W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 10:38 AM BST

PDB ID	:	5B0W
Title	:	Crystal structure of the 11-cis isomer of pharaonis halorhodopsin in the absence of halide ions
Authors	:	Kouyama, T.; Chan, S.K.
Deposited on	:	2015-11-11
Resolution	:	1.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

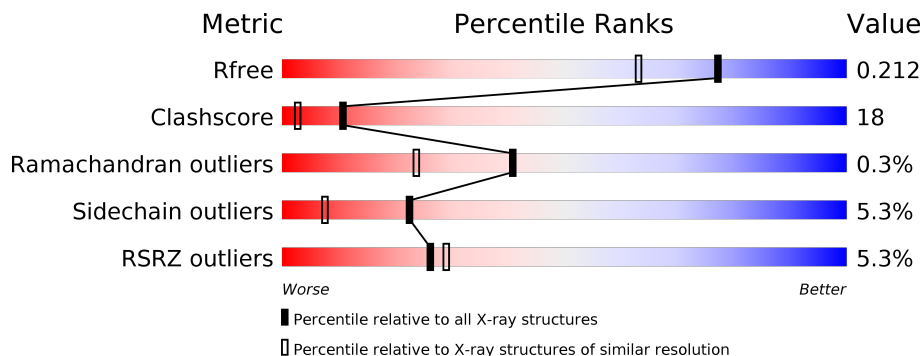|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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		0.212
Clashscore		18
Ramachandran outliers		0.3%
Sidechain outliers		5.3%
RSRZ outliers		5.3%

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	291	4% 60% 25% • 10%
1	B	291	4% 56% 31% • 11%
1	D	291	6% 63% 24% • 11%
1	E	291	3% 73% 15% • 11%
1	F	291	5% 73% 16% • 11%
1	G	291	5% 73% 15% • 11%

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
3	22B	A	302	-	-	X	-
4	L3P	A	303	-	-	-	X
4	L3P	A	304	-	-	-	X
4	L3P	B	302	-	-	-	X
4	L3P	F	302	-	-	-	X
4	L3P	F	303	-	-	-	X
4	L3P	G	302	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12650 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 Halorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	261	0
			1971	1308	300	352	11			
1	B	260	Total	C	N	O	S	0	260	0
			1963	1302	299	351	11			
1	D	259	Total	C	N	O	S	0	259	0
			1957	1299	298	349	11			
1	E	260	Total	C	N	O	S	0	260	0
			1963	1302	299	351	11			
1	F	260	Total	C	N	O	S	0	260	0
			1963	1302	299	351	11			
1	G	259	Total	C	N	O	S	0	259	0
			1957	1299	298	349	11			

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).
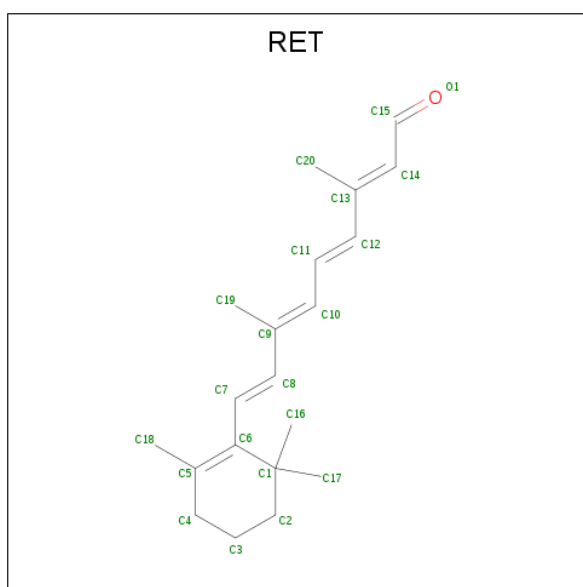
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 20	C 20	0	1
2	B	1	Total 20	C 20	0	1
2	D	1	Total 20	C 20	0	1
2	E	1	Total 20	C 20	0	1
2	F	1	Total 20	C 20	0	1
2	G	1	Total 20	C 20	0	1

- Molecule 3 is BACTERIORUBERIN (three-letter code: 22B) (formula: $C_{50}H_{76}O_4$).

22B
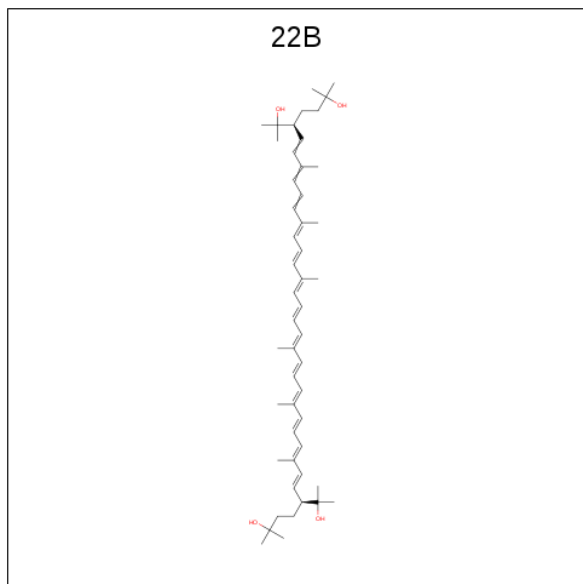
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 37	C 35	O 2	0	0

- Molecule 4 is 2,3-DI-O-PHYTANLY-3-SN-GLYCERO-1-PHOSPHORYL-3'-SN-GLYCER OL-1'-PHOSPHATE (three-letter code: L3P) (formula: $C_{46}H_{94}O_{11}P_2$).
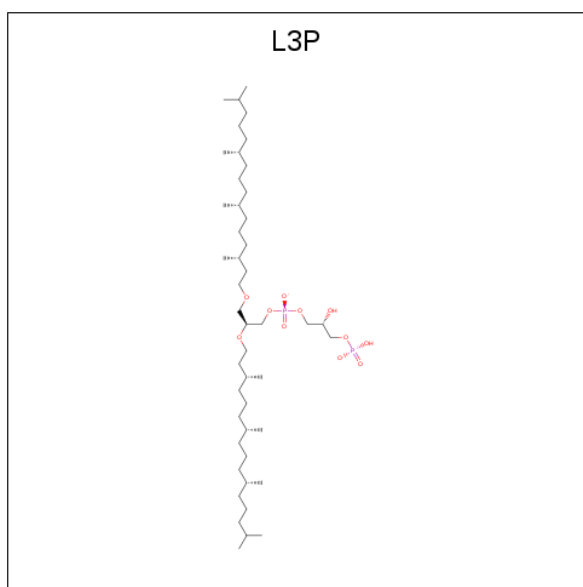
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 20	C 20	0	0
4	A	1	Total 20	C 20	0	0
4	B	1	Total 20	C 20	0	0
4	F	1	Total 20	C 20	0	0
4	F	1	Total 20	C 20	0	0
4	G	1	Total 20	C 20	0	0

- Molecule 5 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).

BNG
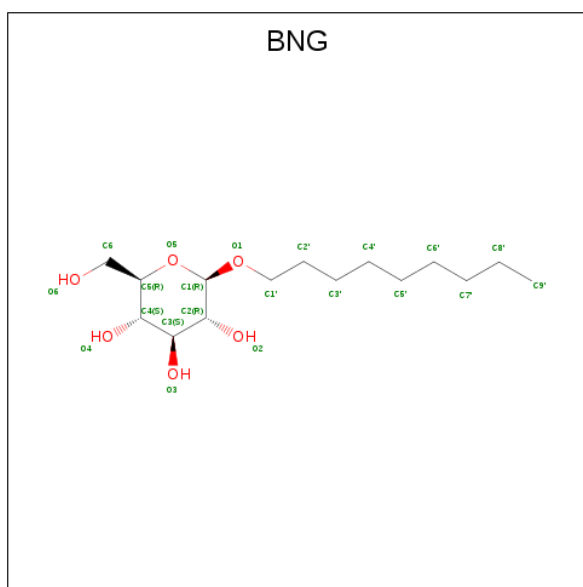
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 21	C 15	O 6	0	0
5	A	1	Total 21	C 15	O 6	0	0
5	A	1	Total 21	C 15	O 6	0	0
5	B	1	Total 21	C 15	O 6	0	0
5	F	1	Total 21	C 15	O 6	0	0
5	G	1	Total 21	C 15	O 6	0	0
5	G	1	Total 21	C 15	O 6	0	0

- Molecule 6 is ISOLEUCINE (three-letter code: ILE) (formula: $C_6H_{13}NO_2$).

