wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID	:	8B19
Title	:	DtpB-Nb132-AFA
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Deposited on	:	2022-09-09
Resolution	:	2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

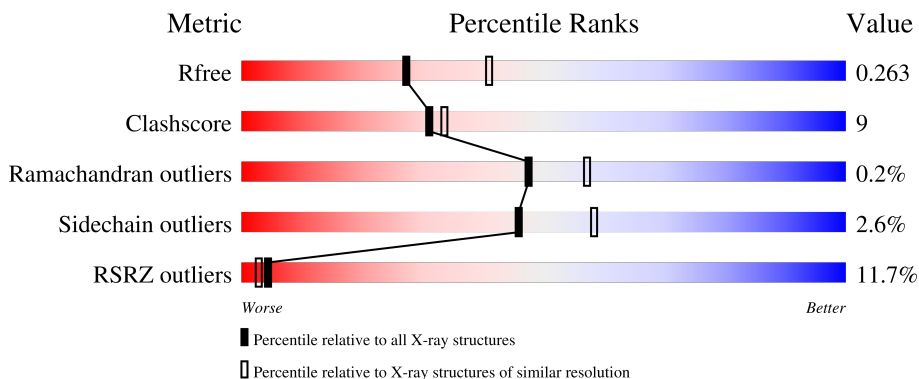|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.45 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		9
Ramachandran outliers		0.2%
Sidechain outliers		2.6%
RSRZ outliers		11.7%

Worse　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	13% — 71% — 20% — · — 8%
2	B	127	5% — 83% — 17%
3	C	3	33% — 67%

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
11	HEX	A	814	-	-	-	X
11	HEX	A	815	-	-	-	X
5	OCT	A	802	-	-	-	X
6	PG4	A	806	-	-	-	X
8	D12	A	809	-	-	-	X

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 4793 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
			Total	C	N	O	S			
1	A	451	3480	2349	531	573	27	4	0	0

- Molecule 2 is a protein called Nanobody 132.

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

- Molecule 3 is a protein called ALA-PHE-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	22	15	3	4	0	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).
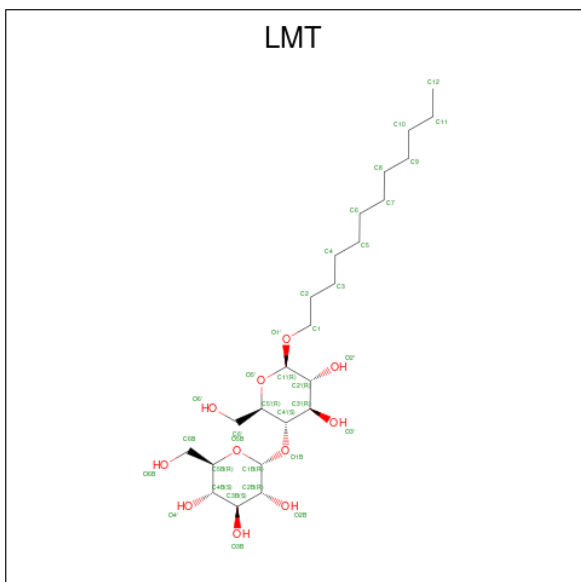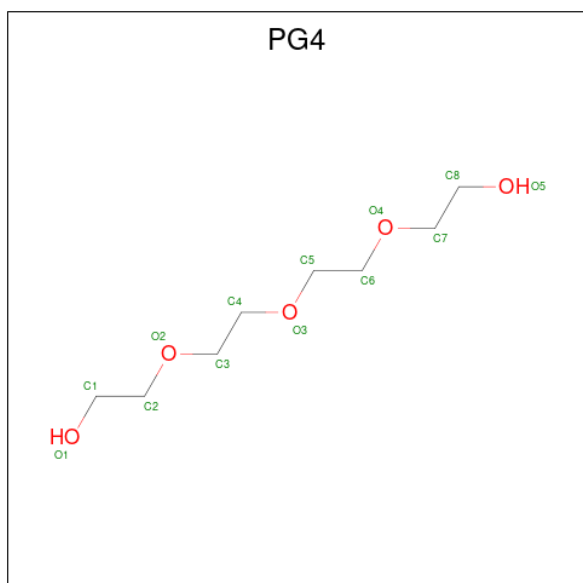
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 35	C 24	O 11	0	0

- Molecule 5 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}) (labeled as "Ligand of Interest" by depositor).
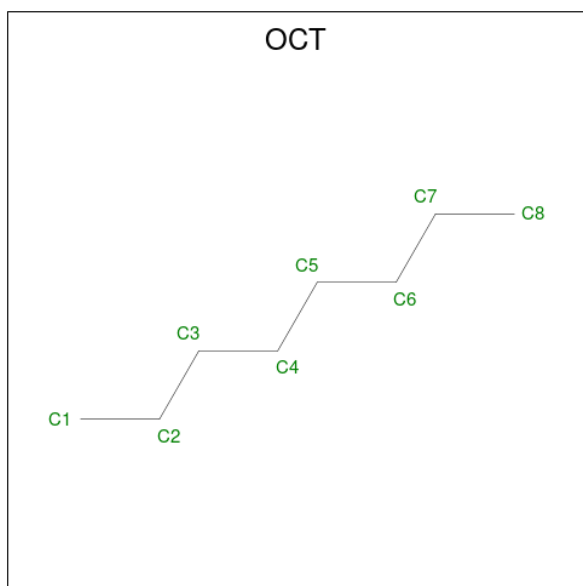
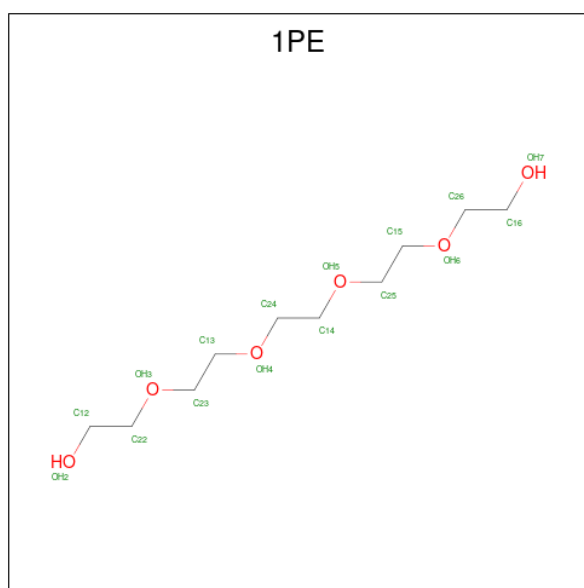| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 8	C 8	0	0

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

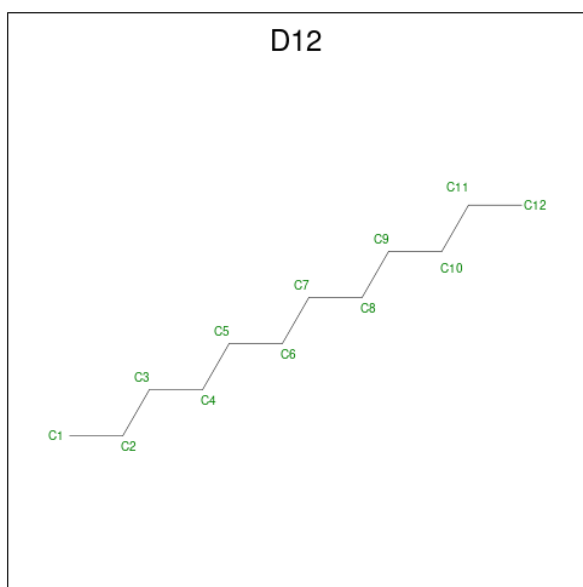| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 13	C 8	O 5	0	0
6	A	1	Total 13	C 8	O 5	0	0
6	A	1	Total 13	C 8	O 5	0	0
6	A	1	Total 13	C 8	O 5	0	0
6	A	1	Total 13	C 8	O 5	0	0

