W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2021 – 06:07 PM JST

PDB ID	:	7CQM
Title	:	PlsY grown in LCP soaked with selenourea for 22 min
Authors	:	Luo, Z.P.; Li, D.F.
Deposited on	:	2020-08-11
Resolution	:	1.80 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 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	:	2.23.1
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)	:	2.23.1

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
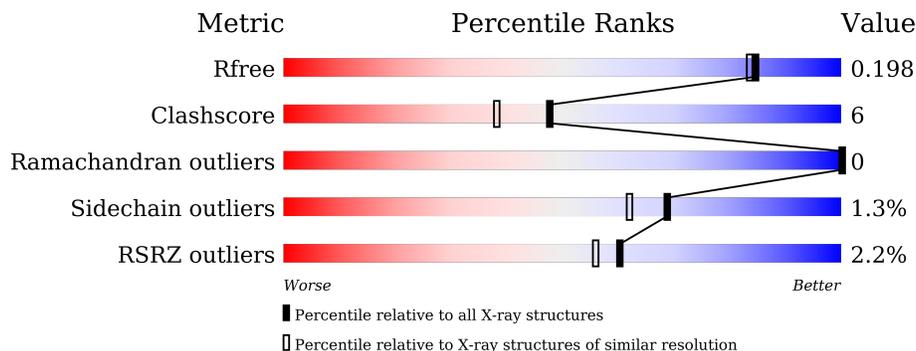
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	201	2% · 88% 11%
1	B	201	2% · 89% 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
2	SEY	A	304	-	-	X	-
2	SEY	A	305	-	-	X	-
3	SO4	A	312	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 3687 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 Glycerol-3-phosphate acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total 1539	C 1039	N 249	O 249	S 2	0	1	0
1	B	200	Total 1531	C 1033	N 248	O 248	S 2	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP O66905
A	1	GLY	-	expression tag	UNP O66905
A	2	SER	-	expression tag	UNP O66905
A	193	GLY	-	expression tag	UNP O66905
A	194	THR	-	expression tag	UNP O66905
A	195	LEU	-	expression tag	UNP O66905
A	196	GLU	-	expression tag	UNP O66905
A	197	VAL	-	expression tag	UNP O66905
A	198	LEU	-	expression tag	UNP O66905
A	199	PHE	-	expression tag	UNP O66905
A	200	GLN	-	expression tag	UNP O66905
B	0	MET	-	expression tag	UNP O66905
B	1	GLY	-	expression tag	UNP O66905
B	2	SER	-	expression tag	UNP O66905
B	193	GLY	-	expression tag	UNP O66905
B	194	THR	-	expression tag	UNP O66905
B	195	LEU	-	expression tag	UNP O66905
B	196	GLU	-	expression tag	UNP O66905
B	197	VAL	-	expression tag	UNP O66905
B	198	LEU	-	expression tag	UNP O66905
B	199	PHE	-	expression tag	UNP O66905
B	200	GLN	-	expression tag	UNP O66905

- Molecule 2 is selenourea (three-letter code: SEY) (formula: CH_4N_2Se) (labeled as "Ligand of Interest" by depositor).
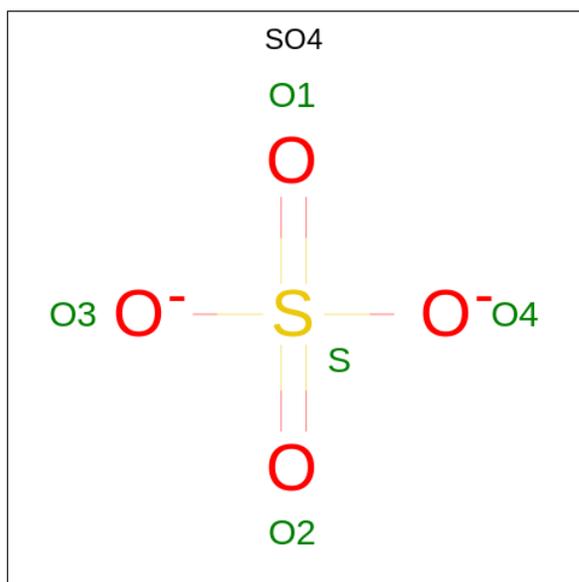
SEY

SE

Se

NH$_2$ N2

C

H$_2$N

N1

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	A	1	Total 7	C 2	N 4	Se 1	0	1
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	A	1	Total 4	C 1	N 2	Se 1	0	0
2	B	1	Total 4	C 1	N 2	Se 1	0	0
2	B	1	Total 4	C 1	N 2	Se 1	0	0
2	B	1	Total 4	C 1	N 2	Se 1	0	0
2	B	1	Total 4	C 1	N 2	Se 1	0	0
2	B	1	Total 4	C 1	N 2	Se 1	0	0
2	B	1	Total 7	C 2	N 4	Se 1	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	Se		
2	B	1	4	1	2	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	A	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0

- Molecule 4 is (2R)-2,3-dihydroxypropyl (7Z)-hexadec-7-enoate (three-letter code: 79M) (formula: $C_{19}H_{36}O_4$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 19	C 15	O 4	0	0
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 12	C 8	O 4	0	0
4	A	1	Total 23	C 19	O 4	0	0
4	A	1	Total 11	C 7	O 4	0	0
4	A	1	Total 11	C 7	O 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 23	C 19	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0
4	B	1	Total 19	C 15	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0
4	B	1	Total 23	C 19	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total 65	O 65	0	0
5	B	55	Total 55	O 55	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: Glycerol-3-phosphate acyltransferase
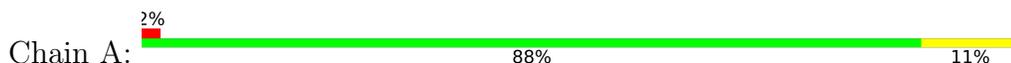
• Molecule 1: Glycerol-3-phosphate acyltransferase
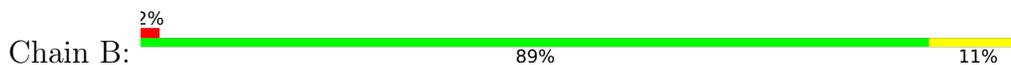
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.88Å 88.99Å 53.98Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	36.37 – 1.80 36.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.4 (36.37-1.80) 89.4 (36.37-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.156 , 0.190 0.170 , 0.198	Depositor DCC
R_{free} test set	2070 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 51.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
Reported twinning fraction	0.564 for H, K, L 0.436 for -L, -K, -H	Depositor
Outliers	0 of 42117 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3687	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.45% 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: 79M, SEY, SO4

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	0.78	0/1578	0.78	0/2141
1	B	0.79	0/1570	0.78	0/2130
All	All	0.79	0/3148	0.78	0/4271

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	1539	0	1607	29	0
1	B	1531	0	1597	18	0
2	A	35	0	0	5	0
2	B	31	0	0	4	0
3	A	30	0	0	2	0
3	B	30	0	0	0	0
4	A	191	0	276	7	0
4	B	180	0	277	7	0
5	A	65	0	0	1	0
5	B	55	0	0	2	0
All	All	3687	0	3757	45	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 6.

The worst 5 of 45 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:137:TYR:CE1	1:A:191:ARG:HG3	2.27	0.69
1:A:131:ILE:HD11	4:B:320:79M:H62C	1.76	0.66
1:A:131:ILE:HD12	1:B:155:VAL:HG11	1.80	0.64
1:B:32:ASN:ND2	5:B:401:HOH:O	2.31	0.62
1:A:45:ARG:NH2	3:A:312:SO4:O2	2.32	0.59

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	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
1	B	198/201 (98%)	196 (99%)	2 (1%)	0	100	100
All	All	397/402 (99%)	392 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	157/160 (98%)	154 (98%)	3 (2%)	57	46
1	B	156/160 (98%)	155 (99%)	1 (1%)	86	84
All	All	313/320 (98%)	309 (99%)	4 (1%)	69	62

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	98	PHE
1	A	190	HIS
1	B	77	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS

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 ⓘ

47 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	$\#\|Z\| > 2$
3	SO4	A	311	-	4,4,4	0.35	0	6,6,6	0.09	0
4	79M	A	321	-	10,10,22	0.32	0	11,11,23	0.26	0
4	79M	B	320	-	22,22,22	0.29	0	23,23,23	0.41	0
4	79M	A	320	-	22,22,22	0.60	0	23,23,23	0.53	0
2	SEY	B	306	-	3,3,3	0.38	0	3,3,3	0.61	0
4	79M	A	315	-	18,18,22	0.25	0	19,19,23	0.32	0
4	79M	A	324	-	22,22,22	0.29	0	23,23,23	0.39	0
2	SEY	A	306[B]	-	3,3,3	0.47	0	3,3,3	0.57	0
3	SO4	A	313	-	4,4,4	0.33	0	6,6,6	0.07	0
4	79M	A	322	-	10,10,22	0.33	0	11,11,23	0.30	0
2	SEY	A	301	-	3,3,3	0.65	0	3,3,3	1.01	0
2	SEY	B	308	-	3,3,3	0.51	0	3,3,3	0.41	0
3	SO4	B	313	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SEY	B	307[B]	-	3,3,3	0.45	0	3,3,3	0.54	0
3	SO4	A	312	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	B	312	-	4,4,4	0.34	0	6,6,6	0.11	0
4	79M	B	317	-	22,22,22	0.43	0	23,23,23	0.34	0
4	79M	A	319	-	11,11,22	0.27	0	12,12,23	0.40	0
3	SO4	A	308	-	4,4,4	0.36	0	6,6,6	0.45	0
2	SEY	A	303	-	3,3,3	0.48	0	3,3,3	0.36	0
2	SEY	B	303	-	3,3,3	0.53	0	3,3,3	0.37	0
3	SO4	B	310	-	4,4,4	0.28	0	6,6,6	0.41	0
3	SO4	A	309	-	4,4,4	0.34	0	6,6,6	0.31	0
4	79M	B	316	-	18,18,22	0.22	0	19,19,23	0.26	0
3	SO4	B	309	-	4,4,4	0.25	0	6,6,6	0.30	0
2	SEY	A	302	-	3,3,3	0.49	0	3,3,3	0.84	0
2	SEY	B	305	-	3,3,3	0.46	0	3,3,3	0.45	0
3	SO4	B	311	-	4,4,4	0.38	0	6,6,6	0.29	0
4	79M	A	317	-	22,22,22	0.39	0	23,23,23	0.42	0
4	79M	B	315	-	22,22,22	0.44	0	23,23,23	0.48	0
2	SEY	B	304	-	3,3,3	0.49	0	3,3,3	0.34	0
2	SEY	A	304	-	3,3,3	0.52	0	3,3,3	0.32	0
4	79M	A	318	-	22,22,22	0.40	0	23,23,23	0.36	0
4	79M	B	318	-	22,22,22	0.26	0	23,23,23	0.20	0
2	SEY	A	307	-	3,3,3	0.59	0	3,3,3	0.18	0
2	SEY	A	306[A]	-	3,3,3	0.43	0	3,3,3	0.43	0
4	79M	B	302	-	22,22,22	0.27	0	23,23,23	0.26	0
4	79M	A	316	-	22,22,22	0.27	0	23,23,23	0.25	0
2	SEY	A	305	-	3,3,3	0.35	0	3,3,3	0.69	0
3	SO4	B	314	-	4,4,4	0.31	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	79M	A	314	-	22,22,22	0.50	0	23,23,23	0.62	0
2	SEY	B	307[A]	-	3,3,3	0.39	0	3,3,3	0.63	0
4	79M	B	321	-	22,22,22	0.28	0	23,23,23	0.29	0
4	79M	B	319	-	22,22,22	0.36	0	23,23,23	0.34	0
2	SEY	A	323	-	3,3,3	0.36	0	3,3,3	0.67	0
3	SO4	A	310	-	4,4,4	0.32	0	6,6,6	0.22	0
2	SEY	B	301	-	3,3,3	0.56	0	3,3,3	0.40	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	79M	B	316	-	-	5/18/18/22	-
4	79M	A	318	-	-	8/22/22/22	-
4	79M	A	322	-	-	7/10/10/22	-
4	79M	B	318	-	-	11/22/22/22	-
4	79M	A	321	-	-	3/10/10/22	-
4	79M	A	317	-	-	10/22/22/22	-
4	79M	B	315	-	-	1/22/22/22	-
4	79M	B	302	-	-	8/22/22/22	-
4	79M	A	316	-	-	6/22/22/22	-
4	79M	B	319	-	-	4/22/22/22	-
4	79M	B	321	-	-	12/22/22/22	-
4	79M	B	320	-	-	7/22/22/22	-
4	79M	A	314	-	-	8/22/22/22	-
4	79M	A	319	-	-	2/11/11/22	-
4	79M	A	320	-	-	8/22/22/22	-
4	79M	A	315	-	-	6/18/18/22	-
4	79M	B	317	-	-	7/22/22/22	-
4	79M	A	324	-	-	8/22/22/22	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	317	79M	C21-C22-C24-O25
4	A	319	79M	O20-C21-C22-O23
4	A	322	79M	O20-C21-C22-C24
4	A	322	79M	O20-C21-C22-O23
4	A	324	79M	O20-C21-C22-C24

There are no ring outliers.

