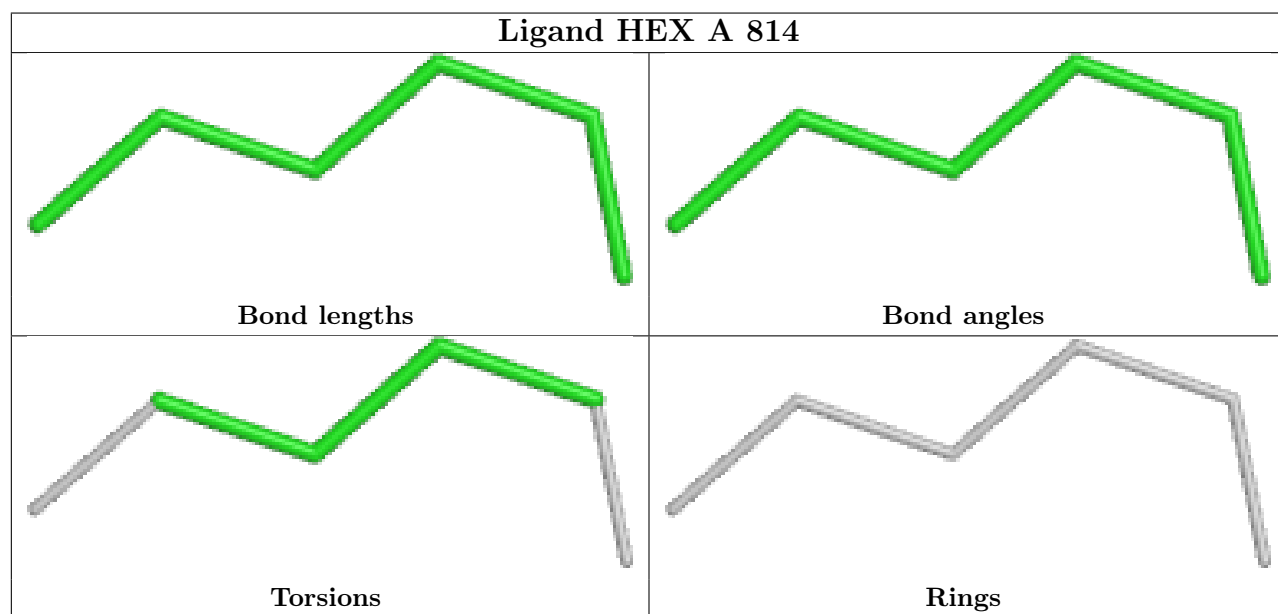
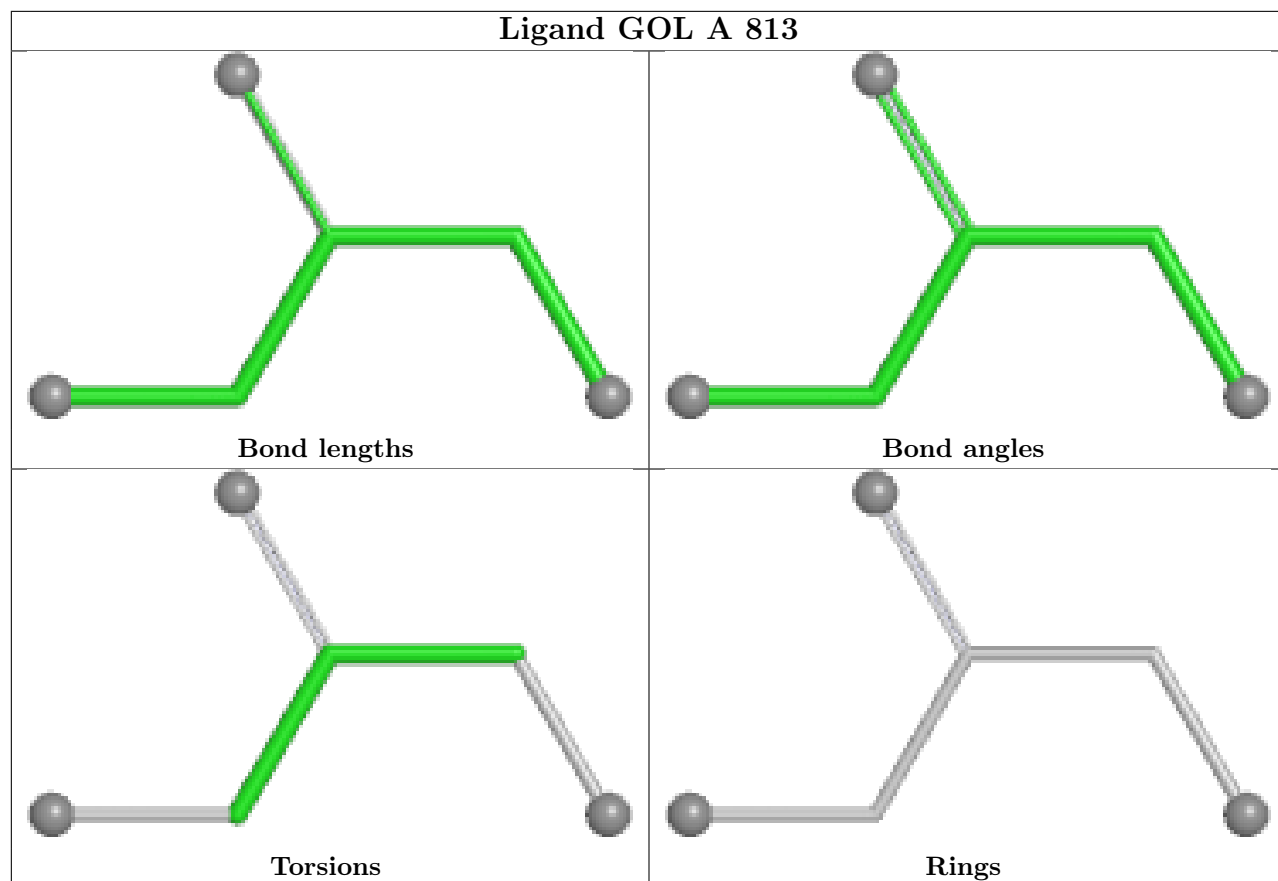
There are no ring outliers.

