



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 02:30 PM JST

PDB ID : 6AK3  
Title : Crystal structure of the human prostaglandin E receptor EP3 bound to prostaglandin E2  
Authors : Morimoto, K.; Suno, R.; Iwata, S.; Kobayashi, T.  
Deposited on : 2018-08-29  
Resolution : 2.90 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

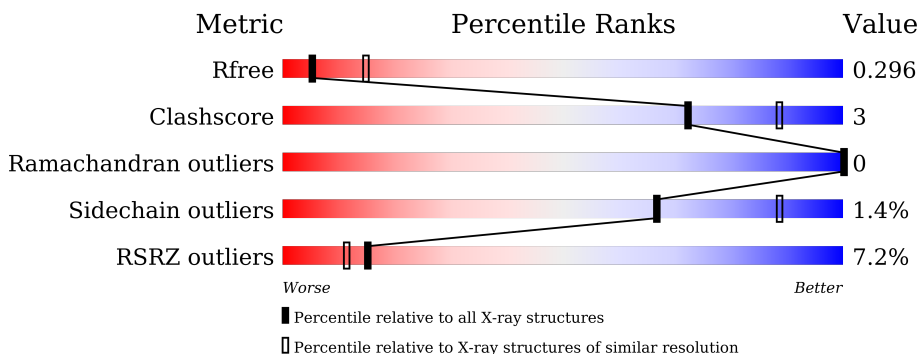
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	418	 4% 61% 5% 30%
1	B	418	 5% 59% 5% 31%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4251 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 Prostaglandin E2 receptor EP3 subtype,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	272	2038	1347	337	337	17	0	0	0
1	A	272	2071	1372	345	337	17	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

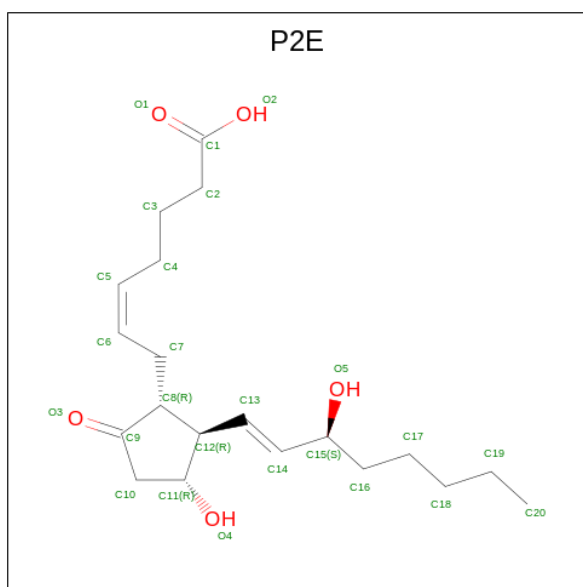
Chain	Residue	Modelled	Actual	Comment	Reference
B	39	GLY	-	expression tag	UNP P43115
B	40	PRO	-	expression tag	UNP P43115
B	41	THR	-	expression tag	UNP P43115
B	42	SER	-	expression tag	UNP P43115
B	173	ILE	ALA	engineered mutation	UNP P43115
B	185	SER	VAL	engineered mutation	UNP P43115
B	217	GLN	ASN	engineered mutation	UNP P43115
B	258	ASP	SER	engineered mutation	UNP P43115
B	289	LEU	CYS	engineered mutation	UNP P43115
B	308	GLN	ASN	engineered mutation	UNP P43115
B	360	LEU	-	linker	UNP P43115
B	361	GLU	-	linker	UNP P43115
B	362	LEU	-	linker	UNP P43115
B	363	GLU	-	linker	UNP P43115
B	364	VAL	-	linker	UNP P43115
B	365	LEU	-	linker	UNP P43115
B	366	PHE	-	linker	UNP P43115
B	367	GLN	-	linker	UNP P43115
B	1007	TRP	MET	engineered mutation	UNP P0ABE7
B	1041	GLY	-	linker	UNP P0ABE7
B	1042	SER	-	linker	UNP P0ABE7
B	1043	GLY	-	linker	UNP P0ABE7
B	1044	SER	-	linker	UNP P0ABE7
B	1045	GLY	-	linker	UNP P0ABE7