19 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	321	79M	1	0
4	B	320	79M	2	0
2	B	306	SEY	1	0
4	A	315	79M	2	0
2	A	301	SEY	1	0
2	B	308	SEY	1	0
3	A	312	SO4	2	0
4	B	317	79M	1	0
2	B	303	SEY	1	0
4	B	316	79M	1	0
2	A	302	SEY	1	0
4	A	317	79M	1	0
2	A	304	SEY	2	0
4	A	318	79M	2	0
2	A	305	SEY	2	0
4	A	314	79M	1	0
2	B	307[A]	SEY	1	0
4	B	321	79M	1	0
4	B	319	79M	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 79M A 321

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 320

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 320

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 306

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 315

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 324

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 306 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 322

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 308

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 307 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 317

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 319

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 316

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 305

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 317

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 315

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 304

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 304

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 318

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 318

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 307

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 306 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 316

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M A 314

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 307 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 321

Bond lengths

Bond angles

Torsions

Rings

Ligand 79M B 319

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY A 323

Bond lengths

Bond angles

Torsions

Rings

Ligand SEY B 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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	200/201 (99%)	-0.24	4 (2%)	65	61	12, 20, 37, 60	0
1	B	200/201 (99%)	-0.24	5 (2%)	57	52	12, 20, 40, 76	0
All	All	400/402 (99%)	-0.24	9 (2%)	60	56	12, 20, 39, 76	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	LEU	5.3
1	B	199	PHE	4.8
1	A	199	PHE	4.3
1	B	98	PHE	4.0
1	A	97	PHE	3.8