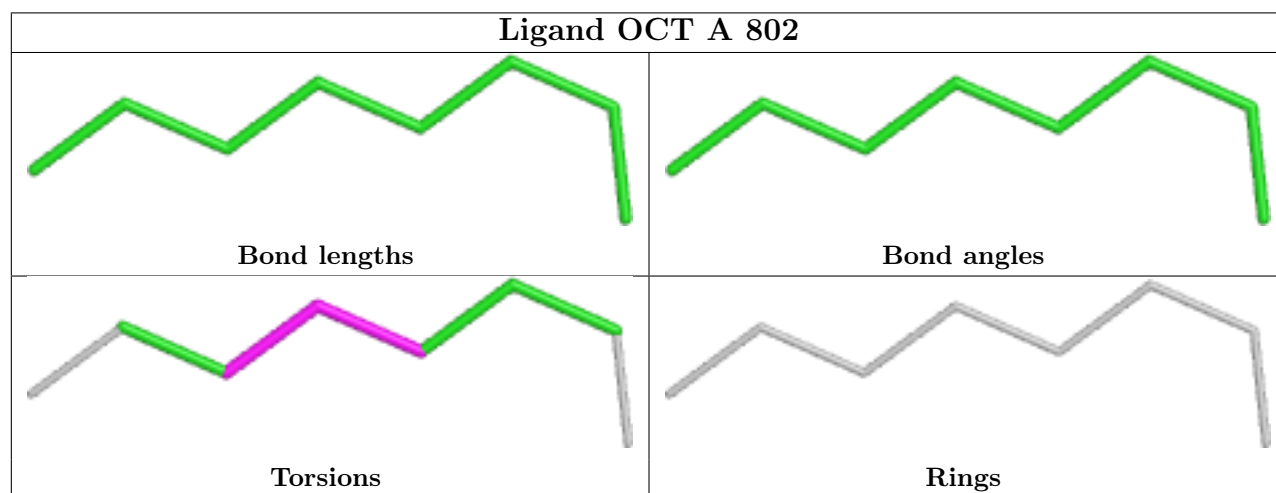
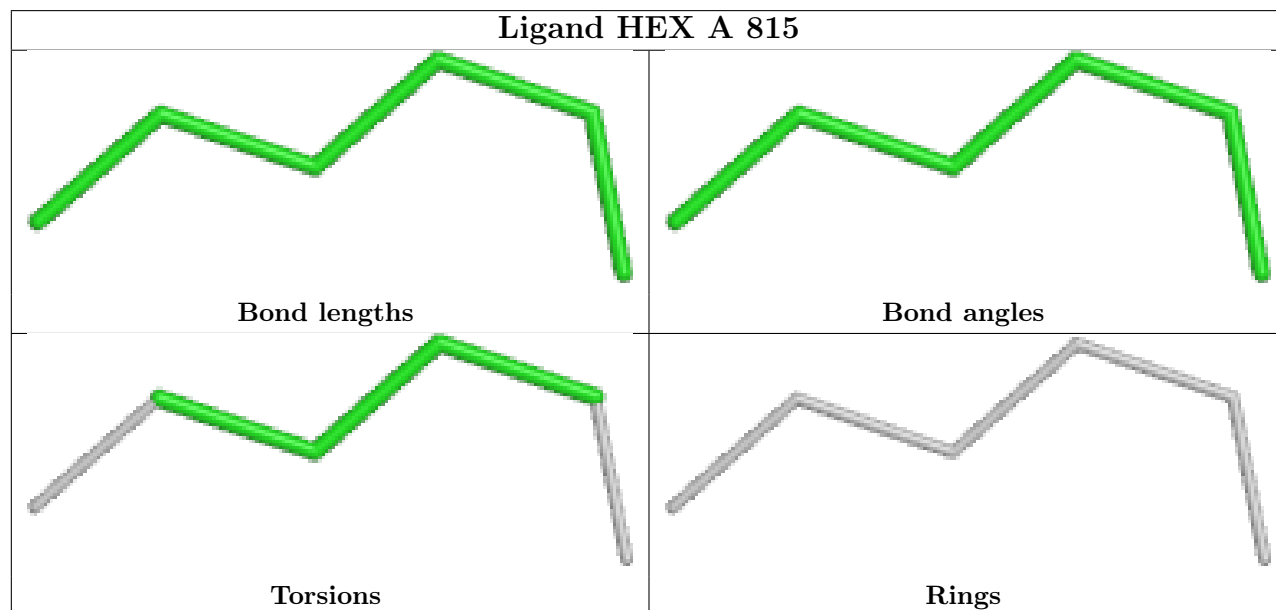
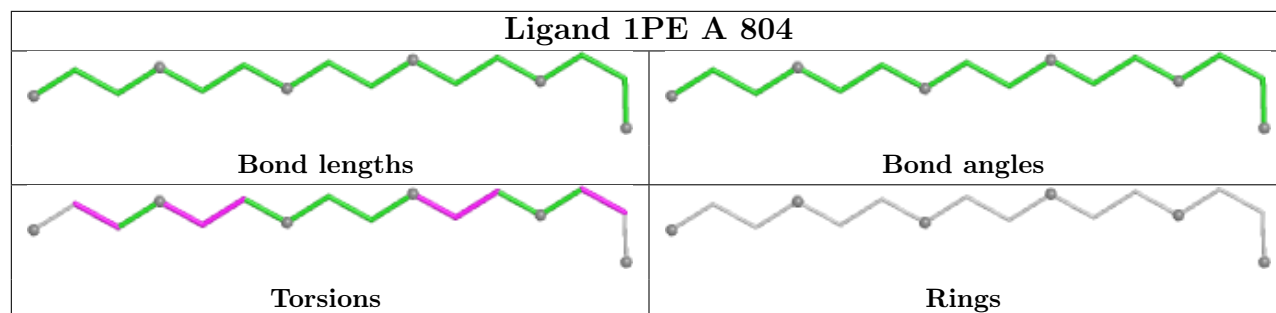
3 monomers are involved in 7 short contacts:

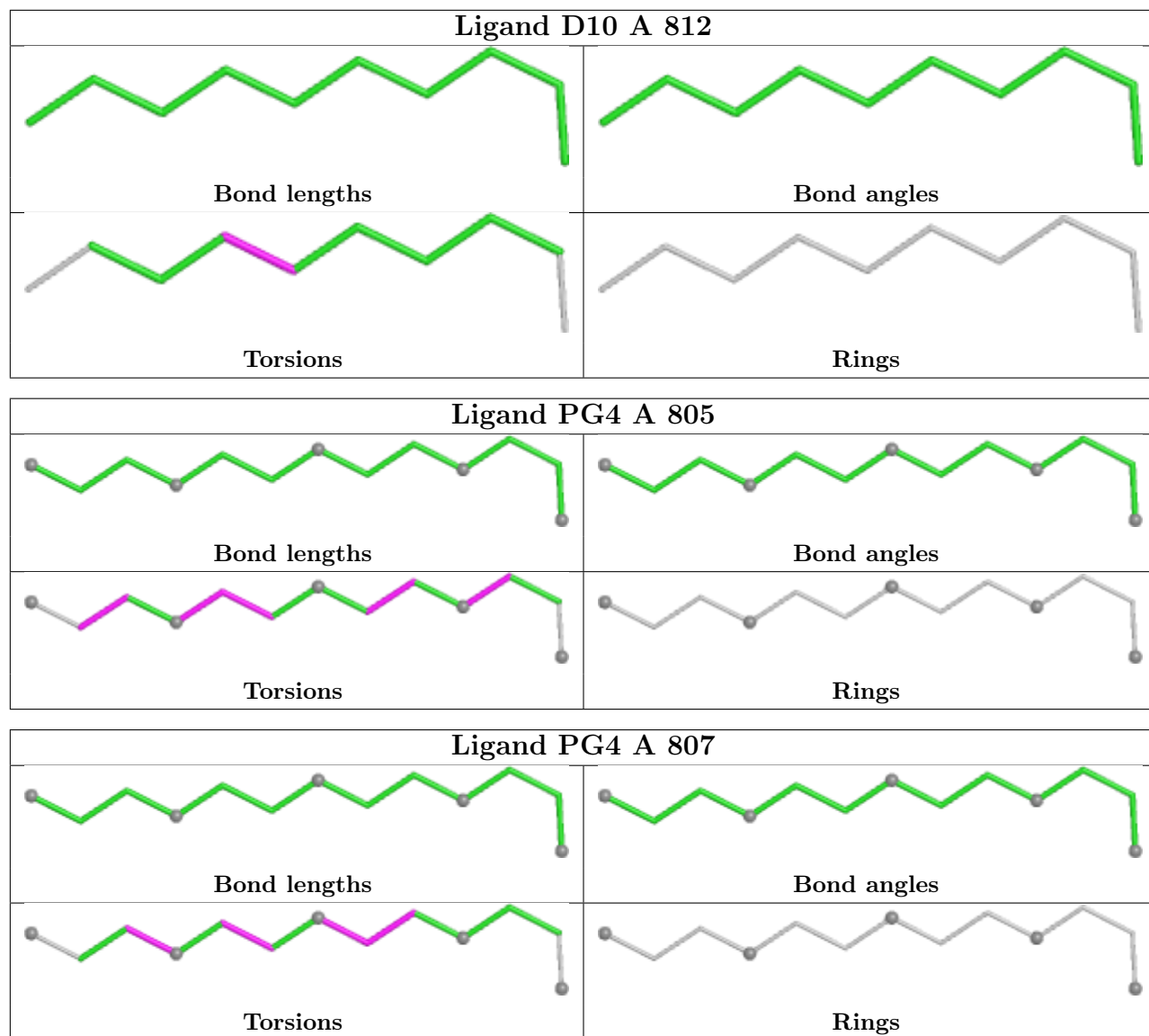
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	LMT	5	0
10	A	812	D10	1	0
6	A	807	PG4	1	0