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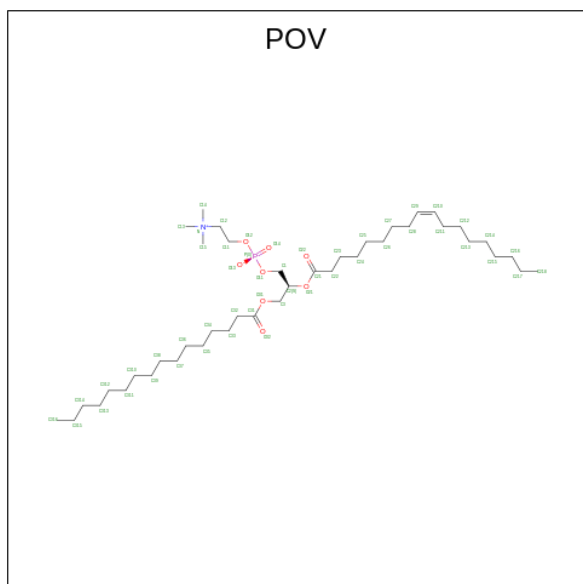
Chain	Residue	Modelled	Actual	Comment	Reference
B	1098	ILE	ARG	engineered mutation	UNP P0ABE7
B	1102	ILE	HIS	engineered mutation	UNP P0ABE7
B	1106	GLY	-	expression tag	UNP P0ABE7
A	39	GLY	-	expression tag	UNP P43115
A	40	PRO	-	expression tag	UNP P43115
A	41	THR	-	expression tag	UNP P43115
A	42	SER	-	expression tag	UNP P43115
A	173	ILE	ALA	engineered mutation	UNP P43115
A	185	SER	VAL	engineered mutation	UNP P43115
A	217	GLN	ASN	engineered mutation	UNP P43115
A	258	ASP	SER	engineered mutation	UNP P43115
A	289	LEU	CYS	engineered mutation	UNP P43115
A	308	GLN	ASN	engineered mutation	UNP P43115
A	360	LEU	-	linker	UNP P43115
A	361	GLU	-	linker	UNP P43115
A	362	LEU	-	linker	UNP P43115
A	363	GLU	-	linker	UNP P43115
A	364	VAL	-	linker	UNP P43115
A	365	LEU	-	linker	UNP P43115
A	366	PHE	-	linker	UNP P43115
A	367	GLN	-	linker	UNP P43115
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1041	GLY	-	linker	UNP P0ABE7
A	1042	SER	-	linker	UNP P0ABE7
A	1043	GLY	-	linker	UNP P0ABE7
A	1044	SER	-	linker	UNP P0ABE7
A	1045	GLY	-	linker	UNP P0ABE7
A	1098	ILE	ARG	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	GLY	-	expression tag	UNP P0ABE7

- Molecule 2 is (Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(E,3S)-3-hydroxyoct-1-enyl]-5-oxo-cyclopentyl]hept-5-enoic acid (three-letter code: P2E) (formula: C<sub>20</sub>H<sub>32</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			25	20	5		
2	A	1	Total	C	O	0	0
			25	20	5		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C<sub>42</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			46	37	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	46	37	8	1	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.09Å 42.28Å 161.30Å 90.00° 96.09° 90.00°	Depositor
Resolution (Å)	48.38 – 2.90 48.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.38-2.90) 99.9 (48.38-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, $R_{free}$	0.251 , 0.295 0.251 , 0.296	Depositor DCC
$R_{free}$ test set	967 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.759	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 80.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: POV, P2E

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	0.23	0/2110	0.36	0/2854
1	B	0.23	0/2077	0.37	0/2810
All	All	0.23	0/4187	0.37	0/5664

