WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2023 – 02:10 PM EST

PDB ID	:	4OPM
Title	:	Crystal structure of a putative lipase (lip1) from Acinetobacter baumannii AYE at 1.70 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2014-02-05
Resolution	:	1.70 Å(reported)

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

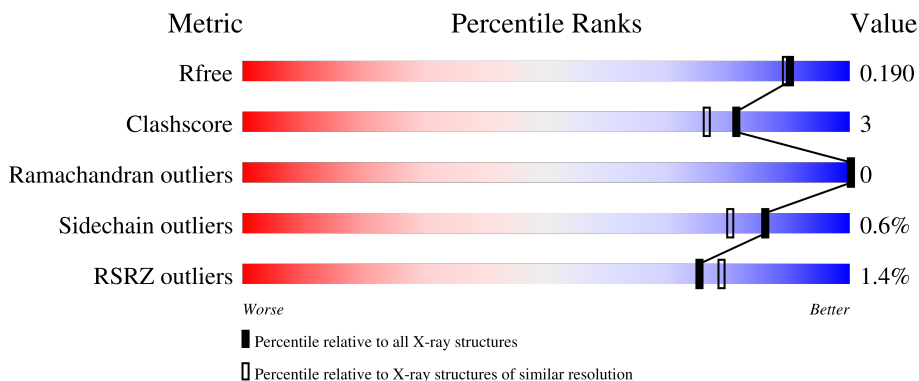|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.70 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		0.190
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		1.4%

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 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	306	2% 90% 8% ·
1	B	306	% 92% 6% ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5805 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.
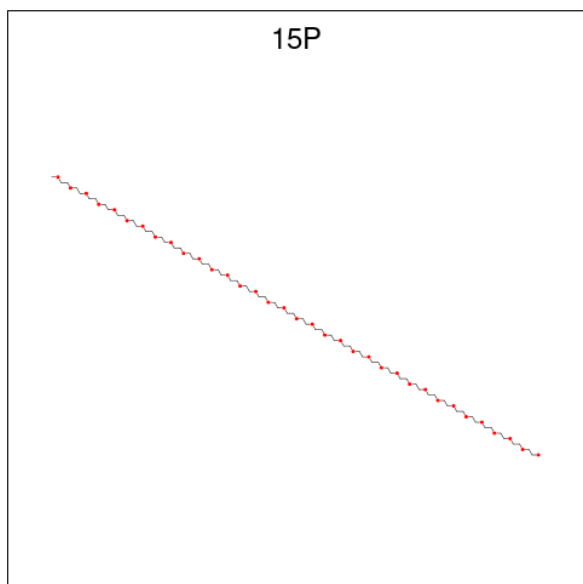
- Molecule 1 is a protein called Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	Se	0	20	0
			2459	1605	399	451	4			
1	B	299	Total	C	N	O	Se	0	20	0
			2457	1603	399	451	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B0V9K7
B	0	GLY	-	expression tag	UNP B0V9K7

- Molecule 2 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).

15P

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			91	60	31		

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- Molecule 3 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).
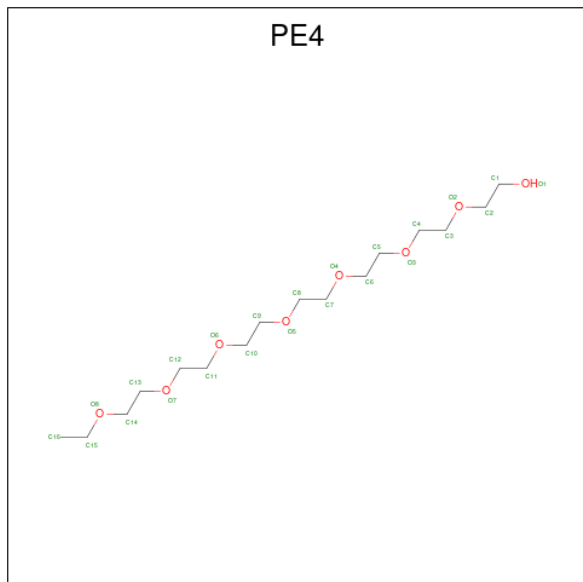
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			22	14	8		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	338	Total 344	O 344	0	7
6	B	347	Total 357	O 357	0	10

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: Lipase

Chain A:

• Molecule 1: Lipase

Chain B:
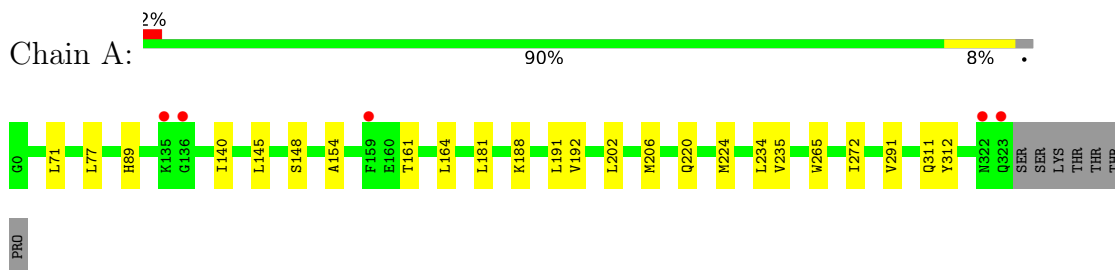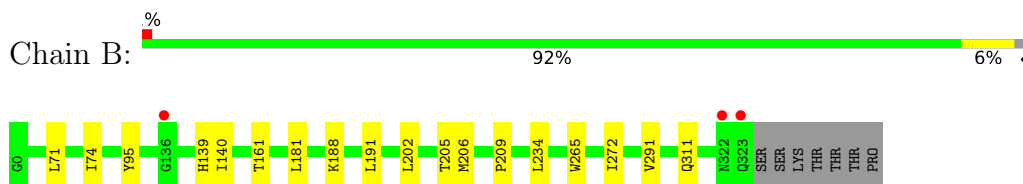
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	100.40Å 66.90Å 110.38Å 90.00° 95.58° 90.00°	Depositor
Resolution (Å)	48.56 – 1.70 48.56 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.56-1.70) 97.1 (48.56-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 1.70Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.161 , 0.185 0.168 , 0.190	Depositor DCC
R_{free} test set	3893 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5805	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 15P, GOL, PE4, 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	0.48	0/2569	0.54	0/3490
1	B	0.50	0/2567	0.54	0/3484
All	All	0.49	0/5136	0.54	0/6974

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 ⓘ

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	2459	0	2571	16	0
1	B	2457	0	2561	11	0
2	A	91	0	121	3	0
3	A	57	0	74	1	0
3	B	24	0	31	0	0
4	B	6	0	8	0	0
5	B	10	0	0	0	0
6	A	344	0	0	0	0
6	B	357	0	0	0	0
All	All	5805	0	5366	27	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 3.

All (27) 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:192[B]:VAL:CG2	1:A:224:MSE:HB3	2.27	0.63
1:B:71[A]:LEU:HG	1:B:95:TYR:HB3	1.80	0.63
1:A:154:ALA:HB2	1:A:164[B]:LEU:HD21	1.86	0.57
1:A:148:SER:HB3	2:A:401:15P:H28	1.87	0.56
1:A:77:LEU:HD13	1:A:234[B]:LEU:HD22	1.89	0.55
1:B:74:ILE:HD11	1:B:140[B]:ILE:HD11	1.91	0.52
1:B:140[A]:ILE:HD12	1:B:161:THR:HG23	1.93	0.51
1:A:145:LEU:HD21	1:A:234[B]:LEU:HD21	1.93	0.50
1:A:202:LEU:HD22	1:A:206:MSE:CE	2.41	0.50
1:A:192[B]:VAL:HG21	1:A:224:MSE:HB3	1.94	0.49
1:B:188:LYS:HA	1:B:191[A]:LEU:HD12	1.94	0.49
1:A:181:LEU:HD11	1:A:272:ILE:HG23	1.94	0.48
1:A:291:VAL:HG11	1:A:311:GLN:HG3	1.96	0.47
1:A:191[A]:LEU:HD11	1:A:235:VAL:HG21	1.97	0.47
2:A:401:15P:H452	1:B:205:THR:HG21	1.97	0.47
1:B:291:VAL:HG11	1:B:311:GLN:HG3	1.97	0.46
1:A:140:ILE:HD12	1:A:161:THR:HG23	1.98	0.45
1:A:192[B]:VAL:HG21	1:A:224:MSE:CB	2.46	0.45
1:A:71[B]:LEU:HD11	1:A:312:TYR:OH	2.17	0.45
1:A:220:GLN:HG2	2:A:401:15P:H252	2.00	0.44
1:A:188:LYS:HA	1:A:191[A]:LEU:HD13	1.99	0.43
1:B:206:MSE:HE3	1:B:209:PRO:HB3	2.01	0.43
1:B:71[A]:LEU:CD2	1:B:139:HIS:HB2	2.49	0.43
1:B:202:LEU:HD22	1:B:206:MSE:CE	2.48	0.42
1:B:181[B]:LEU:HD11	1:B:272:ILE:HG23	2.00	0.42
1:B:188:LYS:HA	1:B:191[B]:LEU:HD13	2.01	0.42
1:A:89:HIS:CE1	3:A:405:PE4:H22	2.55	0.41

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	317/306 (104%)	313 (99%)	4 (1%)	0	100	100
1	B	317/306 (104%)	315 (99%)	2 (1%)	0	100	100
All	All	634/612 (104%)	628 (99%)	6 (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	281/265 (106%)	280 (100%)	1 (0%)	91	87
1	B	279/265 (105%)	277 (99%)	2 (1%)	84	77
All	All	560/530 (106%)	557 (100%)	3 (0%)	86	83

