



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:04 AM UTC

PDB ID : 1TJJ / pdb_00001tjj
Title : Human GM2 Activator Protein PAF complex
Authors : Wright, C.S.; Mi, L.-Z.; Rastinejad, F.
Deposited on : 2004-06-04
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

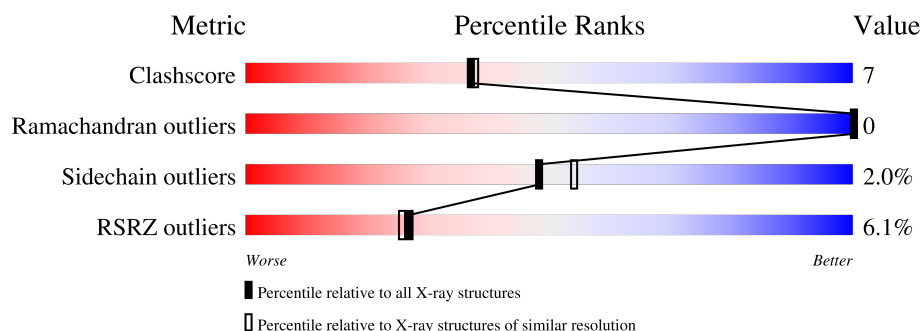
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	164	6% 87% 12% .
1	B	164	7% 83% 16% .
1	C	164	5% 86% 13% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4578 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 Ganglioside GM2 activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1241	797	195	239	10			
1	B	164	Total	C	N	O	S	0	0	0
			1241	797	195	239	10			
1	C	163	Total	C	N	O	S	0	0	0
			1234	793	194	238	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P17900
A	2	MET	-	expression tag	UNP P17900
B	1	HIS	-	expression tag	UNP P17900
B	2	MET	-	expression tag	UNP P17900
C	1	HIS	-	expression tag	UNP P17900
C	2	MET	-	expression tag	UNP P17900

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).

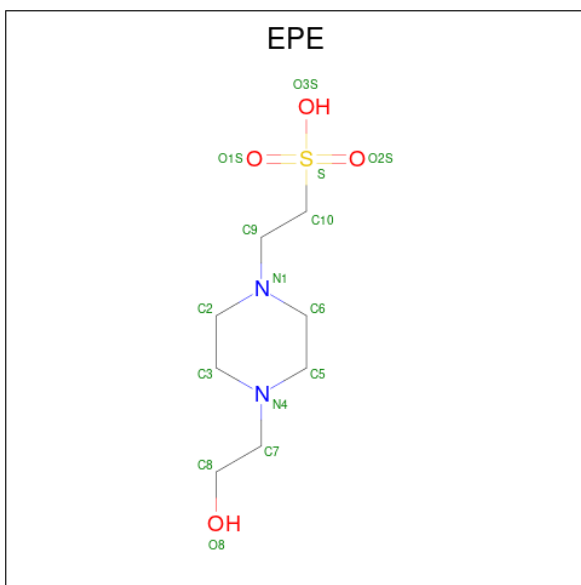


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

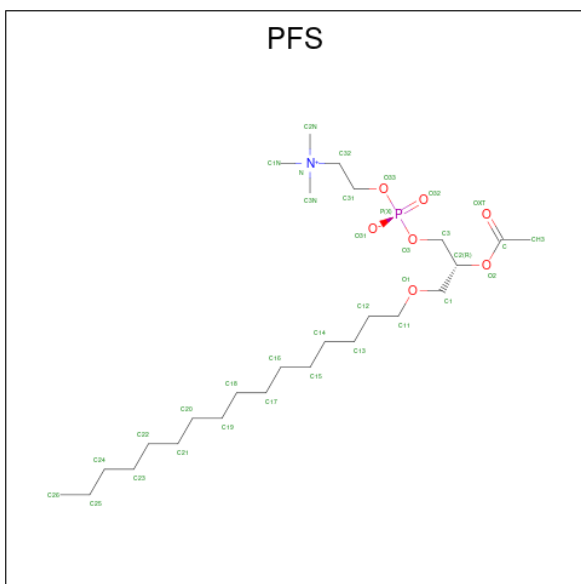
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 15	C 8	N 2	O 4	S 1	0	0
4	C	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 5 is (2R)-2-(acetyloxy)-3-(hexadecyloxy)propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: PFS) (formula: $\text{C}_{26}\text{H}_{54}\text{NO}_7\text{P}$).