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	2071	0	2162	11	0
1	B	2038	0	2105	14	0
2	A	25	0	31	2	0
2	B	25	0	31	1	0
3	A	46	0	69	3	0
3	B	46	0	69	1	0
All	All	4251	0	4467	30	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 (30) 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)
3:A:1202:POV:H21C	3:A:1202:POV:H31C	1.72	0.70
1:A:260:CYS:HB2	1:A:277:THR:HG21	1.74	0.69
1:B:59:LEU:HB2	1:B:107:THR:HG21	1.83	0.60
1:A:59:LEU:HB2	1:A:107:THR:HG21	1.83	0.60
1:A:78:ARG:HD2	1:A:90:LEU:HD21	1.83	0.60
1:B:263:LYS:NZ	1:B:1106:GLY:O	2.35	0.58
1:B:260:CYS:HB2	1:B:277:THR:HG21	1.90	0.54
1:A:50:VAL:HG22	1:A:204:PRO:HG3	1.94	0.49
1:B:290:VAL:HG21	1:B:345:VAL:HG11	1.95	0.48
1:B:271:ALA:N	1:B:1104:LYS:O	2.46	0.47
1:B:53:ALA:HB2	3:B:1202:POV:H3A	1.96	0.47
1:A:283:GLN:NE2	1:A:345:VAL:O	2.39	0.47
1:A:262:ALA:O	1:A:1001:ALA:N	2.48	0.47
1:A:290:VAL:HG21	1:A:345:VAL:HG11	1.98	0.46
3:A:1202:POV:H24A	3:A:1202:POV:H36A	1.99	0.46
2:B:1201:P2E:H12	2:B:1201:P2E:H6	1.72	0.44
1:B:78:ARG:HD2	1:B:90:LEU:HD21	1.99	0.44
2:A:1201:P2E:H4	2:A:1201:P2E:H7	1.63	0.44
1:A:78:ARG:HG3	1:A:90:LEU:HD11	1.98	0.43
1:B:49:SER:O	1:B:333:ARG:NH2	2.46	0.43
2:A:1201:P2E:H6	2:A:1201:P2E:H12	1.80	0.43
1:A:150:ALA:O	1:A:154:GLU:HG2	2.19	0.42
1:A:53:ALA:HB2	3:A:1202:POV:H3A	2.02	0.42
1:A:86:LYS:HA	1:A:86:LYS:HD3	1.89	0.42
1:B:262:ALA:O	1:B:1001:ALA:N	2.53	0.41
1:B:150:ALA:O	1:B:154:GLU:HG2	2.20	0.41
1:B:78:ARG:HG3	1:B:90:LEU:HD11	2.02	0.41
1:B:50:VAL:HG22	1:B:204:PRO:HG3	2.03	0.40
1:B:90:LEU:HD23	1:B:90:LEU:HA	1.97	0.40
1:B:117:LYS:O	1:B:119:ARG:N	2.55	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	253/418 (60%)	253 (100%)	0	0	100	100
1	B	257/418 (62%)	256 (100%)	1 (0%)	0	100	100
All	All	510/836 (61%)	509 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

### 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	218/345 (63%)	215 (99%)	3 (1%)	67	89
1	B	213/345 (62%)	210 (99%)	3 (1%)	67	89
All	All	431/690 (62%)	425 (99%)	6 (1%)	67	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78	ARG
1	B	128	ARG
1	B	263	LYS
1	A	78	ARG
1	A	128	ARG
1	A	263	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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
2	P2E	A	1201	-	25,25,25	4.01	8 (32%)	26,31,31	0.95	1 (3%)
3	POV	A	1202	-	45,45,51	1.16	7 (15%)	49,50,59	1.29	3 (6%)
2	P2E	B	1201	-	25,25,25	4.02	8 (32%)	26,31,31	0.98	1 (3%)
3	POV	B	1202	-	45,45,51	1.16	7 (15%)	49,50,59	1.30	3 (6%)

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	P2E	A	1201	-	-	7/19/35/35	0/1/1/1
3	POV	A	1202	-	-	23/47/47/55	-
2	P2E	B	1201	-	-	9/19/35/35	0/1/1/1
3	POV	B	1202	-	-	19/47/47/55	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	P2E	C10-C11	-14.28	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	P2E	C10-C11	-14.27	1.35	1.52
2	A	1201	P2E	C8-C9	-8.62	1.37	1.52
2	B	1201	P2E	C8-C9	-8.62	1.37	1.52
2	B	1201	P2E	C10-C9	6.42	1.60	1.51
2	A	1201	P2E	C10-C9	6.39	1.60	1.51
2	B	1201	P2E	C12-C11	5.37	1.67	1.55
2	A	1201	P2E	C12-C11	5.30	1.66	1.55
2	A	1201	P2E	C7-C8	4.14	1.60	1.54
2	B	1201	P2E	C7-C8	4.13	1.60	1.54
3	A	1202	POV	C29-C210	3.72	1.53	1.31
3	B	1202	POV	C29-C210	3.71	1.53	1.31
2	A	1201	P2E	O5-C15	-2.79	1.38	1.43
2	B	1201	P2E	O5-C15	-2.74	1.38	1.43
3	A	1202	POV	P-O12	2.68	1.65	1.54
3	B	1202	POV	P-O12	2.68	1.65	1.54
3	B	1202	POV	O31-C31	2.39	1.40	1.33
3	A	1202	POV	O31-C31	2.37	1.40	1.33
3	B	1202	POV	O21-C21	2.36	1.41	1.34
3	A	1202	POV	O21-C2	-2.34	1.40	1.46
3	A	1202	POV	O21-C21	2.33	1.40	1.34
3	B	1202	POV	O21-C2	-2.31	1.40	1.46
3	A	1202	POV	O31-C3	-2.14	1.40	1.45
3	B	1202	POV	P-O13	-2.13	1.46	1.54
3	B	1202	POV	O31-C3	-2.12	1.40	1.45
3	A	1202	POV	P-O13	-2.12	1.46	1.54
2	A	1201	P2E	C14-C13	2.08	1.38	1.32
2	B	1201	P2E	O3-C9	-2.08	1.18	1.21
2	B	1201	P2E	C14-C13	2.06	1.38	1.32
2	A	1201	P2E	O3-C9	-2.02	1.18	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	POV	O21-C21-C22	4.55	121.30	111.50
3	B	1202	POV	O21-C21-C22	4.53	121.26	111.50
3	B	1202	POV	O31-C31-C32	2.61	120.10	111.91
3	A	1202	POV	O31-C31-C32	2.48	119.70	111.91
3	A	1202	POV	O13-P-O14	-2.47	101.01	110.68
3	B	1202	POV	O13-P-O14	-2.42	101.19	110.68
2	B	1201	P2E	C15-C14-C13	-2.02	119.84	125.09
2	A	1201	P2E	C7-C6-C5	-2.01	118.94	126.40