WORLDWIDE
PDB
PROTEIN DATA BANK
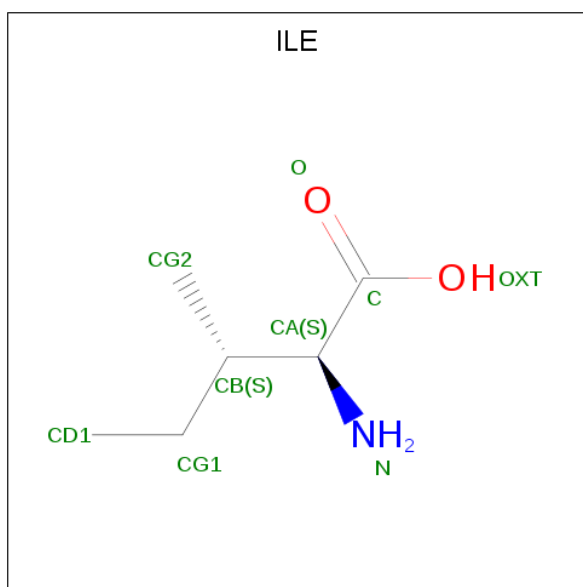
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	E	1	8	6	1	1	0	1

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	94	Total 94	O 94	0	94
7	B	78	Total 78	O 78	0	78
7	D	68	Total 68	O 68	0	68
7	E	69	Total 69	O 69	0	69
7	F	64	Total 64	O 64	0	64
7	G	71	Total 71	O 71	0	71

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: Halorhodopsin
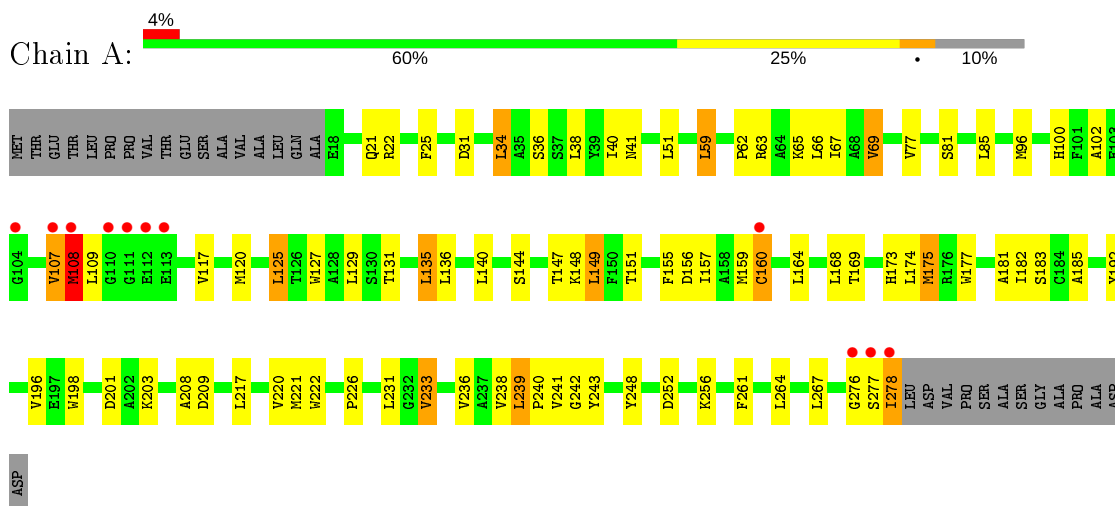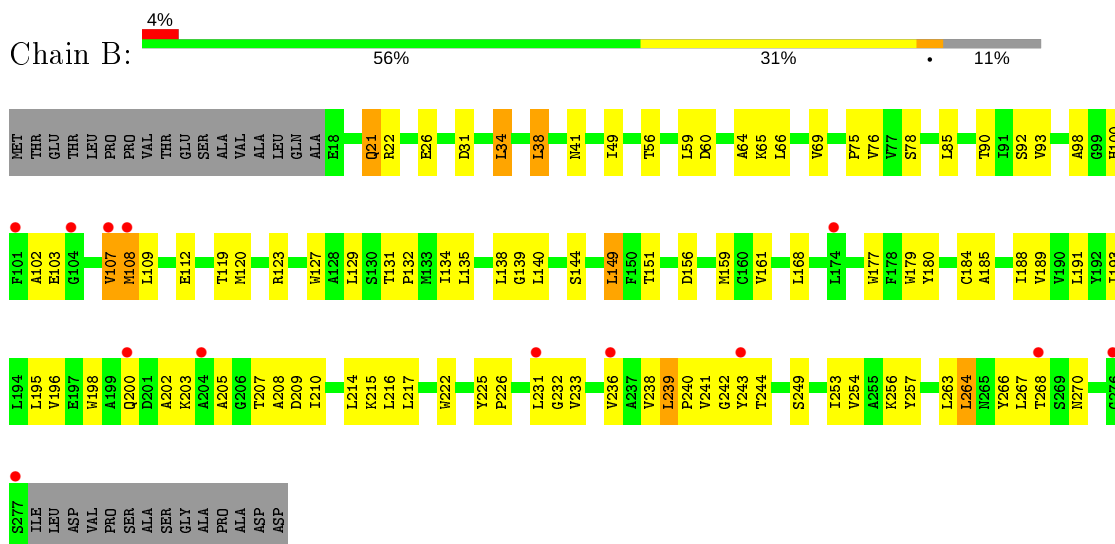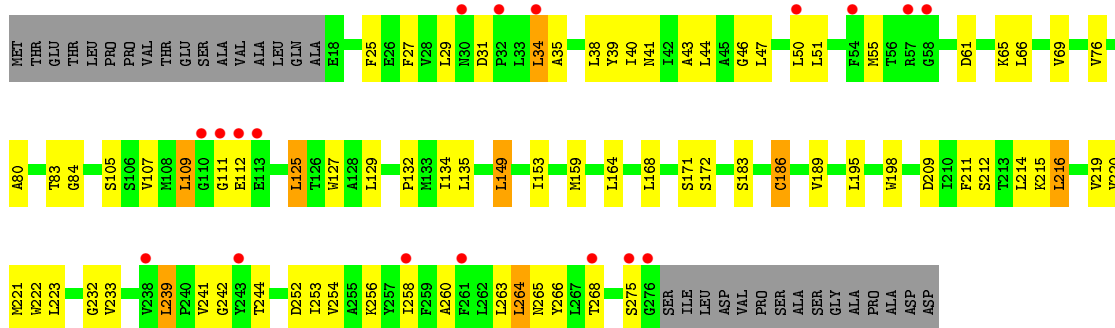
- Molecule 1: Halorhodopsin

- Molecule 1: Halorhodopsin

• Molecule 1: Halorhodopsin

Chain E:

• Molecule 1: Halorhodopsin

Chain F:

• Molecule 1: Halorhodopsin

Chain G:
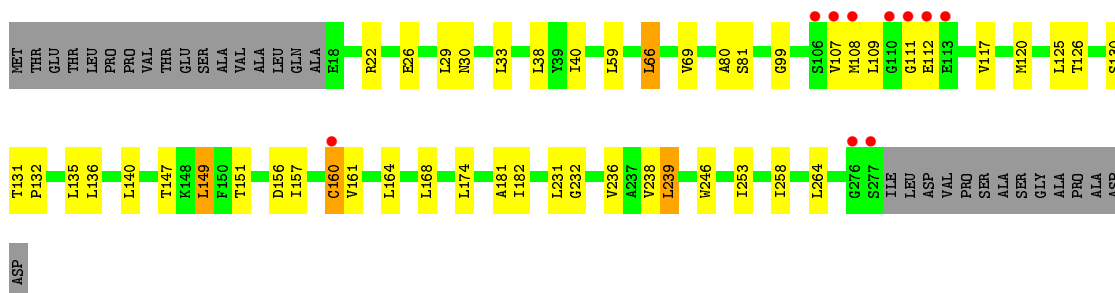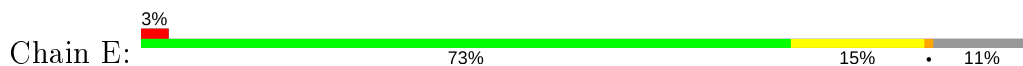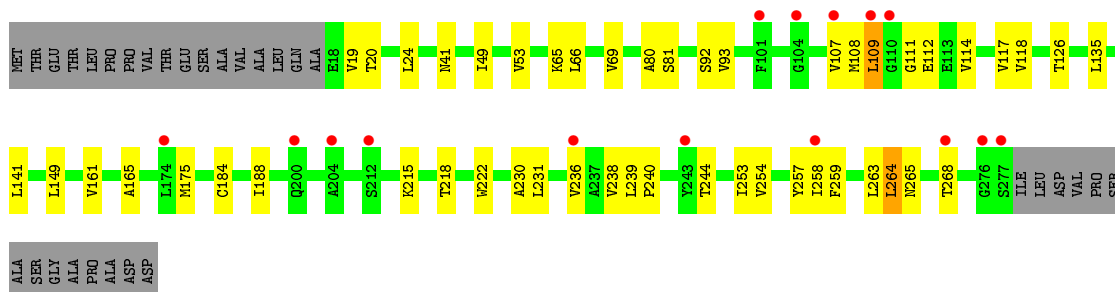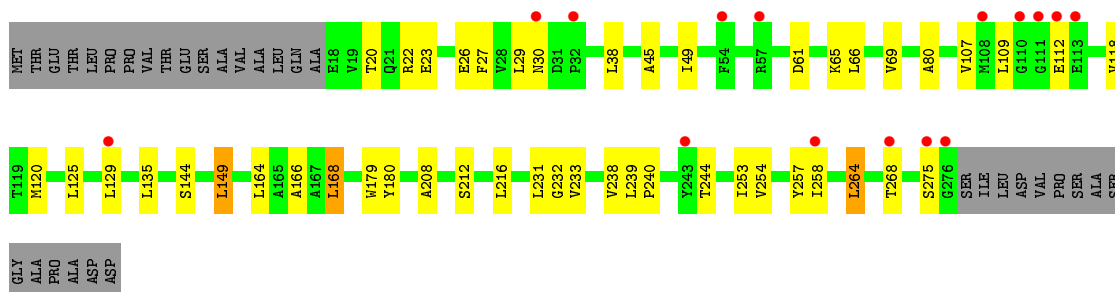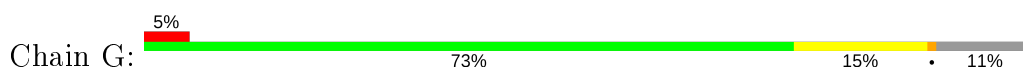
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.32Å 97.93Å 101.53Å 90.00° 128.67° 90.00°	Depositor
Resolution (Å)	15.00 – 1.70 41.68 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (15.00-1.70) 96.7 (41.68-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 1.70Å)	Xtriage
Refinement program	CNS 1.21	Depositor
R, R_{free}	0.202 , 0.215 0.197 , 0.212	Depositor DCC
R_{free} test set	5465 reflections (4.37%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 68.5	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.012 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12650	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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:
BNG, RET, L3P, 22B

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	0.66	1/2017 (0.0%)	0.78	1/2762 (0.0%)
1	B	0.52	0/2009	0.71	0/2751
1	D	0.57	1/2003 (0.0%)	0.70	0/2743
1	E	0.54	0/2009	0.65	1/2751 (0.0%)
1	F	0.44	0/2009	0.59	0/2751
1	G	0.47	0/2003	0.58	0/2743
All	All	0.54	2/12050 (0.0%)	0.67	2/16501 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if
the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected
by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a
sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186[A]	CYS	CB-SG	-5.68	1.72	1.81
1	A	160[A]	CYS	CB-SG	-5.34	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149[B]	LEU	CA-CB-CG	5.57	128.11	115.30
1	A	107[A]	VAL	N-CA-C	5.48	125.80	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248[A]	TYR	Sidechain

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	1971	0	1898	122	0
1	B	1963	0	1871	107	0
1	D	1957	0	1900	81	0
1	E	1963	0	1868	54	0
1	F	1963	0	1836	39	0
1	G	1957	0	1850	34	0
2	A	20	0	17	5	0
2	B	20	0	14	5	0
2	D	20	0	18	2	0
2	E	20	0	13	0	0
2	F	20	0	13	0	0
2	G	20	0	15	2	0
3	A	37	0	49	46	0
4	A	40	0	78	11	0
4	B	20	0	39	1	0
4	F	40	0	78	14	0
4	G	20	0	39	6	0
5	A	63	0	90	3	0
5	B	21	0	30	3	0
5	F	21	0	30	2	0
5	G	42	0	60	2	0
6	E	8	0	10	0	0
7	A	94	0	0	8	0
7	B	78	0	0	7	0
7	D	68	0	0	3	0
7	E	69	0	0	3	0
7	F	64	0	0	5	0
7	G	71	0	0	2	0
All	All	12650	0	11816	439	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 18.

The worst 5 of 439 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:147[A]:THR:CG2	3:A:302:22B:H241	1.72	1.19
1:B:233[A]:VAL:H	1:B:244[A]:THR:HG21	1.06	1.15
1:D:254[A]:VAL:HG13	1:D:258[A]:ILE:HD11	1.18	1.12
1:A:147[A]:THR:HG22	3:A:302:22B:H241	1.14	1.12
1:D:164[A]:LEU:O	1:D:168[A]:LEU:HD13	1.57	1.04

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	259/291 (89%)	256 (99%)	2 (1%)	1 (0%)	34	18
1	B	258/291 (89%)	248 (96%)	8 (3%)	2 (1%)	19	6
1	D	257/291 (88%)	251 (98%)	6 (2%)	0	100	100
1	E	258/291 (89%)	251 (97%)	6 (2%)	1 (0%)	34	18
1	F	258/291 (89%)	253 (98%)	5 (2%)	0	100	100
1	G	257/291 (88%)	253 (98%)	4 (2%)	0	100	100
All	All	1547/1746 (89%)	1512 (98%)	31 (2%)	4 (0%)	41	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108[A]	MET
1	B	108[A]	MET
1	E	111[B]	GLY
1	B	196[A]	VAL

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	209/233 (90%)	192 (92%)	17 (8%)	11	2
1	B	208/233 (89%)	197 (95%)	11 (5%)	22	7
1	D	207/233 (89%)	194 (94%)	13 (6%)	18	5
1	E	208/233 (89%)	197 (95%)	11 (5%)	22	7
1	F	208/233 (89%)	201 (97%)	7 (3%)	37	18
1	G	207/233 (89%)	200 (97%)	7 (3%)	37	18
All	All	1247/1398 (89%)	1181 (95%)	66 (5%)	22	7

