Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 04:03 pm GMT

PDB ID	:	4A8P
Title	:	Crystal structure of putrescine transcarbamylase from Enterococcus faecalis with N5-(phosphonoacetyl)-L-ornithine
Authors	:	Polo, L.M.; Gil-Ortiz, F.; Rubio, V.
Deposited on	:	2011-11-21
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

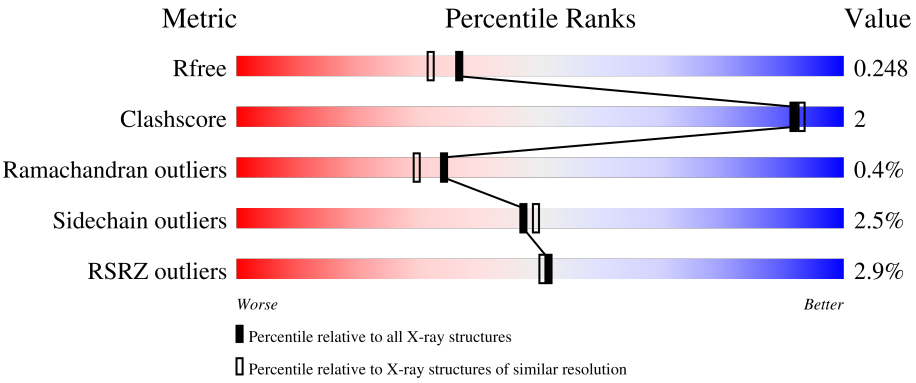
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	355	89% 6% • 5%
1	B	355	90% 5% 5%
1	C	355	88% 6% • 5%
1	D	355	5% 89% 5% 6%
1	E	355	5% 89% 5% 6%

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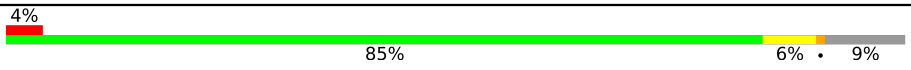
Mol	Chain	Length	Quality of chain
1	F	355	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16128 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 PUTRESCINE CARBAMOYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2628	1656	440	510	22			
1	B	338	Total	C	N	O	S	0	0	0
			2627	1653	441	511	22			
1	C	339	Total	C	N	O	S	0	0	0
			2640	1661	441	517	21			
1	D	334	Total	C	N	O	S	0	0	0
			2553	1605	430	497	21			
1	E	333	Total	C	N	O	S	0	0	0
			2551	1608	428	494	21			
1	F	323	Total	C	N	O	S	0	0	0
			2480	1560	415	483	22			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	SER	-	expression tag	UNP Q837U7
A	341	ALA	-	expression tag	UNP Q837U7
A	342	ALA	-	expression tag	UNP Q837U7
A	343	LYS	-	expression tag	UNP Q837U7
A	344	LEU	-	expression tag	UNP Q837U7
A	345	ALA	-	expression tag	UNP Q837U7
A	346	ALA	-	expression tag	UNP Q837U7
A	347	ALA	-	expression tag	UNP Q837U7
A	348	LEU	-	expression tag	UNP Q837U7
A	349	GLU	-	expression tag	UNP Q837U7
A	350	HIS	-	expression tag	UNP Q837U7
A	351	HIS	-	expression tag	UNP Q837U7
A	352	HIS	-	expression tag	UNP Q837U7
A	353	HIS	-	expression tag	UNP Q837U7
A	354	HIS	-	expression tag	UNP Q837U7
A	355	HIS	-	expression tag	UNP Q837U7
B	340	SER	-	expression tag	UNP Q837U7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	341	ALA	-	expression tag	UNP Q837U7
B	342	ALA	-	expression tag	UNP Q837U7
B	343	LYS	-	expression tag	UNP Q837U7
B	344	LEU	-	expression tag	UNP Q837U7
B	345	ALA	-	expression tag	UNP Q837U7
B	346	ALA	-	expression tag	UNP Q837U7
B	347	ALA	-	expression tag	UNP Q837U7
B	348	LEU	-	expression tag	UNP Q837U7
B	349	GLU	-	expression tag	UNP Q837U7
B	350	HIS	-	expression tag	UNP Q837U7
B	351	HIS	-	expression tag	UNP Q837U7
B	352	HIS	-	expression tag	UNP Q837U7
B	353	HIS	-	expression tag	UNP Q837U7
B	354	HIS	-	expression tag	UNP Q837U7
B	355	HIS	-	expression tag	UNP Q837U7
C	340	SER	-	expression tag	UNP Q837U7
C	341	ALA	-	expression tag	UNP Q837U7
C	342	ALA	-	expression tag	UNP Q837U7
C	343	LYS	-	expression tag	UNP Q837U7
C	344	LEU	-	expression tag	UNP Q837U7
C	345	ALA	-	expression tag	UNP Q837U7
C	346	ALA	-	expression tag	UNP Q837U7
C	347	ALA	-	expression tag	UNP Q837U7
C	348	LEU	-	expression tag	UNP Q837U7
C	349	GLU	-	expression tag	UNP Q837U7
C	350	HIS	-	expression tag	UNP Q837U7
C	351	HIS	-	expression tag	UNP Q837U7
C	352	HIS	-	expression tag	UNP Q837U7
C	353	HIS	-	expression tag	UNP Q837U7
C	354	HIS	-	expression tag	UNP Q837U7
C	355	HIS	-	expression tag	UNP Q837U7
D	340	SER	-	expression tag	UNP Q837U7
D	341	ALA	-	expression tag	UNP Q837U7
D	342	ALA	-	expression tag	UNP Q837U7
D	343	LYS	-	expression tag	UNP Q837U7
D	344	LEU	-	expression tag	UNP Q837U7
D	345	ALA	-	expression tag	UNP Q837U7
D	346	ALA	-	expression tag	UNP Q837U7
D	347	ALA	-	expression tag	UNP Q837U7
D	348	LEU	-	expression tag	UNP Q837U7
D	349	GLU	-	expression tag	UNP Q837U7
D	350	HIS	-	expression tag	UNP Q837U7

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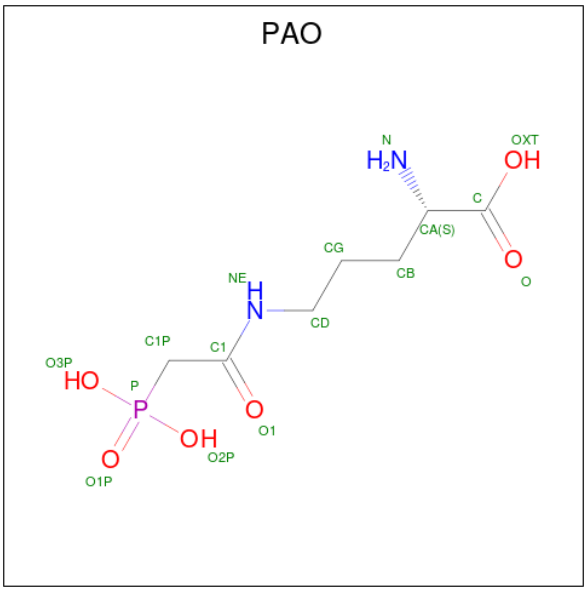
Chain	Residue	Modelled	Actual	Comment	Reference
D	351	HIS	-	expression tag	UNP Q837U7
D	352	HIS	-	expression tag	UNP Q837U7
D	353	HIS	-	expression tag	UNP Q837U7
D	354	HIS	-	expression tag	UNP Q837U7
D	355	HIS	-	expression tag	UNP Q837U7
E	340	SER	-	expression tag	UNP Q837U7
E	341	ALA	-	expression tag	UNP Q837U7
E	342	ALA	-	expression tag	UNP Q837U7
E	343	LYS	-	expression tag	UNP Q837U7
E	344	LEU	-	expression tag	UNP Q837U7
E	345	ALA	-	expression tag	UNP Q837U7
E	346	ALA	-	expression tag	UNP Q837U7
E	347	ALA	-	expression tag	UNP Q837U7
E	348	LEU	-	expression tag	UNP Q837U7
E	349	GLU	-	expression tag	UNP Q837U7
E	350	HIS	-	expression tag	UNP Q837U7
E	351	HIS	-	expression tag	UNP Q837U7
E	352	HIS	-	expression tag	UNP Q837U7
E	353	HIS	-	expression tag	UNP Q837U7
E	354	HIS	-	expression tag	UNP Q837U7
E	355	HIS	-	expression tag	UNP Q837U7
F	340	SER	-	expression tag	UNP Q837U7
F	341	ALA	-	expression tag	UNP Q837U7
F	342	ALA	-	expression tag	UNP Q837U7
F	343	LYS	-	expression tag	UNP Q837U7
F	344	LEU	-	expression tag	UNP Q837U7
F	345	ALA	-	expression tag	UNP Q837U7
F	346	ALA	-	expression tag	UNP Q837U7
F	347	ALA	-	expression tag	UNP Q837U7
F	348	LEU	-	expression tag	UNP Q837U7
F	349	GLU	-	expression tag	UNP Q837U7
F	350	HIS	-	expression tag	UNP Q837U7
F	351	HIS	-	expression tag	UNP Q837U7
F	352	HIS	-	expression tag	UNP Q837U7
F	353	HIS	-	expression tag	UNP Q837U7
F	354	HIS	-	expression tag	UNP Q837U7
F	355	HIS	-	expression tag	UNP Q837U7

- Molecule 2 is N-(PHOSPHONOACETYL)-L-ORNITHINE (three-letter code: PAO) (formula: $C_7H_{15}N_2O_6P$).