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1202	POV	O22-C21-O21-C2
3	A	1202	POV	O22-C21-O21-C2
3	B	1202	POV	O32-C31-O31-C3
3	B	1202	POV	C32-C31-O31-C3
3	A	1202	POV	O32-C31-O31-C3
3	A	1202	POV	C32-C31-O31-C3
3	B	1202	POV	C22-C21-O21-C2
3	A	1202	POV	C22-C21-O21-C2
3	A	1202	POV	C311-C310-C39-C38
3	A	1202	POV	C311-C312-C313-C314
3	B	1202	POV	C26-C27-C28-C29
3	B	1202	POV	C23-C24-C25-C26
2	A	1201	P2E	C16-C17-C18-C19
3	B	1202	POV	C211-C212-C213-C214
3	A	1202	POV	C39-C310-C311-C312
3	A	1202	POV	C34-C35-C36-C37
3	B	1202	POV	C33-C34-C35-C36
3	A	1202	POV	C33-C34-C35-C36
3	A	1202	POV	C211-C210-C29-C28
3	B	1202	POV	C211-C210-C29-C28
3	B	1202	POV	C213-C214-C215-C216
3	B	1202	POV	C37-C38-C39-C310
2	B	1201	P2E	C8-C12-C13-C14
3	B	1202	POV	C212-C213-C214-C215
3	A	1202	POV	C21-C22-C23-C24
2	B	1201	P2E	C16-C17-C18-C19
3	A	1202	POV	C214-C215-C216-C217
3	A	1202	POV	C212-C213-C214-C215
2	A	1201	P2E	C1-C2-C3-C4
2	B	1201	P2E	C6-C7-C8-C12
2	B	1201	P2E	C1-C2-C3-C4
2	A	1201	P2E	C14-C15-C16-C17
3	B	1202	POV	C311-C310-C39-C38
3	B	1202	POV	O11-C1-C2-O21
3	A	1202	POV	O11-C1-C2-O21
2	A	1201	P2E	C17-C18-C19-C20
3	B	1202	POV	O11-C1-C2-C3
3	A	1202	POV	O11-C1-C2-C3
3	A	1202	POV	C29-C210-C211-C212
3	A	1202	POV	C27-C28-C29-C210