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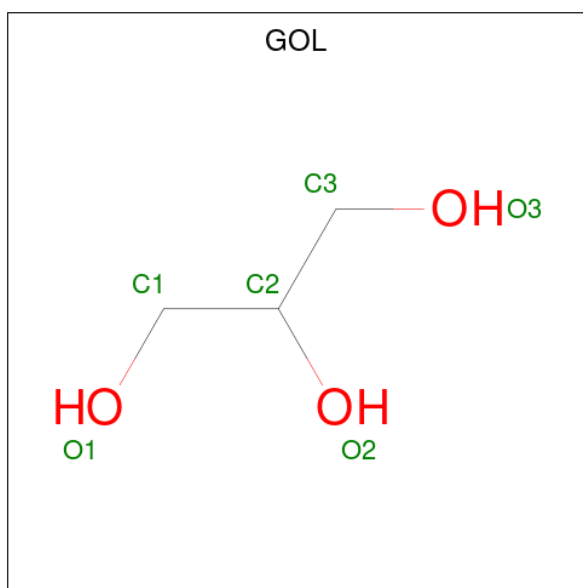

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 16	C 10	O 6	0	0
7	A	1	Total 16	C 10	O 6	0	0

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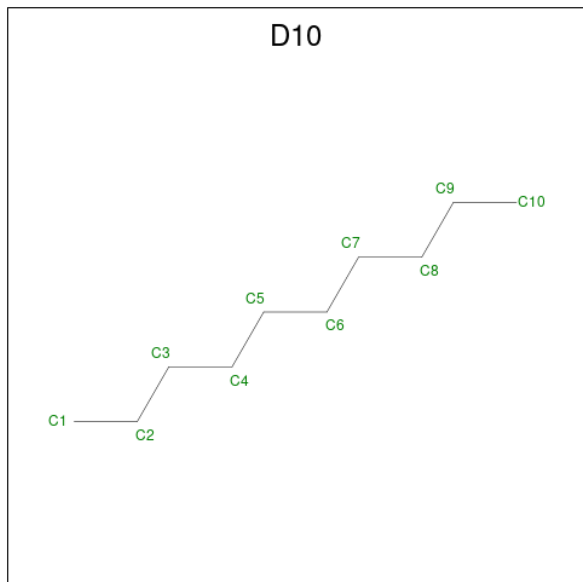
D12

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

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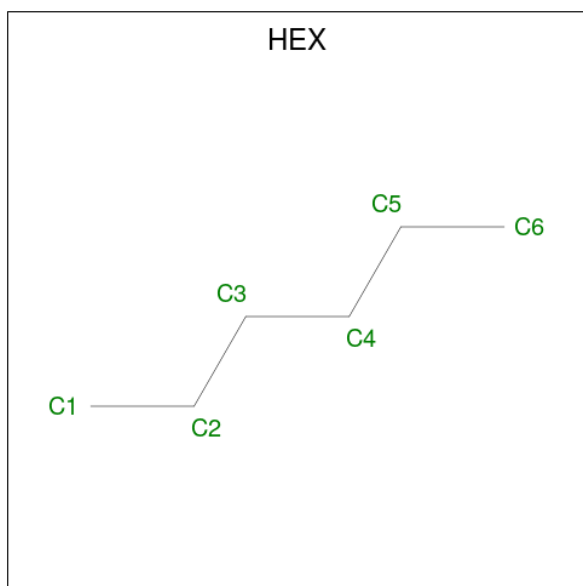
GOL

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

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

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

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

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	72	Total 72	O 72	0	0
12	B	56	Total 56	O 56	0	0
12	C	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dipeptide and tripeptide permease B

Chain A:
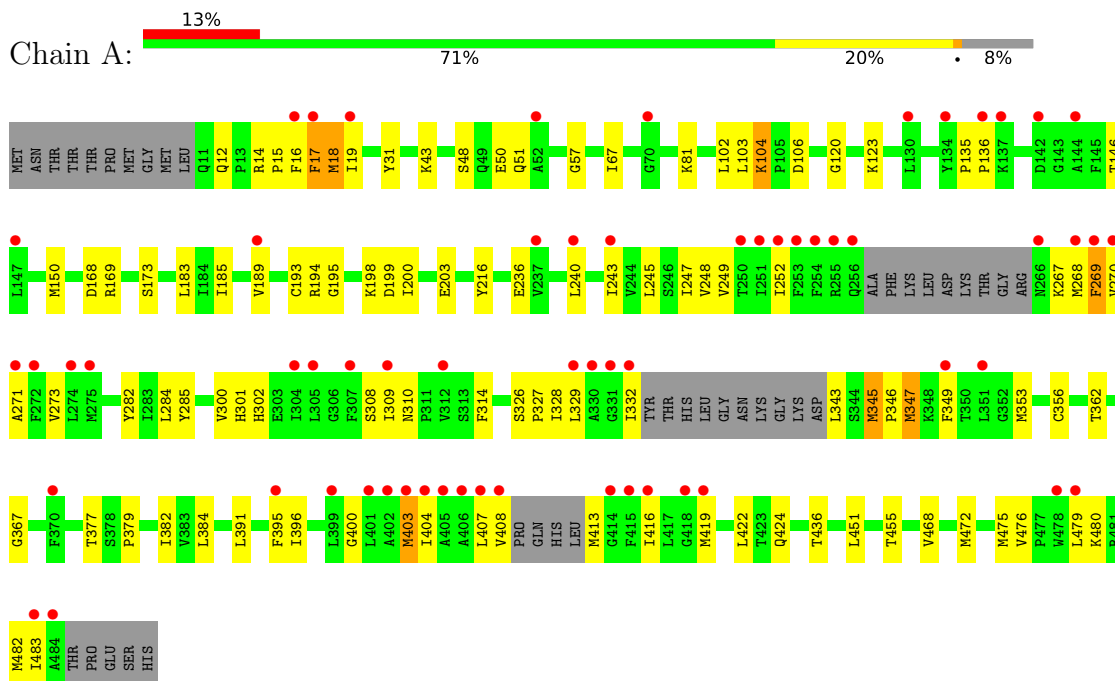
• Molecule 2: Nanobody 132

Chain B:
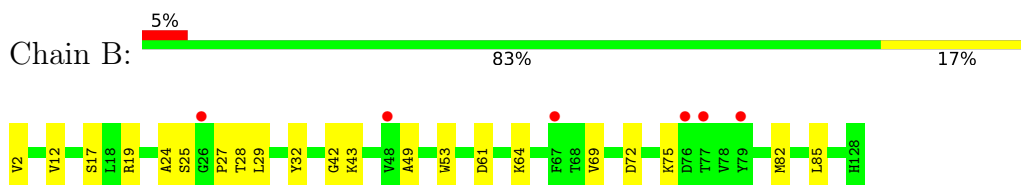
• Molecule 3: ALA-PHE-ALA

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.70Å 125.51Å 169.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.30 – 2.45 100.91 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.30-2.45) 93.4 (100.91-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.268 0.221 , 0.263	Depositor DCC
R_{free} test set	2223 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 80.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4793	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LMT, D10, 1PE, OCT, GOL, D12, HEX, PG4