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

Mol	Chain	Res	Type
1	A	265	TRP
1	B	234	LEU
1	B	265	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	218	GLN
1	B	295	ASN

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 ⓘ

13 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	PE4	B	403	-	6,6,23	0.43	0	5,5,22	0.26	0
3	PE4	B	401	-	9,9,23	0.49	0	8,8,22	0.44	0
5	SO4	B	406	-	4,4,4	0.29	0	6,6,6	0.22	0
3	PE4	A	404	-	6,6,23	0.46	0	5,5,22	0.20	0
3	PE4	A	406	-	6,6,23	0.50	0	5,5,22	0.20	0
3	PE4	A	405	-	6,6,23	0.47	0	5,5,22	0.23	0
3	PE4	A	407	-	6,6,23	0.43	0	5,5,22	0.31	0
3	PE4	A	403	-	21,21,23	0.48	0	20,20,22	0.27	0
2	15P	A	401	-	90,90,103	0.50	0	89,89,102	0.28	0
4	GOL	B	404	-	5,5,5	0.05	0	5,5,5	0.25	0
5	SO4	B	405	-	4,4,4	0.16	0	6,6,6	0.33	0
3	PE4	A	402	-	6,6,23	0.46	0	5,5,22	0.25	0
3	PE4	B	402	-	6,6,23	0.45	0	5,5,22	0.16	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
3	PE4	B	403	-	-	1/4/4/21	-
3	PE4	B	401	-	-	6/7/7/21	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PE4	A	404	-	-	1/4/4/21	-
3	PE4	A	406	-	-	1/4/4/21	-
3	PE4	A	405	-	-	2/4/4/21	-
3	PE4	A	407	-	-	3/4/4/21	-
3	PE4	A	403	-	-	9/19/19/21	-
2	15P	A	401	-	-	60/88/88/101	-
4	GOL	B	404	-	-	0/4/4/4	-
3	PE4	A	402	-	-	3/4/4/21	-
3	PE4	B	402	-	-	2/4/4/21	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	PE4	O4-C7-C8-O5
2	A	401	15P	O18-C37-C38-O19
2	A	401	15P	O14-C29-C30-O15
2	A	401	15P	O5-C10-C9-O4
2	A	401	15P	O16-C33-C34-O17
3	A	405	PE4	O1-C1-C2-O2
2	A	401	15P	O25-C51-C52-O26
2	A	401	15P	O5-C11-C12-O6
2	A	401	15P	O19-C39-C40-O20
2	A	401	15P	O22-C45-C46-O23
3	A	403	PE4	O3-C5-C6-O4
2	A	401	15P	OXT-C1-C2-O1
2	A	401	15P	O17-C35-C36-O18
2	A	401	15P	O7-C15-C16-O8
3	A	403	PE4	O7-C13-C14-O8
3	A	406	PE4	O1-C1-C2-O2
3	B	403	PE4	O1-C1-C2-O2
3	B	401	PE4	O1-C1-C2-O2
3	B	401	PE4	O3-C5-C6-O4
2	A	401	15P	O2-C5-C6-O3
3	A	402	PE4	O1-C1-C2-O2
2	A	401	15P	O3-C7-C8-O4
2	A	401	15P	O12-C25-C26-O13

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Mol	Chain	Res	Type	Atoms
2	A	401	15P	O23-C47-C48-O24
2	A	401	15P	O20-C41-C42-O21
2	A	401	15P	C11-C12-O6-C13
3	A	403	PE4	C9-C10-O6-C11
3	B	401	PE4	C3-C4-O3-C5
2	A	401	15P	C23-C24-O12-C25
3	A	405	PE4	C4-C3-O2-C2
2	A	401	15P	C30-C29-O14-C28
2	A	401	15P	C31-C32-O16-C33
2	A	401	15P	C37-C38-O19-C39
2	A	401	15P	C41-C42-O21-C43
2	A	401	15P	C60-C59-O29-C58
2	A	401	15P	C1-C2-O1-C3
2	A	401	15P	C39-C40-O20-C41
3	A	403	PE4	C4-C3-O2-C2
2	A	401	15P	C56-C55-O27-C54
3	A	404	PE4	C4-C3-O2-C2
3	A	407	PE4	C1-C2-O2-C3
2	A	401	15P	C28-C27-O13-C26
3	A	402	PE4	C4-C3-O2-C2
2	A	401	15P	C15-C16-O8-C17
3	A	403	PE4	C1-C2-O2-C3
2	A	401	15P	O13-C27-C28-O14
2	A	401	15P	C13-C14-O7-C15
2	A	401	15P	C51-C52-O26-C53
2	A	401	15P	C14-C13-O6-C12
2	A	401	15P	C44-C43-O21-C42
2	A	401	15P	C8-C7-O3-C6
2	A	401	15P	C40-C39-O19-C38
3	B	401	PE4	C6-C5-O3-C4
2	A	401	15P	C35-C36-O18-C37
2	A	401	15P	C48-C47-O23-C46
2	A	401	15P	C33-C34-O17-C35
2	A	401	15P	C53-C54-O27-C55
2	A	401	15P	C20-C19-O9-C18
3	B	402	PE4	C1-C2-O2-C3
2	A	401	15P	C29-C30-O15-C31
2	A	401	15P	C21-C22-O11-C23
2	A	401	15P	O24-C49-C50-O25
2	A	401	15P	C12-C11-O5-C10
2	A	401	15P	C36-C35-O17-C34
2	A	401	15P	C6-C5-O2-C4