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
4	79M	A	324	23/23	0.65	0.20	51,66,85,87	0
2	SEY	B	308	4/4	0.66	0.32	25,34,36,49	4
4	79M	B	319	23/23	0.69	0.30	37,57,74,76	0
4	79M	B	302	23/23	0.71	0.23	41,63,100,108	0
3	SO4	B	314	5/5	0.74	0.22	47,50,73,86	0
4	79M	A	318	23/23	0.75	0.28	36,57,70,72	0
3	SO4	A	312	5/5	0.79	0.26	39,64,82,97	0
2	SEY	B	306	4/4	0.79	0.24	14,41,49,49	4
3	SO4	A	311	5/5	0.80	0.20	55,79,91,94	0
4	79M	A	316	23/23	0.80	0.17	35,44,52,69	0
4	79M	A	315	19/23	0.81	0.14	45,56,72,73	0
4	79M	A	321	11/23	0.82	0.19	40,50,65,77	0
2	SEY	B	307[A]	4/4	0.82	0.26	21,27,32,72	3
2	SEY	B	307[B]	4/4	0.82	0.26	54,55,61,72	3
4	79M	B	316	19/23	0.82	0.18	46,62,80,81	0
4	79M	B	318	23/23	0.82	0.26	37,57,79,83	0
2	SEY	A	305	4/4	0.82	0.27	14,34,34,41	4
4	79M	A	322	11/23	0.83	0.16	47,54,66,69	0
3	SO4	B	312	5/5	0.84	0.19	37,66,81,87	0
4	79M	B	317	23/23	0.85	0.19	30,42,53,57	0
4	79M	B	320	23/23	0.85	0.21	32,46,58,67	0
4	79M	A	320	23/23	0.86	0.26	30,51,78,87	0
3	SO4	A	313	5/5	0.86	0.29	46,60,71,81	0
4	79M	A	317	23/23	0.88	0.25	26,52,70,81	0
4	79M	B	321	23/23	0.88	0.29	24,58,88,98	0
2	SEY	A	306[A]	4/4	0.89	0.17	34,35,44,80	3
2	SEY	A	306[B]	4/4	0.89	0.17	31,36,42,80	3
2	SEY	A	307	4/4	0.89	0.18	21,30,35,49	4
2	SEY	B	305	4/4	0.89	0.16	38,48,57,57	4
4	79M	A	319	12/23	0.90	0.16	42,54,69,71	0
3	SO4	B	313	5/5	0.90	0.23	35,48,66,79	0
4	79M	B	315	23/23	0.92	0.11	19,24,34,37	0
4	79M	A	314	23/23	0.93	0.10	16,26,35,40	0
2	SEY	A	302	4/4	0.94	0.20	11,23,23,30	4
2	SEY	A	304	4/4	0.95	0.13	30,31,34,38	4
2	SEY	B	303	4/4	0.95	0.16	22,45,50,55	4
3	SO4	B	311	5/5	0.95	0.14	38,38,44,66	0
2	SEY	B	301	4/4	0.96	0.12	12,25,25,37	4
2	SEY	A	303	4/4	0.97	0.14	26,28,29,34	4
2	SEY	A	323	4/4	0.97	0.07	14,28,30,45	4
2	SEY	B	304	4/4	0.97	0.28	43,44,50,51	4
3	SO4	A	310	5/5	0.98	0.12	28,43,54,60	0
3	SO4	B	309	5/5	0.99	0.05	17,18,18,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	310	5/5	0.99	0.06	14,14,15,15	0
2	SEY	A	301	4/4	0.99	0.06	21,30,32,43	0
3	SO4	A	309	5/5	0.99	0.07	12,14,15,16	0
3	SO4	A	308	5/5	1.00	0.05	13,16,18,20	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 79M A 324:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
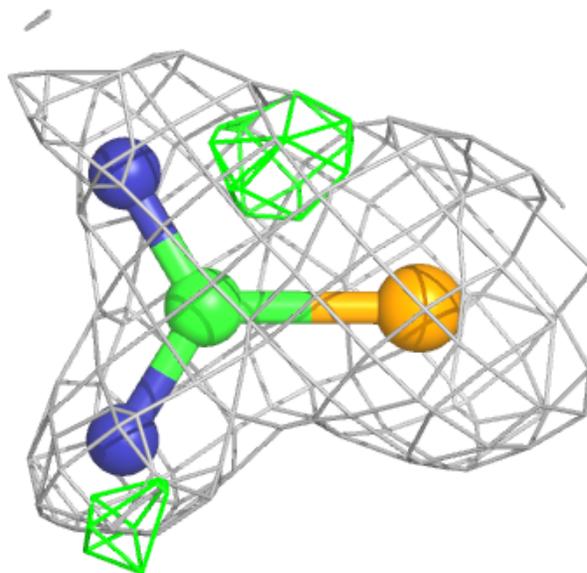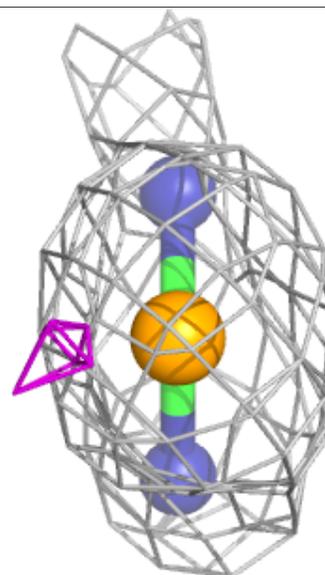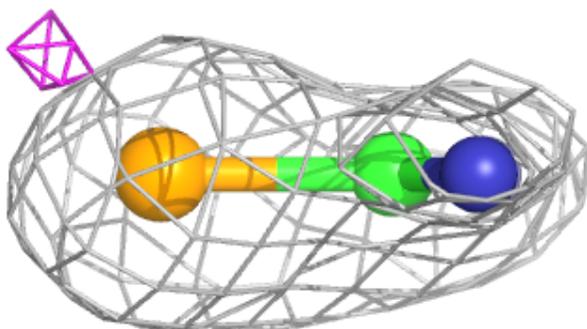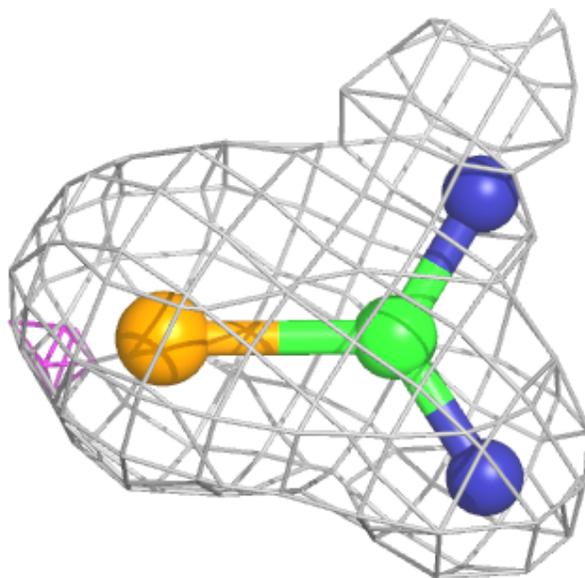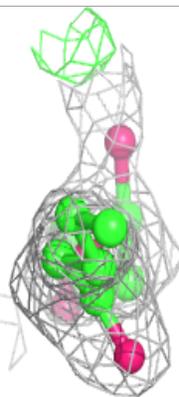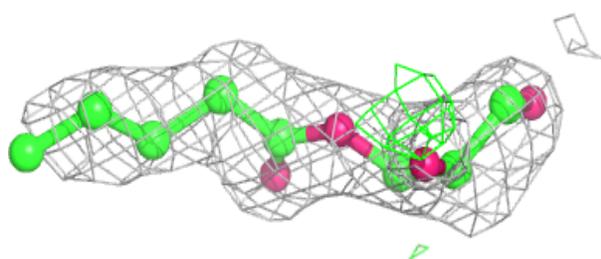and green (positive)
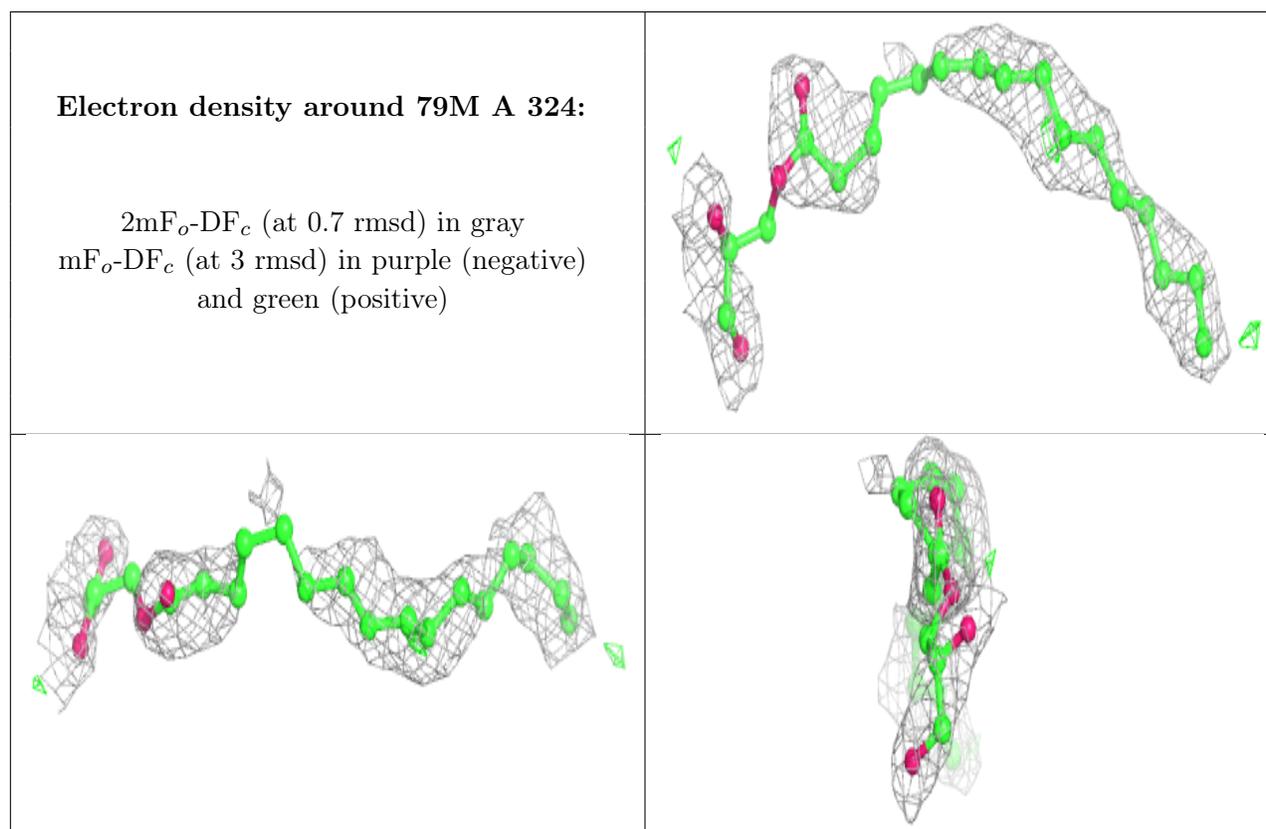
Electron density around SEY B 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
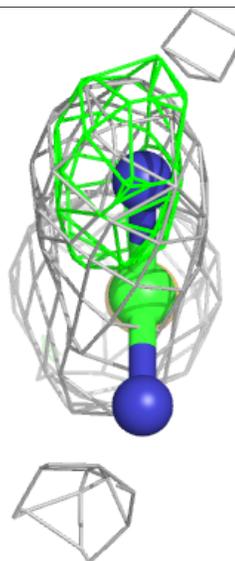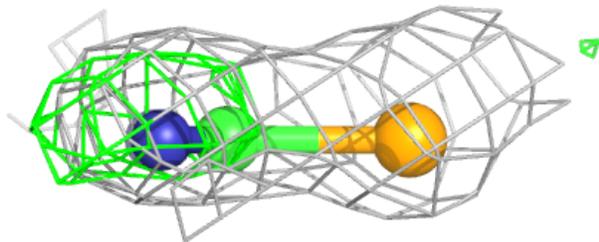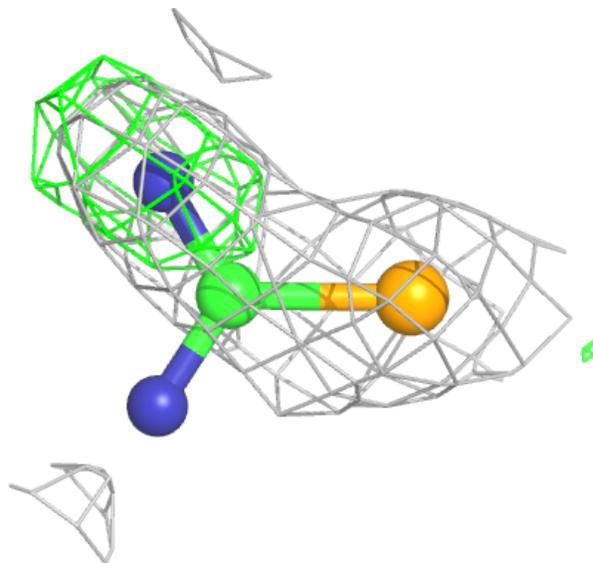
Electron density around 79M B 319:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
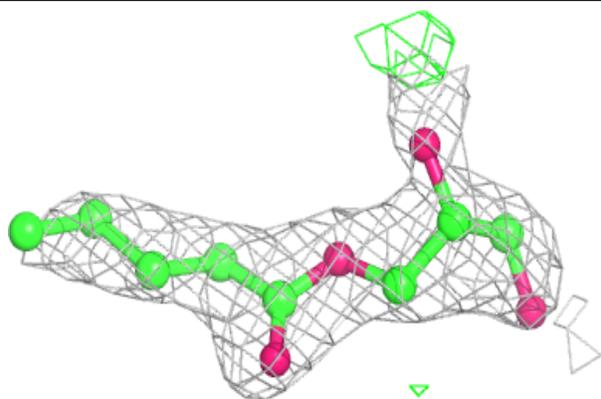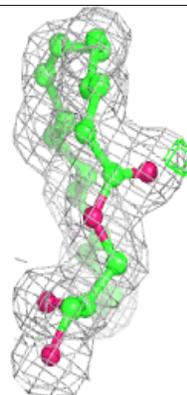and green (positive)
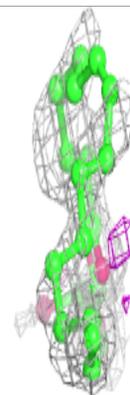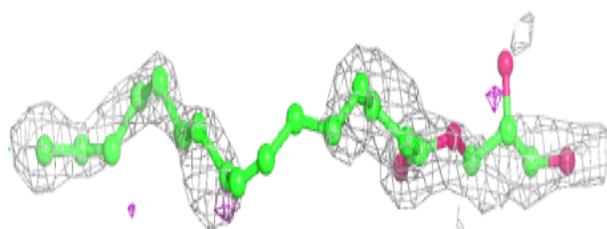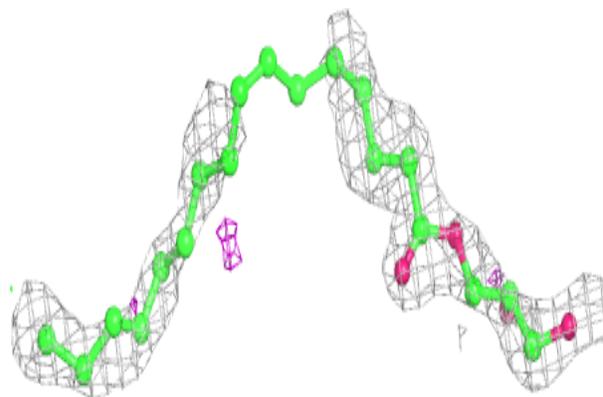
Electron density around 79M B 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
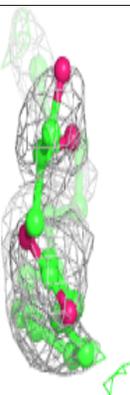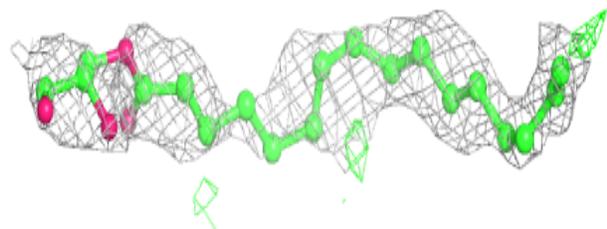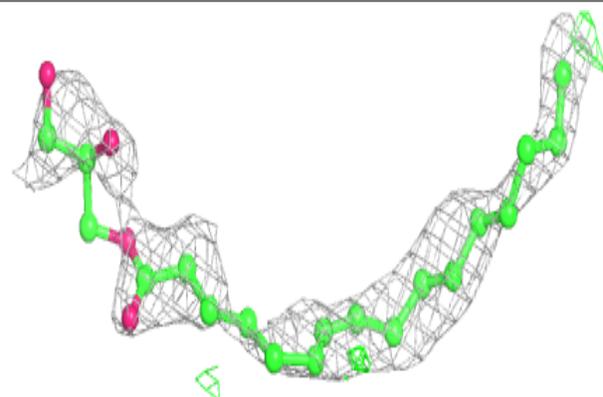
Electron density around 79M A 318:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
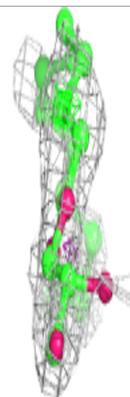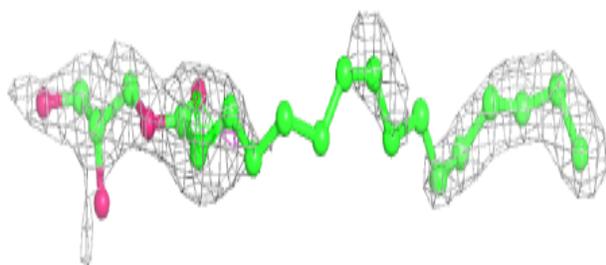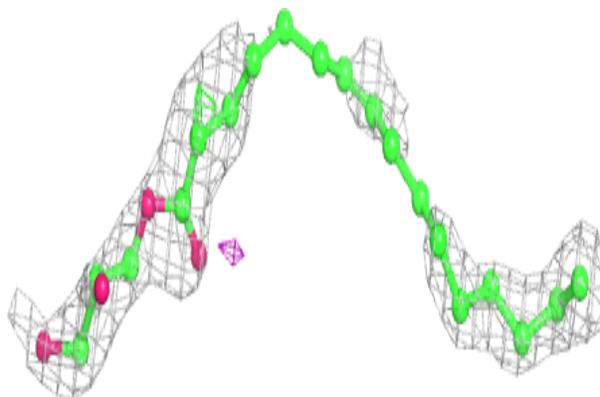
Electron density around SEY B 306:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
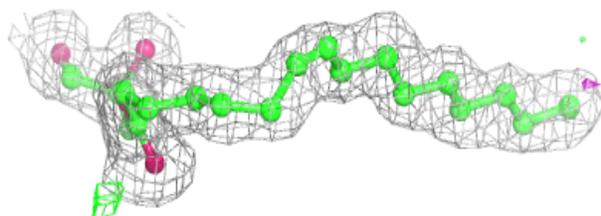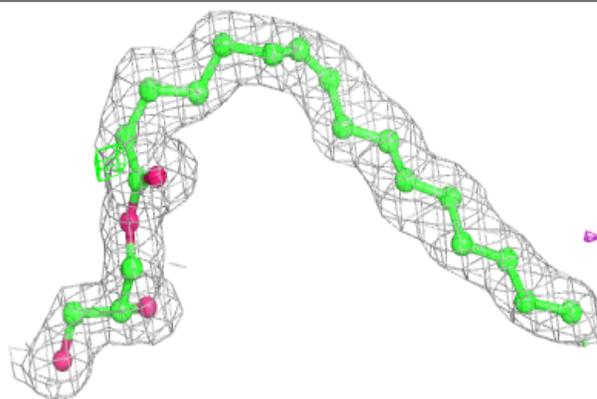and green (positive)
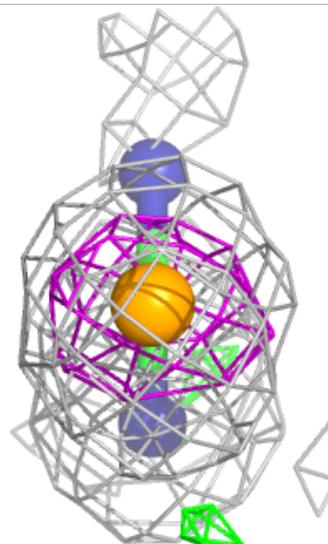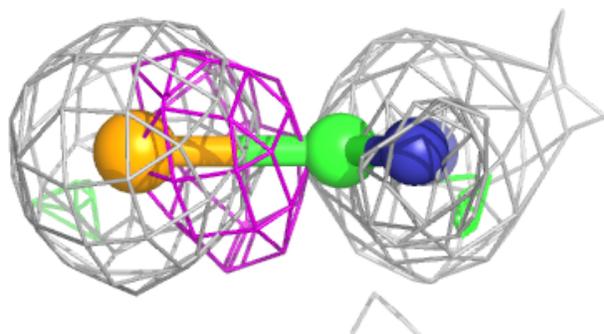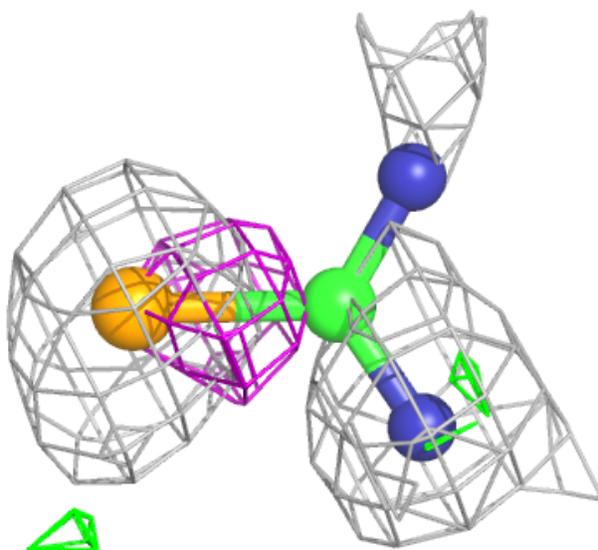
Electron density around 79M A 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
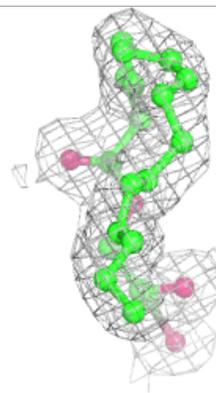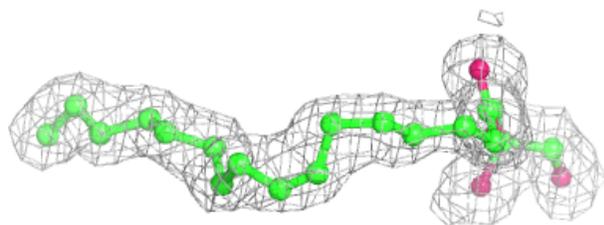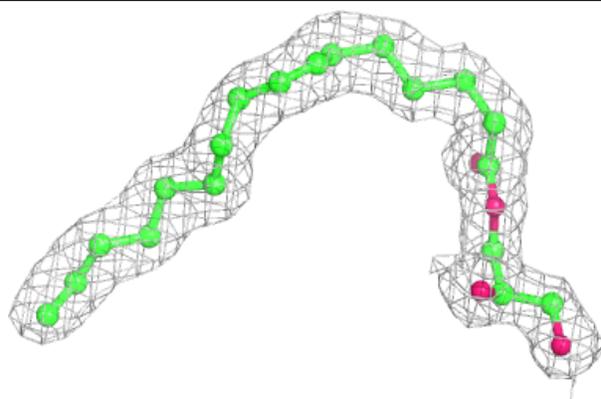and green (positive)
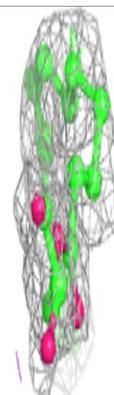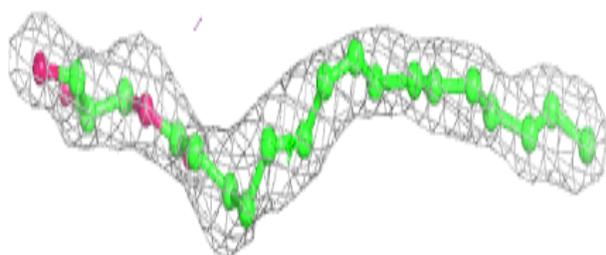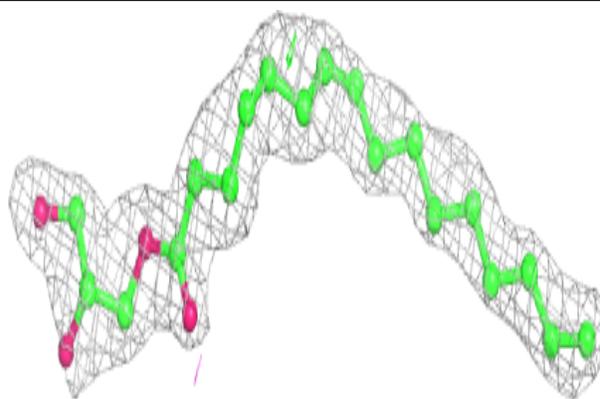
Electron density around 79M A 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
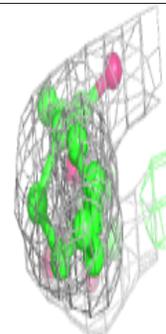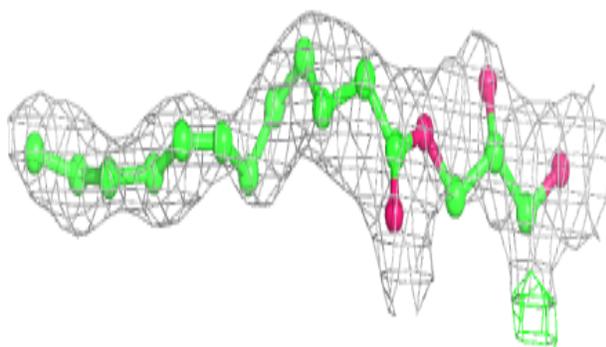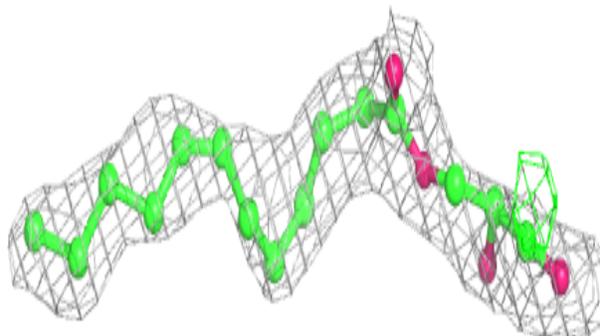
Electron density around 79M A 321:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
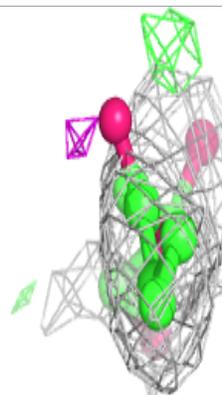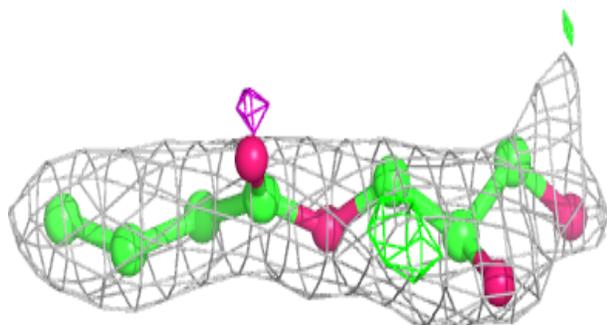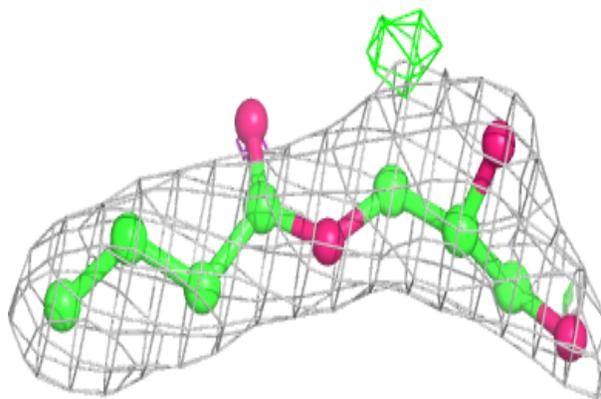
Electron density around SEY B 307 (A):