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	0.51	0/3572	0.71	5/4859 (0.1%)
2	B	0.51	0/1004	0.70	0/1361
3	C	0.84	0/22	0.84	0/27
All	All	0.52	0/4598	0.71	5/6247 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	345	MET	CB-CG-SD	-8.39	87.24	112.40
1	A	345	MET	CG-SD-CE	-7.25	88.61	100.20
1	A	102	LEU	CA-CB-CG	-6.11	101.25	115.30
1	A	347	MET	CG-SD-CE	5.58	109.13	100.20
1	A	403	MET	CA-CB-CG	-5.29	104.31	113.30

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	75	0
2	B	976	0	939	11	0
3	C	22	0	21	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	46	6	0
5	A	8	0	18	0	0
6	A	65	0	90	1	0
7	A	32	0	44	2	0
8	A	12	0	26	0	0
9	A	12	0	16	0	0
10	A	10	0	22	1	0
11	A	12	0	28	0	0
12	A	72	0	0	4	0
12	B	56	0	0	2	0
12	C	1	0	0	0	0
All	All	4793	0	4855	86	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.

The worst 5 of 86 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:273:VAL:HG11	1:A:475:MET:HE1	1.41	1.02
2:B:19:ARG:NH1	12:B:201:HOH:O	2.11	0.80
1:A:81:LYS:NZ	1:A:200:ILE:O	2.15	0.79
1:A:123:LYS:HE3	3:C:3:ALA:O	1.85	0.76
1:A:271:ALA:HB2	1:A:407:LEU:HD11	1.69	0.73

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	443/489 (91%)	438 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	126/127 (99%)	118 (94%)	7 (6%)	1 (1%)	19	22
3	C	1/3 (33%)	1 (100%)	0	0	100	100
All	All	570/619 (92%)	557 (98%)	12 (2%)	1 (0%)	47	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/401 (92%)	357 (97%)	11 (3%)	41	52
2	B	102/101 (101%)	101 (99%)	1 (1%)	76	84
3	C	1/1 (100%)	1 (100%)	0	100	100
All	All	471/503 (94%)	459 (98%)	12 (2%)	46	60

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	PHE
1	A	349	PHE
2	B	53	TRP
1	A	419	MET
1	A	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	389	GLN
1	A	424	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 monosaccharides 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	$\#|Z| > 2$
6	PG4	A	807	-	12,12,12	0.22	0	11,11,11	0.50	0
7	1PE	A	811	-	15,15,15	0.14	0	14,14,14	0.19	0
4	LMT	A	801	-	36,36,36	1.24	4 (11%)	47,47,47	1.46	7 (14%)
11	HEX	A	814	-	5,5,5	0.33	0	4,4,4	0.60	0
9	GOL	A	813	-	5,5,5	0.93	0	5,5,5	0.97	0
8	D12	A	809	-	11,11,11	0.40	0	10,10,10	0.67	0
6	PG4	A	803	-	12,12,12	0.23	0	11,11,11	0.54	0
11	HEX	A	815	-	5,5,5	0.36	0	4,4,4	0.53	0
6	PG4	A	805	-	12,12,12	0.20	0	11,11,11	0.59	0
6	PG4	A	808	-	12,12,12	0.28	0	11,11,11	0.63	0
9	GOL	A	810	-	5,5,5	1.02	0	5,5,5	0.78	0
10	D10	A	812	-	9,9,9	0.34	0	8,8,8	0.99	0
5	OCT	A	802	-	7,7,7	0.33	0	6,6,6	0.75	0
6	PG4	A	806	-	12,12,12	0.27	0	11,11,11	0.46	0
7	1PE	A	804	-	15,15,15	0.19	0	14,14,14	0.29	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
6	PG4	A	807	-	-	4/10/10/10	-
7	1PE	A	811	-	-	7/13/13/13	-
4	LMT	A	801	-	-	15/21/61/61	0/2/2/2
11	HEX	A	814	-	-	0/3/3/3	-
9	GOL	A	813	-	-	0/4/4/4	-
8	D12	A	809	-	-	2/9/9/9	-
6	PG4	A	803	-	-	4/10/10/10	-
11	HEX	A	815	-	-	0/3/3/3	-
6	PG4	A	805	-	-	4/10/10/10	-
6	PG4	A	808	-	-	4/10/10/10	-
9	GOL	A	810	-	-	0/4/4/4	-
10	D10	A	812	-	-	1/7/7/7	-
5	OCT	A	802	-	-	3/5/5/5	-
6	PG4	A	806	-	-	5/10/10/10	-
7	1PE	A	804	-	-	4/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O5B-C1B	3.80	1.51	1.41
4	A	801	LMT	O5'-C1'	3.32	1.50	1.41
4	A	801	LMT	O5B-C5B	2.24	1.49	1.44
4	A	801	LMT	O1B-C4'	2.09	1.49	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	C1'-C2'-C3'	3.70	117.69	110.00
4	A	801	LMT	C1'-O5'-C5'	-3.30	107.20	113.69
4	A	801	LMT	C2'-C3'-C4'	3.19	116.96	109.68
4	A	801	LMT	C3'-C4'-C5'	2.36	116.33	110.93
4	A	801	LMT	O1B-C4'-C5'	2.30	115.75	109.45

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C2'-C1'-O1'-C1
4	A	801	LMT	O5'-C1'-O1'-C1
4	A	801	LMT	O5B-C5B-C6B-O6B
4	A	801	LMT	O5'-C5'-C6'-O6'
4	A	801	LMT	C4B-C5B-C6B-O6B

There are no ring outliers.