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Mol	Chain	Res	Type	Atoms
3	A	403	PE4	C10-C9-O5-C8
3	A	403	PE4	C7-C8-O5-C9
3	A	407	PE4	O2-C3-C4-O3
3	A	407	PE4	O1-C1-C2-O2
2	A	401	15P	C3-C4-O2-C5
3	A	402	PE4	C1-C2-O2-C3
2	A	401	15P	C4-C3-O1-C2
2	A	401	15P	O11-C23-C24-O12
2	A	401	15P	C18-C17-O8-C16
2	A	401	15P	C55-C56-O28-C57
2	A	401	15P	C26-C25-O12-C24
2	A	401	15P	O21-C43-C44-O22
2	A	401	15P	C22-C21-O10-C20
3	B	401	PE4	O2-C3-C4-O3
3	A	403	PE4	C5-C6-O4-C7
2	A	401	15P	O6-C13-C14-O7
2	A	401	15P	O10-C21-C22-O11
3	B	402	PE4	C4-C3-O2-C2
3	B	401	PE4	C4-C3-O2-C2
2	A	401	15P	O15-C31-C32-O16
2	A	401	15P	C52-C51-O25-C50
2	A	401	15P	O27-C55-C56-O28
2	A	401	15P	O1-C3-C4-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	PE4	1	0
2	A	401	15P	3	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 PE4 B 403

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 A 404

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 A 406

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 A 405

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 A 407

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 A 403

| Bond lengths | Bond angles |

| Torsions | Rings |

Ligand 15P A 401

| Bond lengths | Bond angles |

| Torsions | Rings |

Ligand PE4 A 402

| Bond lengths | Bond angles |

| Torsions | Rings |

Ligand PE4 B 402

| Bond lengths | Bond angles |

| Torsions | Rings |

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	296/306 (96%)	-0.26	5 (1%)	70	74	15, 23, 41, 95	0
1	B	296/306 (96%)	-0.27	3 (1%)	82	85	14, 22, 38, 81	0
All	All	592/612 (96%)	-0.26	8 (1%)	75	79	14, 23, 39, 95	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	GLY	4.2
1	A	136	GLY	4.2
1	B	322	ASN	3.2
1	A	323	GLN	3.0
1	B	323	GLN	2.6
1	A	135	LYS	2.1
1	A	159	PHE	2.1
1	A	322	ASN	2.0

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
3	PE4	A	407	7/24	0.63	0.23	65,69,73,74	0
3	PE4	A	406	7/24	0.69	0.17	54,56,59,59	0
4	GOL	B	404	6/6	0.73	0.27	69,70,71,71	0
3	PE4	B	403	7/24	0.74	0.19	60,61,63,63	0
3	PE4	B	402	7/24	0.75	0.19	60,60,62,62	0
3	PE4	A	402	7/24	0.76	0.14	55,56,61,61	0
3	PE4	A	403	22/24	0.76	0.29	67,70,74,75	0
3	PE4	B	401	10/24	0.76	0.17	46,47,49,49	0
2	15P	A	401	91/104	0.78	0.15	43,55,60,62	0
3	PE4	A	404	7/24	0.79	0.15	60,60,60,61	0
3	PE4	A	405	7/24	0.81	0.12	50,54,58,59	0
5	SO4	B	405	5/5	0.93	0.14	20,24,25,26	5
5	SO4	B	406	5/5	0.95	0.22	31,33,35,36	5

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.
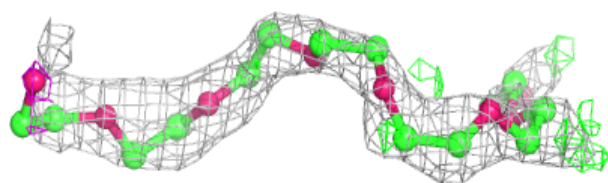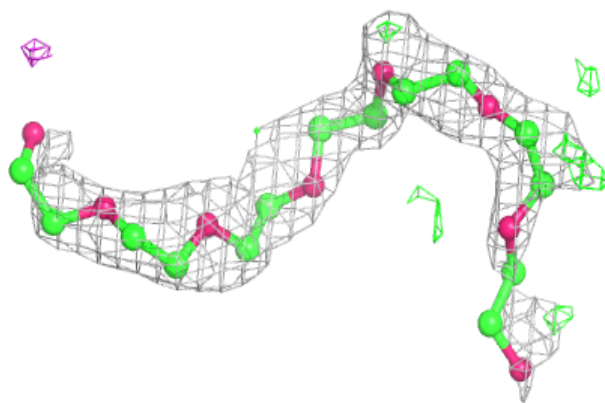