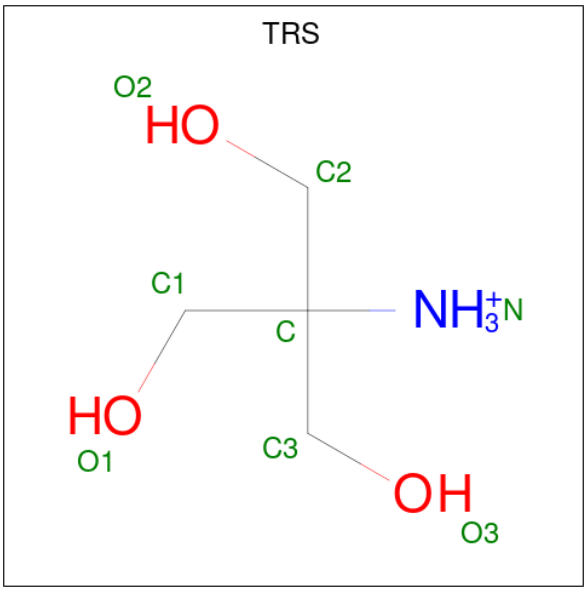


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P 16 7 2 6 1	0	0
2	B	1	Total C N O P 16 7 2 6 1	0	0
2	C	1	Total C N O P 16 7 2 6 1	0	0
2	D	1	Total C N O P 16 7 2 6 1	0	0
2	E	1	Total C N O P 16 7 2 6 1	0	0
2	F	1	Total C N O P 16 7 2 6 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	D	1	Total Ni 1 1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 8 4 1 3	0	0
4	C	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is water.

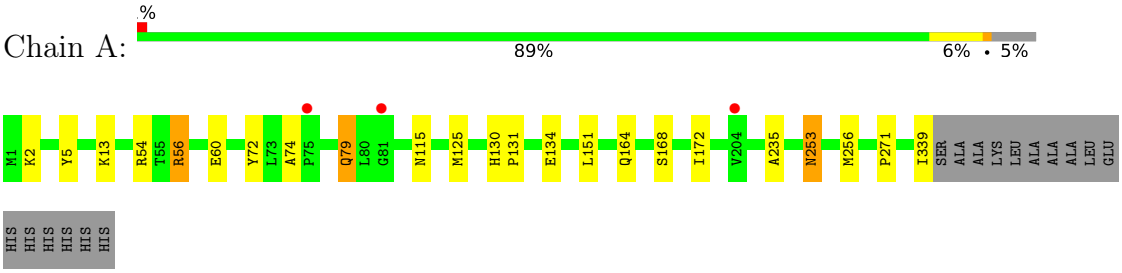
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	130	Total O 130 130	0	0
5	B	113	Total O 113 113	0	0
5	C	91	Total O 91 91	0	0
5	D	102	Total O 102 102	0	0
5	E	50	Total O 50 50	0	0
5	F	49	Total O 49 49	0	0

3 Residue-property plots (i)

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

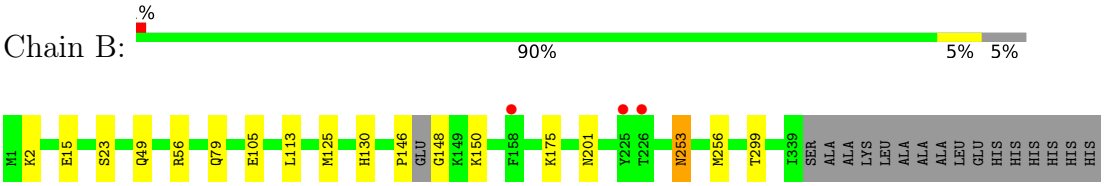
• Molecule 1: PUTRESCINE CARBAMOYLTRANSFERASE

Chain A:



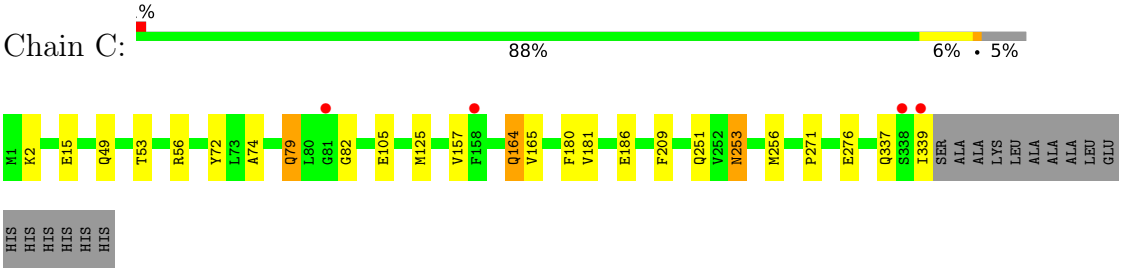
• Molecule 1: PUTRESCINE CARBAMOYLTRANSFERASE

Chain B:



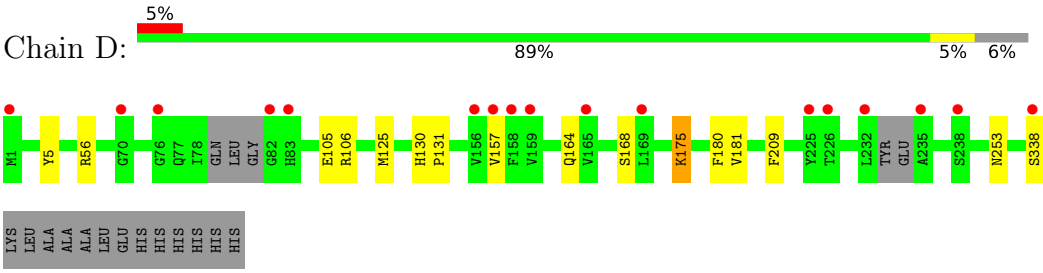
• Molecule 1: PUTRESCINE CARBAMOYLTRANSFERASE

Chain C:



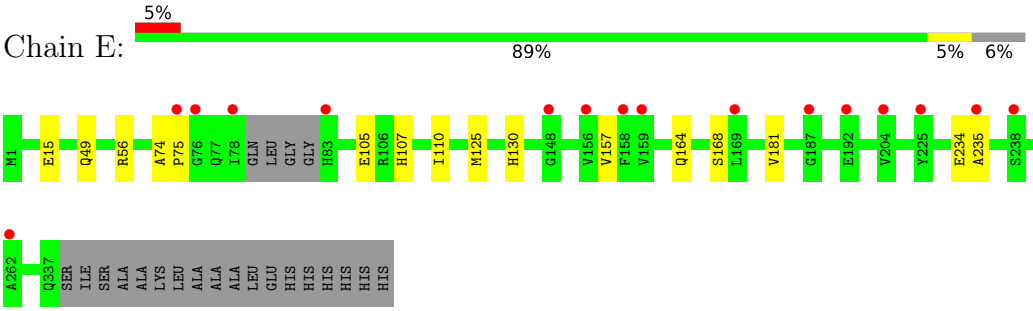
• Molecule 1: PUTRESCINE CARBAMOYLTRANSFERASE

Chain D:



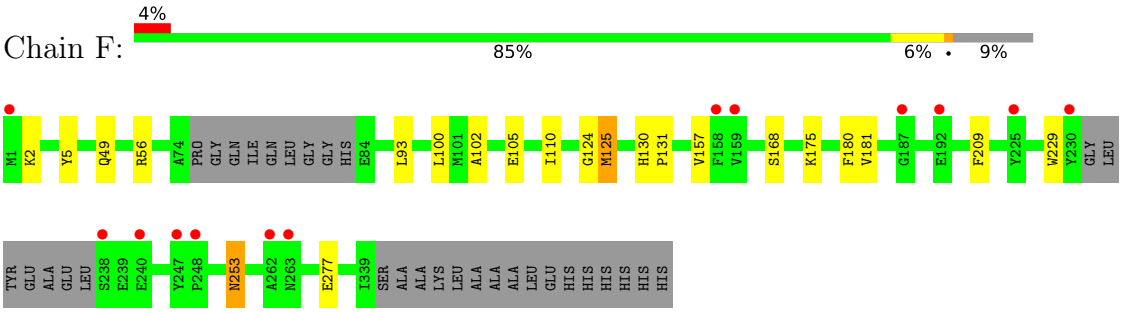
• Molecule 1: PUTRESCINE CARBAMOYLTRANSFERASE

Chain E:



• Molecule 1: PUTRESCINE CARBAMOYLTRANSFERASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.52Å 81.71Å 82.28Å 105.43° 102.80° 100.75°	Depositor
Resolution (Å)	25.00 – 2.00 24.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.6 (25.00-2.00) 83.9 (24.82-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.196 , 0.237 0.207 , 0.248	Depositor DCC
R_{free} test set	5541 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16128	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NI, PAO, TRS

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	0.41	0/2676	0.53	1/3619 (0.0%)
1	B	0.41	0/2673	0.52	0/3611
1	C	0.41	0/2688	0.51	0/3635
1	D	0.39	0/2598	0.50	0/3517
1	E	0.38	0/2597	0.49	0/3518
1	F	0.38	0/2523	0.48	0/3416
All	All	0.40	0/15755	0.51	1/21316 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	LEU	CA-CB-CG	5.01	126.82	115.30

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	2628	0	2536	11	0
1	B	2627	0	2545	9	0
1	C	2640	0	2545	14	0
1	D	2553	0	2417	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2551	0	2426	7	0
1	F	2480	0	2352	10	0
2	A	16	0	12	0	0
2	B	16	0	12	0	0
2	C	16	0	12	0	0
2	D	16	0	12	0	0
2	E	16	0	12	0	0
2	F	16	0	12	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
5	A	130	0	0	0	0
5	B	113	0	0	0	0
5	C	91	0	0	0	0
5	D	102	0	0	1	0
5	E	50	0	0	0	0
5	F	49	0	0	1	0
All	All	16128	0	14917	50	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 2.