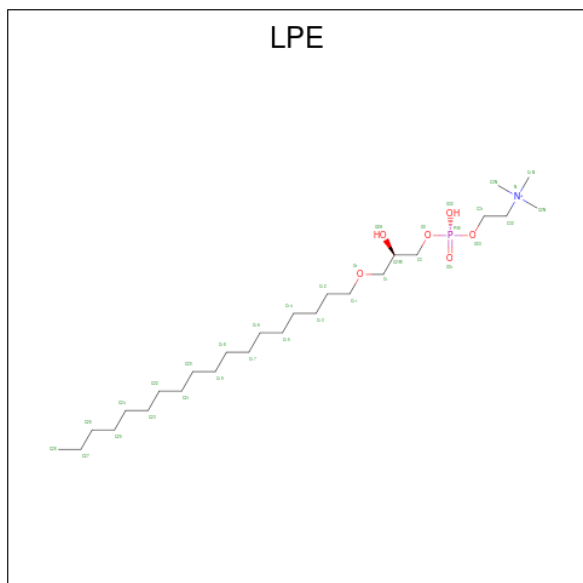
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			35	26	1	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			35	26	1	7	1		
5	C	1	Total	C	N	O	P	0	0
			35	26	1	7	1		

- Molecule 6 is 1-O-OCTADECYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: LPE) (formula: $C_{26}H_{57}NO_6P$).



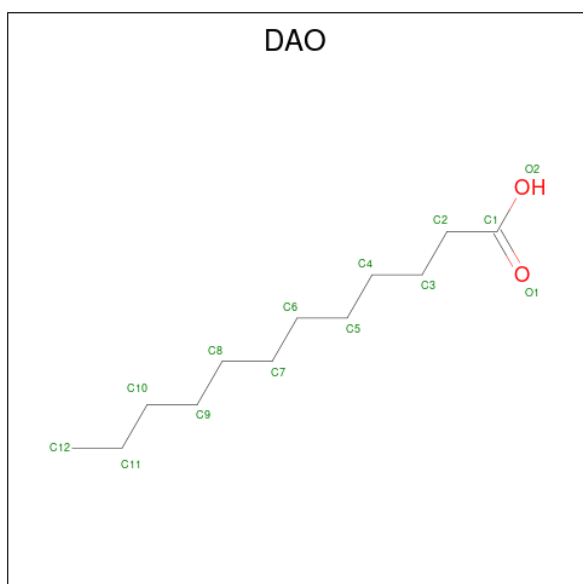
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			34	26	1	6	1		
6	B	1	Total	C	N	O	P	0	0
			34	26	1	6	1		
6	C	1	Total	C	N	O	P	0	0
			34	26	1	6	1		

- Molecule 7 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



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

- Molecule 8 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			14	12	2		

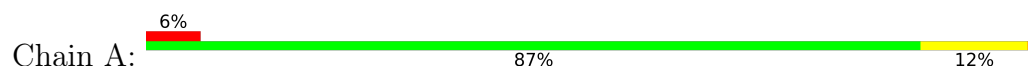
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	185	Total	O	0	0
			185	185		
9	B	205	Total	O	0	0
			205	205		
9	C	178	Total	O	0	0
			178	178		

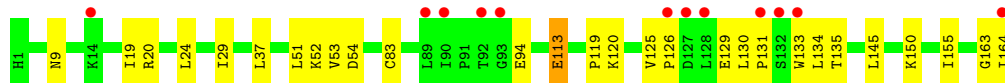
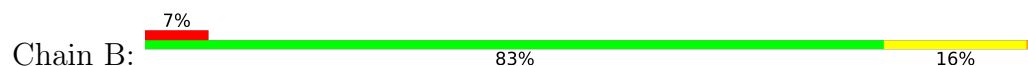
3 Residue-property plots [i](#)

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.