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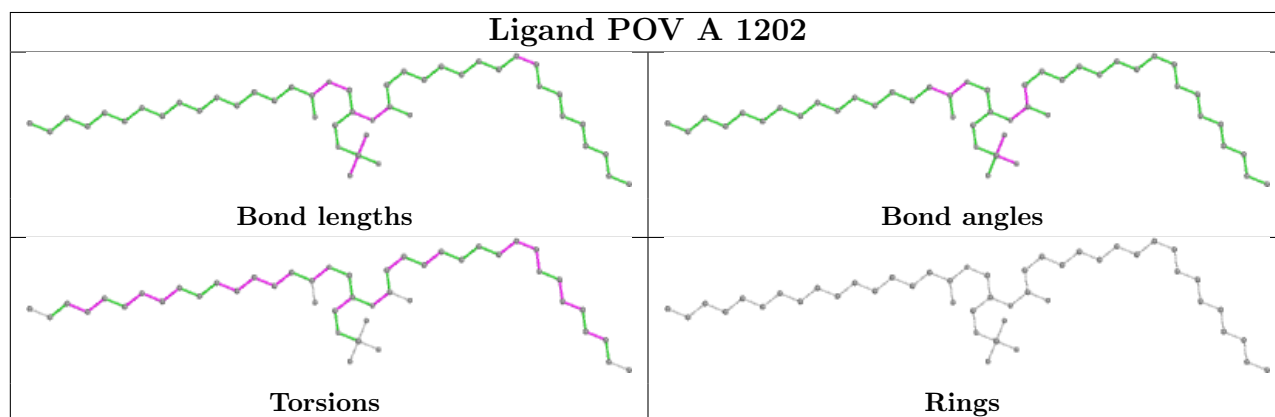
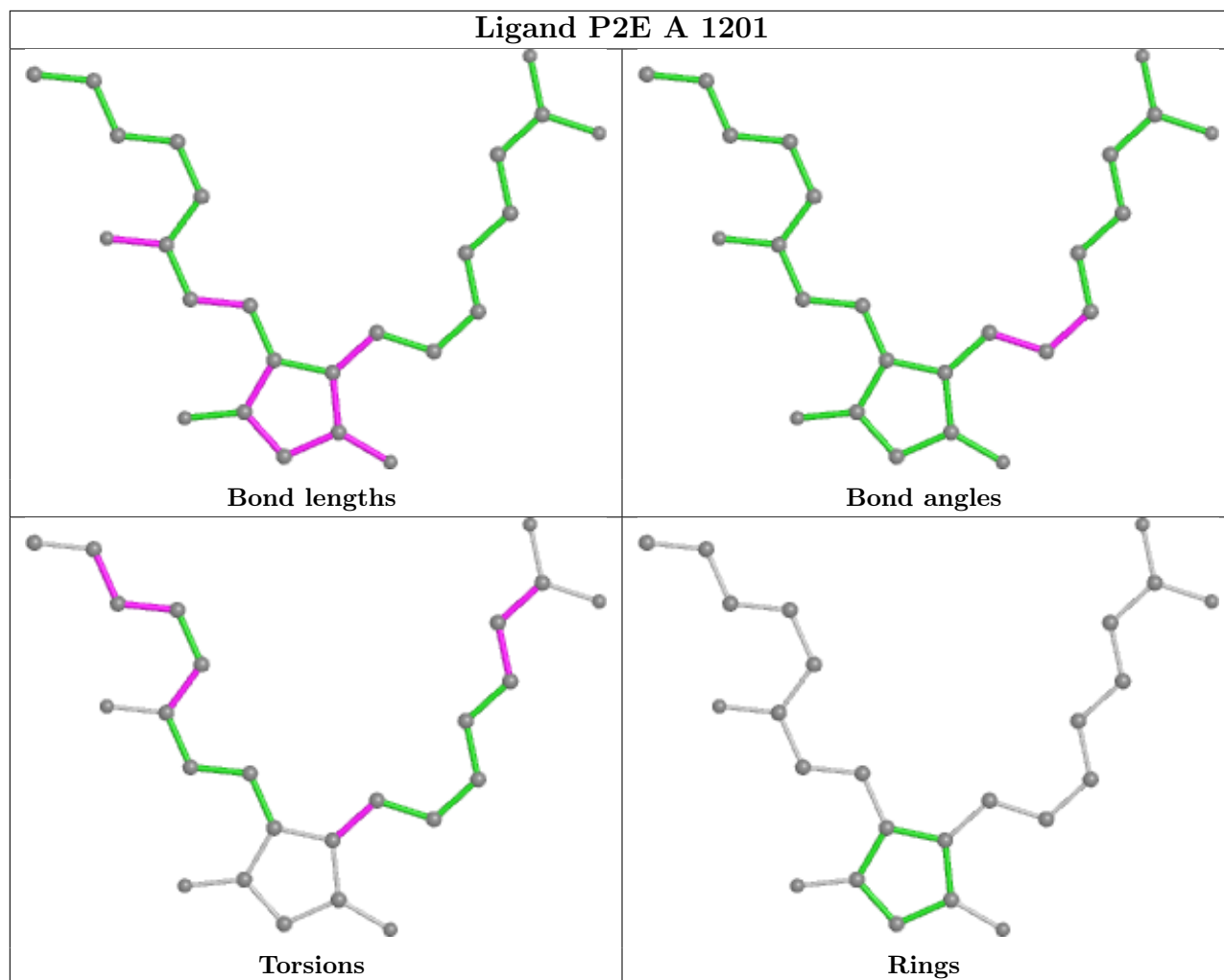
Mol	Chain	Res	Type	Atoms
3	B	1202	POV	C24-C25-C26-C27
3	A	1202	POV	C32-C33-C34-C35
2	B	1201	P2E	O1-C1-C2-C3
2	A	1201	P2E	O1-C1-C2-C3
3	A	1202	POV	C23-C24-C25-C26
3	B	1202	POV	C312-C313-C314-C315
3	A	1202	POV	C312-C313-C314-C315
3	B	1202	POV	C34-C35-C36-C37
2	B	1201	P2E	O2-C1-C2-C3
2	A	1201	P2E	O2-C1-C2-C3
3	A	1202	POV	C31-C32-C33-C34
2	B	1201	P2E	C17-C18-C19-C20
2	A	1201	P2E	C6-C7-C8-C12
3	A	1202	POV	C37-C38-C39-C310
2	B	1201	P2E	C14-C15-C16-C17
3	B	1202	POV	C1-C2-C3-O31
2	B	1201	P2E	C11-C12-C13-C14
3	A	1202	POV	C211-C212-C213-C214

There are no ring outliers.