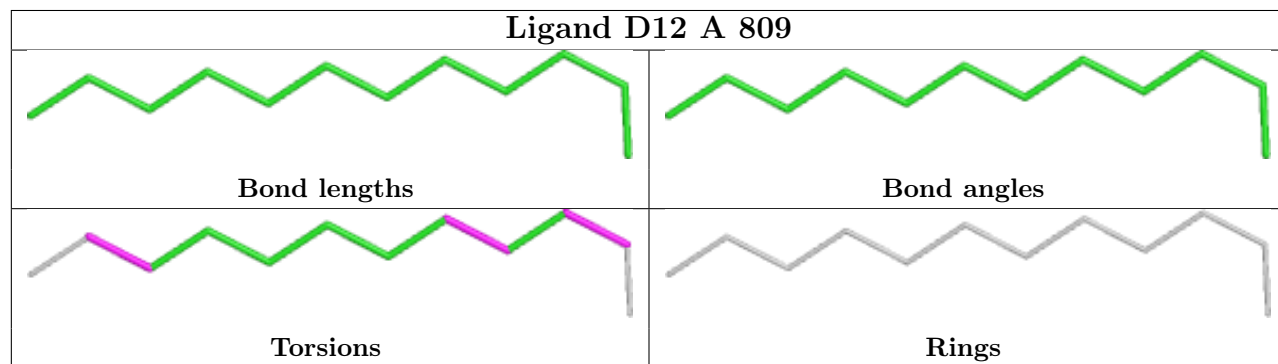
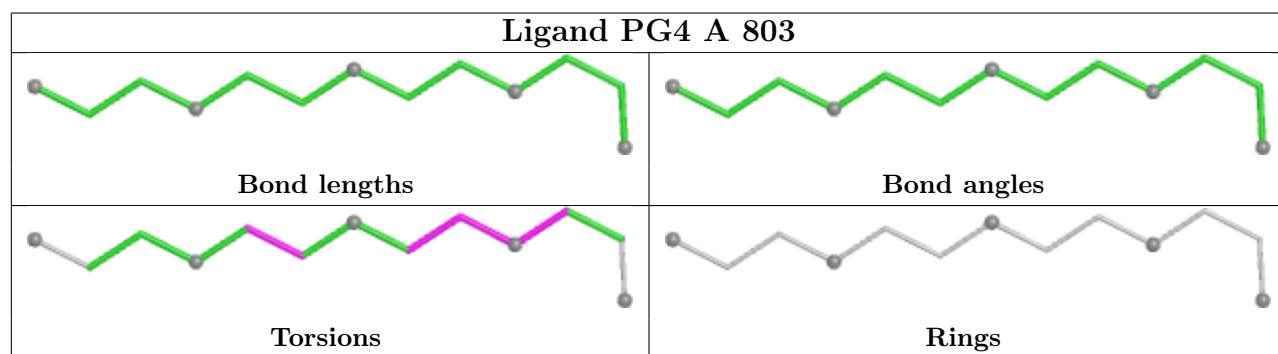
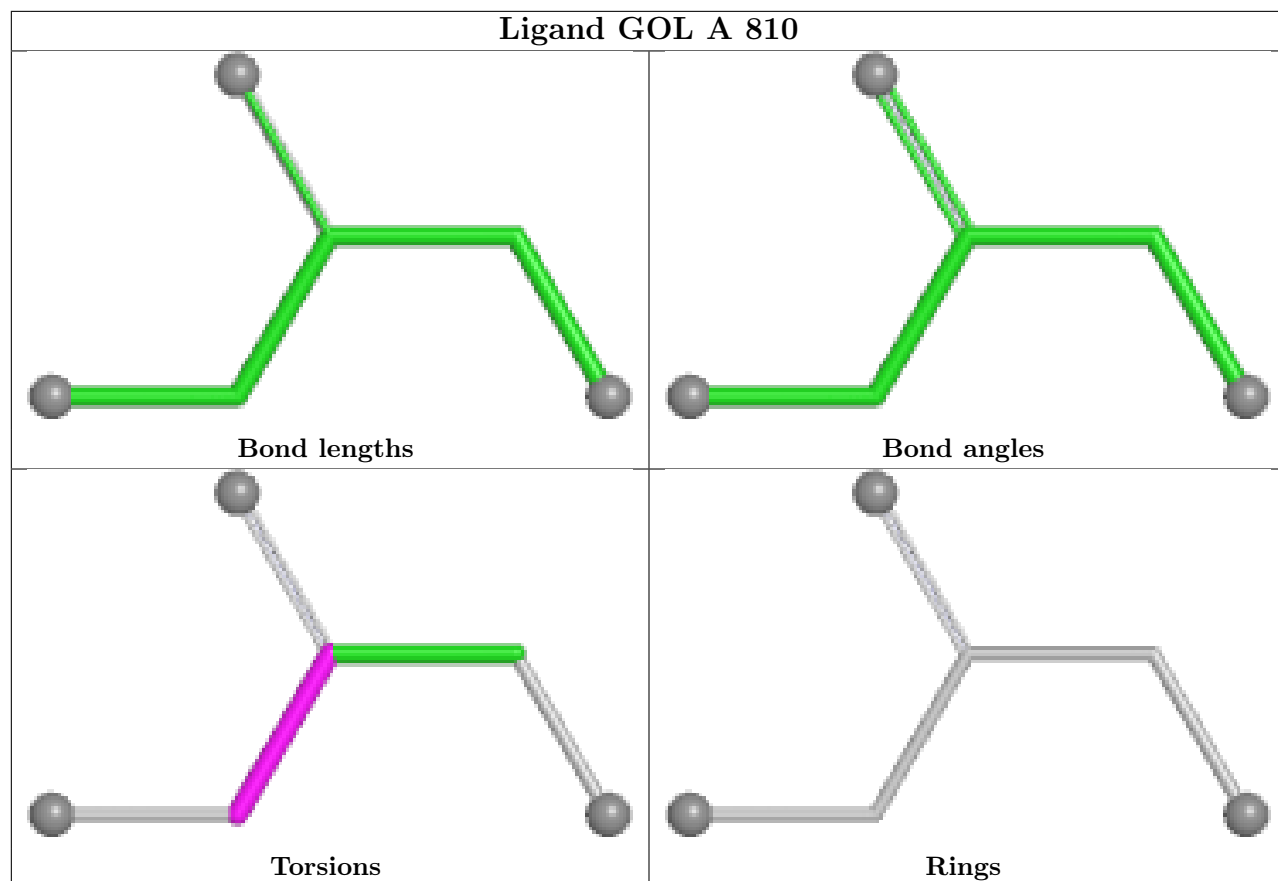
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