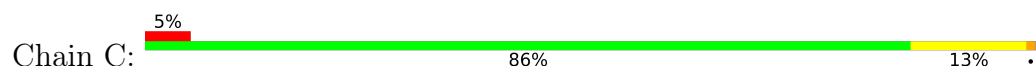
- Molecule 1: Ganglioside GM2 activator



- Molecule 1: Ganglioside GM2 activator



- Molecule 1: Ganglioside GM2 activator



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.47Å 86.51Å 120.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 2.00 19.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.79-2.00) 99.1 (19.79-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.03 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.234 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4578	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EPE, CL, DAO, ACT, PFS, IPA, LPE

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	0.58	0/1273	0.88	1/1739 (0.1%)
1	B	0.57	0/1273	0.96	3/1739 (0.2%)
1	C	0.53	0/1266	0.89	3/1731 (0.2%)
All	All	0.56	0/3812	0.91	7/5209 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	9	ASN	N-CA-C	-6.97	99.23	110.32
1	C	9	ASN	N-CA-C	-6.21	100.38	110.20
1	A	9	ASN	N-CA-C	-6.08	101.48	110.48
1	B	94	GLU	CA-C-N	5.39	125.33	119.78
1	B	94	GLU	C-N-CA	5.39	125.33	119.78
1	C	73	TYR	N-CA-C	5.29	119.03	112.47
1	C	15	ASP	N-CA-C	5.02	116.20	109.83

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	1241	0	1240	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1241	0	1240	18	0
1	C	1234	0	1229	18	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
2	C	4	0	3	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	0	0
4	A	15	0	17	0	0
4	C	15	0	17	2	0
5	A	35	0	54	6	0
5	B	35	0	54	2	0
5	C	35	0	54	1	0
6	A	34	0	56	5	0
6	B	34	0	56	3	0
6	C	34	0	56	1	0
7	A	4	0	8	1	0
7	B	4	0	8	0	0
7	C	12	0	24	0	0
8	B	14	0	23	0	0
9	A	185	0	0	3	0
9	B	205	0	0	2	0
9	C	178	0	0	3	0
All	All	4578	0	4151	58	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 7.