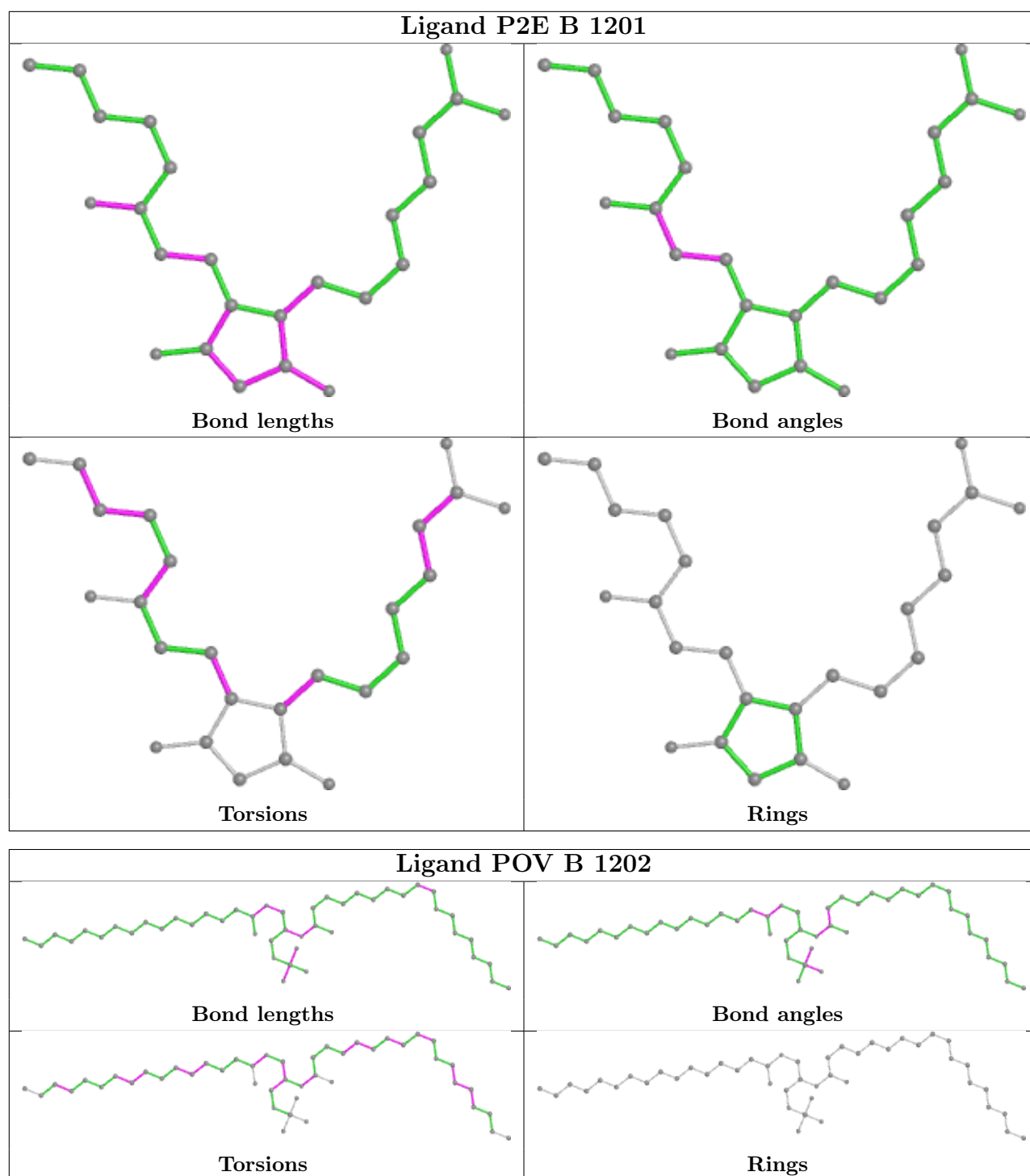
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	P2E	2	0
3	A	1202	POV	3	0
2	B	1201	P2E	1	0
3	B	1202	POV	1	0