All (50) 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:79:GLN:HG3	1:C:271:PRO:HG3	1.65	0.77
1:A:72:TYR:CE2	1:A:74:ALA:HB2	2.28	0.68
1:D:339:ILE:HG12	1:E:15:GLU:HG2	1.81	0.62
1:A:79:GLN:NE2	1:C:53:THR:OG1	2.36	0.59
1:B:15:GLU:HG2	1:C:339:ILE:HG12	1.83	0.58
1:C:79:GLN:HE21	1:C:79:GLN:H	1.53	0.56
1:C:253:ASN:HD22	1:C:253:ASN:C	2.09	0.53
1:F:180:PHE:O	1:F:209:PHE:HA	2.08	0.53
1:F:5:TYR:CE2	1:F:131:PRO:HB2	2.44	0.52
1:F:157:VAL:HG22	1:F:181:VAL:HB	1.90	0.52
1:B:49:GLN:HE21	1:B:105:GLU:H	1.57	0.52
1:A:271:PRO:HG3	1:B:79:GLN:HG3	1.92	0.51
1:D:105:GLU:HG3	1:D:106:ARG:HG2	1.93	0.51
1:C:49:GLN:NE2	1:C:105:GLU:H	2.11	0.49
1:C:72:TYR:CE2	1:C:74:ALA:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ASN:ND2	1:C:256:MET:H	2.12	0.48
1:D:5:TYR:CE2	1:D:131:PRO:HB2	2.49	0.48
1:A:235:ALA:HB1	1:E:235:ALA:HB1	1.95	0.47
1:E:157:VAL:HG22	1:E:181:VAL:HB	1.96	0.47
1:A:79:GLN:NE2	1:A:79:GLN:H	2.12	0.47
1:F:49:GLN:HE21	1:F:105:GLU:H	1.63	0.47
1:F:253:ASN:C	1:F:253:ASN:HD22	2.18	0.46
1:E:253:ASN:ND2	1:E:253:ASN:H	2.14	0.46
1:D:175:LYS:HE3	5:D:2008:HOH:O	2.16	0.46
1:D:180:PHE:O	1:D:209:PHE:HA	2.17	0.45
1:B:23:SER:HB3	1:B:299:THR:HG22	1.99	0.45
1:E:107:HIS:O	1:E:110:ILE:HG22	2.17	0.44
1:C:157:VAL:HG22	1:C:181:VAL:HB	2.00	0.44
1:E:74:ALA:HB1	1:E:75:PRO:HD2	1.98	0.43
1:C:49:GLN:HE21	1:C:105:GLU:H	1.65	0.43
1:A:134:GLU:OE1	1:A:172:ILE:HB	2.18	0.43
1:C:251:GLN:HG3	1:C:276:GLU:O	2.19	0.43
1:F:93:LEU:HD13	1:F:100:LEU:HD11	2.00	0.43
1:B:253:ASN:HD22	1:B:256:MET:H	1.66	0.42
1:B:49:GLN:NE2	1:B:105:GLU:H	2.17	0.42
1:E:49:GLN:HE21	1:E:105:GLU:H	1.68	0.42
1:C:164:GLN:HE21	1:C:165:VAL:H	1.69	0.41
1:F:102:ALA:HB3	1:F:110:ILE:CD1	2.51	0.41
1:F:175:LYS:HE2	5:F:2006:HOH:O	2.19	0.41
1:D:157:VAL:HG22	1:D:181:VAL:HB	2.02	0.41
1:B:253:ASN:ND2	1:B:256:MET:H	2.19	0.41
1:C:180:PHE:O	1:C:209:PHE:HA	2.21	0.41
1:A:56:ARG:NE	1:A:60:GLU:OE2	2.41	0.41
1:A:253:ASN:HD22	1:A:256:MET:H	1.67	0.41
1:A:339:ILE:HG12	1:C:15:GLU:HG2	2.03	0.41
1:F:124:GLY:O	1:F:125:MET:CB	2.69	0.40
1:B:146:PRO:O	1:B:148:GLY:HA2	2.21	0.40
1:B:150:LYS:HB2	1:B:150:LYS:HE3	1.89	0.40
1:A:5:TYR:CE2	1:A:131:PRO:HB2	2.56	0.40
1:F:229:TRP:CZ2	1:F:277:GLU:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	337/355 (95%)	329 (98%)	7 (2%)	1 (0%)	41	37
1	B	334/355 (94%)	325 (97%)	8 (2%)	1 (0%)	41	37
1	C	337/355 (95%)	329 (98%)	6 (2%)	2 (1%)	25	19
1	D	328/355 (92%)	323 (98%)	4 (1%)	1 (0%)	41	37
1	E	329/355 (93%)	321 (98%)	7 (2%)	1 (0%)	41	37
1	F	317/355 (89%)	311 (98%)	5 (2%)	1 (0%)	41	37
All	All	1982/2130 (93%)	1938 (98%)	37 (2%)	7 (0%)	34	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	MET
1	B	125	MET
1	C	125	MET
1	D	125	MET
1	E	125	MET
1	F	125	MET
1	C	82	GLY

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	282/307 (92%)	272 (96%)	10 (4%)	36	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	284/307 (92%)	277 (98%)	7 (2%)	47 49
1	C	285/307 (93%)	278 (98%)	7 (2%)	47 49
1	D	268/307 (87%)	261 (97%)	7 (3%)	46 48
1	E	268/307 (87%)	262 (98%)	6 (2%)	52 55
1	F	263/307 (86%)	258 (98%)	5 (2%)	57 61
All	All	1650/1842 (90%)	1608 (98%)	42 (2%)	47 49

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	13	LYS
1	A	54	ARG
1	A	56	ARG
1	A	79	GLN
1	A	115	ASN
1	A	130	HIS
1	A	164	GLN
1	A	168	SER
1	A	253	ASN
1	B	2	LYS
1	B	56	ARG
1	B	113	LEU
1	B	130	HIS
1	B	175	LYS
1	B	201	ASN
1	B	253	ASN
1	C	2	LYS
1	C	56	ARG
1	C	79	GLN
1	C	164	GLN
1	C	186	GLU
1	C	253	ASN
1	C	337	GLN
1	D	56	ARG
1	D	130	HIS
1	D	164	GLN
1	D	168	SER
1	D	175	LYS
1	D	253	ASN

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Mol	Chain	Res	Type
1	D	338	SER
1	E	56	ARG
1	E	130	HIS
1	E	164	GLN
1	E	168	SER
1	E	234	GLU
1	E	253	ASN
1	F	2	LYS
1	F	56	ARG
1	F	130	HIS
1	F	168	SER
1	F	253	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	79	GLN
1	A	115	ASN
1	A	189	GLN
1	A	201	ASN
1	A	253	ASN
1	A	310	ASN
1	A	323	GLN
1	B	41	ASN
1	B	49	GLN
1	B	50	GLN
1	B	115	ASN
1	B	189	GLN
1	B	201	ASN
1	B	253	ASN
1	B	254	GLN
1	B	310	ASN
1	C	41	ASN
1	C	49	GLN
1	C	50	GLN
1	C	79	GLN
1	C	115	ASN
1	C	164	GLN
1	C	189	GLN
1	C	201	ASN
1	C	253	ASN