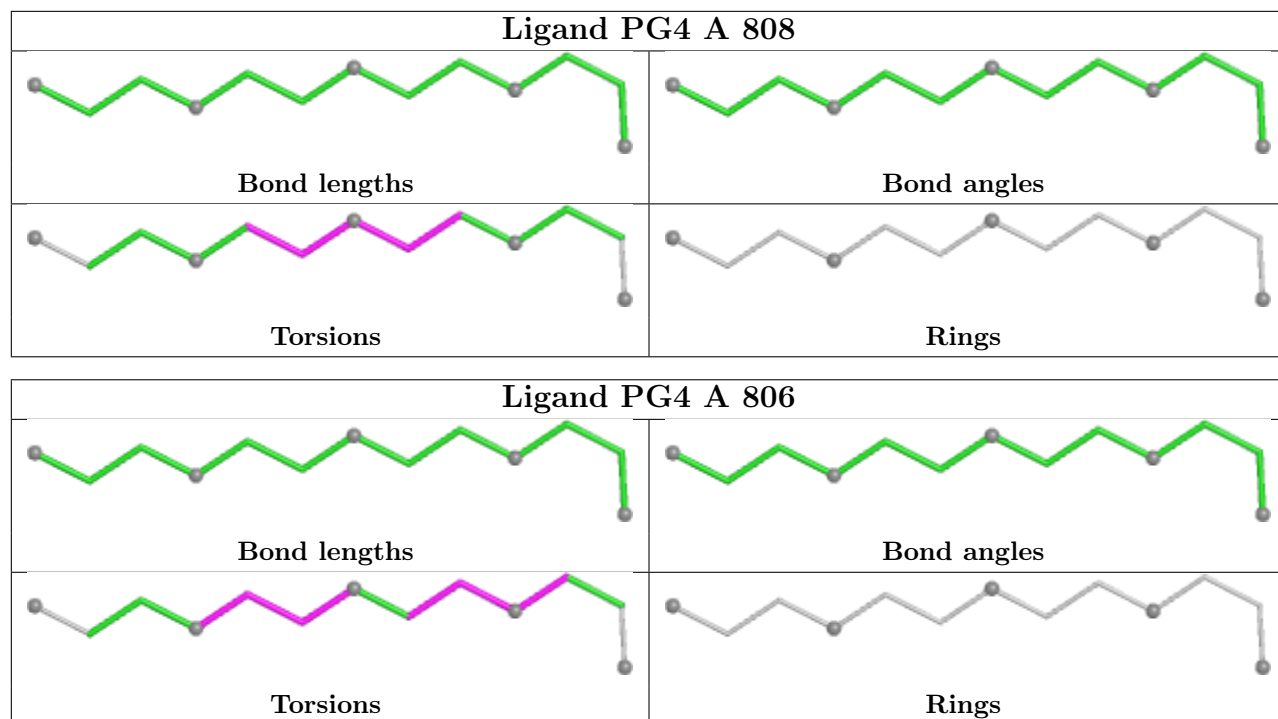












5.7 Other polymers [i](#)

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%)	1.29	93 (20%) 2 3	33, 53, 101, 119	1 (0%)
2	B	127/127 (100%)	0.92	17 (13%) 7 7	34, 53, 79, 92	2 (1%)
3	C	2/2 (100%)	2.27	1 (50%) 0 1	52, 52, 52, 59	0
All	All	580/618 (93%)	1.21	111 (19%) 3 4	33, 53, 95, 119	3 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	PHE	7.8
1	A	343	LEU	7.7
1	A	406	ALA	7.0
1	A	399	LEU	6.5
2	B	2	VAL	6.4
1	A	408	VAL	6.3
1	A	402	ALA	6.0
1	A	253	PHE	5.8
1	A	407	LEU	5.4
1	A	401	LEU	5.4
1	A	398	ALA	5.3
1	A	269	PHE	5.2
1	A	403	MET	5.0
1	A	308	SER	5.0
1	A	254	PHE	5.0
1	A	397	SER	4.9
1	A	305	LEU	4.9
1	A	478	TRP	4.8
1	A	136	PRO	4.8
1	A	199	ASP	4.8
1	A	413	MET	4.7
1	A	236	GLU	4.7
1	A	415	PHE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	344	SER	4.7
1	A	404	ILE	4.6
1	A	400	GLY	4.6
1	A	270	VAL	4.5
1	A	372	ASP	4.4
1	A	249	VAL	4.4
1	A	405	ALA	4.4
1	A	268	MET	4.4
1	A	144	ALA	4.3
2	B	128	HIS	4.1
1	A	345	MET	4.0
1	A	103	LEU	4.0
1	A	332	ILE	3.9
1	A	331	GLY	3.8
1	A	252	ILE	3.8
1	A	484	ALA	3.8
1	A	240	LEU	3.6
1	A	250	THR	3.5
1	A	256	GLN	3.5
1	A	482	MET	3.4
1	A	134	TYR	3.4
1	A	251	ILE	3.4
1	A	330	ALA	3.4
1	A	417	LEU	3.4
1	A	443	ASN	3.4
1	A	416	ILE	3.4
1	A	274	LEU	3.3
1	A	304	ILE	3.3
1	A	433	TYR	3.2
1	A	266	ASN	3.2
1	A	200	ILE	3.2
1	A	139	PRO	3.2
1	A	267	LYS	3.2
1	A	395	PHE	3.1
3	C	2	ILE	3.1
1	A	183	LEU	3.1
1	A	306	GLY	3.0
1	A	255	ARG	3.0
1	A	125	ASN	3.0
1	A	140	ARG	3.0
1	A	198	LYS	3.0
1	A	479	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	76	ASP	3.0
1	A	442	ASP	3.0
2	B	65	GLY	2.9
2	B	26	GLY	2.9
1	A	15	PRO	2.8
2	B	83	ASN	2.8
1	A	424	GLN	2.8
1	A	187	LEU	2.7
1	A	271	ALA	2.6
1	A	483	ILE	2.6
2	B	4	LEU	2.6
2	B	126	HIS	2.6
1	A	349	PHE	2.5
2	B	68	THR	2.5
1	A	141	LEU	2.5
2	B	73	ASN	2.4
1	A	309	ILE	2.4
1	A	420	TRP	2.4
2	B	25	SER	2.4
2	B	86	LYS	2.4
1	A	248	VAL	2.4
1	A	207	ARG	2.3
1	A	272	PHE	2.3
2	B	28	THR	2.3
1	A	50	GLU	2.3
1	A	174	VAL	2.3
1	A	196	MET	2.3
1	A	247	ILE	2.3
1	A	14	ARG	2.2
1	A	203	GLU	2.2
2	B	3	GLN	2.2
1	A	135	PRO	2.2
1	A	105	PRO	2.2
1	A	328	ILE	2.2
1	A	419	MET	2.2
2	B	14	ALA	2.2
2	B	117	THR	2.2
1	A	471	VAL	2.1
1	A	208	PRO	2.1
2	B	67	PHE	2.1
1	A	11	GLN	2.1
1	A	145	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	2.1
1	A	189	VAL	2.0
1	A	324	LEU	2.0
1	A	346	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](#)