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







## 5.7 Other polymers [\(i\)](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	272/418 (65%)	0.17	17 (6%) 20 16	17, 41, 88, 109	0
1	B	272/418 (65%)	0.17	22 (8%) 12 9	18, 42, 94, 108	0
All	All	544/836 (65%)	0.17	39 (7%) 15 11	17, 41, 92, 109	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	CYS	5.0
1	A	1001	ALA	4.9
1	B	164	TRP	4.2
1	B	167	SER	4.2
1	A	166	ALA	4.2
1	A	167	SER	4.2
1	B	166	ALA	4.0
1	B	47	CYS	3.8
1	A	164	TRP	3.8
1	A	196	VAL	3.4
1	A	165	TYR	3.1
1	B	264	ALA	3.1
1	A	273	TRP	3.0
1	B	196	VAL	2.9
1	B	88	PHE	2.9
1	A	1104	LYS	2.9
1	A	88	PHE	2.8
1	B	169	MET	2.7
1	A	213	GLY	2.7
1	B	126	SER	2.7
1	B	121	GLU	2.6
1	A	198	GLN	2.6
1	B	1106	GLY	2.6
1	B	75	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1001	ALA	2.5
1	B	198	GLN	2.4
1	B	212	THR	2.3
1	A	1105	TYR	2.3
1	A	271	ALA	2.3
1	B	159	ILE	2.2
1	B	263	LYS	2.2
1	A	48	GLY	2.1
1	A	121	GLU	2.1
1	B	204	PRO	2.1
1	B	272	GLN	2.1
1	A	263	LYS	2.1
1	B	155	ARG	2.0
1	B	168	HIS	2.0
1	B	77	TYR	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](#)

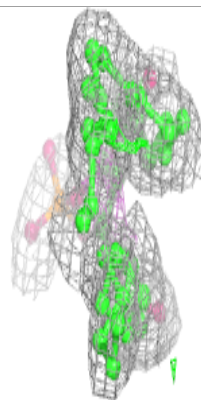
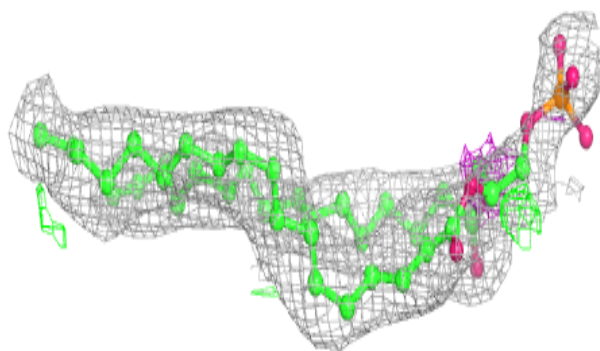
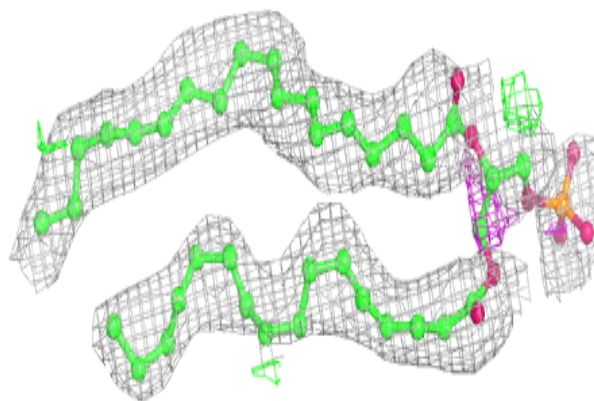
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	POV	A	1202	46/52	0.82	0.29	25,41,123,132	0
3	POV	B	1202	46/52	0.84	0.27	14,49,109,123	0
2	P2E	B	1201	25/25	0.90	0.20	14,28,42,49	0
2	P2E	A	1201	25/25	0.92	0.17	1,20,36,49	0