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	38[A]	LEU
1	D	216[A]	LEU
1	G	66[B]	LEU
1	D	66[A]	LEU
1	D	135[A]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	145[A]	ASN
1	E	41[B]	ASN
1	F	41[B]	ASN
1	D	41[A]	ASN
1	F	30[B]	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	L3P	F	303	-	19,19,58	2.03	11 (57%)	22,22,73	1.60	4 (18%)
2	RET	D	301[A]	1	20,20,21	2.44	7 (35%)	27,27,28	1.56	6 (22%)
2	RET	A	301[A]	1	20,20,21	2.52	7 (35%)	27,27,28	1.62	5 (18%)
2	RET	B	301[A]	1	20,20,21	2.16	6 (30%)	27,27,28	1.56	7 (25%)
5	BNG	G	304	-	21,21,21	1.66	6 (28%)	26,26,26	0.75	0
4	L3P	B	302	-	19,19,58	1.93	8 (42%)	22,22,73	1.44	4 (18%)
4	L3P	G	302	-	19,19,58	1.95	8 (42%)	22,22,73	1.35	2 (9%)
3	22B	A	302	-	35,36,53	3.37	20 (57%)	42,47,72	1.55	7 (16%)
4	L3P	F	302	-	19,19,58	1.89	7 (36%)	22,22,73	1.11	2 (9%)
5	BNG	A	305	-	21,21,21	1.43	5 (23%)	26,26,26	0.71	0
2	RET	E	302[B]	1	20,20,21	2.09	6 (30%)	27,27,28	1.55	5 (18%)
5	BNG	F	304	-	21,21,21	1.25	3 (14%)	26,26,26	0.73	0
4	L3P	A	303	-	19,19,58	1.86	8 (42%)	22,22,73	1.11	1 (4%)
5	BNG	B	303	-	21,21,21	1.79	6 (28%)	26,26,26	0.72	0
5	BNG	A	306	-	21,21,21	1.62	5 (23%)	26,26,26	0.78	1 (3%)
2	RET	F	301[B]	1	20,20,21	2.09	5 (25%)	27,27,28	1.76	8 (29%)
4	L3P	A	304	-	19,19,58	1.79	6 (31%)	22,22,73	1.27	3 (13%)
2	RET	G	301[B]	1	20,20,21	2.00	5 (25%)	27,27,28	1.56	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	BNG	A	307	-	21,21,21	1.56	4 (19%)	26,26,26	0.82	1 (3%)
5	BNG	G	303	-	21,21,21	1.74	7 (33%)	26,26,26	0.75	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	L3P	F	303	-	-	8/20/20/67	-
2	RET	D	301[A]	1	-	1/13/30/31	0/1/1/1
2	RET	A	301[A]	1	-	1/13/30/31	0/1/1/1
2	RET	B	301[A]	1	-	1/13/30/31	0/1/1/1
5	BNG	G	304	-	-	4/12/32/32	0/1/1/1
4	L3P	B	302	-	-	8/20/20/67	-
4	L3P	G	302	-	-	6/20/20/67	-
3	22B	A	302	-	-	16/42/42/65	-
4	L3P	F	302	-	-	12/20/20/67	-
5	BNG	A	305	-	-	1/12/32/32	0/1/1/1
2	RET	E	302[B]	1	-	0/13/30/31	0/1/1/1
5	BNG	F	304	-	-	3/12/32/32	0/1/1/1
4	L3P	A	303	-	-	3/20/20/67	-
5	BNG	B	303	-	-	4/12/32/32	0/1/1/1
5	BNG	A	306	-	-	1/12/32/32	0/1/1/1
2	RET	F	301[B]	1	-	0/13/30/31	0/1/1/1
4	L3P	A	304	-	-	6/20/20/67	-
2	RET	G	301[B]	1	-	0/13/30/31	0/1/1/1
5	BNG	A	307	-	-	4/12/32/32	0/1/1/1
5	BNG	G	303	-	-	1/12/32/32	0/1/1/1

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	22B	C4-C3	9.32	1.54	1.32
2	A	301[A]	RET	C1-C6	7.27	1.63	1.53
3	A	302	22B	C10-C9	6.71	1.44	1.35
2	B	301[A]	RET	C1-C6	6.01	1.62	1.53
2	D	301[A]	RET	C1-C6	5.81	1.61	1.53

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	22B	C50-C43-C44	-4.64	116.43	122.92
4	F	303	L3P	C16-C17-C18	4.44	130.25	115.92
4	G	302	L3P	C26-C25-C23	4.09	129.13	115.92
4	B	302	L3P	C26-C25-C23	3.66	127.74	115.92
2	A	301[A]	RET	C11-C10-C9	-3.61	122.16	127.31

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	22B	C1-C2-C3-C4
3	A	302	22B	C7-C8-C9-C10
3	A	302	22B	C7-C8-C9-C19
3	A	302	22B	C10-C11-C12-C13
3	A	302	22B	C12-C13-C14-C15

There are no ring outliers.

16 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	303	L3P	6	0
2	D	301[A]	RET	2	0
2	A	301[A]	RET	5	0
2	B	301[A]	RET	5	0
5	G	304	BNG	2	0
4	B	302	L3P	1	0
4	G	302	L3P	6	0
3	A	302	22B	46	0
4	F	302	L3P	8	0
5	A	305	BNG	2	0
5	F	304	BNG	2	0
4	A	303	L3P	5	0
5	B	303	BNG	3	0
4	A	304	L3P	6	0
2	G	301[B]	RET	2	0
5	A	307	BNG	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 L3P F 303

Bond lengths

Bond angles

Torsions

Rings

Ligand RET D 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand RET B 301 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG G 304

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P G 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 22B A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P F 302

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand RET E 302 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG F 304

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 306

Bond lengths

Bond angles

Torsions

Rings

Ligand RET F 301 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P A 304

Bond lengths

Bond angles

Torsions

Rings

Ligand RET G 301 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 307 — Bond lengths, Bond angles, Torsions, Rings

Ligand BNG G 303 — Bond lengths, Bond angles, Torsions, Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	261/291 (89%)	0.05	11 (4%)	36	40	9, 13, 30, 47	261 (100%)
1	B	260/291 (89%)	0.34	13 (5%)	28	32	9, 21, 32, 50	260 (100%)
1	D	259/291 (89%)	0.27	18 (6%)	16	19	10, 17, 33, 45	259 (100%)
1	E	260/291 (89%)	-0.02	10 (3%)	40	45	10, 15, 31, 47	260 (100%)
1	F	260/291 (89%)	0.28	15 (5%)	23	25	13, 22, 36, 52	260 (100%)
1	G	259/291 (89%)	0.19	15 (5%)	23	25	11, 19, 34, 47	259 (100%)
All	All	1559/1746 (89%)	0.18	82 (5%)	26	29	9, 18, 33, 52	1559 (100%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277[A]	SER	11.1
1	F	277[B]	SER	10.0
1	D	276[A]	GLY	9.4
1	D	111[A]	GLY	9.1
1	G	276[B]	GLY	7.3

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 monosaccharides 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(Å²)	Q<0.9
4	L3P	G	302	20/59	0.57	0.72	87,89,90,91	0
4	L3P	F	302	20/59	0.57	0.58	66,68,70,70	0
4	L3P	A	303	20/59	0.58	0.77	85,88,90,90	0
5	BNG	G	303	21/21	0.63	0.29	86,88,90,90	0
4	L3P	F	303	20/59	0.65	0.68	75,79,84,85	0
5	BNG	B	303	21/21	0.69	0.20	57,62,65,65	0
5	BNG	A	306	21/21	0.71	0.21	70,73,74,75	0
4	L3P	B	302	20/59	0.71	0.65	77,79,80,81	0
4	L3P	A	304	20/59	0.72	0.65	63,66,70,71	0
3	22B	A	302	37/54	0.72	0.35	41,53,64,65	0
6	ILE	E	301[B]	8/9	0.74	0.17	37,38,40,41	8
5	BNG	A	307	21/21	0.76	0.19	54,60,74,75	0
5	BNG	G	304	21/21	0.84	0.15	27,45,52,53	0
5	BNG	A	305	21/21	0.85	0.15	34,44,68,69	0
5	BNG	F	304	21/21	0.93	0.11	24,27,39,42	0
2	RET	F	301[B]	20/21	0.94	0.10	21,21,26,29	19
2	RET	D	301[A]	20/21	0.95	0.11	8,10,14,14	20
2	RET	E	302[B]	20/21	0.95	0.11	10,12,18,19	20
2	RET	G	301[B]	20/21	0.95	0.11	13,16,22,22	20
2	RET	B	301[A]	20/21	0.96	0.10	15,18,21,22	20
2	RET	A	301[A]	20/21	0.96	0.12	8,11,16,19	20