4 monomers are involved in 10 short contacts:
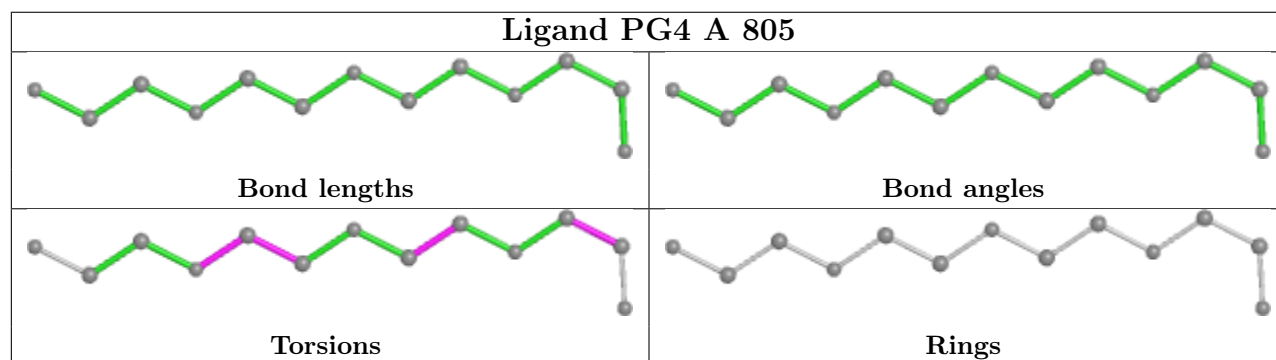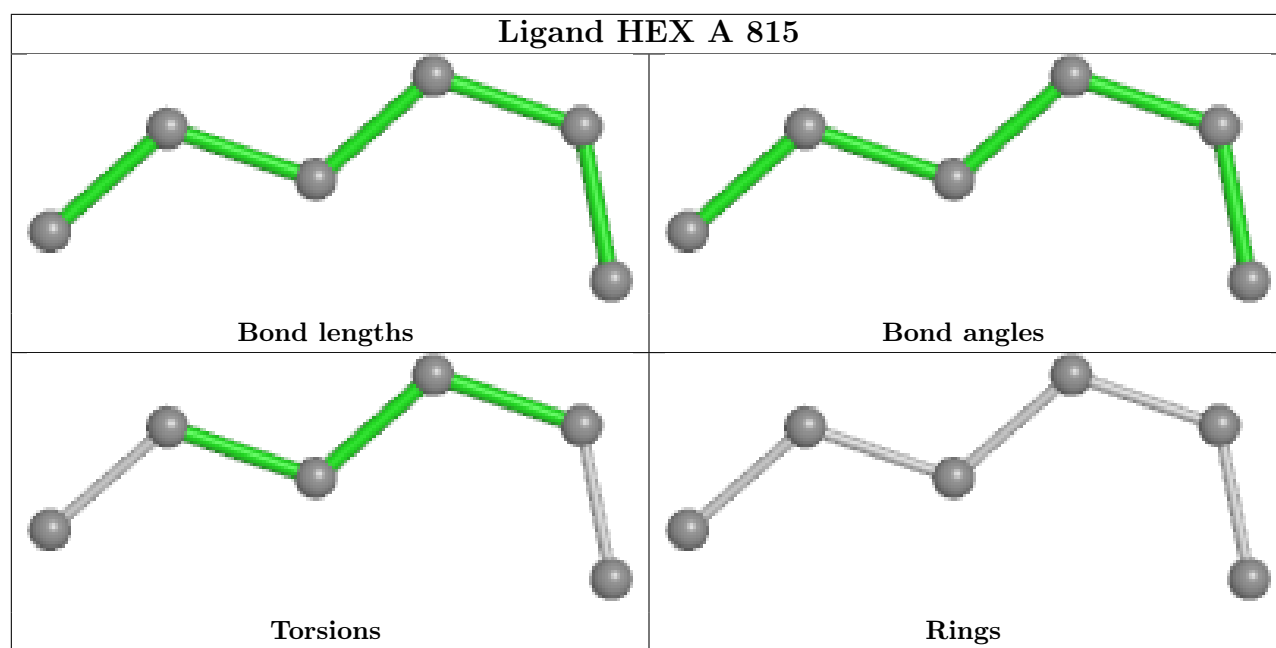
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	807	PG4	1	0
7	A	811	1PE	2	0
4	A	801	LMT	6	0
10	A	812	D10	1	0

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 then 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.

Ligand PG4 A 807

Ligand 1PE A 811

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand HEX A 814

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 813

Bond lengths

Bond angles

Torsions

Rings

Ligand D12 A 809

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 A 803

Bond lengths

Bond angles

Torsions

Rings

Ligand HEX A 815

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 A 805

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 A 808

Bond lengths

Bond angles

Torsions

Rings

Ligand GOL A 810	
Bond lengths	Bond angles
Torsions	Rings

Ligand D10 A 812	
Bond lengths	Bond angles
Torsions	Rings

Ligand OCT A 802

Bond lengths

Bond angles

Torsions

Rings

Ligand PG4 A 806

Bond lengths

Bond angles

Torsions

Rings

Ligand 1PE A 804

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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%)	1.15	62 (13%)	3	2	54, 73, 129, 152	1 (0%)
2	B	127/127 (100%)	0.58	6 (4%)	31	29	57, 74, 104, 110	1 (0%)
3	C	3/3 (100%)	1.03	0	100	100	69, 69, 77, 87	0
All	All	581/619 (93%)	1.02	68 (11%)	4	3	54, 74, 125, 152	2 (0%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	GLY	10.3
1	A	405	ALA	9.3
1	A	254	PHE	8.8
1	A	404	ILE	7.4
1	A	406	ALA	6.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
6	PG4	A	806	13/13	0.42	0.65	94,100,118,121	0
8	D12	A	809	12/12	0.50	1.05	90,97,99,103	0
6	PG4	A	805	13/13	0.55	0.31	86,94,112,115	0
6	PG4	A	808	13/13	0.56	0.32	89,94,104,111	0
9	GOL	A	810	6/6	0.58	0.27	118,121,122,123	0
11	HEX	A	814	6/6	0.63	0.71	92,94,97,98	0
10	D10	A	812	10/10	0.65	0.35	81,83,100,101	0
7	1PE	A	811	16/16	0.66	0.34	90,98,105,106	0
9	GOL	A	813	6/6	0.66	0.15	89,95,95,99	0
11	HEX	A	815	6/6	0.68	0.73	86,91,93,94	0
6	PG4	A	807	13/13	0.74	0.38	81,90,100,104	0
5	OCT	A	802	8/8	0.76	0.44	72,76,83,85	0
6	PG4	A	803	13/13	0.80	0.18	79,88,107,109	0
7	1PE	A	804	16/16	0.83	0.46	69,85,101,110	0
4	LMT	A	801	35/35	0.85	0.45	69,94,110,111	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.
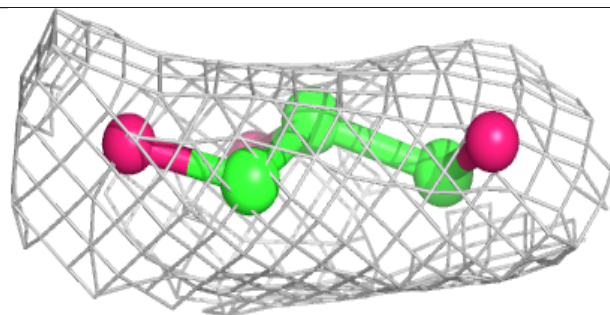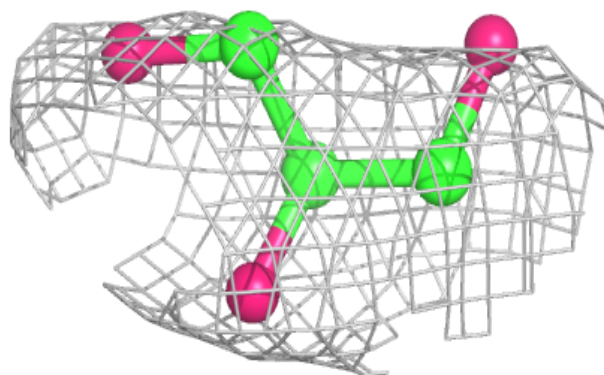