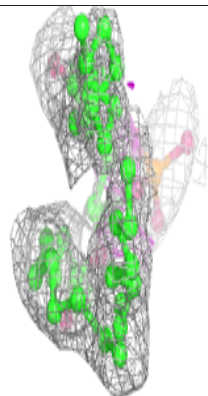
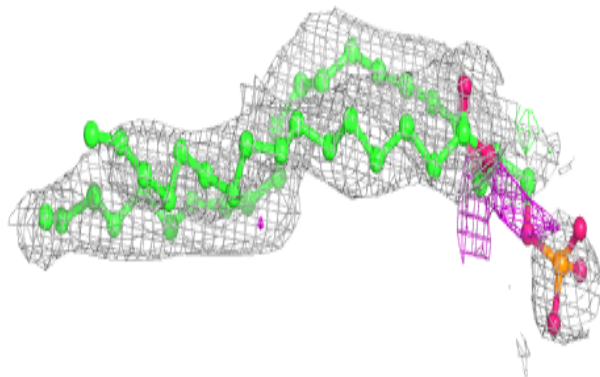
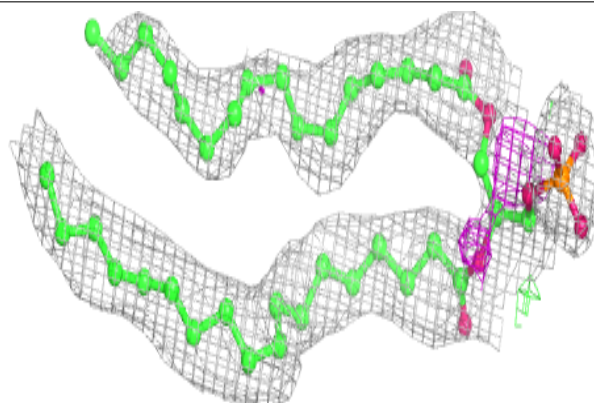
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around POV A 1202:**

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

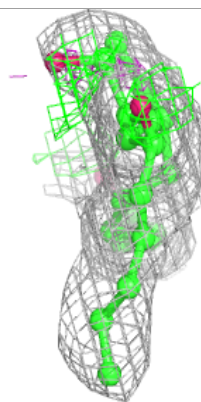
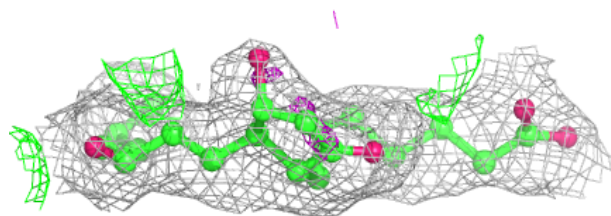
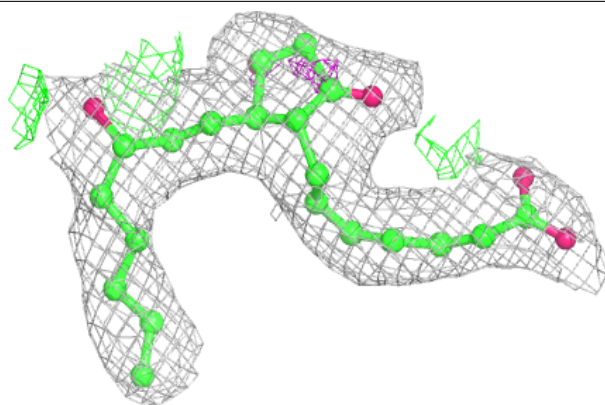
**Electron density around POV B 1202:**

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

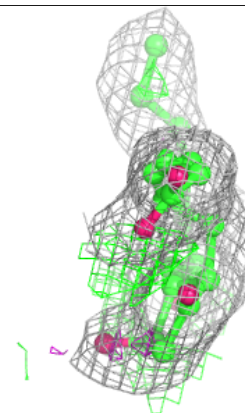
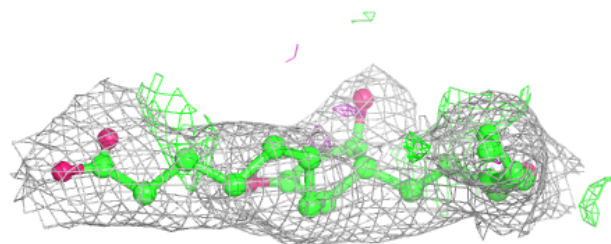
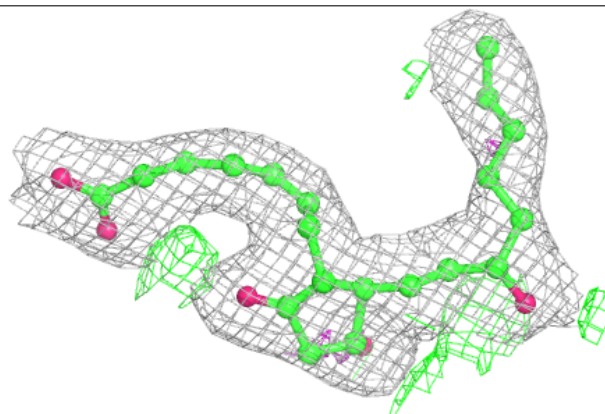


**Electron density around P2E B 1201:**

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

**Electron density around P2E A 1201:**

$2mF_o-DF_c$  (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.