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.
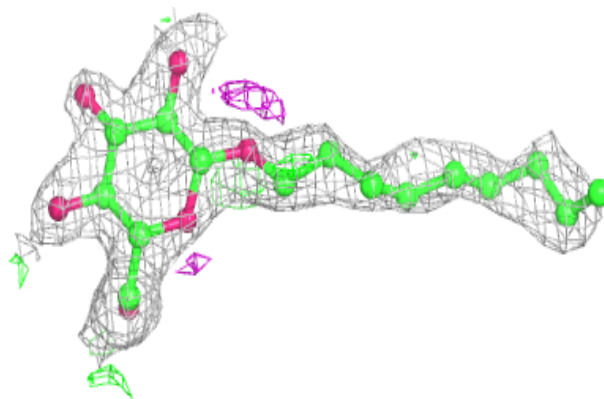
Electron density around L3P G 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
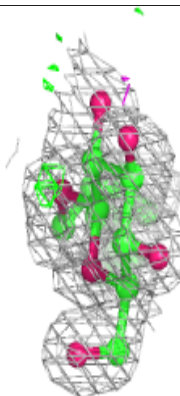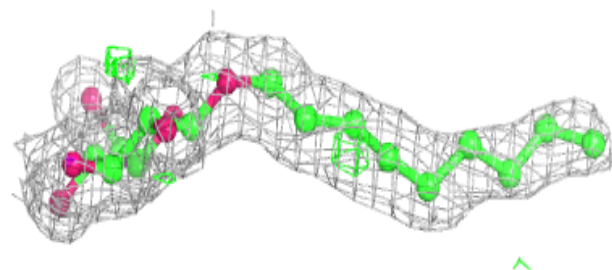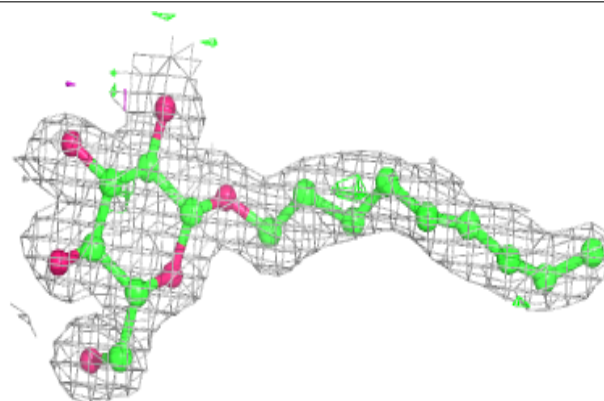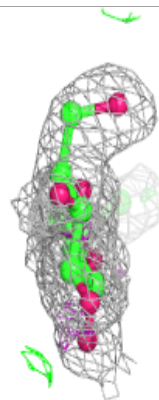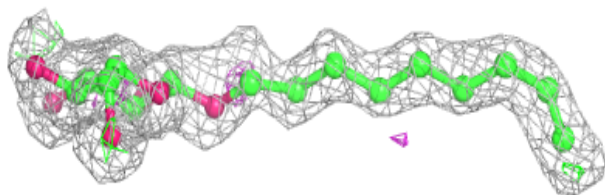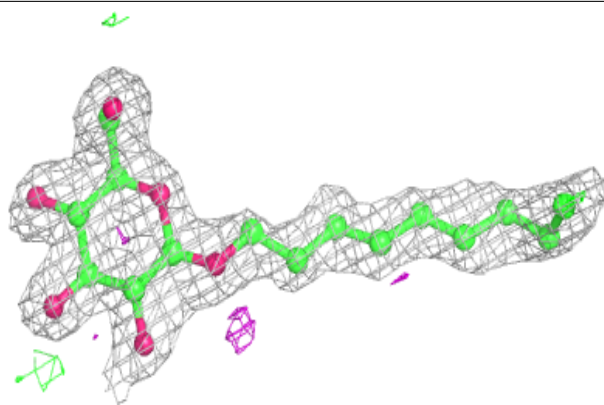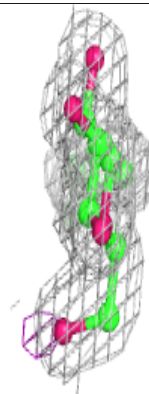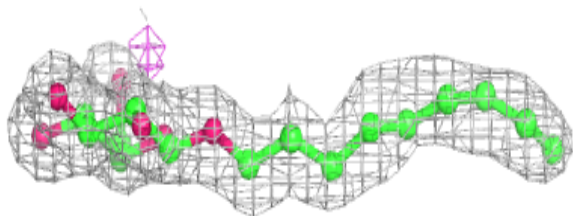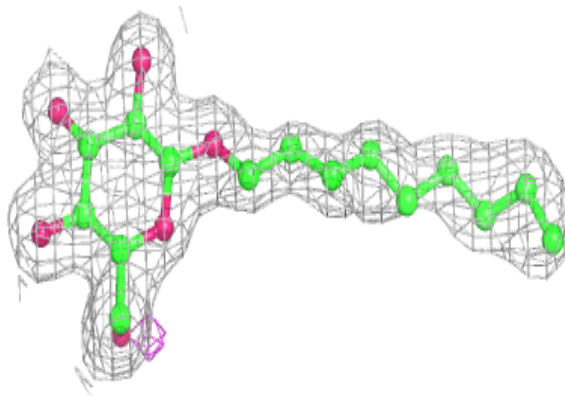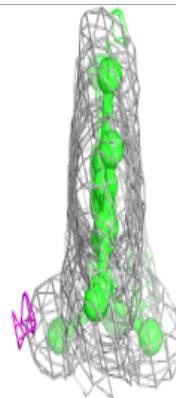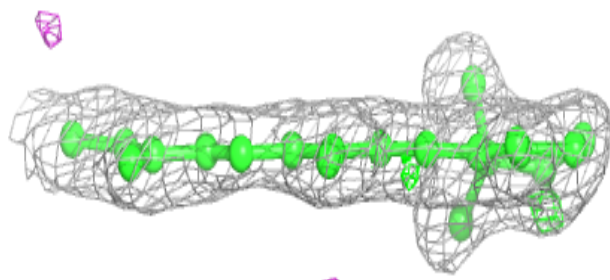mF_o-DF_c (at 3 rmsd) in purple (negative)
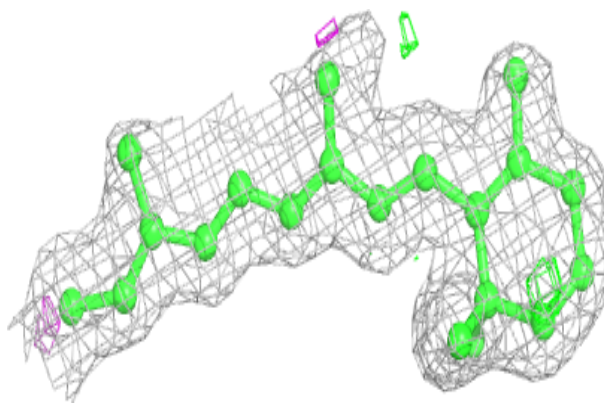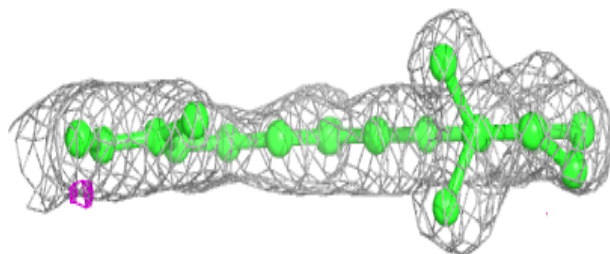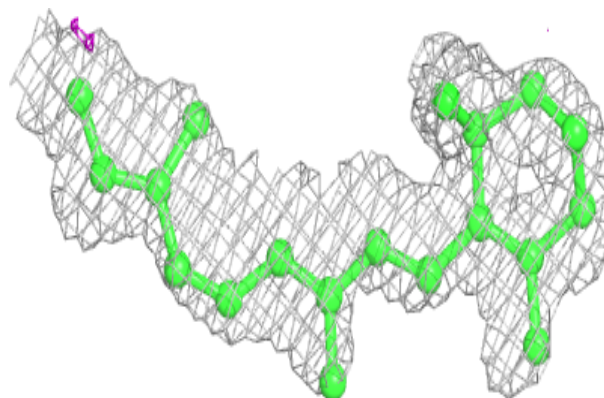and green (positive)
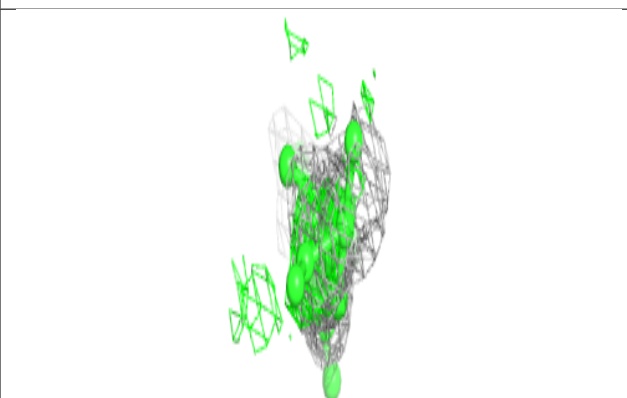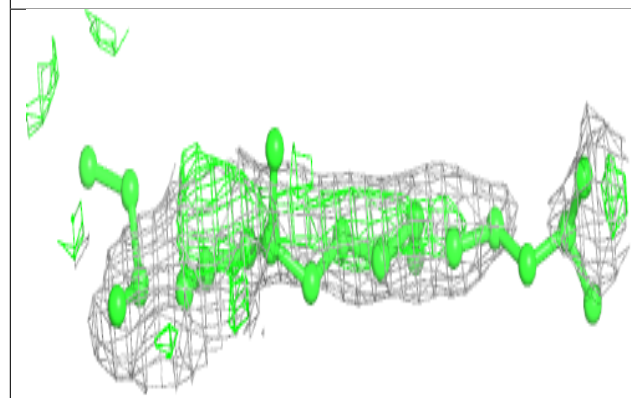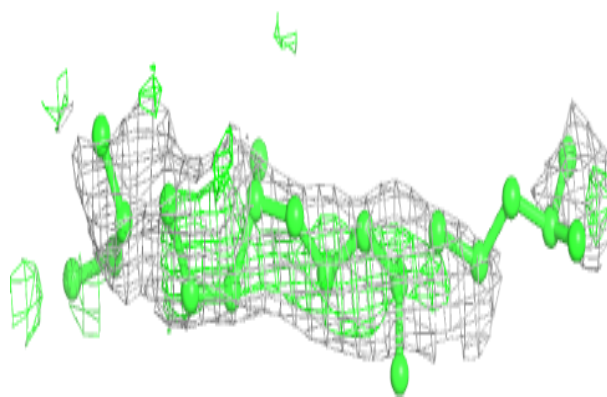
Electron density around L3P F 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
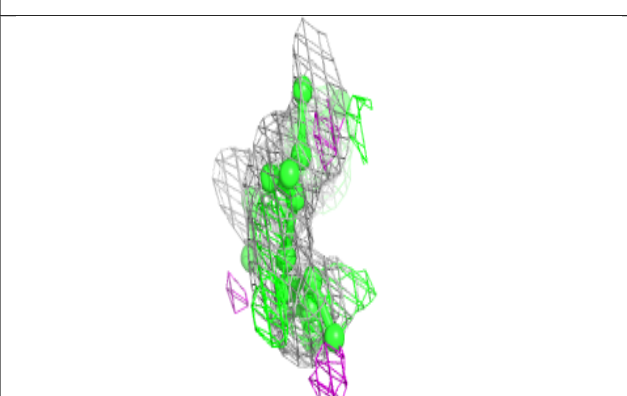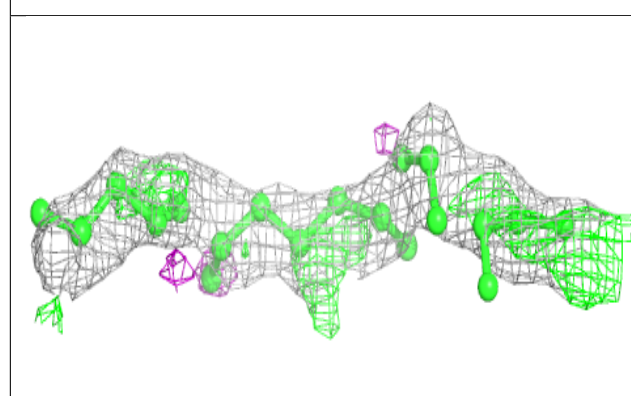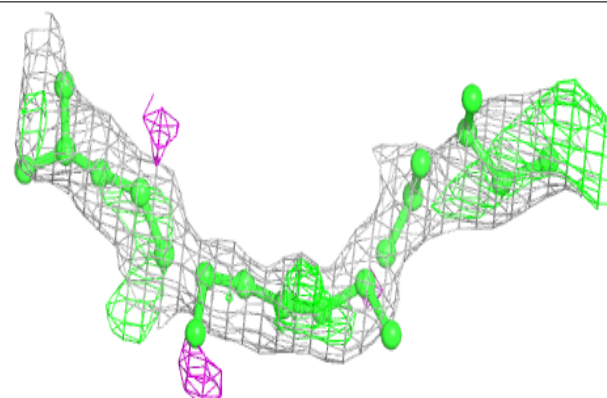