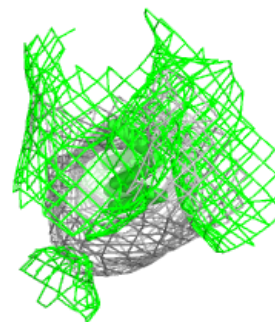
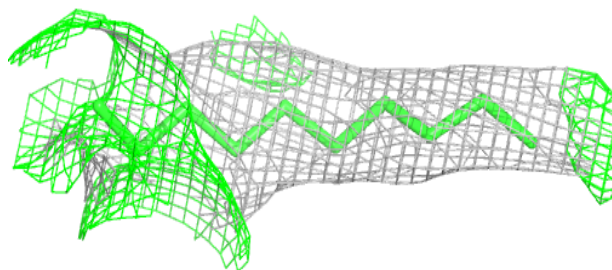
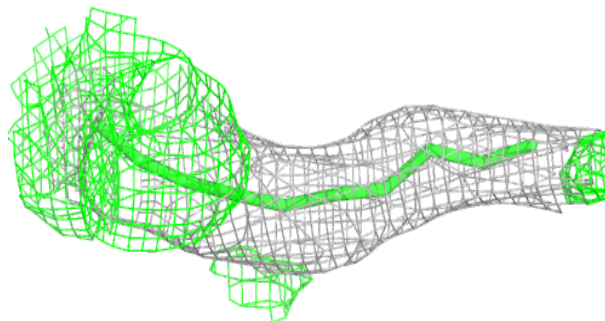
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	D10	A	812	10/10	0.63	0.38	60,64,81,89	0
9	GOL	A	810	6/6	0.65	0.20	89,91,93,94	0
8	D12	A	809	12/12	0.68	0.29	64,71,75,78	0
6	PG4	A	806	13/13	0.70	0.24	67,76,98,99	0
11	HEX	A	815	6/6	0.73	0.32	68,70,74,76	0
6	PG4	A	808	13/13	0.78	0.23	69,75,85,86	0
9	GOL	A	813	6/6	0.78	0.17	73,76,77,80	0
7	1PE	A	811	16/16	0.80	0.22	74,80,86,87	0
4	LMT	A	801	35/35	0.80	0.19	56,73,89,91	0
6	PG4	A	805	13/13	0.80	0.21	68,77,87,88	0
11	HEX	A	814	6/6	0.81	0.28	73,75,79,81	0
6	PG4	A	803	13/13	0.83	0.19	59,68,84,87	0
5	OCT	A	802	8/8	0.85	0.21	57,60,66,67	0
6	PG4	A	807	13/13	0.86	0.17	65,74,86,89	0
7	1PE	A	804	16/16	0.90	0.14	57,65,84,86	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.

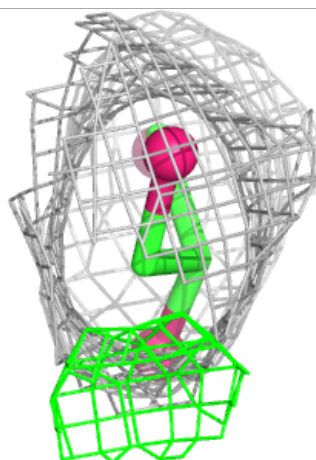
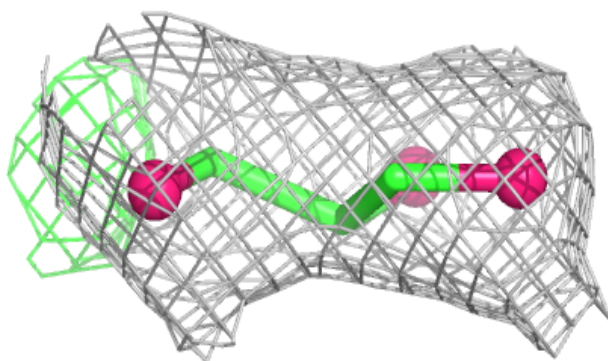
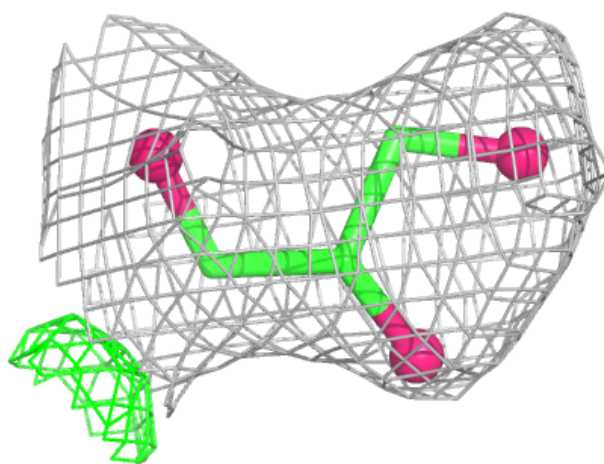
Electron density around D10 A 812:

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



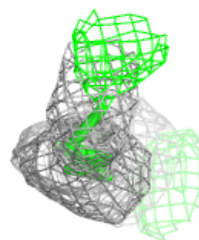
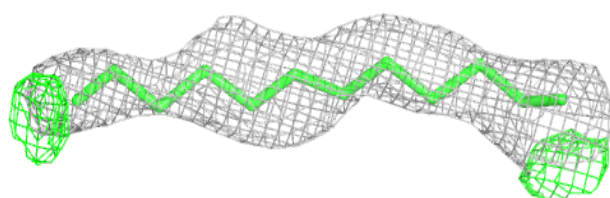
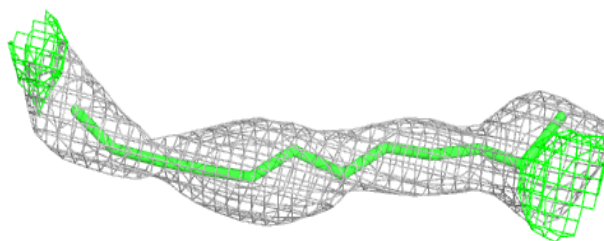
Electron density around GOL A 810:

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

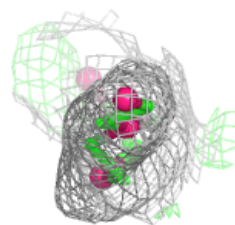
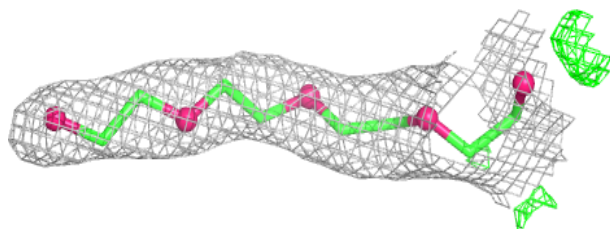


Electron density around D12 A 809:

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

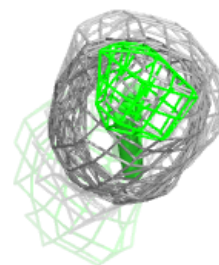
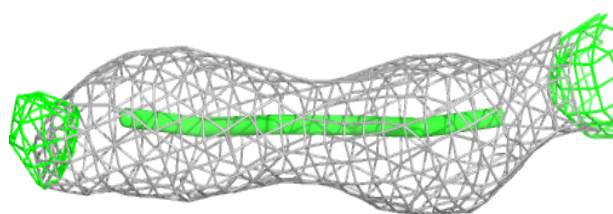
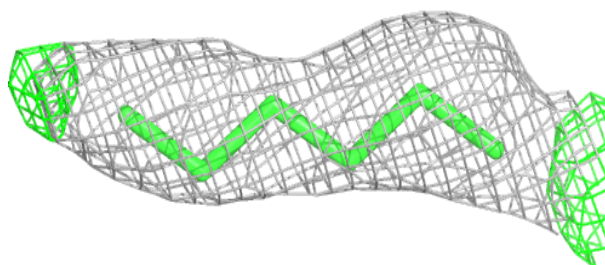
**Electron density around PG4 A 806:**