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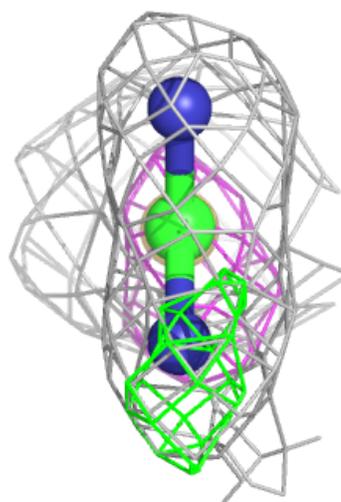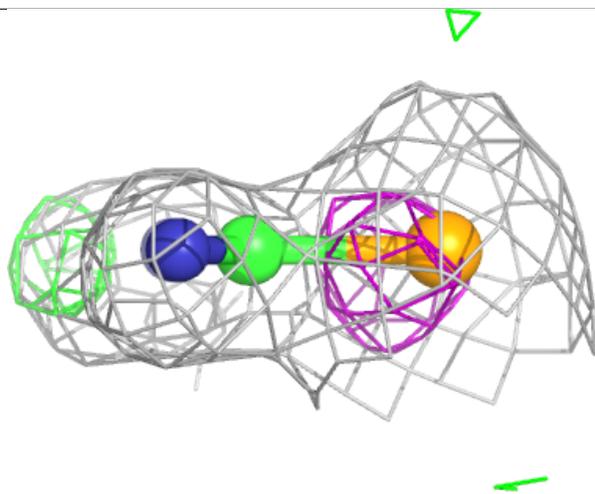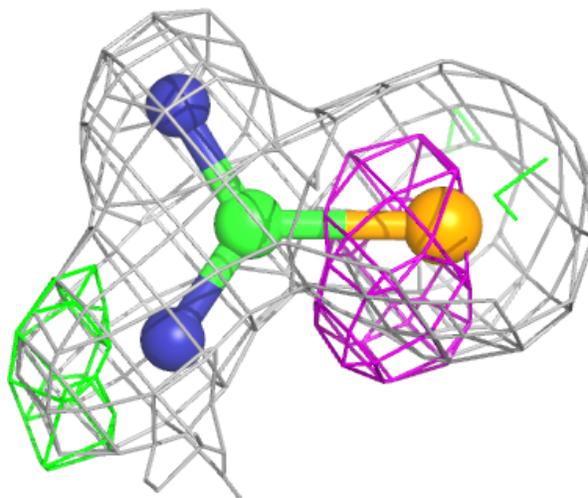
Electron density around SEY B 307 (B):