Electron density around PE4 A 407:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
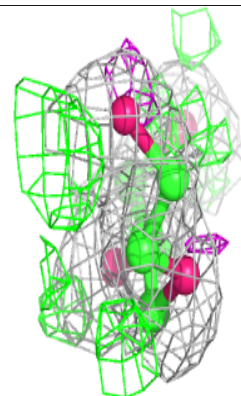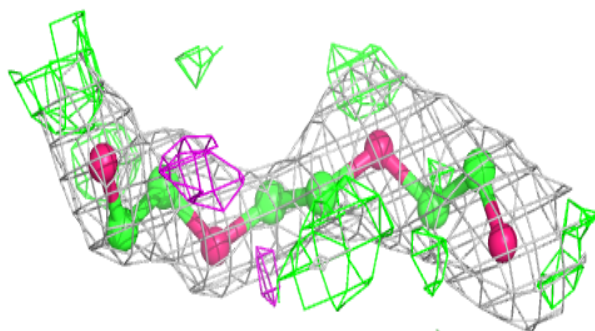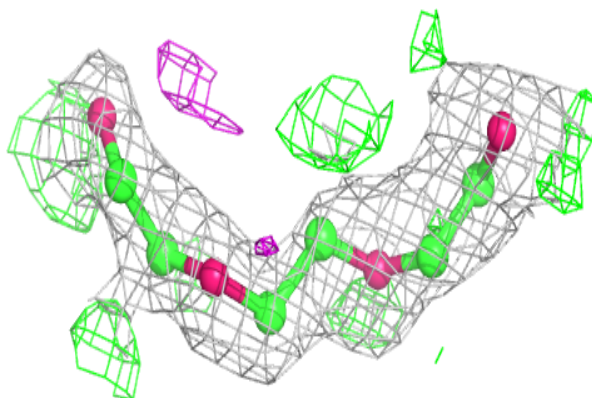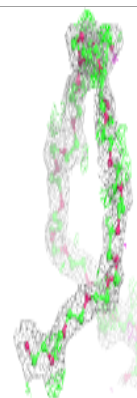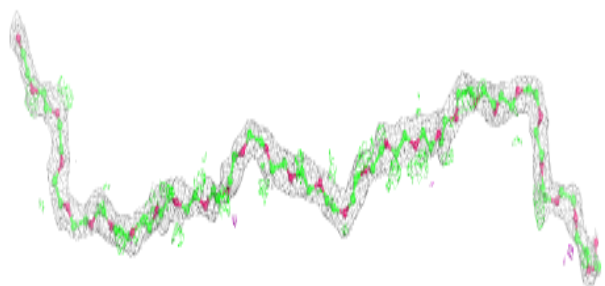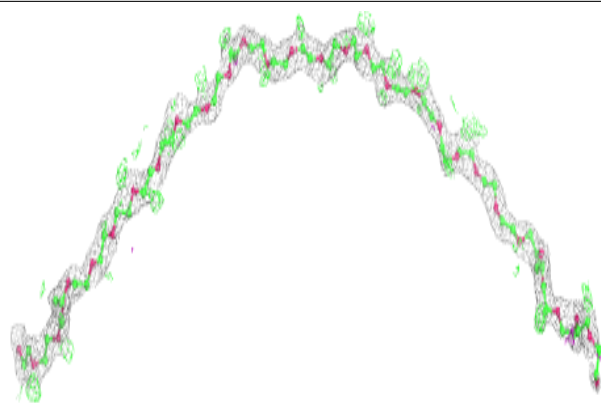mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
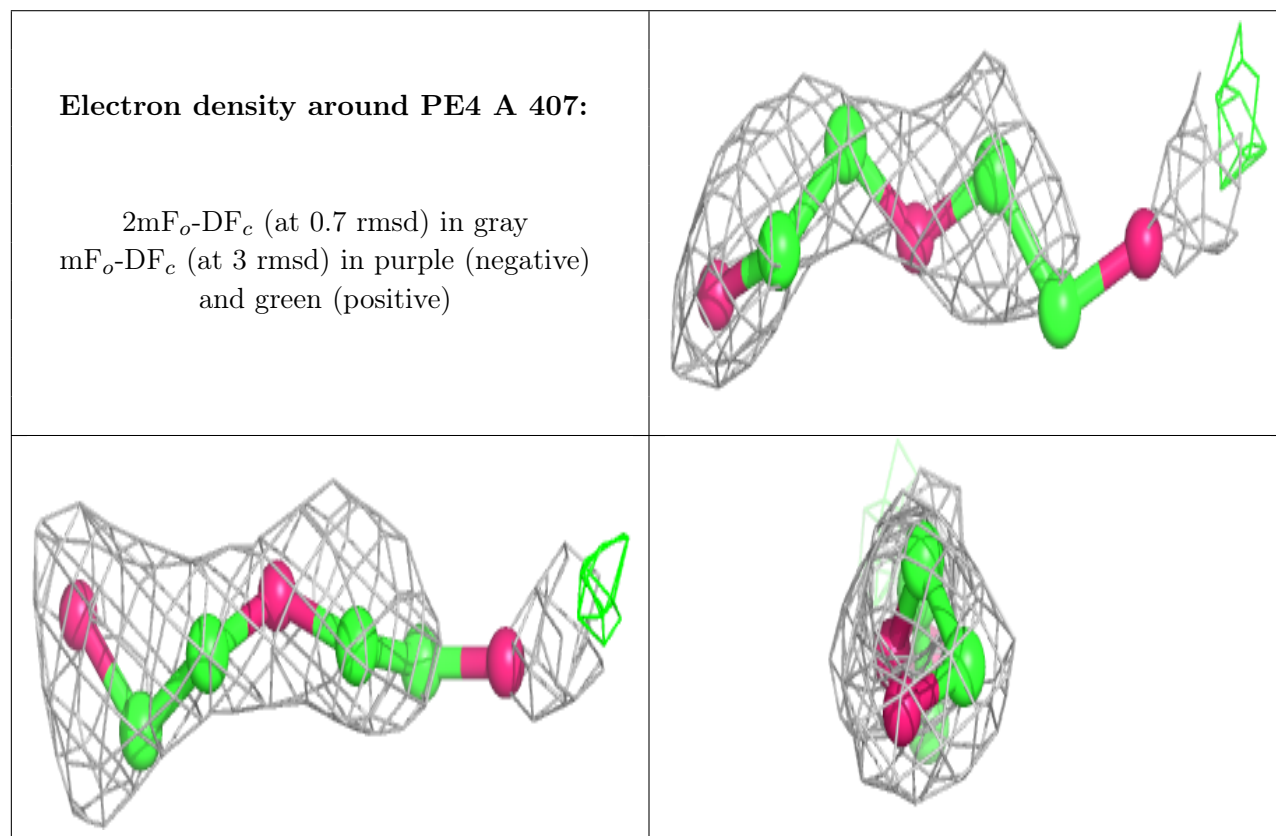
Electron density around PE4 A 406:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