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

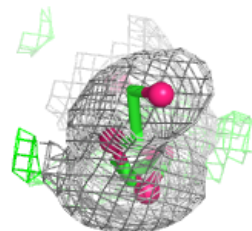
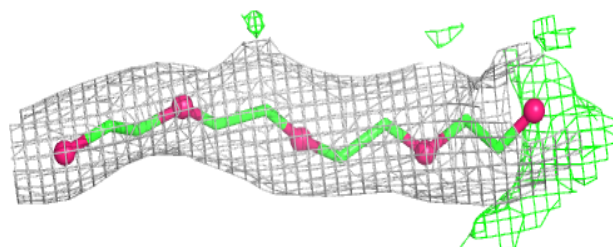
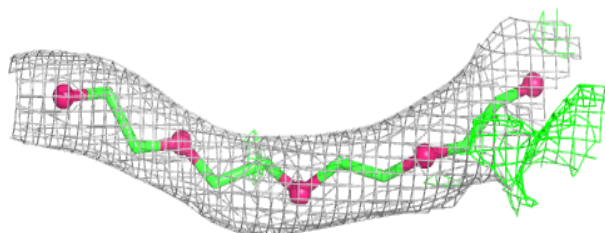


Electron density around HEX A 815:

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

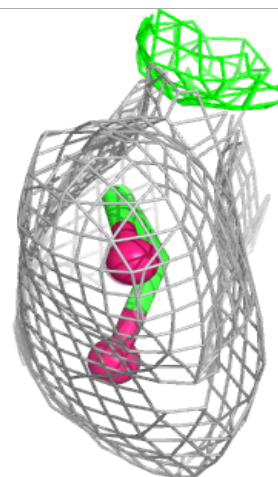
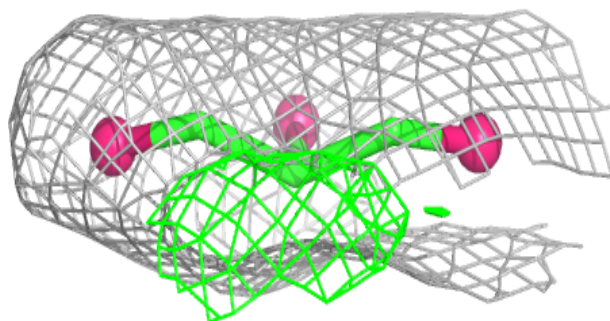
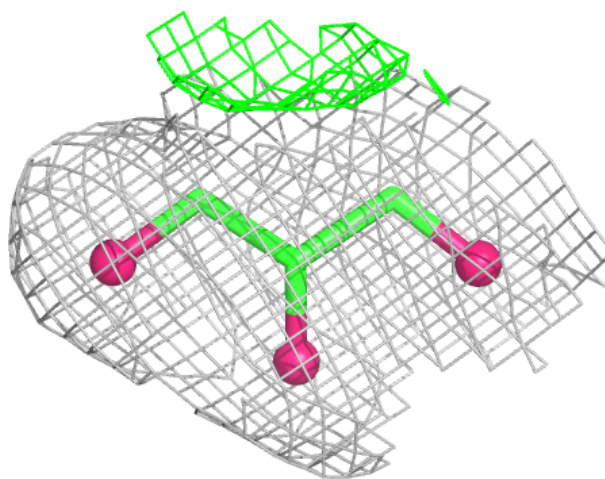
**Electron density around PG4 A 808:**

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



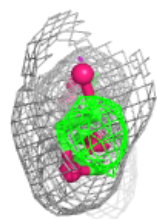
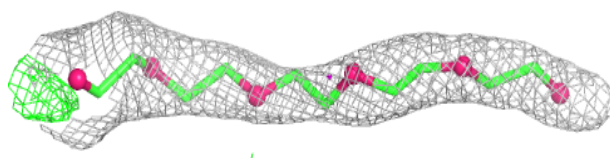
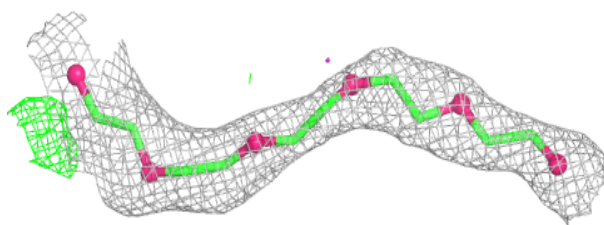
Electron density around GOL A 813:

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

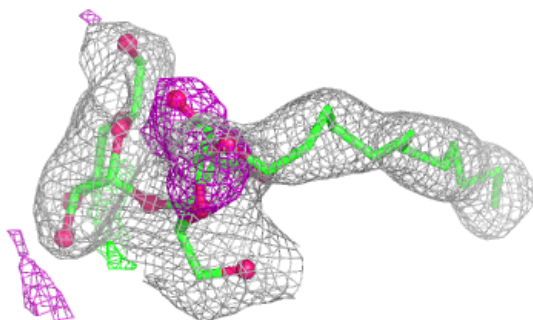
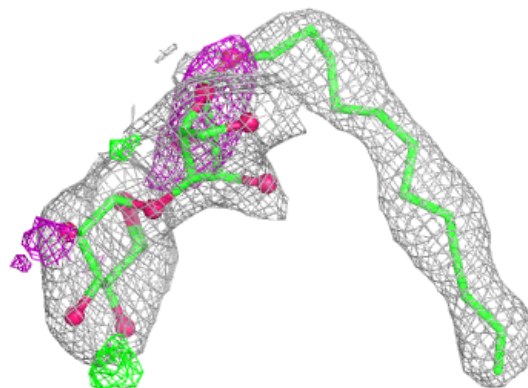


Electron density around 1PE A 811:

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

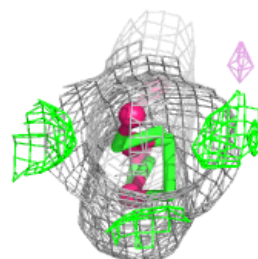
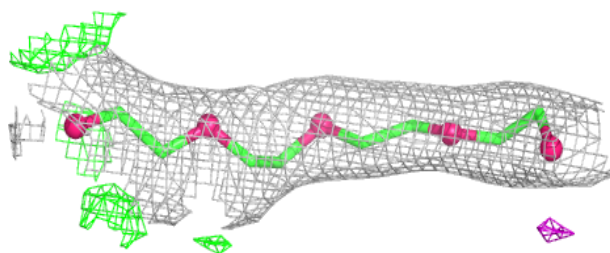
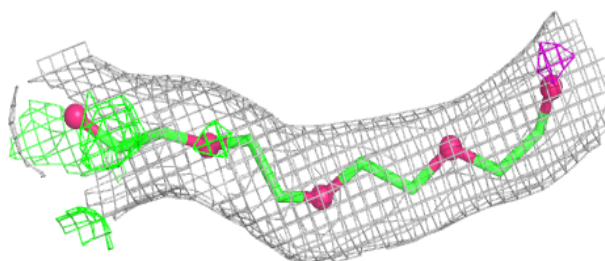
**Electron density around LMT A 801:**

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

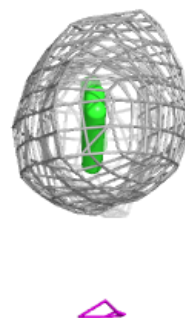
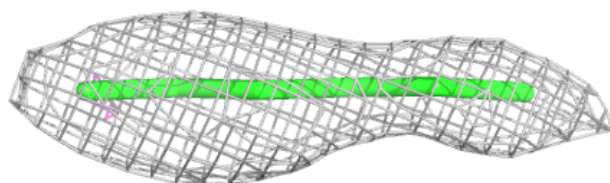
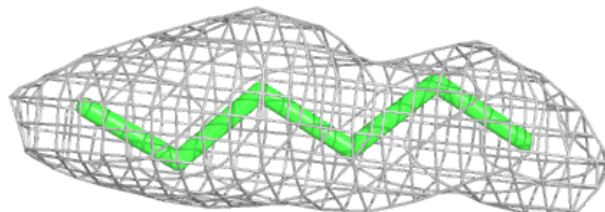


Electron density around PG4 A 805:

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

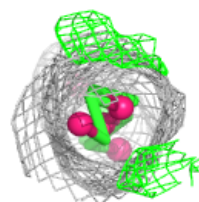
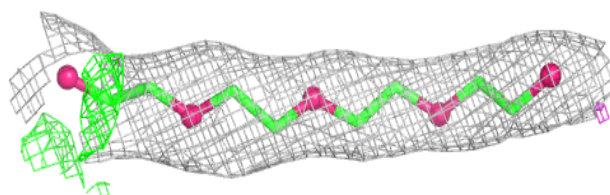
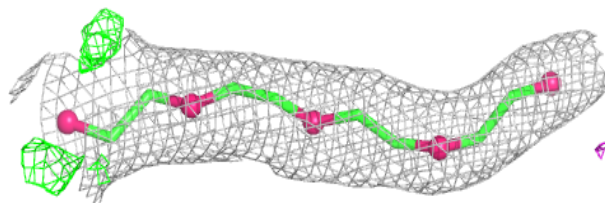
**Electron density around HEX A 814:**

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

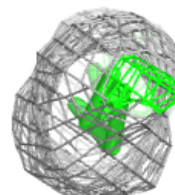
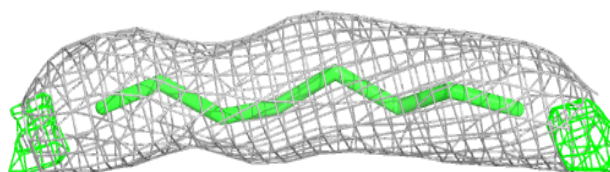
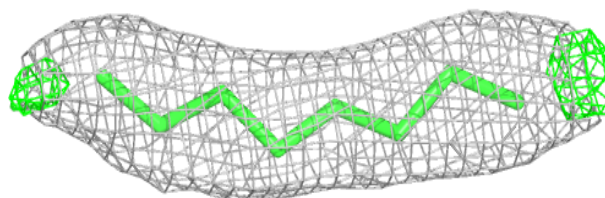


Electron density around PG4 A 803:

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

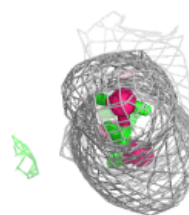
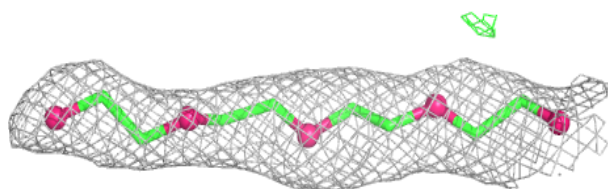
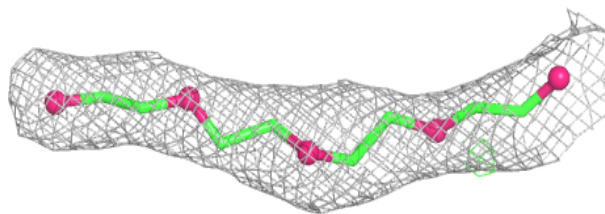
**Electron density around OCT A 802:**

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

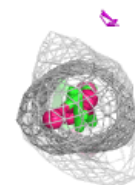
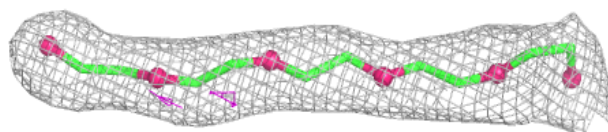
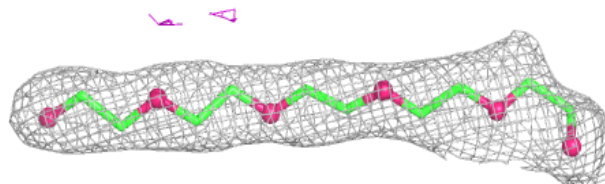


Electron density around PG4 A 807:

$2mF_o-DF_c$ (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.