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
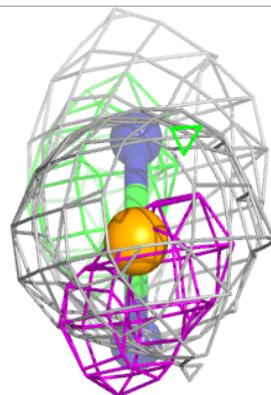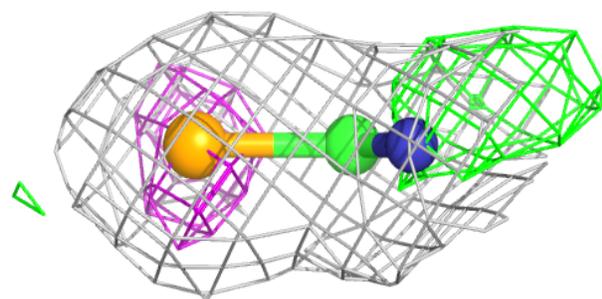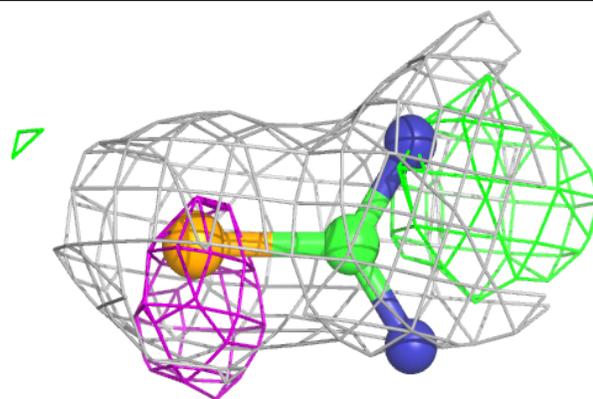
Electron density around 79M B 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
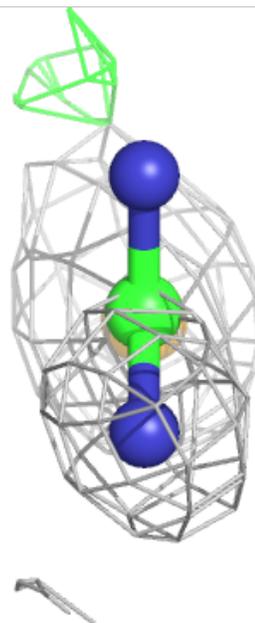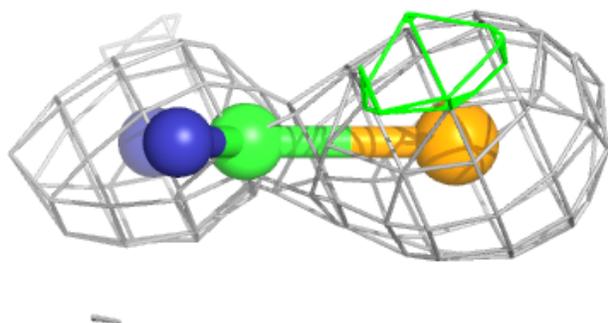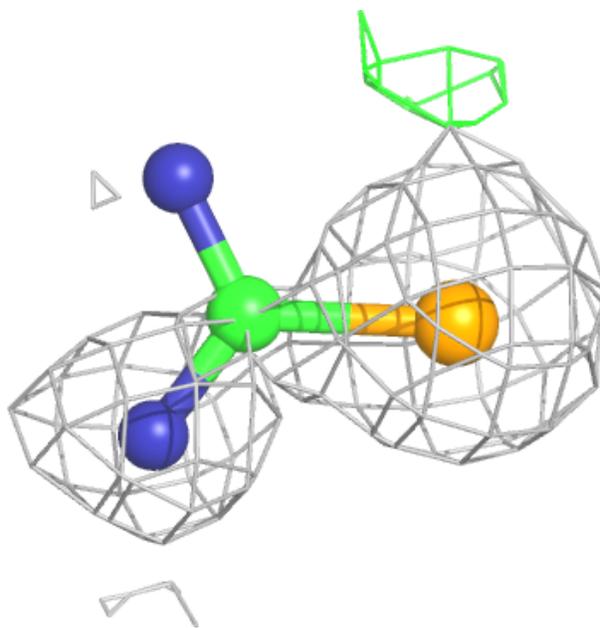and green (positive)
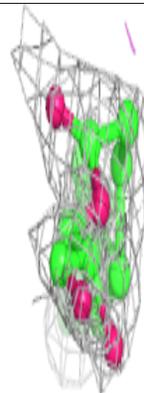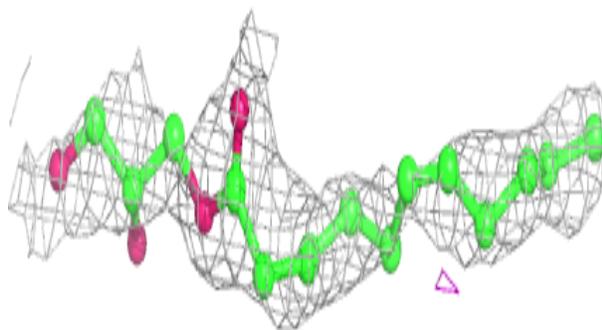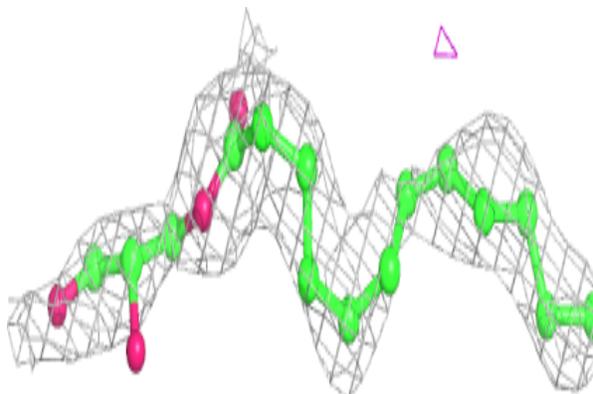
Electron density around 79M B 318:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
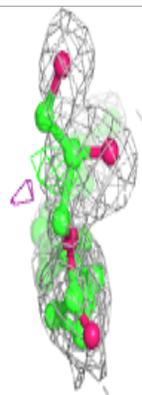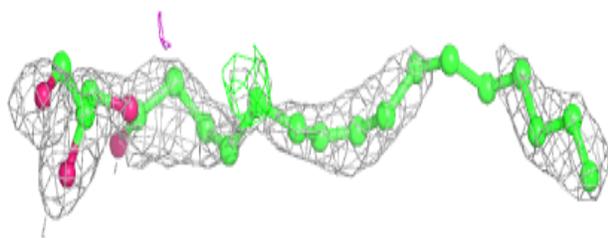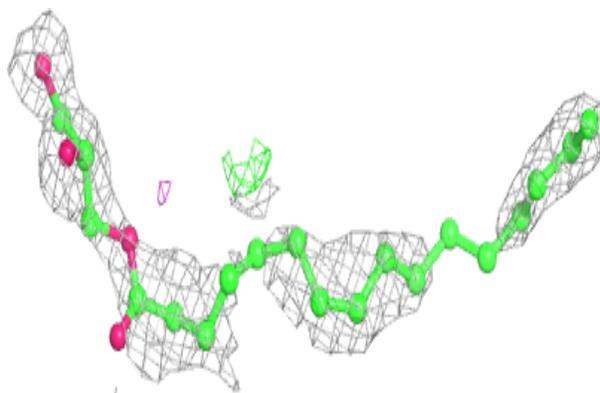
Electron density around SEY A 305:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
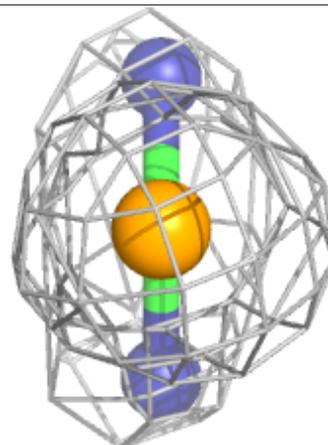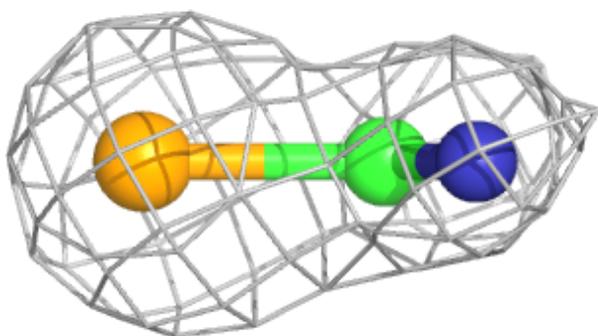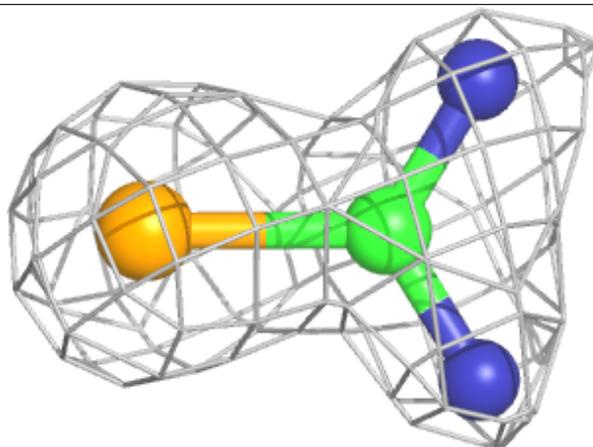and green (positive)
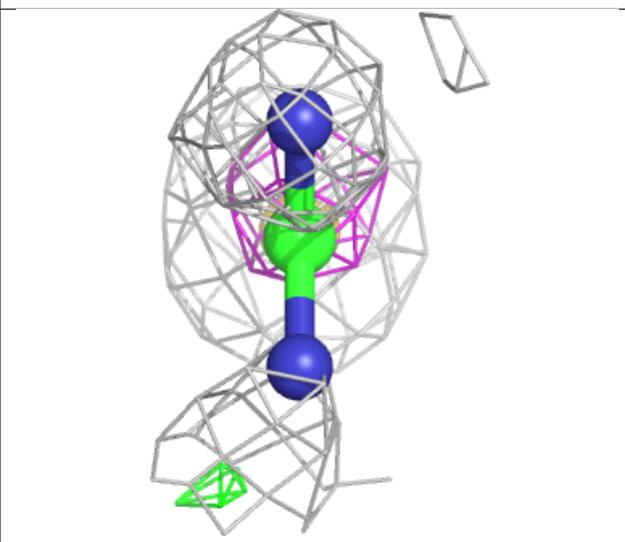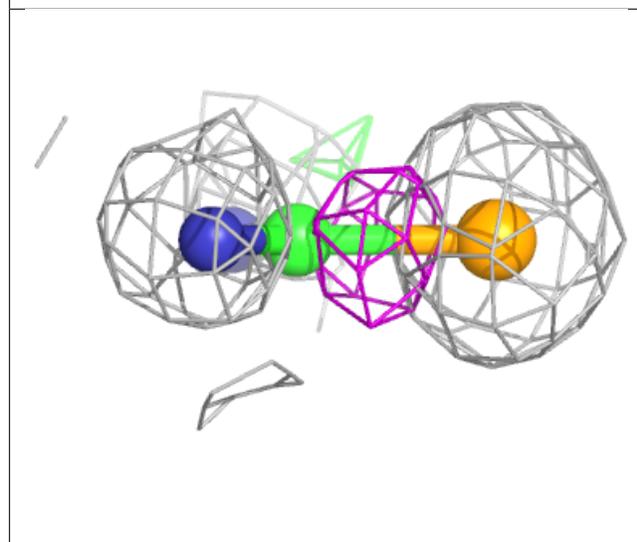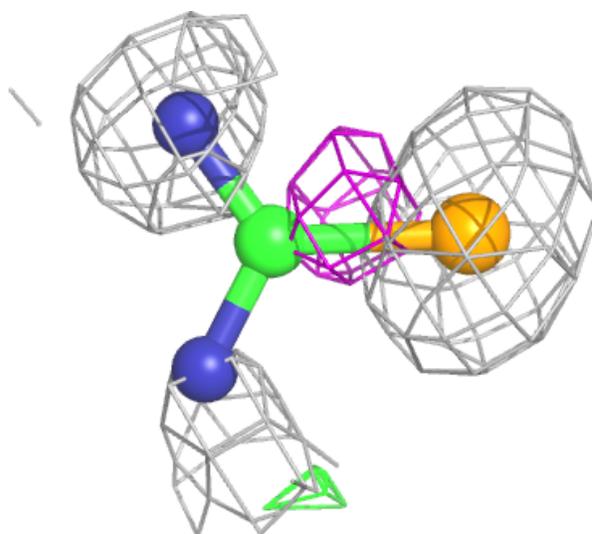
Electron density around 79M A 322:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
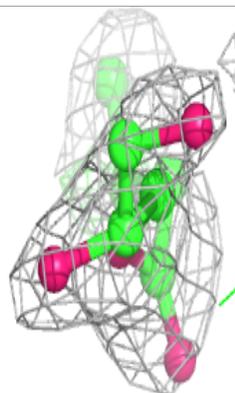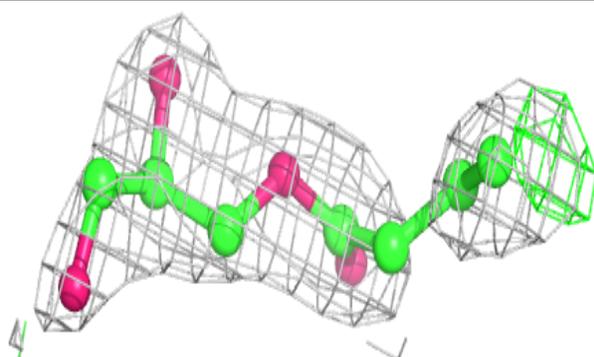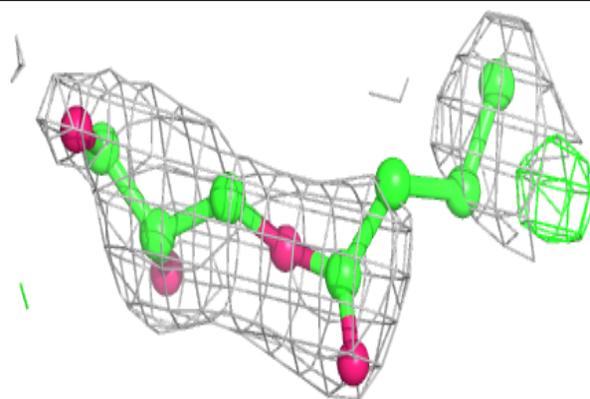
Electron density around 79M B 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
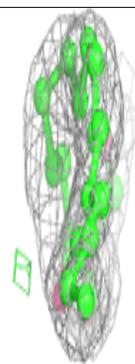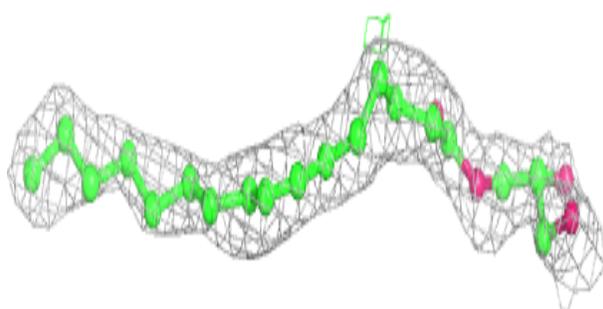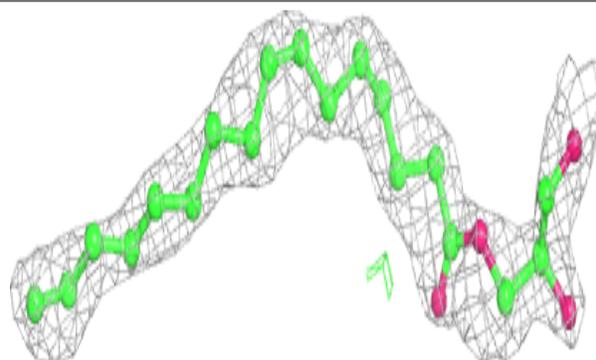
Electron density around 79M B 320:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
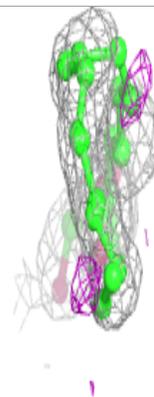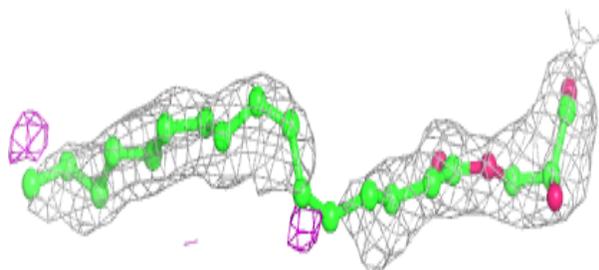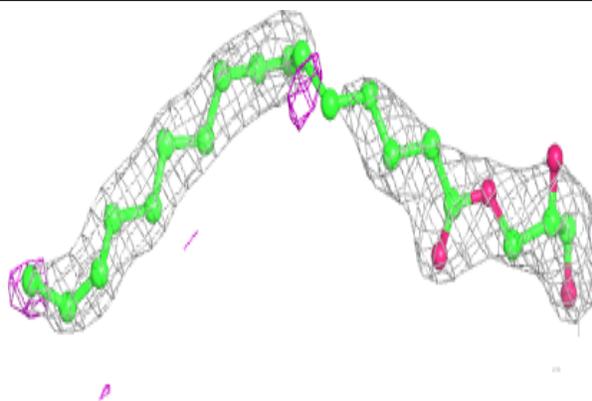
Electron density around 79M A 320:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
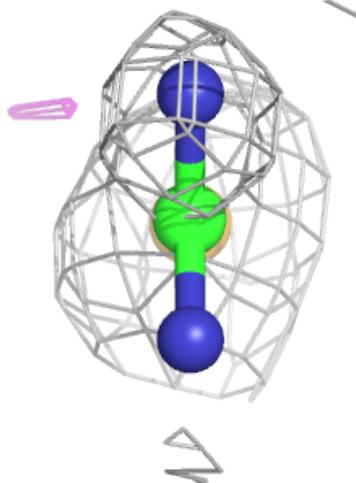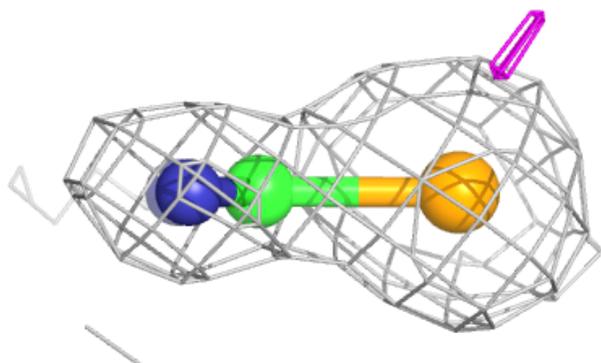$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
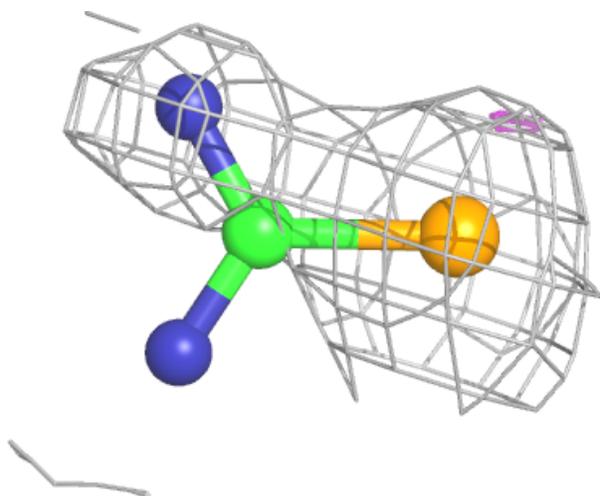and green (positive)
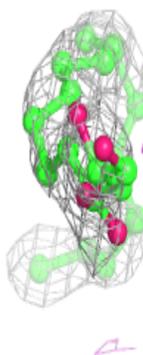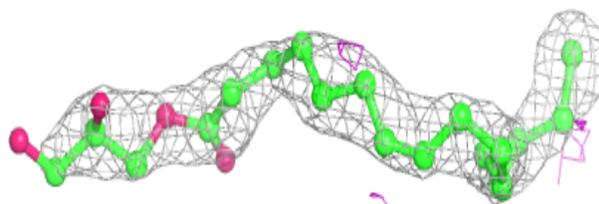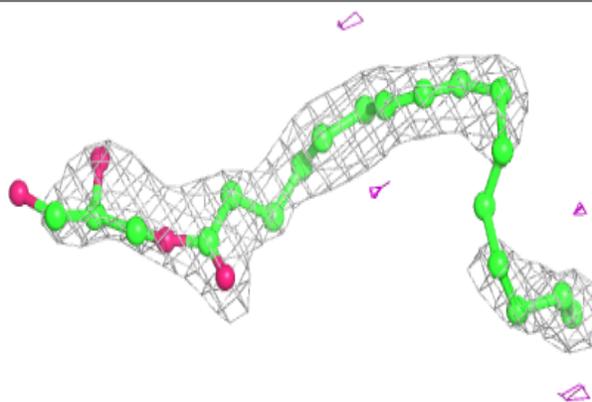
Electron density around 79M A 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
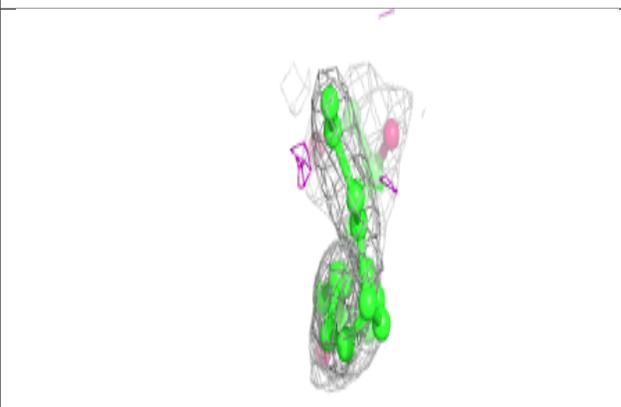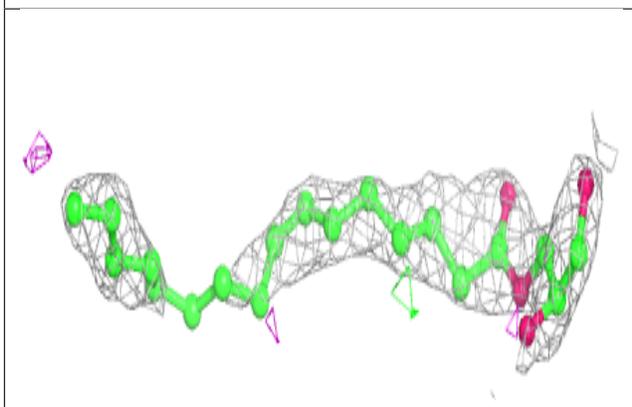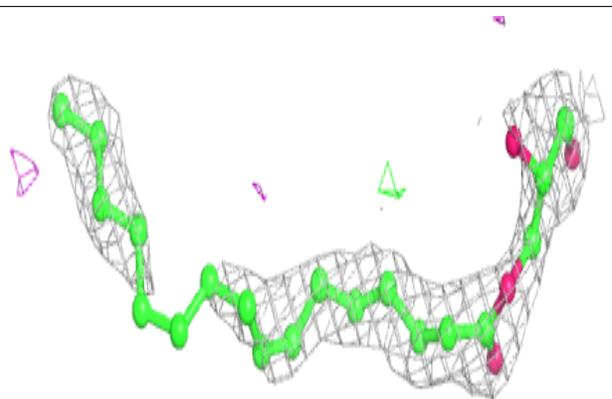
Electron density around 79M B 321:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
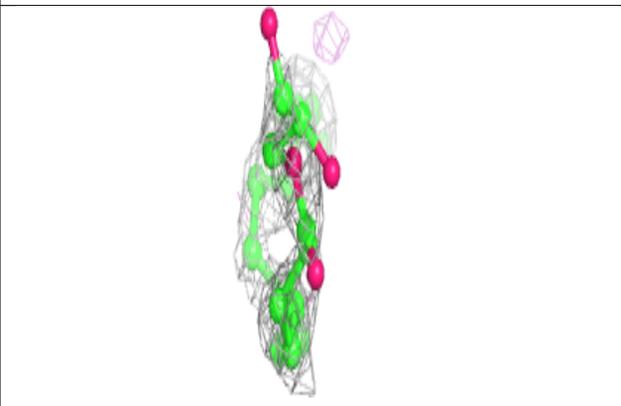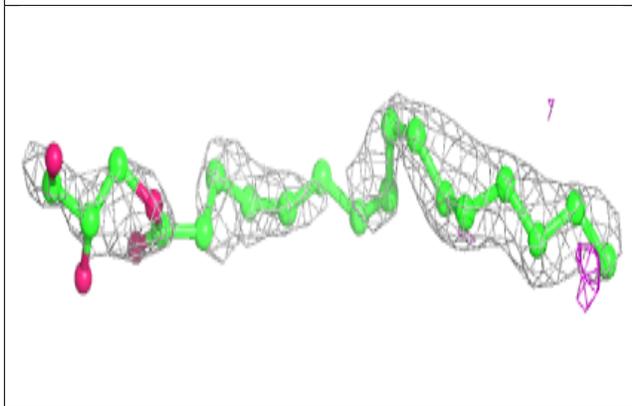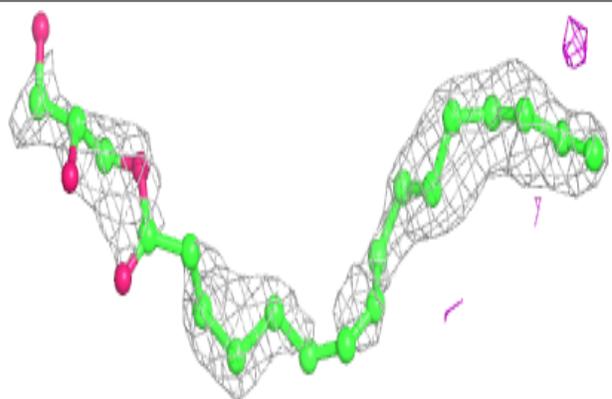
Electron density around SEY A 306 (A):