Electron density around PG4 A 806:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
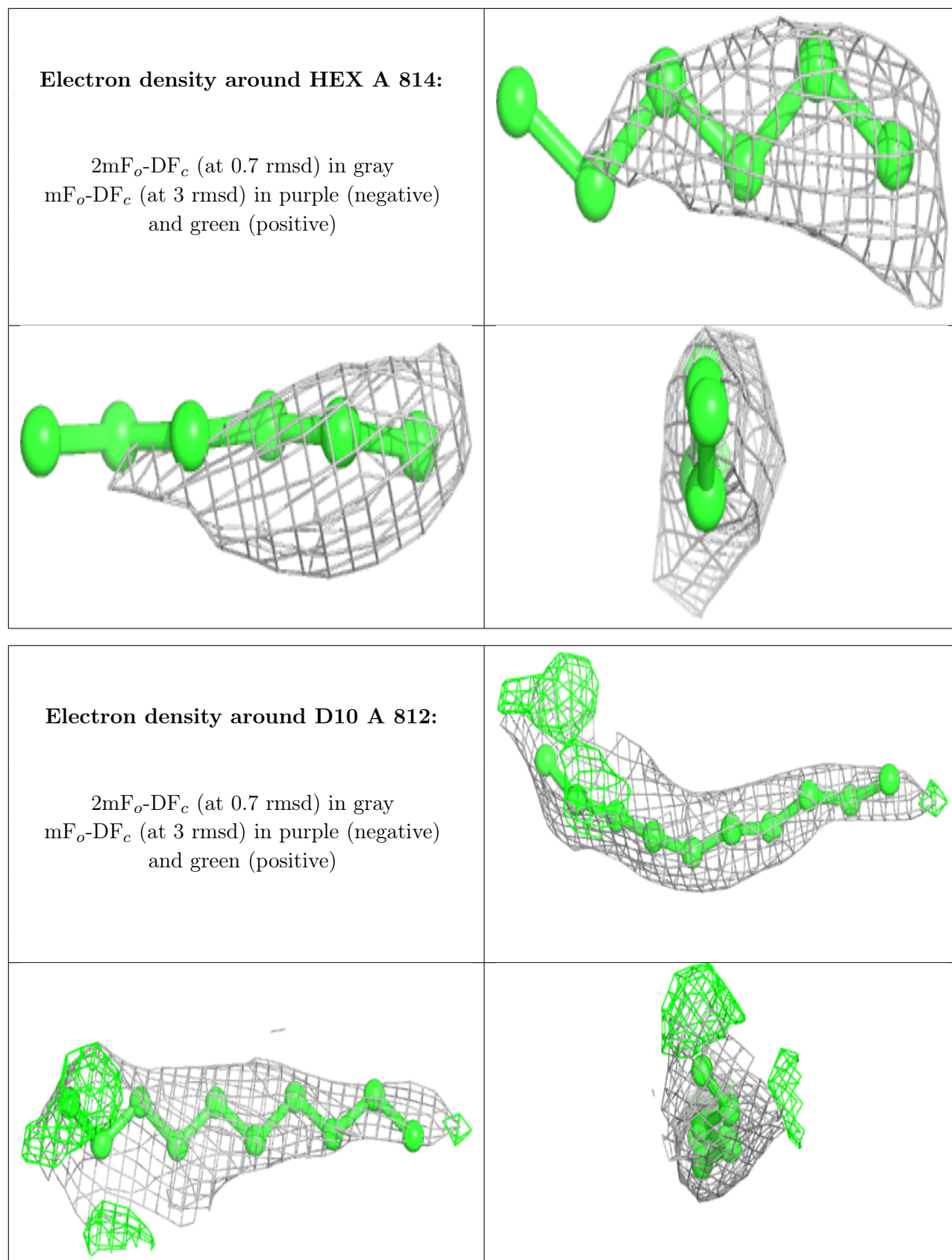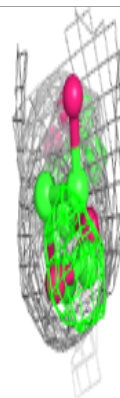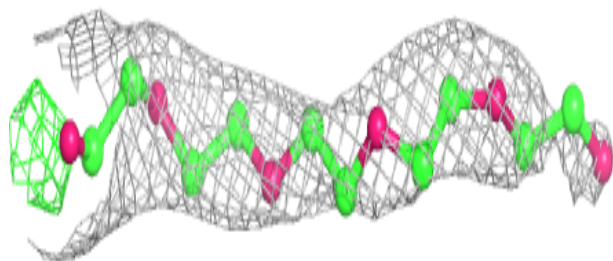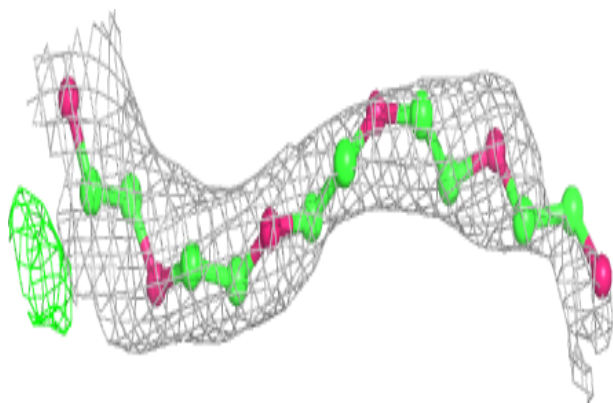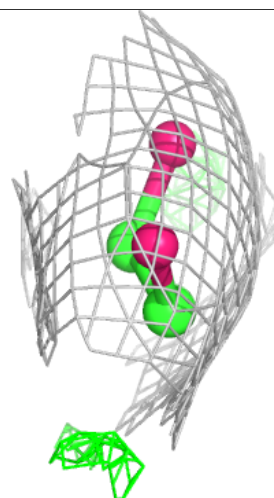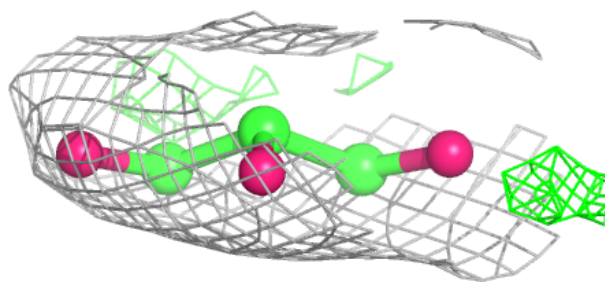$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
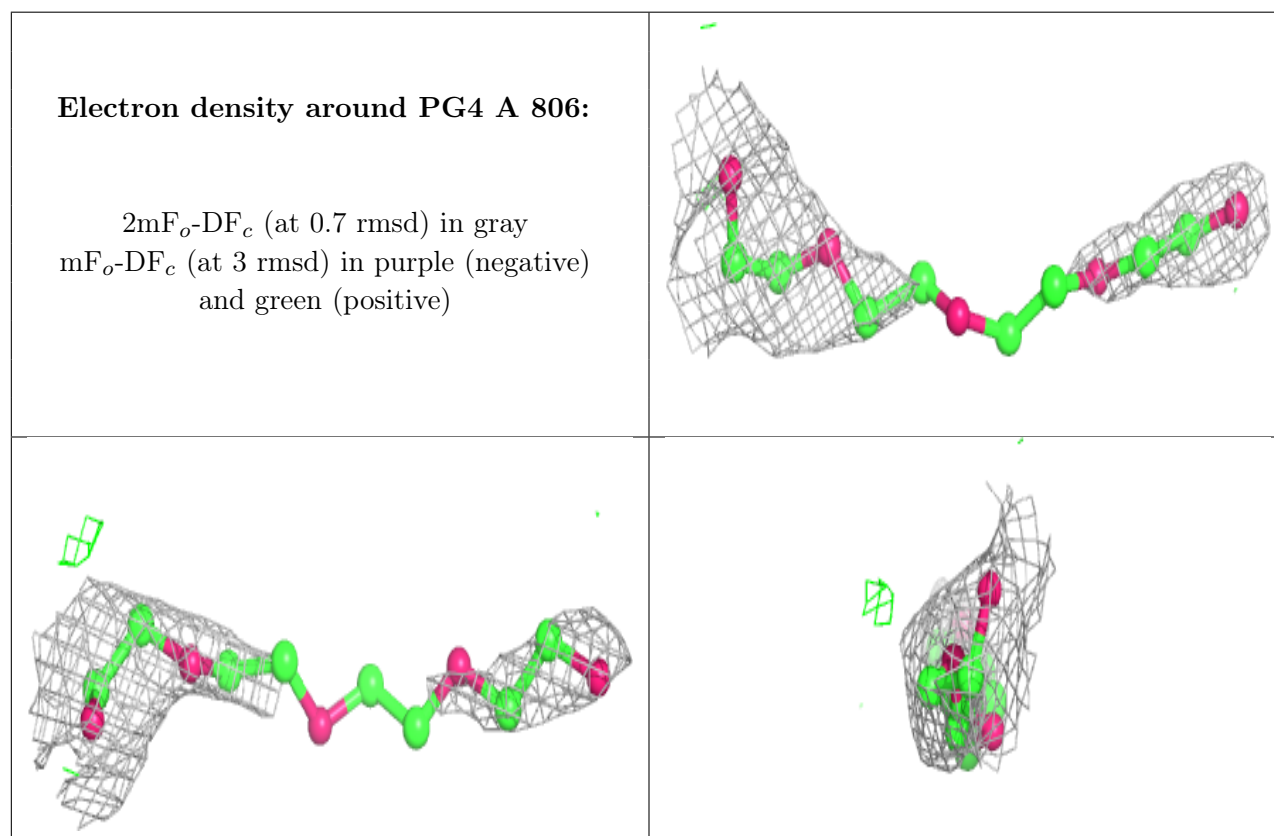