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Mol	Chain	Res	Type
1	C	310	ASN
1	D	41	ASN
1	D	49	GLN
1	D	50	GLN
1	D	115	ASN
1	D	164	GLN
1	D	189	GLN
1	D	201	ASN
1	D	253	ASN
1	D	310	ASN
1	D	323	GLN
1	E	41	ASN
1	E	49	GLN
1	E	50	GLN
1	E	115	ASN
1	E	189	GLN
1	E	201	ASN
1	E	253	ASN
1	E	310	ASN
1	E	323	GLN
1	E	337	GLN
1	F	49	GLN
1	F	50	GLN
1	F	115	ASN
1	F	189	GLN
1	F	201	ASN
1	F	253	ASN
1	F	310	ASN
1	F	337	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
2	PAO	E	1338	-	14,15,15	1.72	3 (21%)	17,20,20	1.34	2 (11%)
2	PAO	D	1340	-	14,15,15	1.89	3 (21%)	17,20,20	1.29	2 (11%)
4	TRS	C	1341	-	7,7,7	0.46	0	9,9,9	0.52	0
2	PAO	C	1340	-	14,15,15	1.95	3 (21%)	17,20,20	1.32	2 (11%)
2	PAO	A	1340	-	14,15,15	1.82	3 (21%)	17,20,20	1.31	2 (11%)
4	TRS	B	1341	-	7,7,7	0.44	0	9,9,9	0.55	0
2	PAO	B	1340	-	14,15,15	2.00	3 (21%)	17,20,20	1.29	1 (5%)
2	PAO	F	1340	-	14,15,15	2.00	3 (21%)	17,20,20	1.50	2 (11%)

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
2	PAO	E	1338	-	-	2/16/16/16	-
2	PAO	D	1340	-	-	2/16/16/16	-
4	TRS	C	1341	-	-	3/9/9/9	-
2	PAO	C	1340	-	-	1/16/16/16	-
2	PAO	A	1340	-	-	1/16/16/16	-
4	TRS	B	1341	-	-	0/9/9/9	-
2	PAO	B	1340	-	-	0/16/16/16	-
2	PAO	F	1340	-	-	2/16/16/16	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1340	PAO	P-O1P	5.88	1.62	1.50
2	C	1340	PAO	P-O1P	5.68	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1340	PAO	P-O1P	5.62	1.62	1.50
2	A	1340	PAO	P-O1P	5.37	1.61	1.50
2	D	1340	PAO	P-O1P	4.93	1.60	1.50
2	E	1338	PAO	P-O1P	4.55	1.59	1.50
2	D	1340	PAO	P-O2P	3.52	1.63	1.54
2	F	1340	PAO	P-O2P	3.39	1.62	1.54
2	C	1340	PAO	P-O2P	2.81	1.61	1.54
2	B	1340	PAO	P-O3P	-2.80	1.48	1.54
2	D	1340	PAO	P-O3P	-2.75	1.48	1.54
2	E	1338	PAO	P-O2P	2.75	1.61	1.54
2	F	1340	PAO	P-O3P	-2.66	1.48	1.54
2	B	1340	PAO	P-O2P	2.65	1.61	1.54
2	E	1338	PAO	P-O3P	-2.60	1.49	1.54
2	C	1340	PAO	P-O3P	-2.45	1.49	1.54
2	A	1340	PAO	P-O3P	-2.44	1.49	1.54
2	A	1340	PAO	P-O2P	2.37	1.60	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1340	PAO	O3P-P-C1P	4.17	115.60	106.84
2	A	1340	PAO	O3P-P-C1P	3.64	114.48	106.84
2	E	1338	PAO	O3P-P-C1P	3.58	114.35	106.84
2	B	1340	PAO	O3P-P-C1P	3.00	113.14	106.84
2	C	1340	PAO	O3P-P-C1P	2.99	113.11	106.84
2	D	1340	PAO	O3P-P-C1P	2.88	112.88	106.84
2	D	1340	PAO	O2P-P-O1P	-2.48	105.83	112.39
2	C	1340	PAO	O1P-P-C1P	-2.29	105.72	110.94
2	A	1340	PAO	O2P-P-O1P	-2.20	106.57	112.39
2	F	1340	PAO	O1P-P-C1P	-2.17	106.00	110.94
2	E	1338	PAO	O1P-P-C1P	-2.11	106.13	110.94

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1338	PAO	C1-C1P-P-O1P
4	C	1341	TRS	C1-C-C3-O3
4	C	1341	TRS	C2-C-C3-O3
4	C	1341	TRS	N-C-C3-O3
2	D	1340	PAO	N-CA-CB-CG
2	A	1340	PAO	C1-C1P-P-O1P

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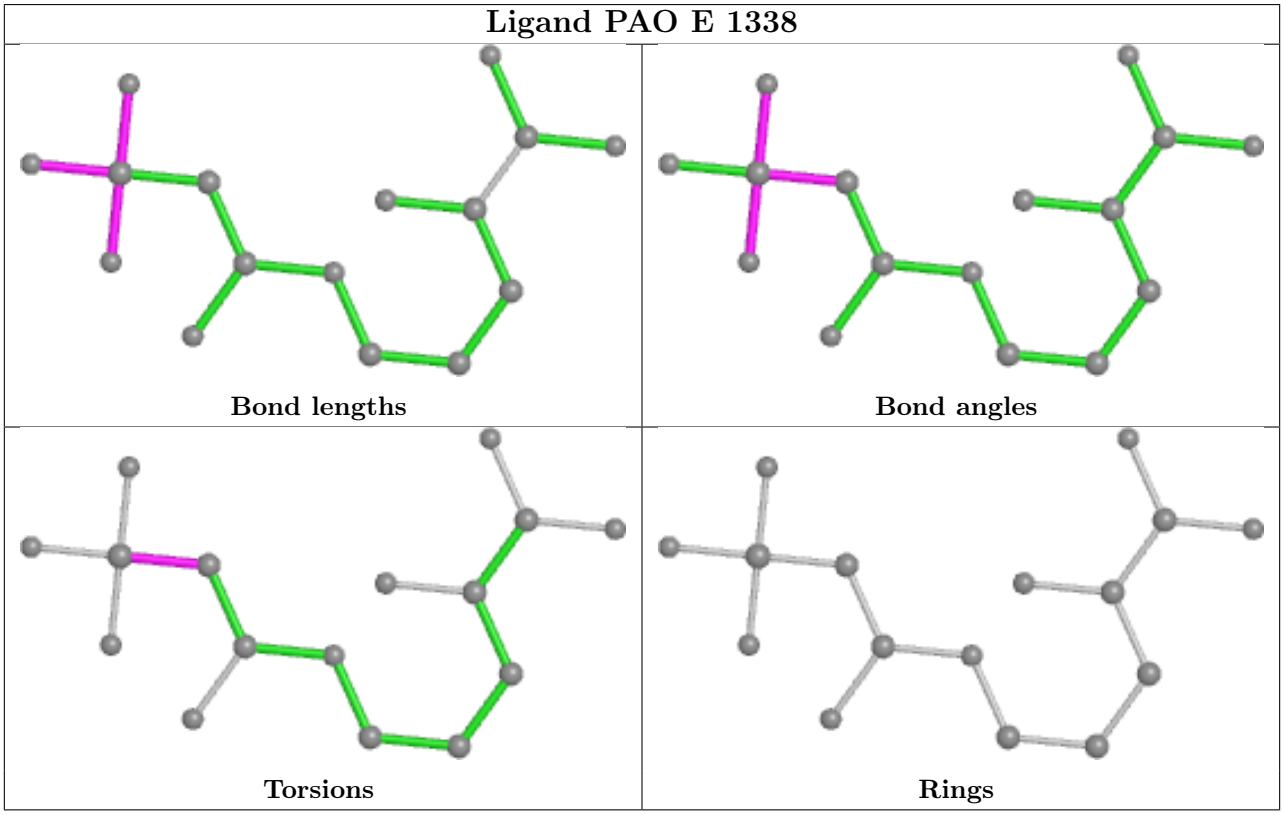
Mol	Chain	Res	Type	Atoms
2	E	1338	PAO	C1-C1P-P-O3P
2	C	1340	PAO	C1-C1P-P-O3P
2	D	1340	PAO	C-CA-CB-CG
2	F	1340	PAO	C-CA-CB-CG
2	F	1340	PAO	N-CA-CB-CG

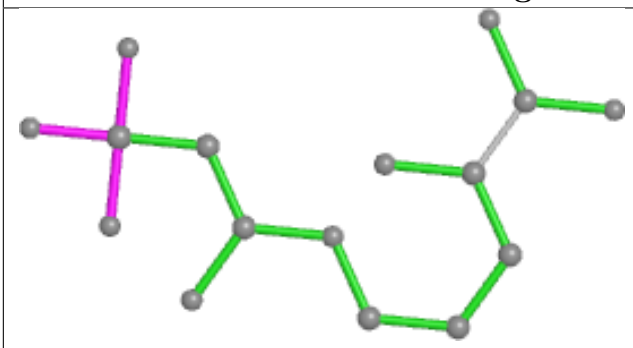
There are no ring outliers.

No monomer is involved in short contacts.