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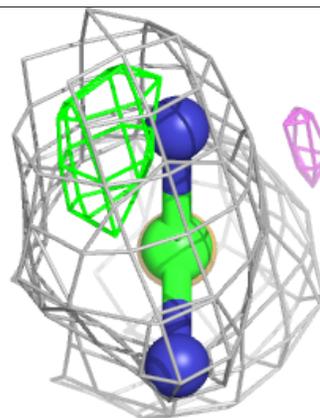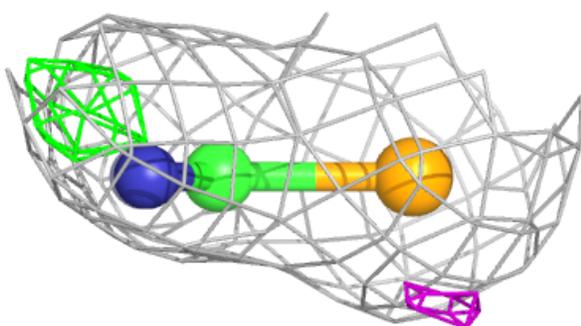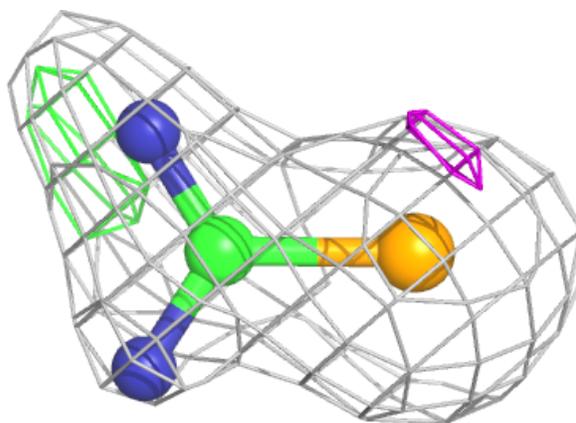
Electron density around SEY A 306 (B):