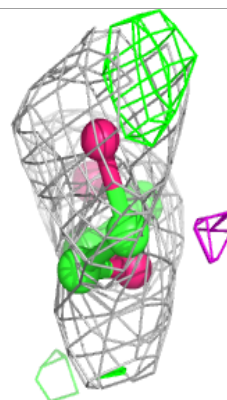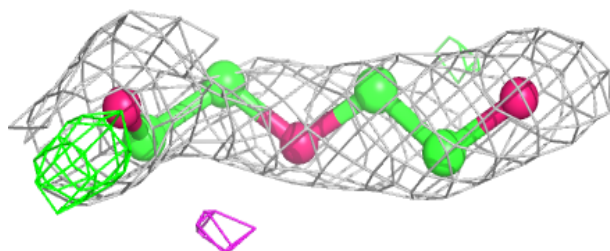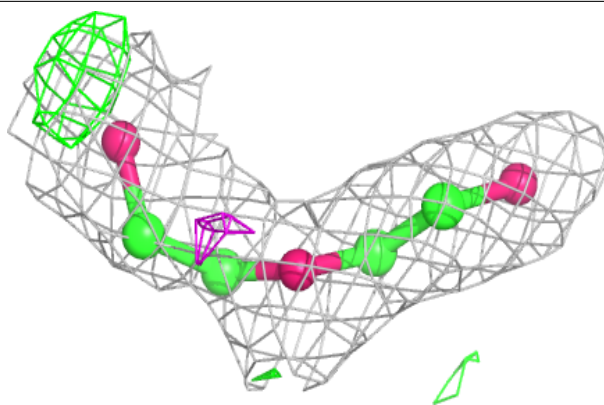
Electron density around PE4 B 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
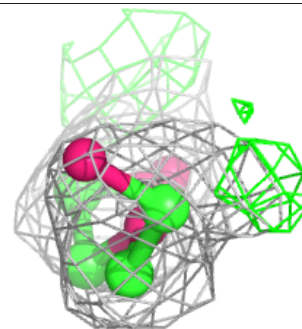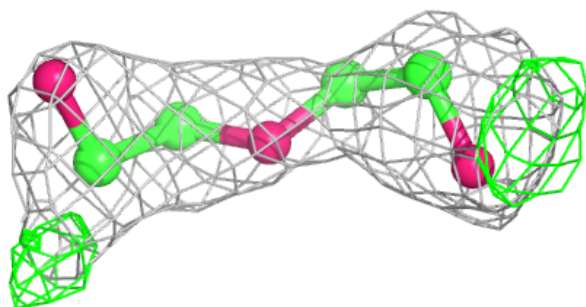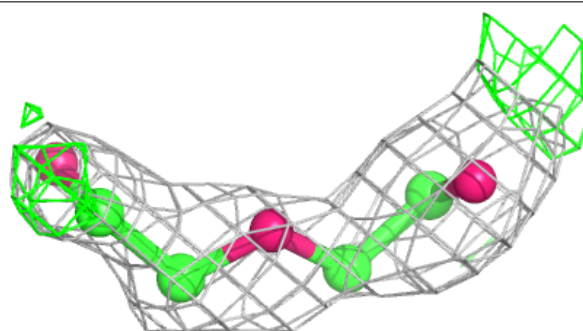
Electron density around PE4 B 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