Electron density around L3P A 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
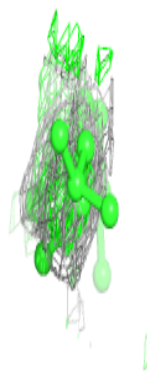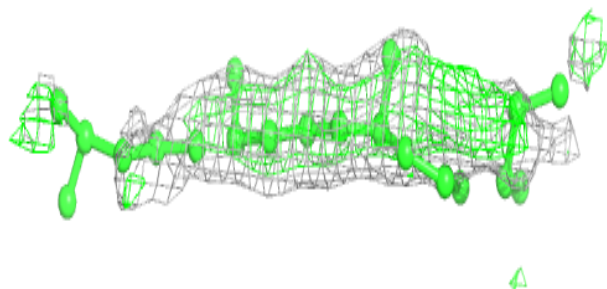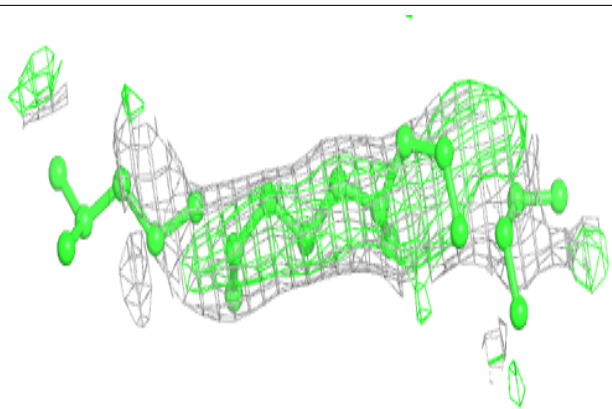
Electron density around BNG G 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
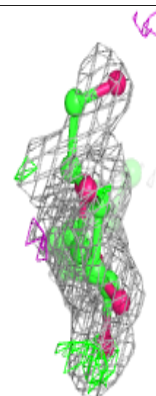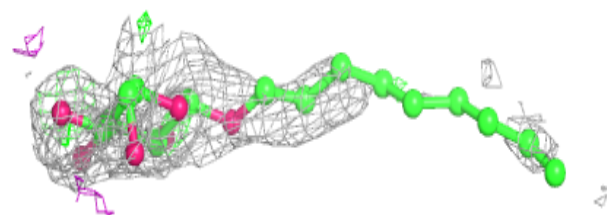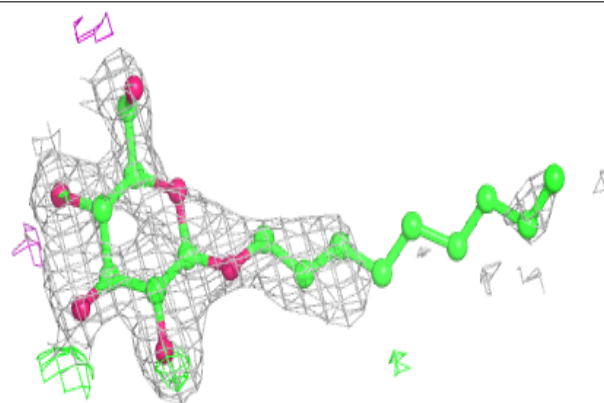
Electron density around L3P F 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
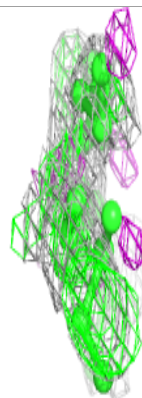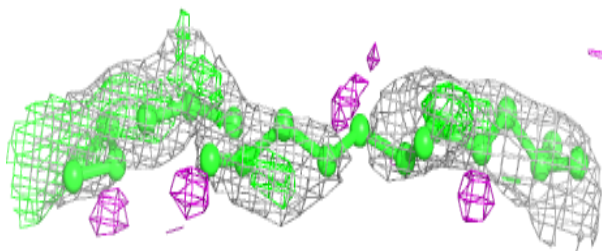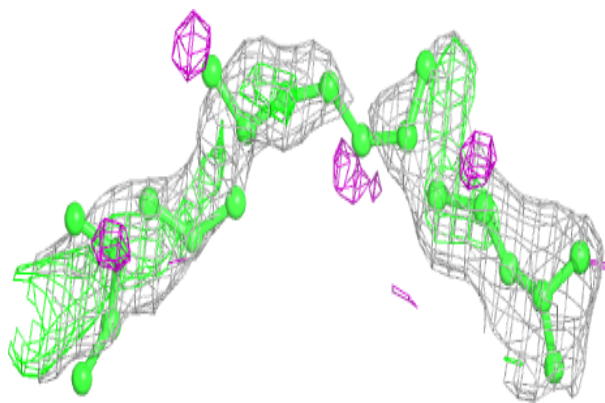
Electron density around BNG B 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
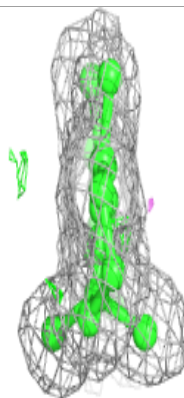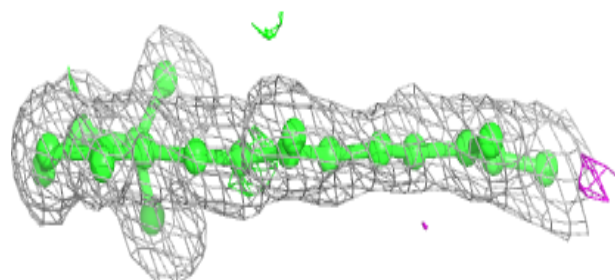$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
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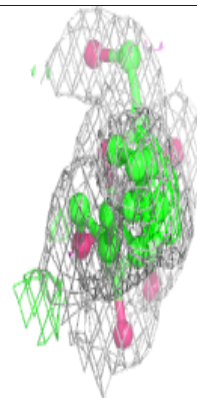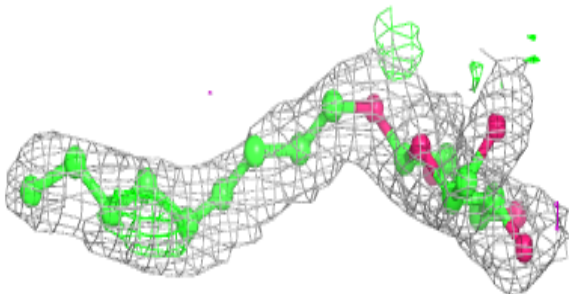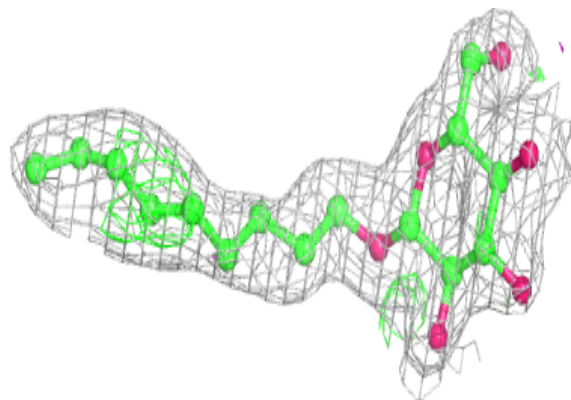
Electron density around BNG A 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