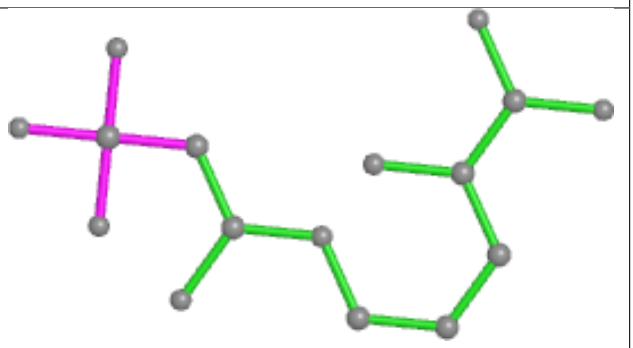
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



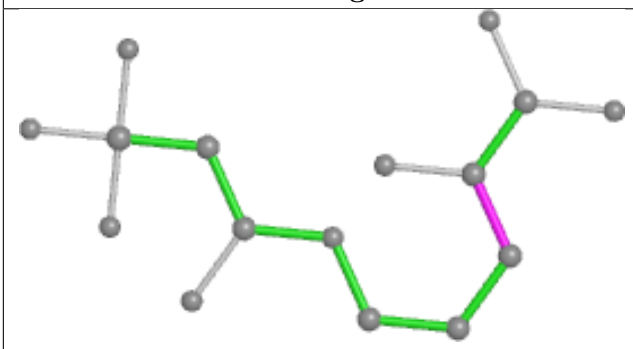
Ligand PAO D 1340



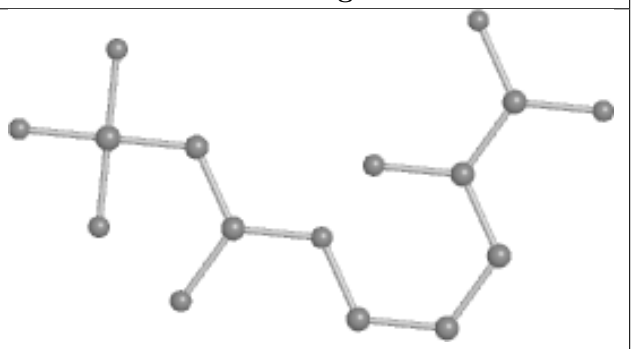
Bond lengths



Bond angles

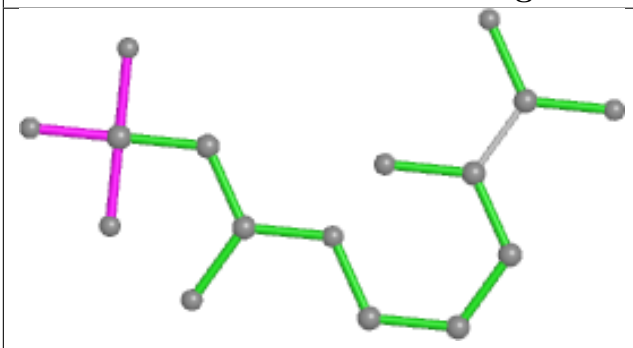


Torsions

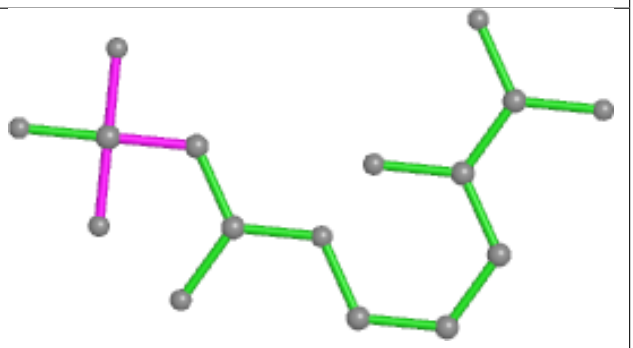


Rings

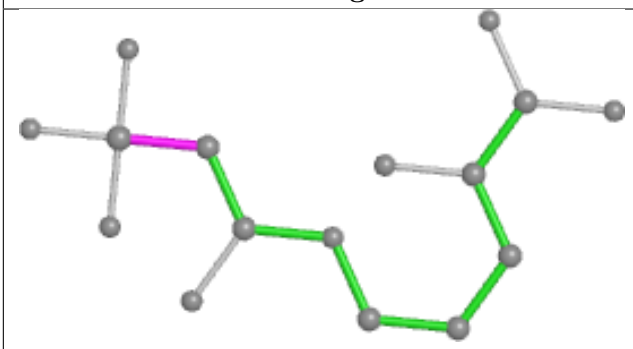
Ligand PAO C 1340



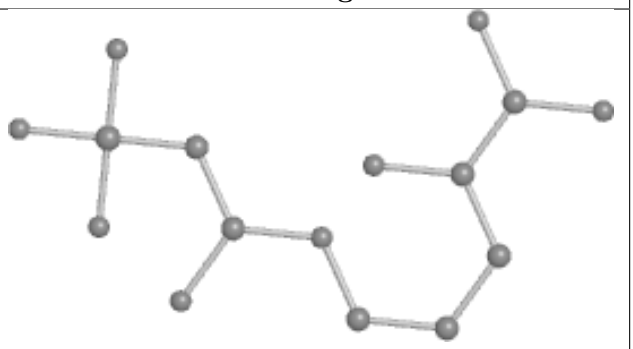
Bond lengths



Bond angles

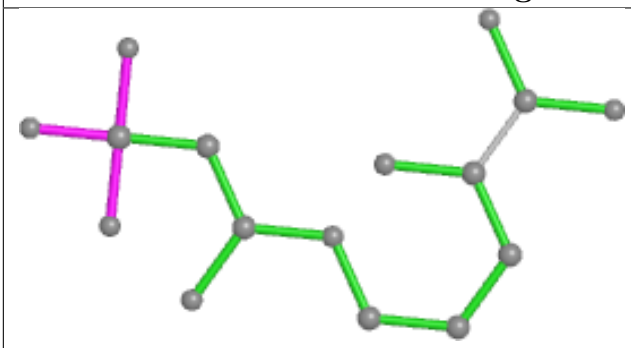


Torsions

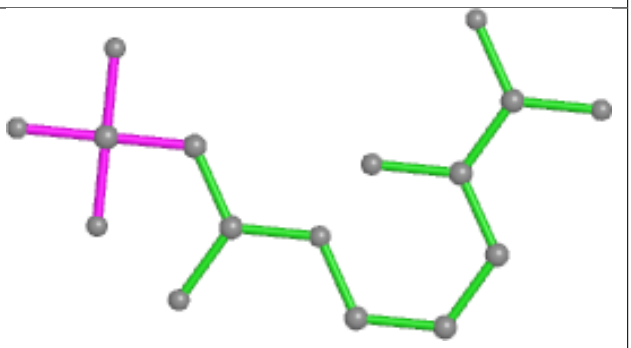


Rings

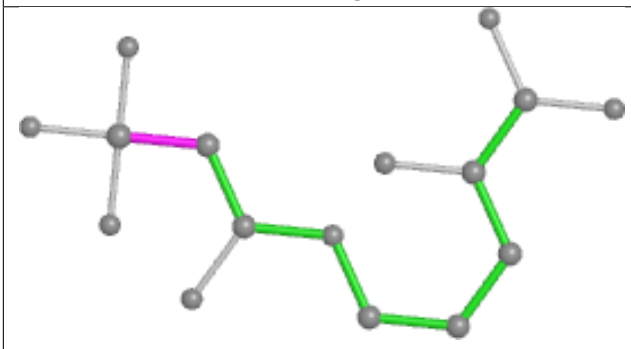
Ligand PAO A 1340



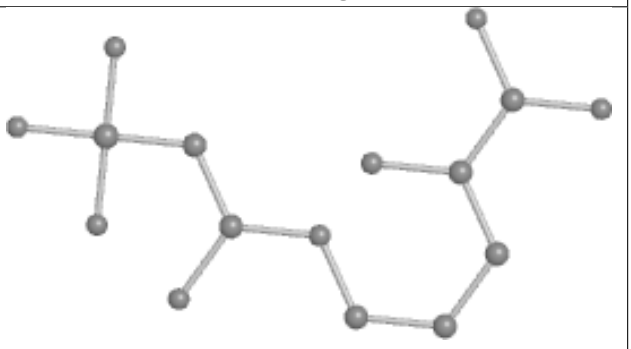
Bond lengths



Bond angles

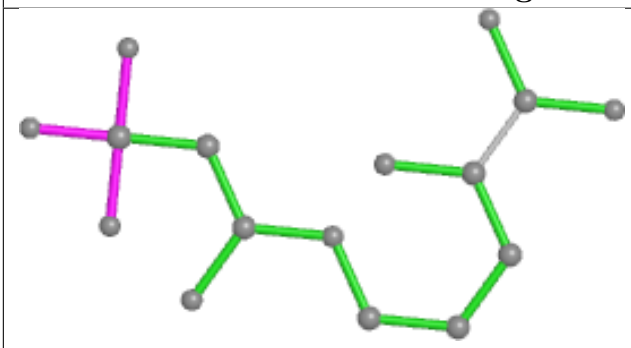


Torsions

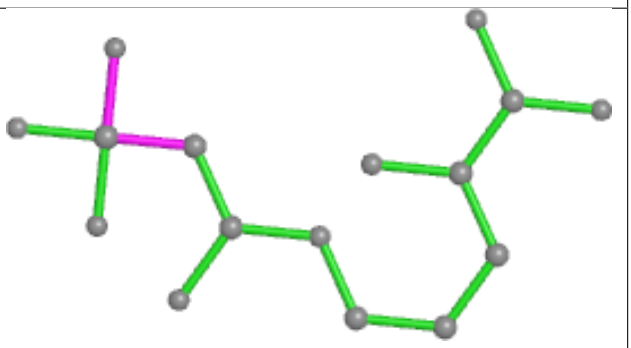


Rings

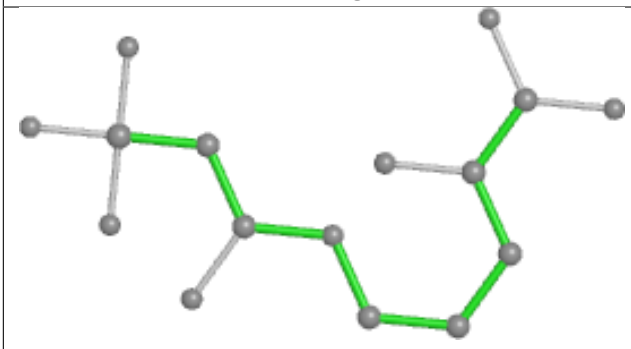
Ligand PAO B 1340



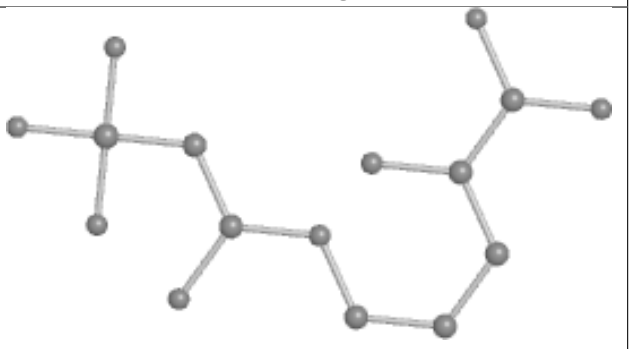
Bond lengths



Bond angles

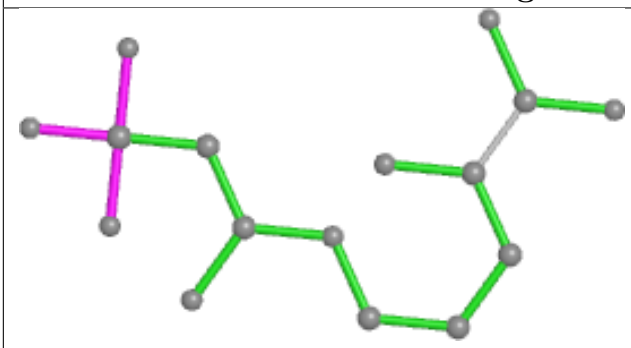


Torsions

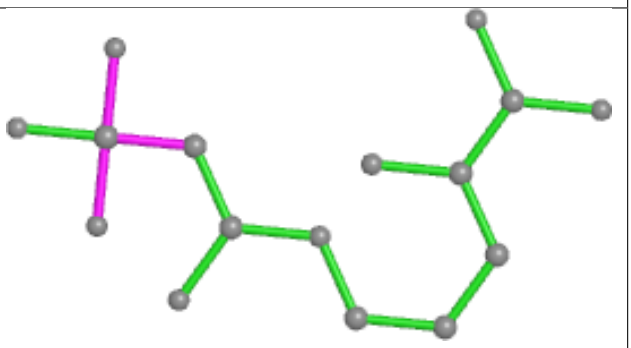


Rings

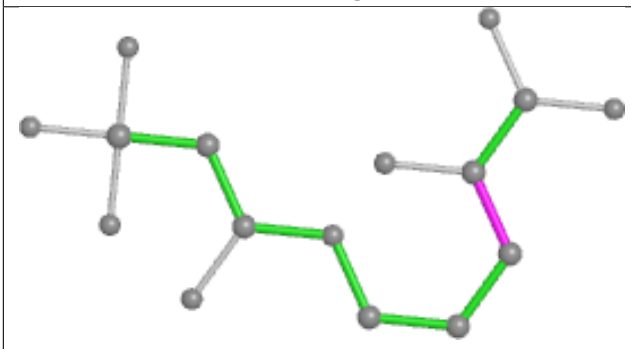
Ligand PAO F 1340



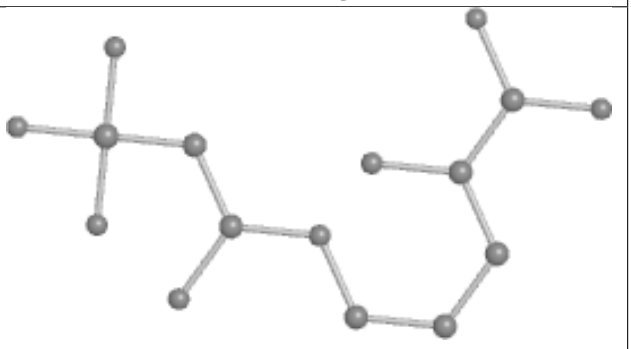
Bond lengths



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, 95^{th} 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	339/355 (95%)	-0.32	3 (0%)	84	83	17, 28, 45, 63	5 (1%)
1	B	338/355 (95%)	-0.29	3 (0%)	84	83	18, 27, 48, 62	4 (1%)