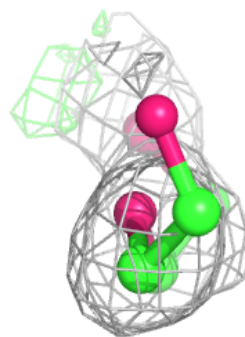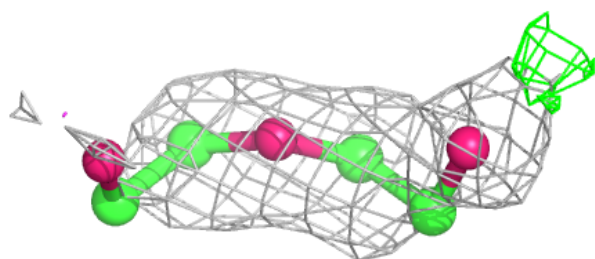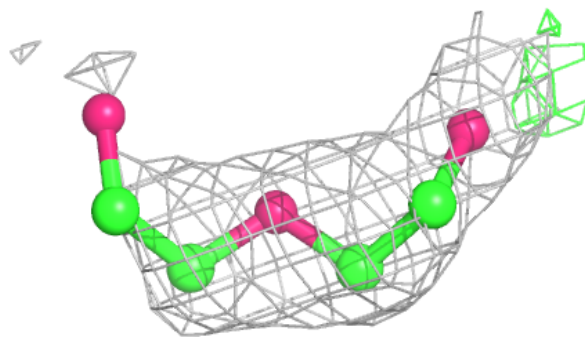
Electron density around PE4 A 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
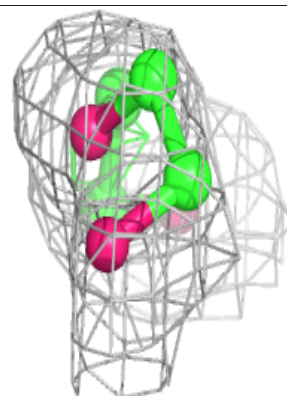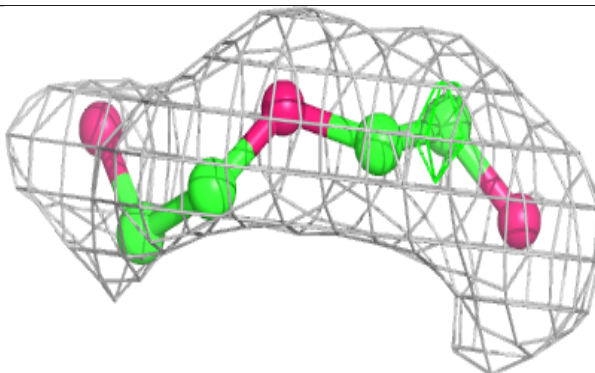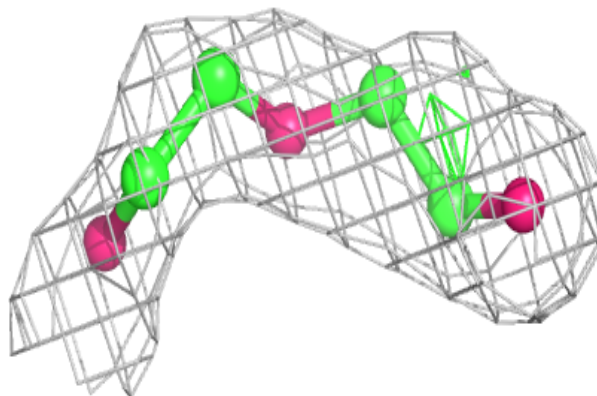
Electron density around PE4 A 403:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
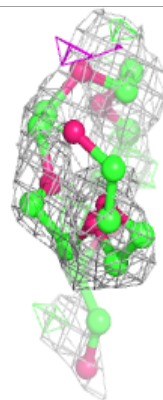
Electron density around PE4 B 401:

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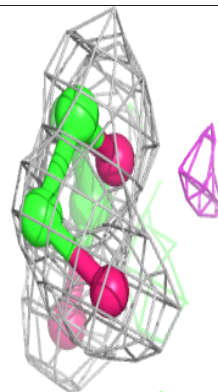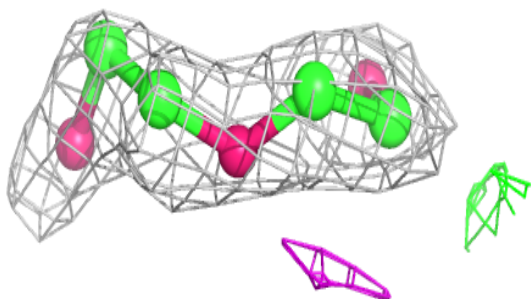mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
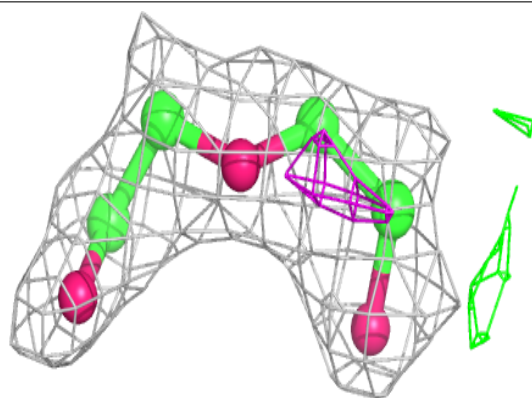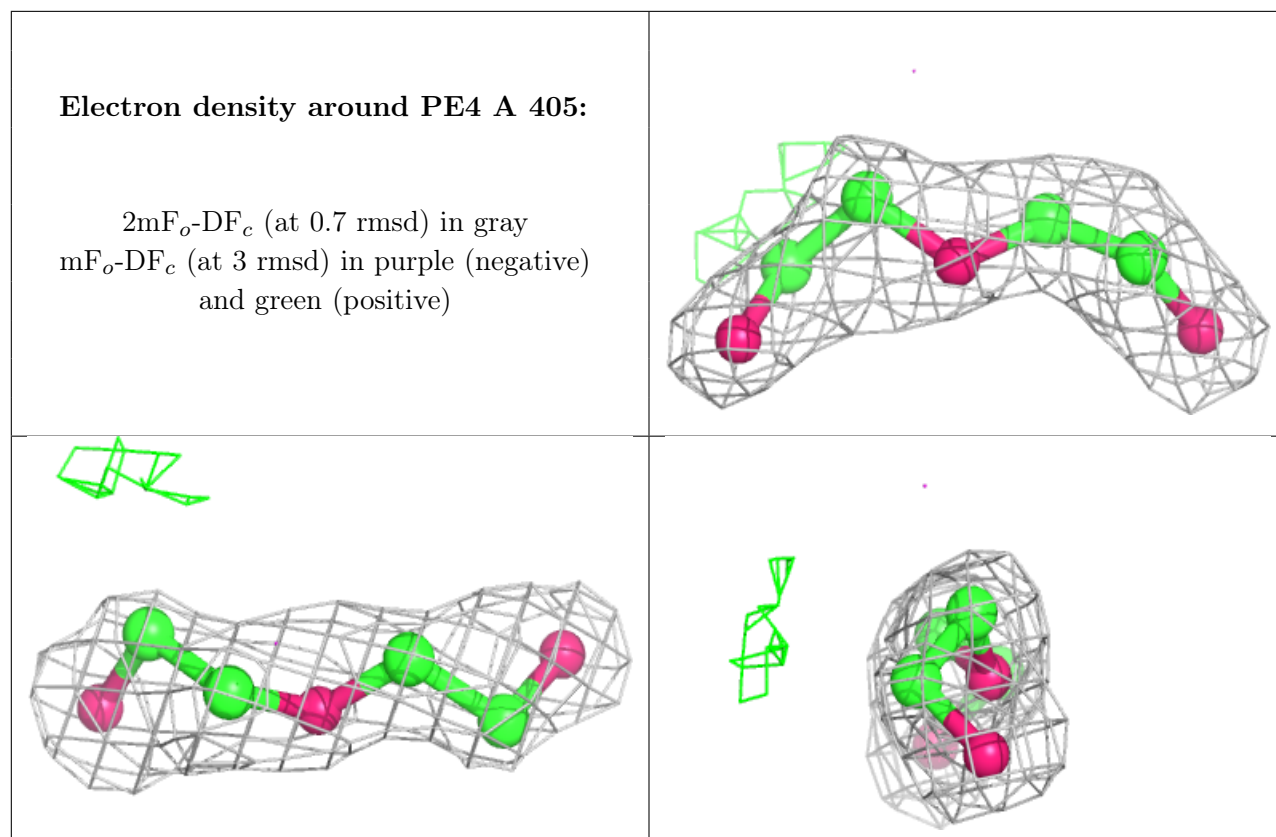and green (positive)

Electron density around 15P A 401:

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 PE4 A 404:

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 PE4 A 405:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.