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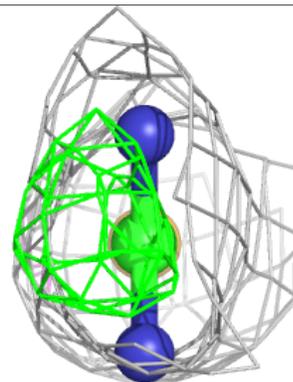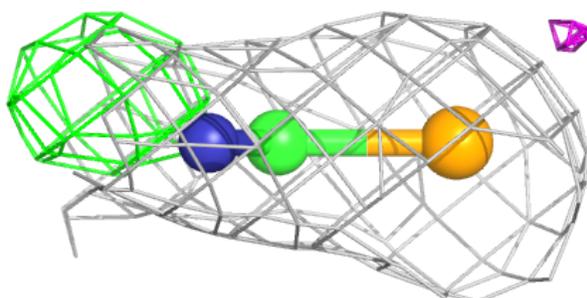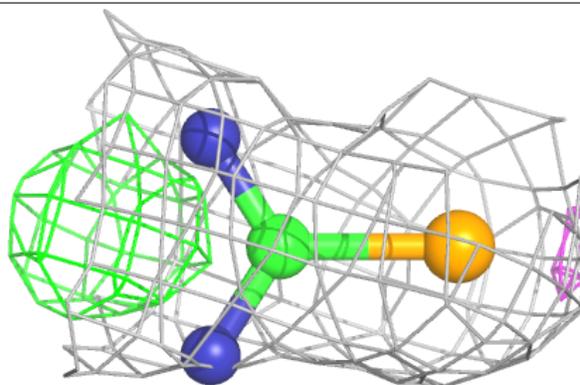
Electron density around SEY A 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
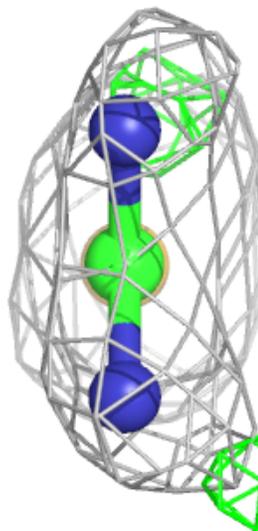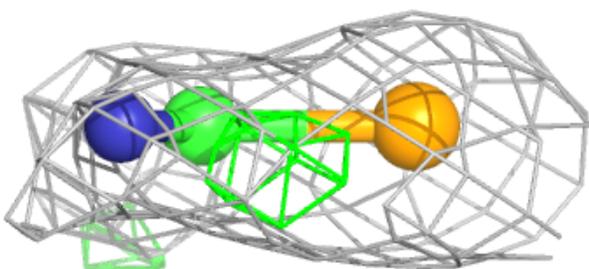
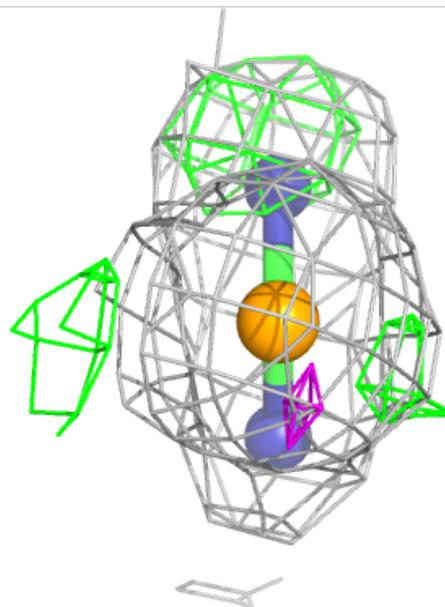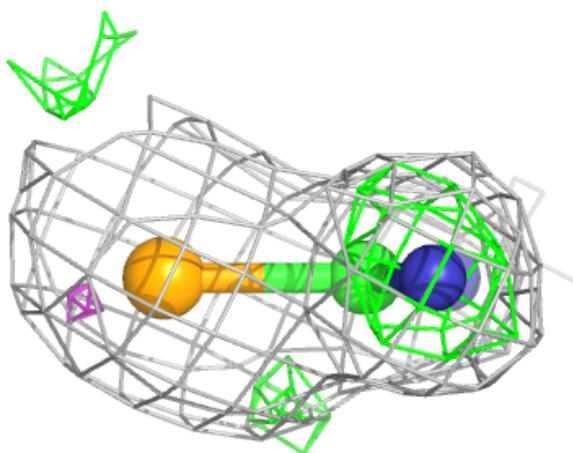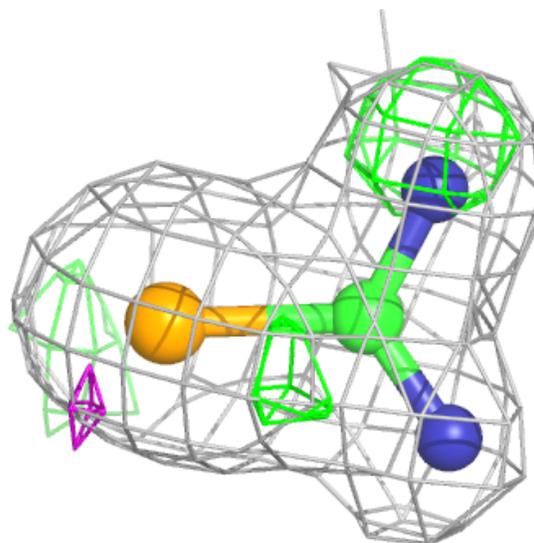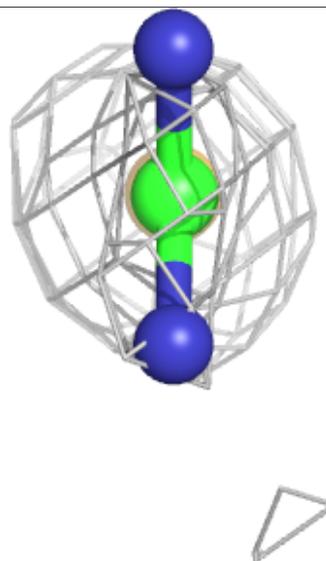**Electron density around SEY B 305:**