1	C	339/355 (95%)	-0.22	4 (1%)	79	78	17, 29, 49, 93	2 (0%)
1	D	334/355 (94%)	-0.01	18 (5%)	25	24	19, 33, 57, 68	2 (0%)
1	E	333/355 (93%)	0.07	17 (5%)	28	27	19, 38, 61, 72	1 (0%)
1	F	323/355 (90%)	0.02	13 (4%)	38	37	19, 37, 58, 77	1 (0%)
All	All	2006/2130 (94%)	-0.13	58 (2%)	51	50	17, 31, 57, 93	15 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	4.1
1	D	157	VAL	3.2
1	C	81	GLY	3.1
1	F	225	TYR	3.1
1	E	235	ALA	3.0
1	E	75	PRO	3.0
1	D	158	PHE	3.0
1	D	338	SER	3.0
1	E	76	GLY	2.9
1	A	75	PRO	2.8
1	D	225	TYR	2.8
1	E	156	VAL	2.8
1	D	159	VAL	2.7
1	D	235	ALA	2.7
1	D	82	GLY	2.7
1	D	226	THR	2.7
1	E	187	GLY	2.6
1	E	158	PHE	2.6
1	F	262	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	1	MET	2.6
1	E	238	SER	2.6
1	D	339	ILE	2.6
1	C	158	PHE	2.6
1	E	148	GLY	2.5
1	F	247	TYR	2.5
1	F	230	TYR	2.5
1	D	83	HIS	2.4
1	D	238	SER	2.4
1	F	187	GLY	2.4
1	F	240	GLU	2.4
1	E	83	HIS	2.4
1	D	76	GLY	2.4
1	B	226	THR	2.4
1	E	262	ALA	2.4
1	E	192	GLU	2.3
1	E	78	ILE	2.3
1	B	158	PHE	2.3
1	F	158	PHE	2.3
1	E	245	VAL	2.2
1	C	338	SER	2.2
1	E	204	VAL	2.2
1	D	169	LEU	2.2
1	A	204	VAL	2.2
1	F	263	ASN	2.2
1	D	70	GLY	2.2
1	D	156	VAL	2.2
1	E	159	VAL	2.1
1	F	159	VAL	2.1
1	C	339	ILE	2.1
1	E	169	LEU	2.1
1	F	192	GLU	2.1
1	D	1	MET	2.0
1	F	248	PRO	2.0
1	D	165	VAL	2.0
1	B	225	TYR	2.0
1	E	225	TYR	2.0
1	F	238	SER	2.0
1	D	232	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