Electron density around D12 A 809:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
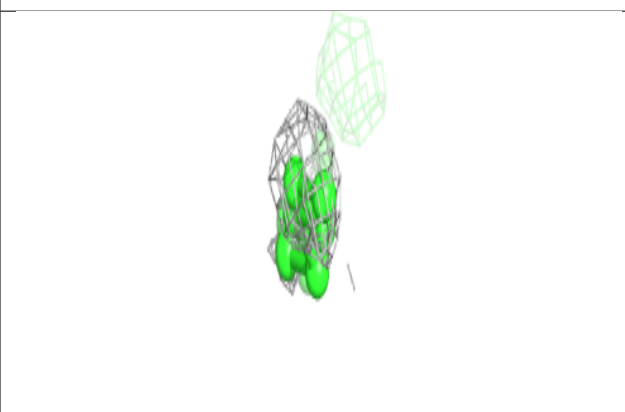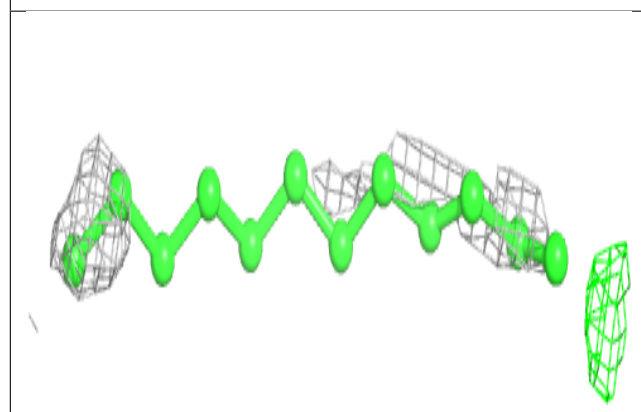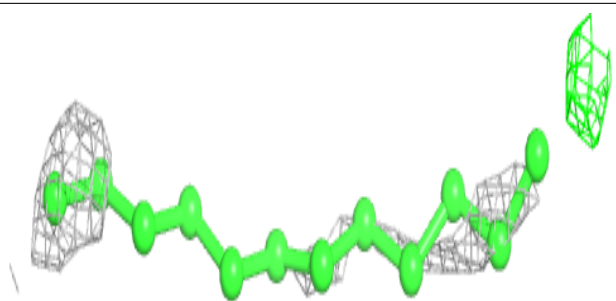
Electron density around PG4 A 805:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
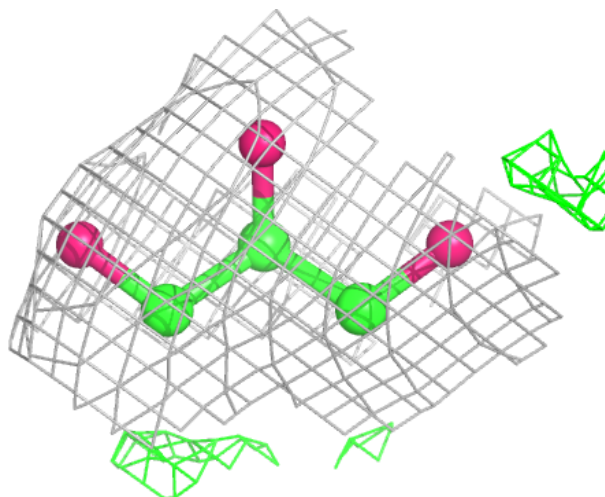$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