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

Electron density around 79M A 319:

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 79M B 315:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
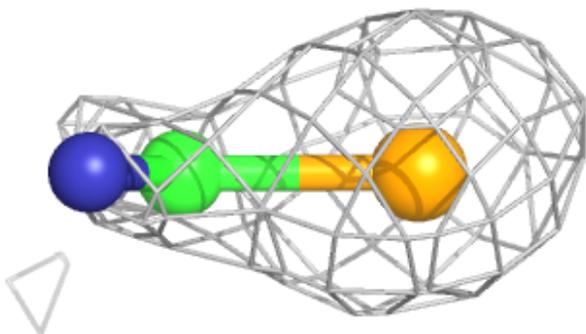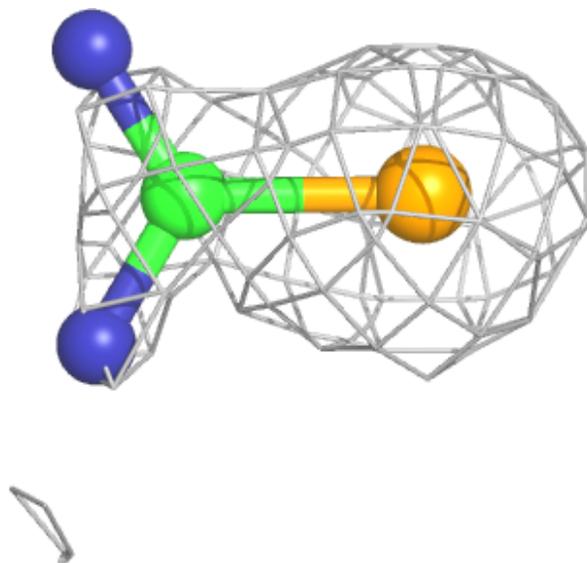and green (positive)

Electron density around 79M A 314:

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

Electron density around SEY A 302:

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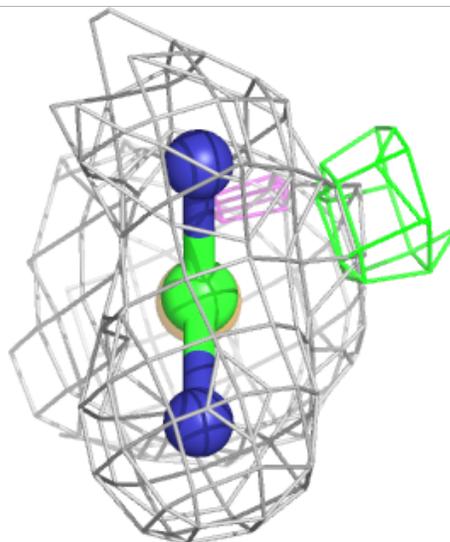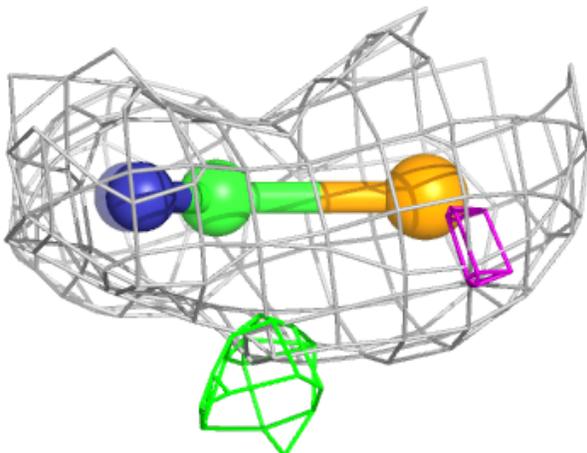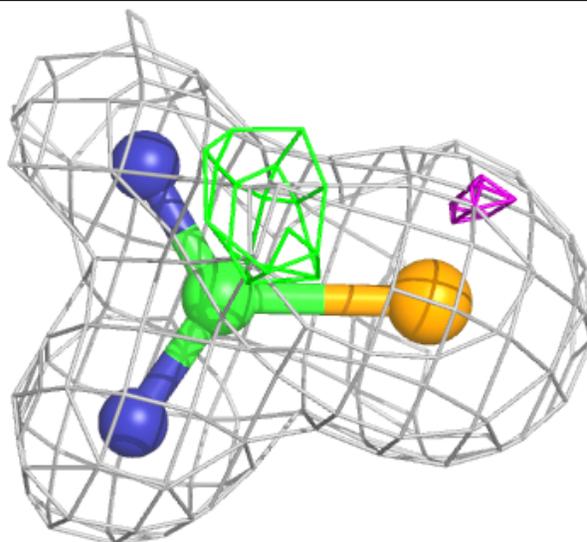and green (positive)

Electron density around SEY 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 SEY B 303:

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

Electron density around SEY B 301:

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

Electron density around SEY A 303:

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

Electron density around SEY A 323:

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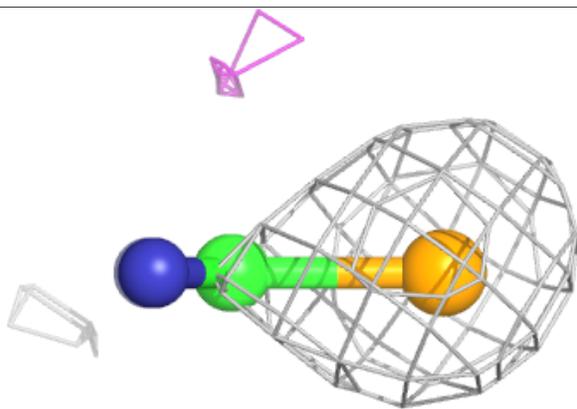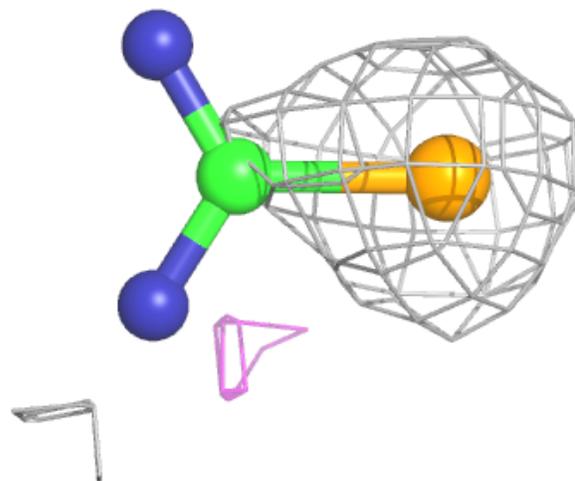and green (positive)

Electron density around SEY B 304:

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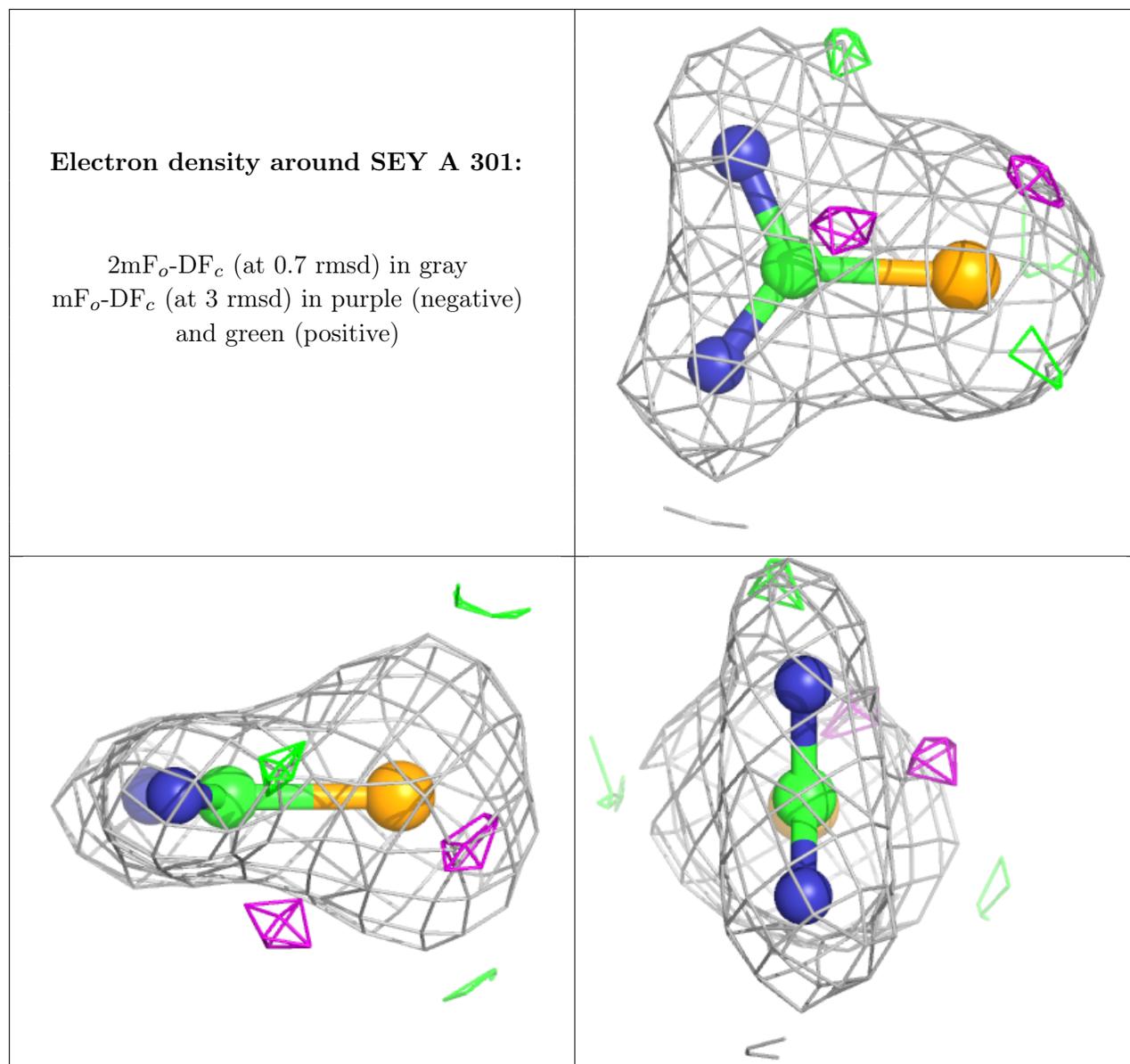and green (positive)

Electron density around SEY A 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
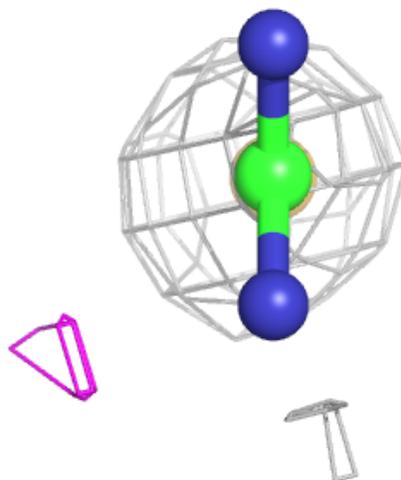
6.5 Other polymers (i)

There are no such residues in this entry.