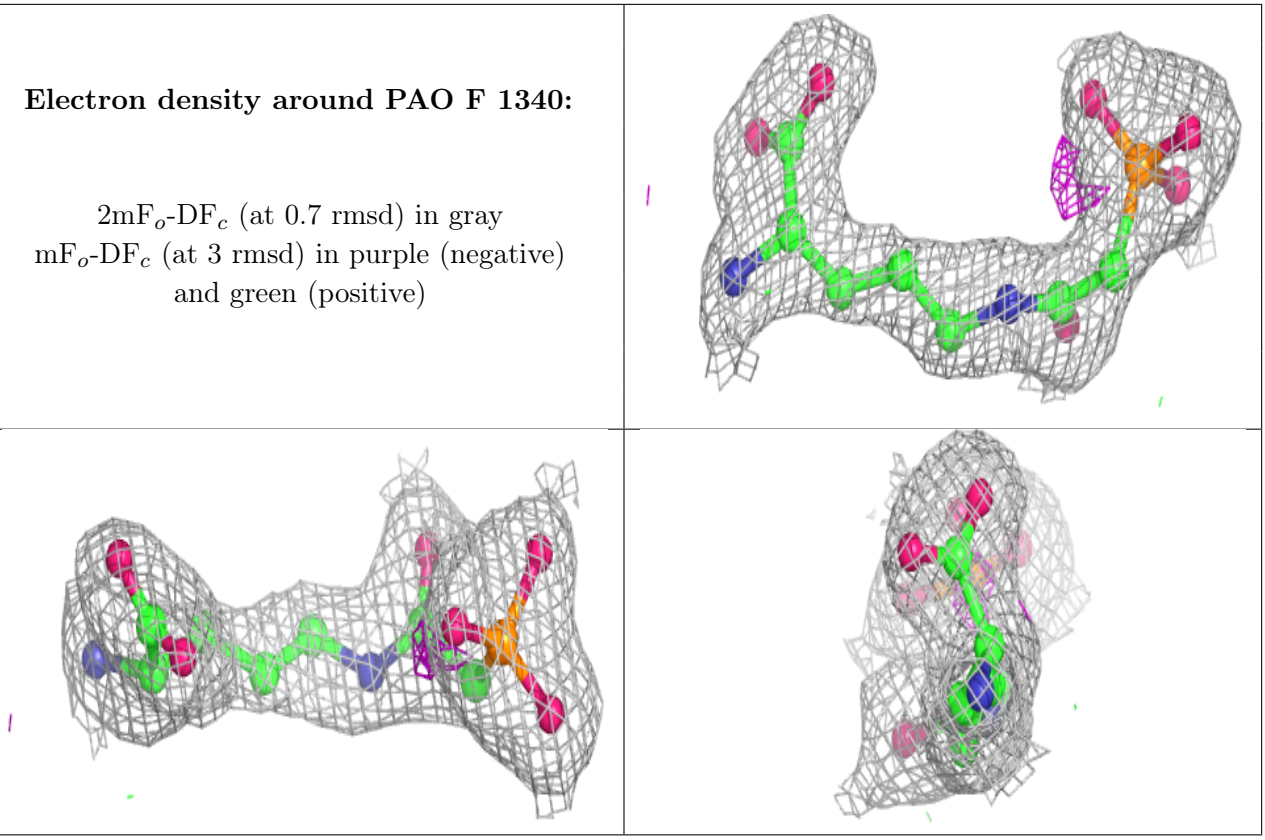
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	TRS	C	1341	8/8	0.86	0.13	39,40,40,40	0
4	TRS	B	1341	8/8	0.92	0.11	37,37,37,38	0
2	PAO	F	1340	16/16	0.94	0.10	30,35,36,36	0
2	PAO	D	1340	16/16	0.96	0.10	28,30,35,35	0
2	PAO	B	1340	16/16	0.97	0.12	23,26,27,27	0
2	PAO	A	1340	16/16	0.97	0.12	23,26,32,32	0
2	PAO	E	1338	16/16	0.97	0.09	30,33,35,35	0
2	PAO	C	1340	16/16	0.98	0.10	22,27,29,29	0
3	NI	D	1341	1/1	0.98	0.06	35,35,35,35	0
3	NI	A	1341	1/1	1.00	0.04	34,34,34,34	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.

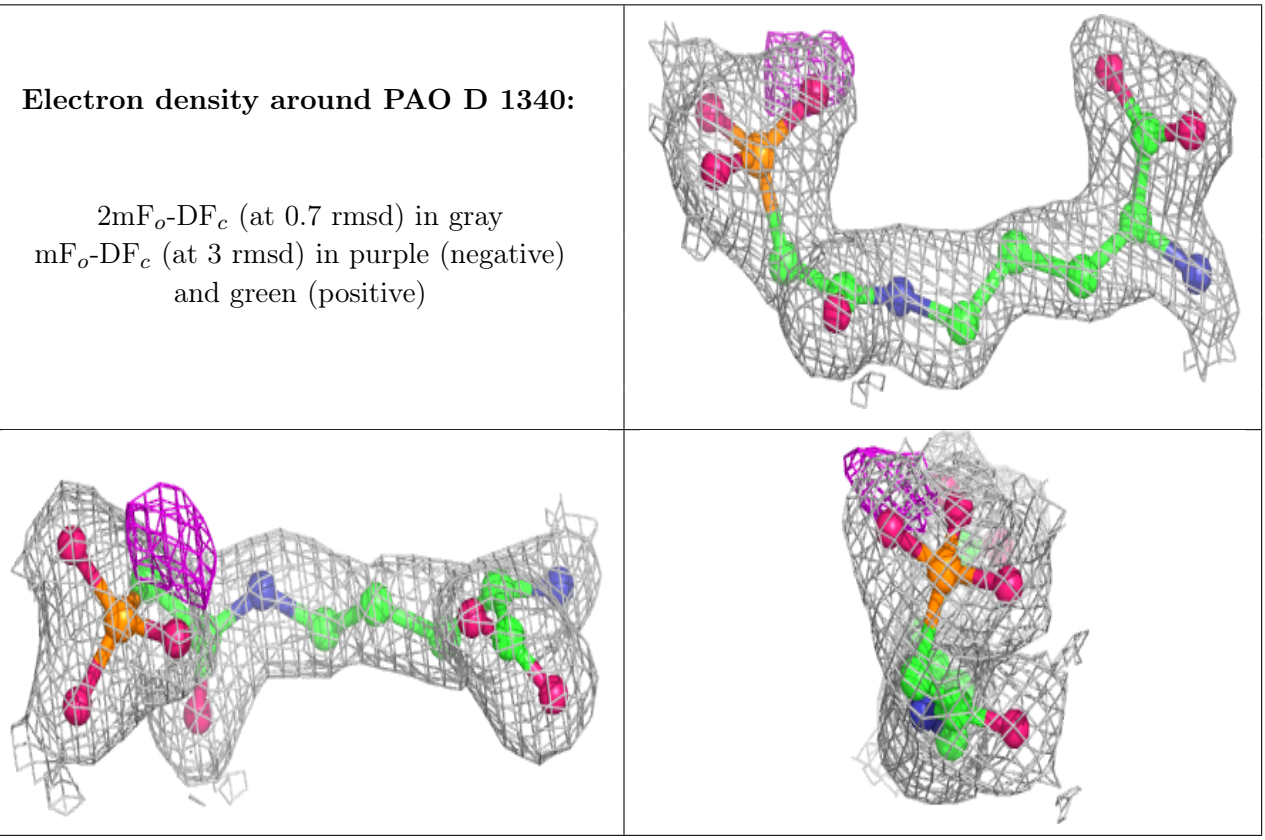
Electron density around PAO F 1340:

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



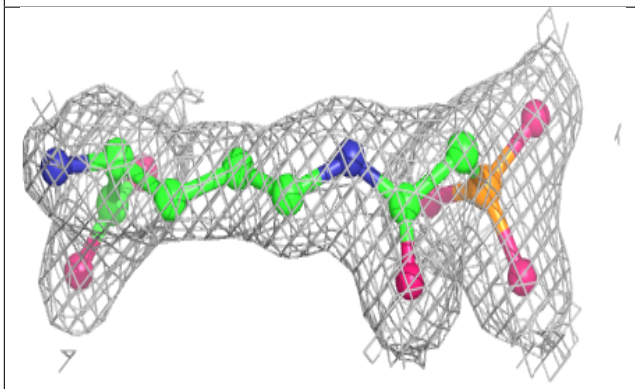
Electron density around PAO D 1340:

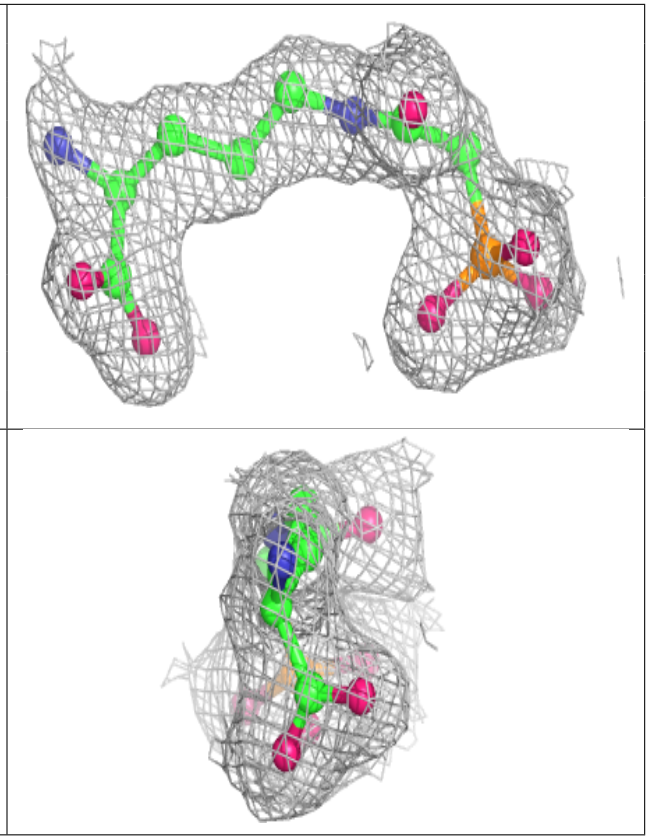
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PAO B 1340:

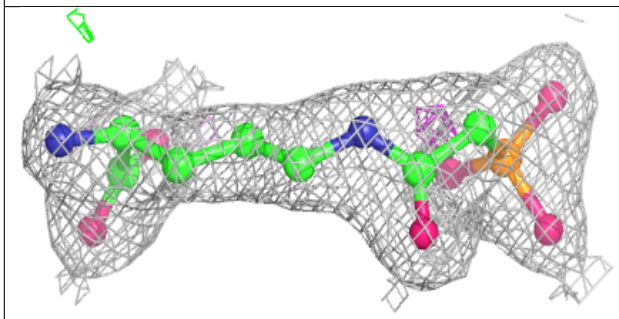
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

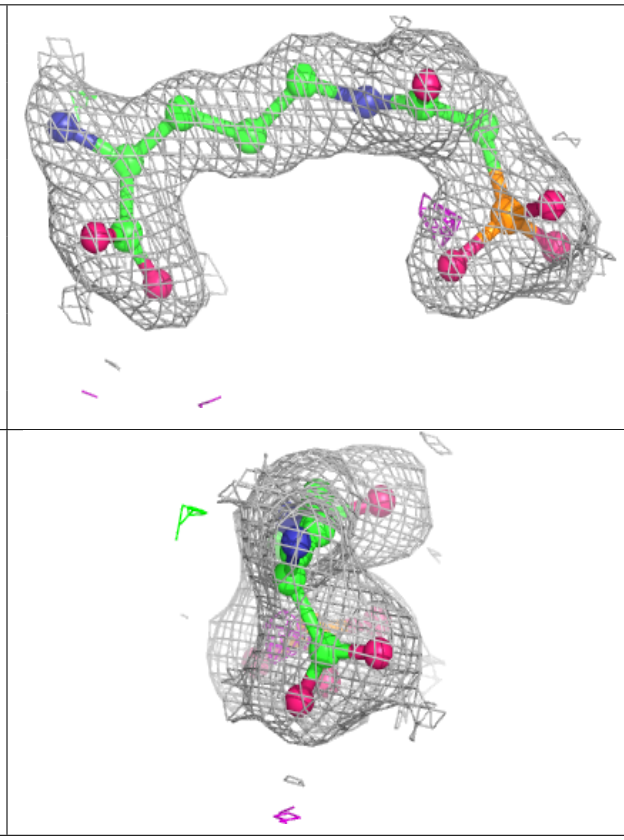




Electron density around PAO A 1340:

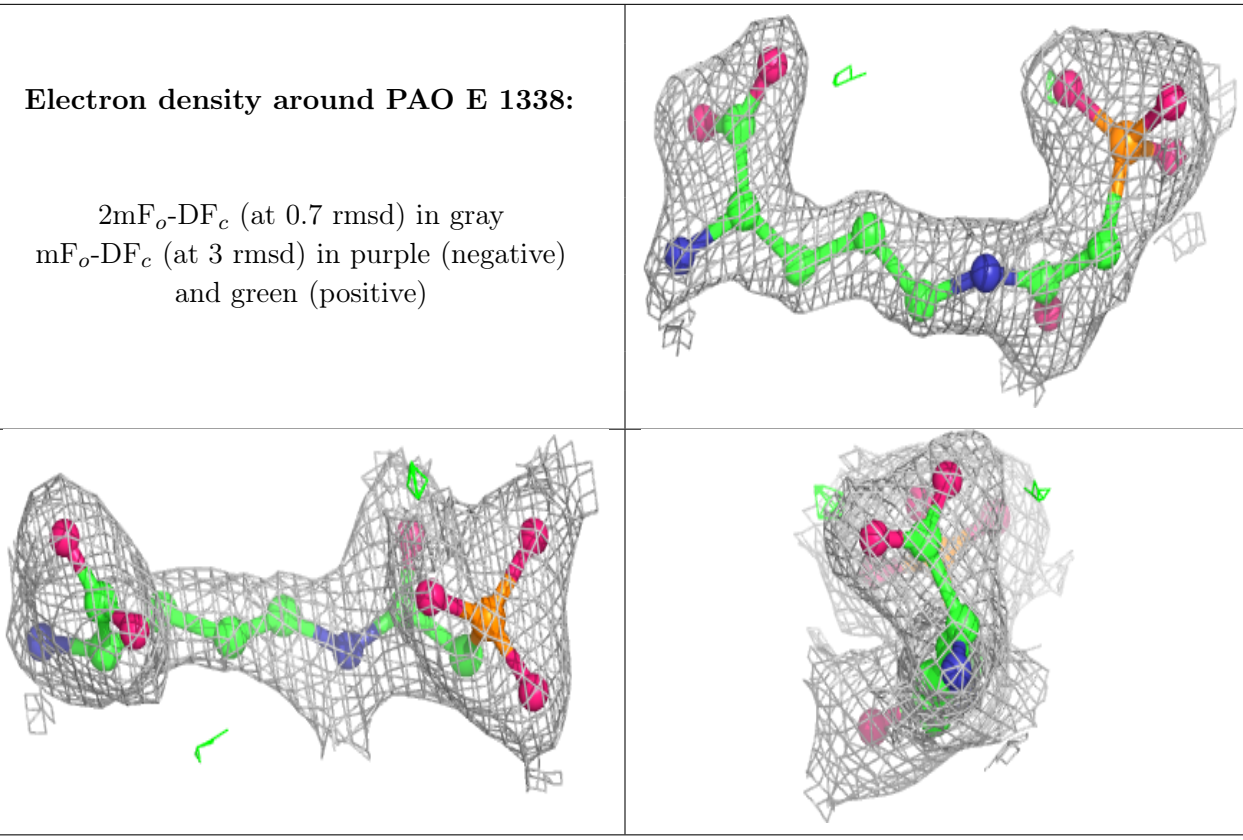
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





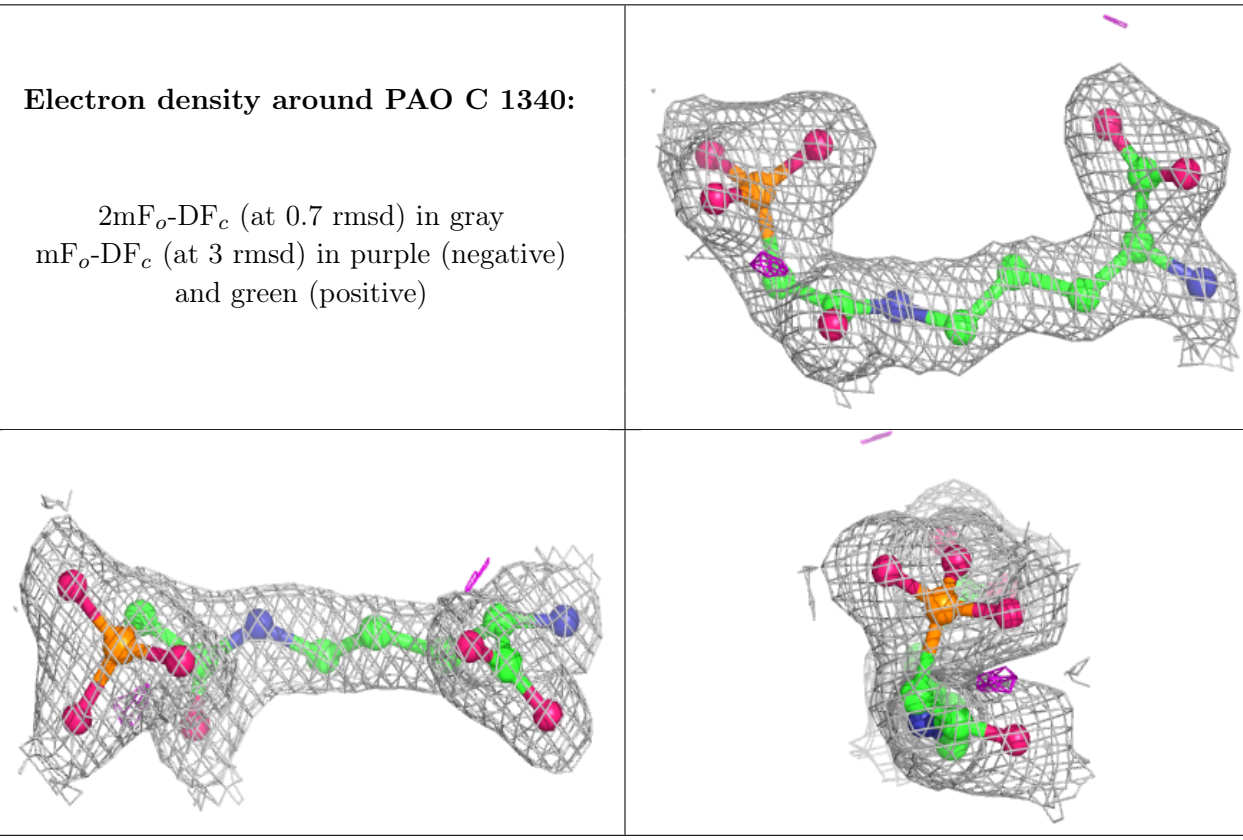
Electron density around PAO E 1338:

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



Electron density around PAO C 1340:

$2mF_o$-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.