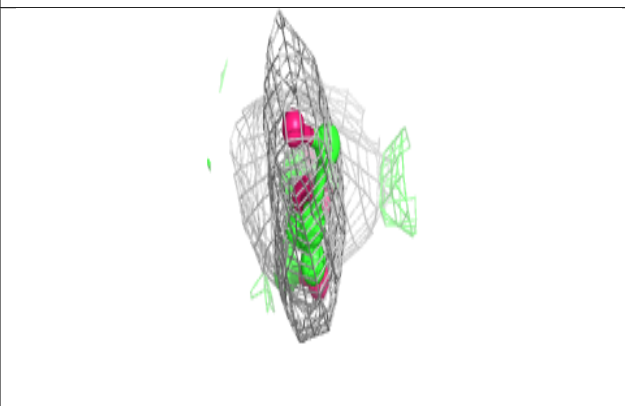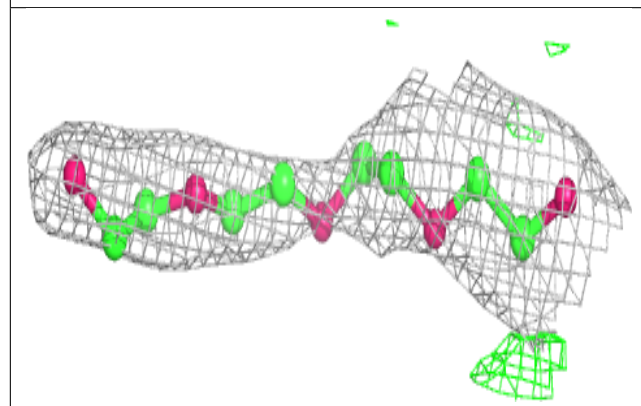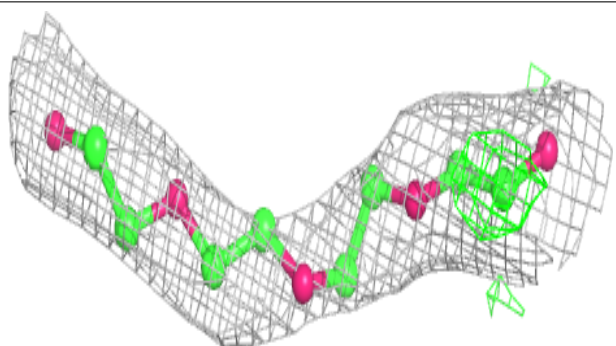
Electron density around PG4 A 808:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
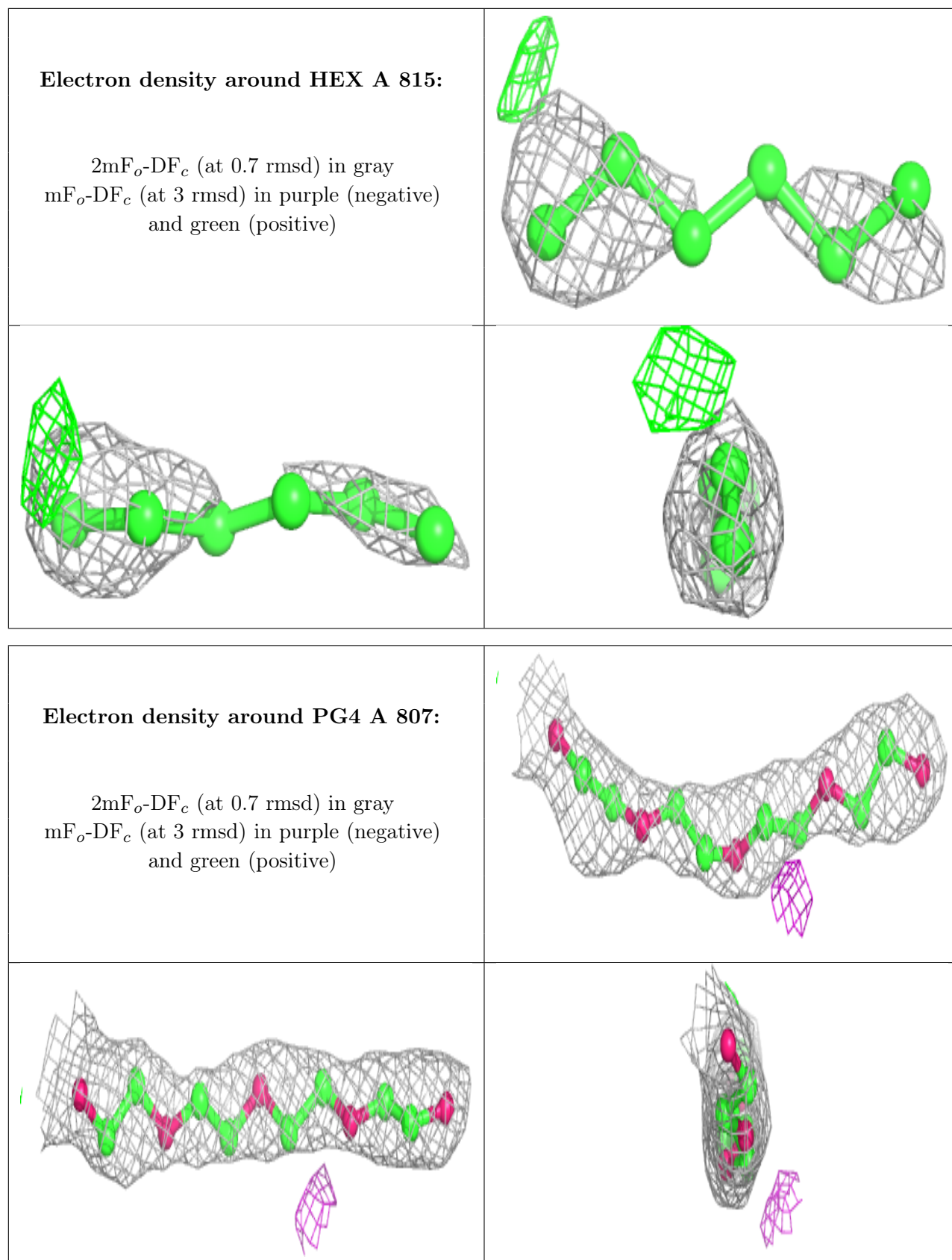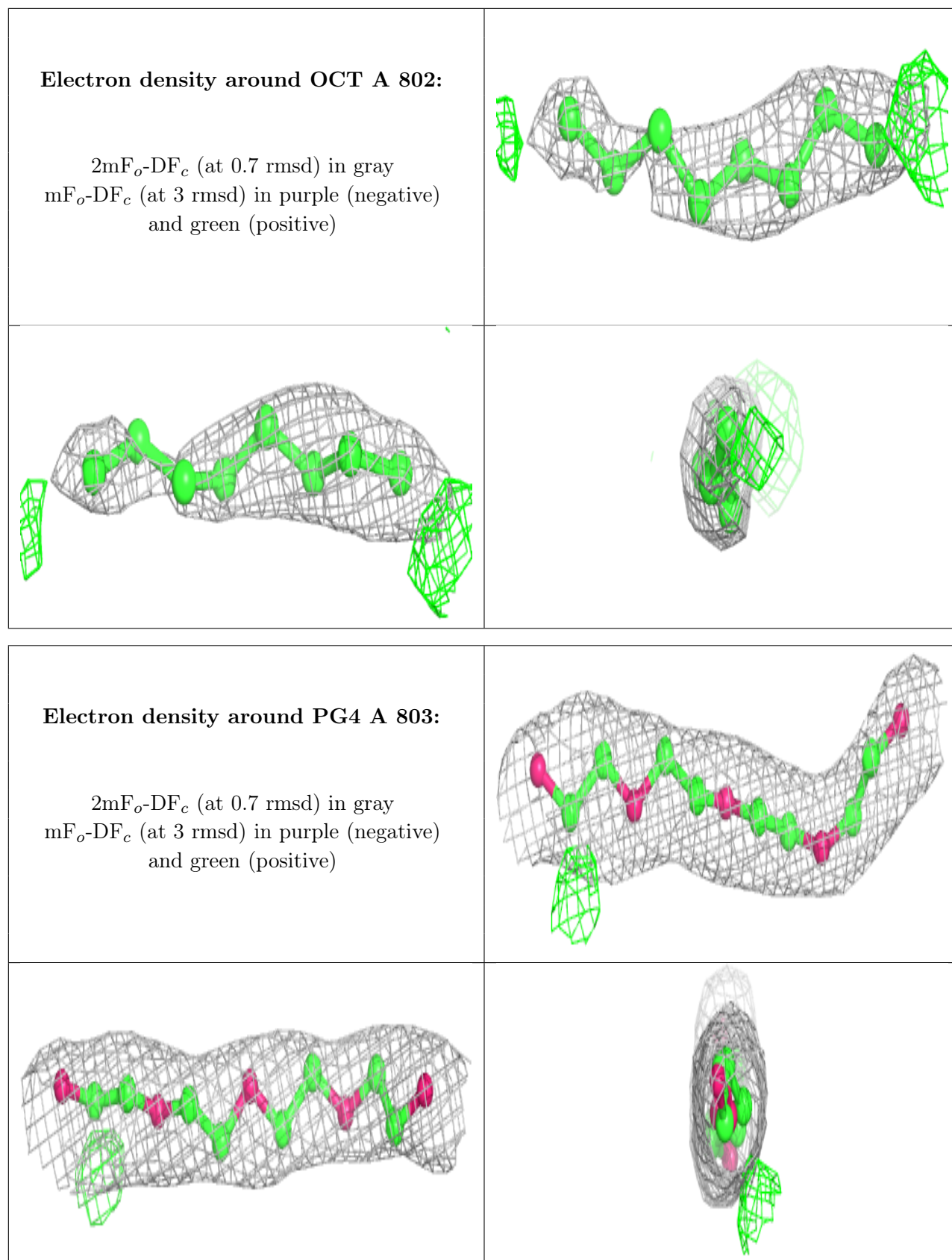and green (positive)
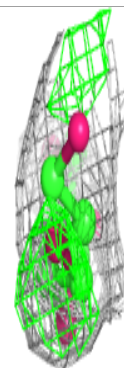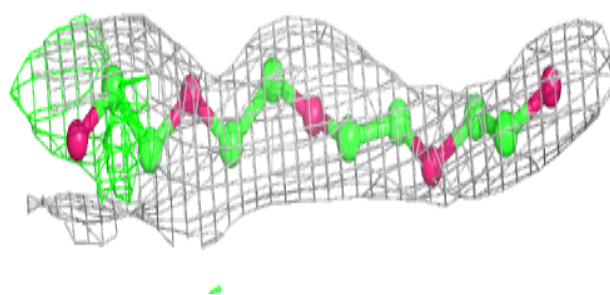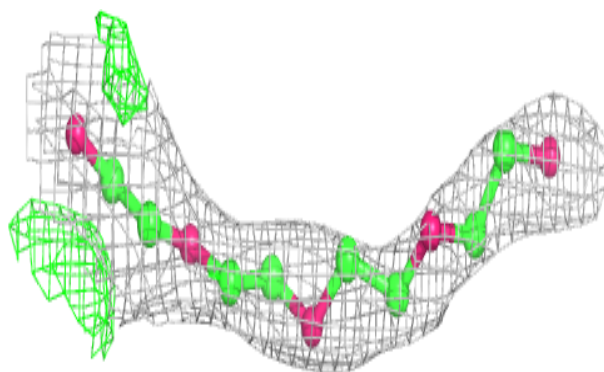
Electron density around GOL A 810:

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

Electron density around 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 D10 A 812:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
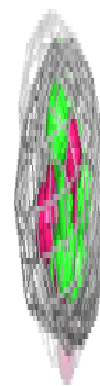mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
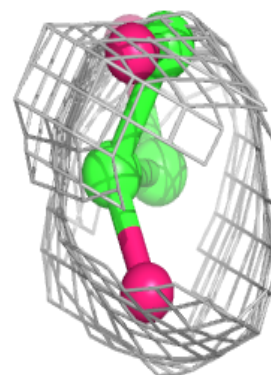
Electron density around 1PE A 811:

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

Electron density around GOL A 813:

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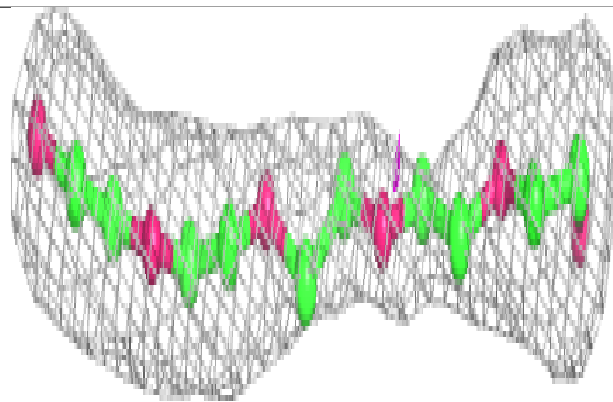$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEX A 815:

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

Electron density around PG4 A 807:

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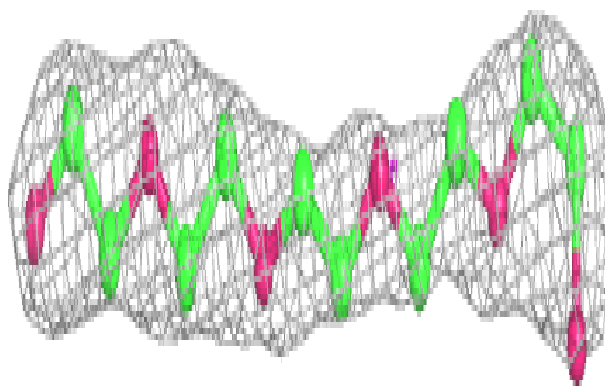and green (positive)

Electron density around OCT A 802:

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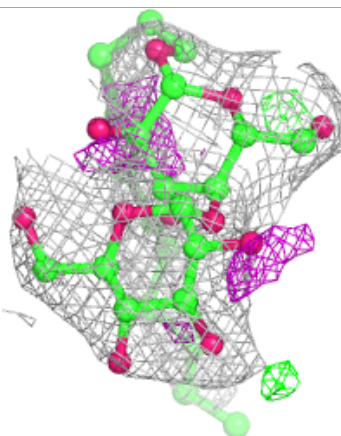mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PG4 A 803:

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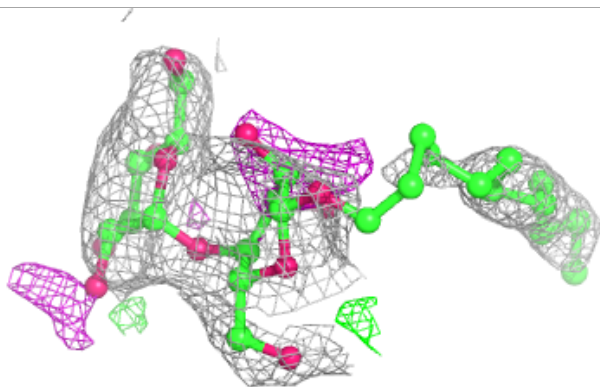mF_o-DF_c (at 3 rmsd) in purple (negative)
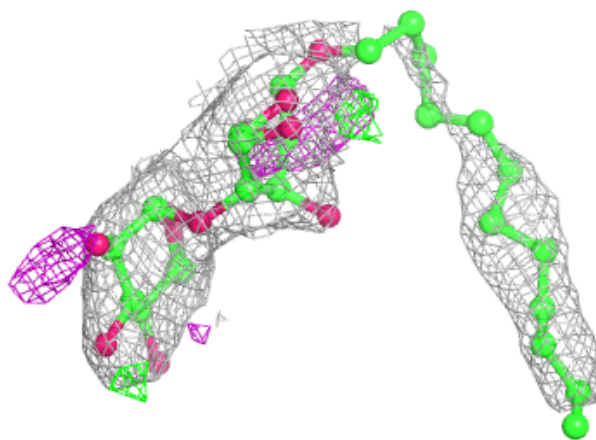and green (positive)

Electron density around 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 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.