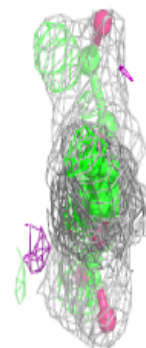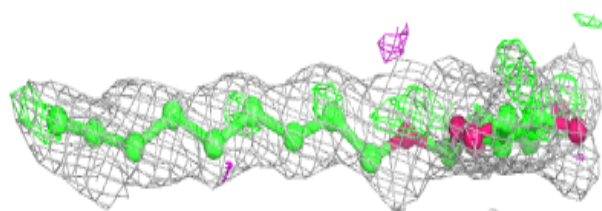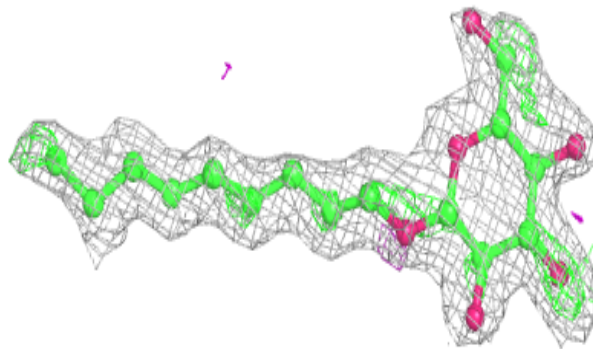
Electron density around L3P B 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
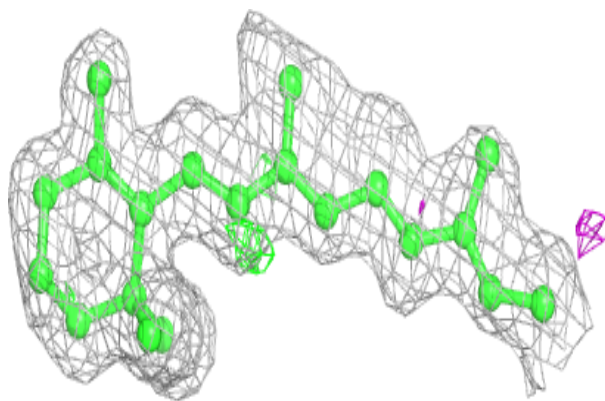and green (positive)
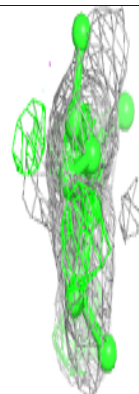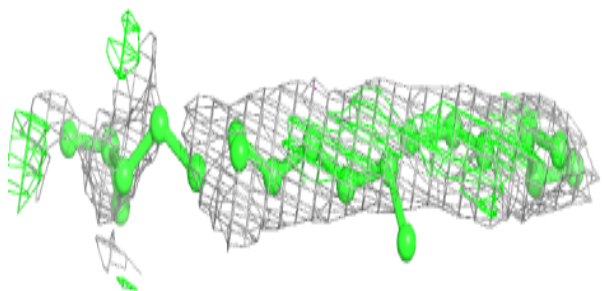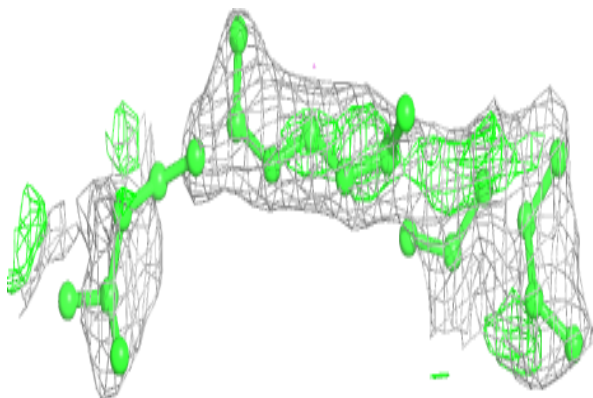
Electron density around L3P A 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
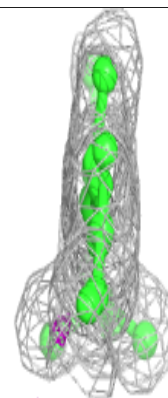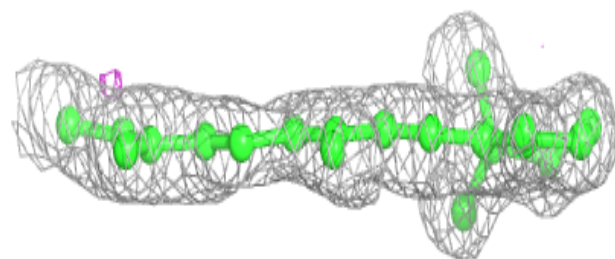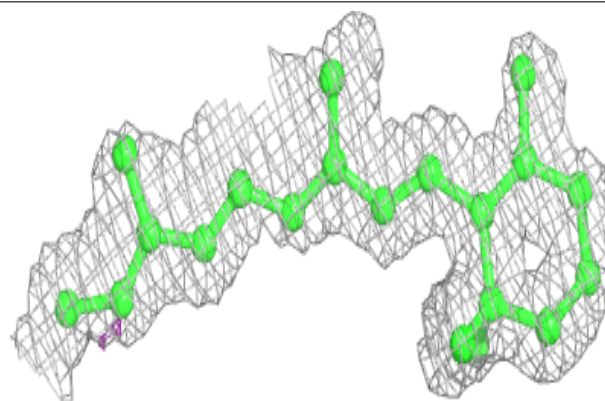and green (positive)
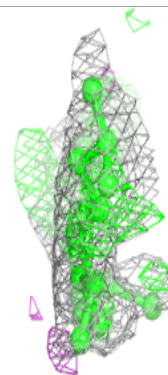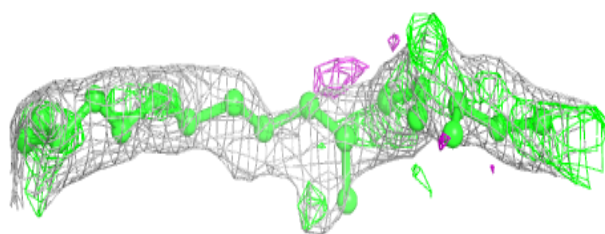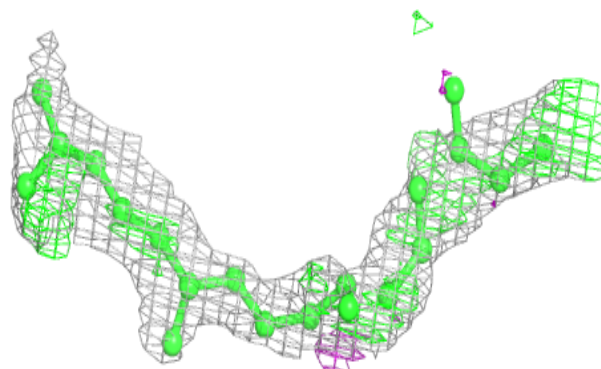
Electron density around 22B A 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
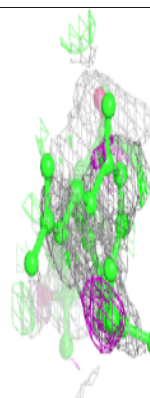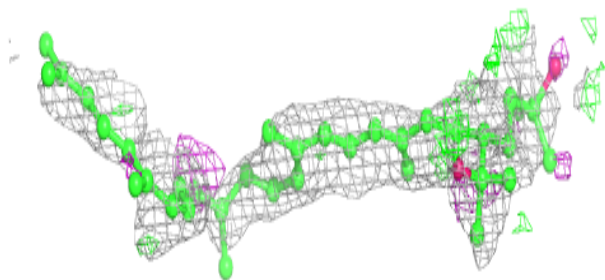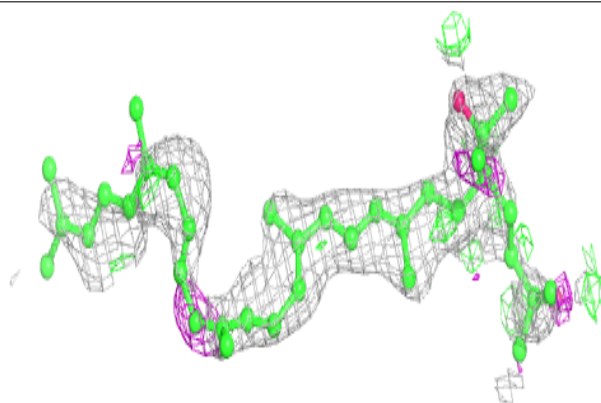
Electron density around BNG A 307:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
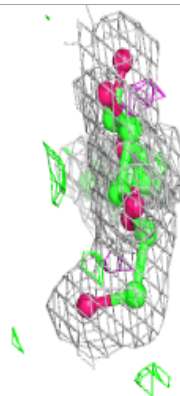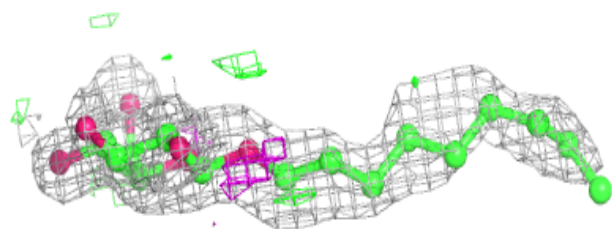
Electron density around BNG G 304:

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

Electron density around BNG A 305:

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

Electron density around BNG F 304:

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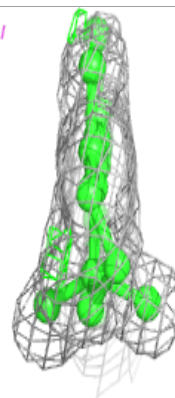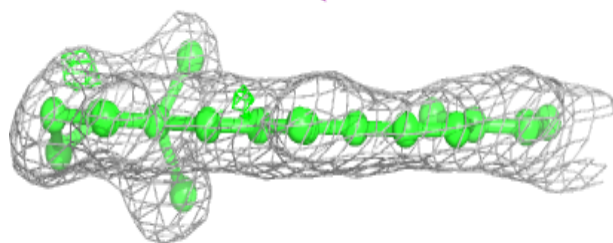$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
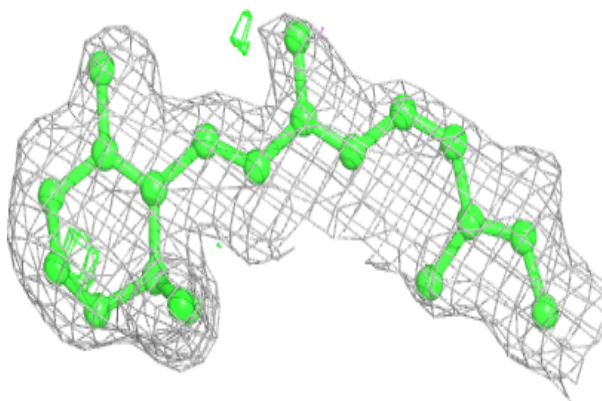and green (positive)

Electron density around RET F 301 (B):

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

Electron density around RET D 301 (A):

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

Electron density around RET E 302 (B):

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

Electron density around RET G 301 (B):

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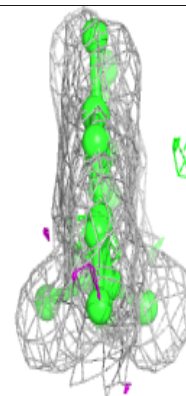$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
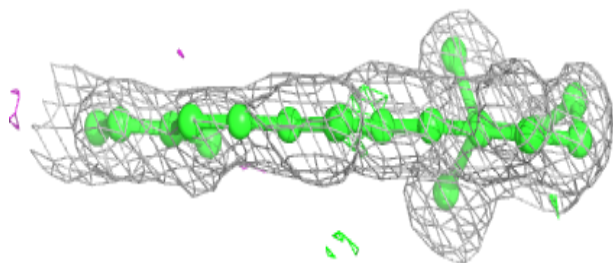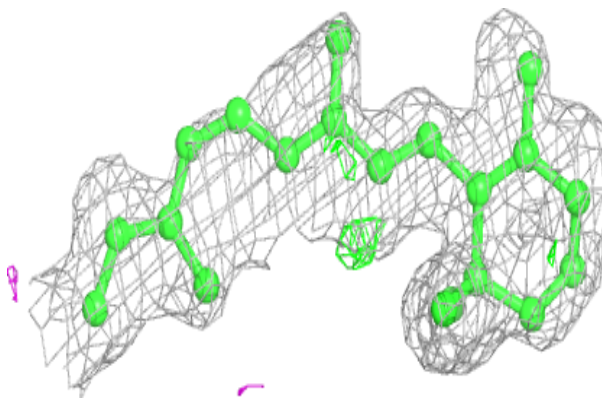and green (positive)

Electron density around RET B 301 (A):

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

Electron density around RET A 301 (A):

$2mF_o$-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.