All (58) 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:B:150:LYS:HE3	9:B:3491:HOH:O	1.78	0.84
1:B:131:PRO:HD2	1:B:134:LEU:HD12	1.65	0.77
1:C:12:GLU:HG3	1:C:13:GLY:H	1.50	0.77
1:C:36:THR:HG23	9:C:3418:HOH:O	1.90	0.72
1:A:53:VAL:HG21	6:A:2483:LPE:H1N2	1.74	0.68
1:A:46:PRO:HG3	1:A:113:GLU:OE2	1.97	0.65
1:B:51:LEU:HD22	1:B:145:LEU:HD11	1.78	0.64
1:A:19:ILE:HD11	5:A:2482:PFS:H202	1.82	0.61
1:C:12:GLU:HG3	1:C:13:GLY:N	2.16	0.61
1:A:39:VAL:HG13	5:A:2482:PFS:H263	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:H	1:A:113:GLU:CD	2.13	0.55
1:C:98:GLU:HA	1:C:98:GLU:OE1	2.08	0.54
1:B:133:TRP:HD1	9:B:3438:HOH:O	1.92	0.53
1:A:57:LEU:HD11	5:A:2482:PFS:O31	2.09	0.53
1:C:12:GLU:CG	1:C:13:GLY:H	2.21	0.52
1:B:37:LEU:HD11	5:B:2484:PFS:H142	1.92	0.52
1:C:90:ILE:O	1:C:108:HIS:HE1	1.92	0.52
1:A:83:CYS:HB2	3:A:801:CL:CL	2.46	0.52
1:B:52:LYS:HD3	1:B:54:ASP:OD2	2.09	0.51
5:B:2484:PFS:O32	5:B:2484:PFS:H2	2.11	0.51
1:A:53:VAL:HG11	6:A:2483:LPE:H2N3	1.92	0.50
9:A:3442:HOH:O	1:C:36:THR:CG2	2.60	0.49
1:C:53:VAL:HG21	6:C:2488:LPE:H2N3	1.94	0.49
1:C:25:GLU:HB2	1:C:36:THR:OG1	2.13	0.49
6:A:2483:LPE:H2N1	9:A:3504:HOH:O	2.14	0.48
1:A:35:VAL:HG21	7:A:1503:IPA:H11	1.97	0.47
1:B:24:LEU:HD21	1:B:29:ILE:HD11	1.97	0.47
1:B:19:ILE:HG12	1:B:155:ILE:HG21	1.96	0.46
1:C:7:TRP:CZ2	4:C:901:EPE:H62	2.50	0.46
1:B:83:CYS:HB2	3:B:802:CL:CL	2.54	0.45
1:A:37:LEU:HG	1:A:38:SER:N	2.32	0.45
9:A:3442:HOH:O	1:C:36:THR:HG22	2.17	0.45
1:A:116:TYR:CD1	6:A:2483:LPE:H141	2.53	0.44
1:B:113:GLU:H	1:B:113:GLU:CD	2.25	0.44
1:B:20:ARG:HH11	1:B:20:ARG:HG3	1.82	0.44
1:A:159:ALA:N	5:A:2482:PFS:HH32	2.33	0.43
1:C:7:TRP:O	4:C:901:EPE:H91	2.18	0.43
1:B:130:LEU:HB2	1:B:135:THR:HG23	2.00	0.43
1:A:98:GLU:HA	1:A:98:GLU:OE1	2.19	0.43
1:B:37:LEU:C	1:B:37:LEU:HD23	2.43	0.42
1:B:163:GLY:O	1:B:164:ILE:C	2.62	0.42
1:A:35:VAL:HG13	1:A:125:VAL:CG2	2.49	0.42
1:C:113:GLU:H	1:C:113:GLU:CD	2.27	0.42
1:C:66:ILE:HD11	9:C:3443:HOH:O	2.18	0.42
1:A:68:ILE:HD13	5:A:2482:PFS:H3N2	2.00	0.41
1:C:147:SER:HB2	1:C:152:LEU:HD11	2.02	0.41
1:A:157:ILE:HG22	5:A:2482:PFS:HH33	2.01	0.41
1:B:145:LEU:HB2	6:B:2485:LPE:O31	2.21	0.41
6:B:2485:LPE:H251	6:B:2485:LPE:H222	1.93	0.41
1:C:132:SER:HB3	1:C:164:ILE:HD13	2.03	0.41
1:B:53:VAL:HG11	6:B:2485:LPE:H1N2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PRO:O	1:B:120:LYS:C	2.64	0.41
1:A:29:ILE:HG23	1:A:35:VAL:CG1	2.50	0.41
1:A:53:VAL:CG1	6:A:2483:LPE:H2N3	2.51	0.41
1:A:90:ILE:O	1:A:91:PRO:C	2.64	0.40
1:C:31:VAL:CG1	9:C:3427:HOH:O	2.70	0.40
1:B:125:VAL:HA	1:B:126:PRO:HD3	1.95	0.40
1:C:139:TYR:CB	5:C:2486:PFS:HH33	2.52	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	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
1	B	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	C	161/164 (98%)	153 (95%)	8 (5%)	0	100	100
All	All	485/492 (99%)	470 (97%)	15 (3%)	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	147/148 (99%)	143 (97%)	4 (3%)	39	42
1	B	147/148 (99%)	145 (99%)	2 (1%)	59	66
1	C	146/148 (99%)	143 (98%)	3 (2%)	47	52
All	All	440/444 (99%)	431 (98%)	9 (2%)	48	54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	66	ILE
1	A	113	GLU
1	A	122	GLU
1	B	113	GLU
1	B	129	GLU
1	C	37	LEU
1	C	118	LEU
1	C	164	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	B	108	HIS
1	C	108	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 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
7	IPA	C	1513	-	3,3,3	0.52	0	3,3,3	0.93	0
4	EPE	A	900	-	15,15,15	1.39	3 (20%)	19,20,20	0.90	0
7	IPA	A	1503	-	3,3,3	0.54	0	3,3,3	0.94	0
8	DAO	B	1364	-	13,13,13	1.43	2 (15%)	13,13,13	1.55	2 (15%)
7	IPA	B	1515	-	3,3,3	0.58	0	3,3,3	0.90	0
2	ACT	A	3321	-	3,3,3	1.32	1 (33%)	3,3,3	0.80	0
2	ACT	B	3322	-	3,3,3	1.30	1 (33%)	3,3,3	0.78	0
2	ACT	B	3323	-	3,3,3	1.33	1 (33%)	3,3,3	0.74	0
7	IPA	C	1514	-	3,3,3	0.60	0	3,3,3	0.92	0
4	EPE	C	901	-	15,15,15	1.27	2 (13%)	19,20,20	0.77	0
5	PFS	B	2484	-	34,34,34	1.38	1 (2%)	39,41,41	2.57	4 (10%)
2	ACT	A	3320	-	3,3,3	1.30	1 (33%)	3,3,3	0.79	0
6	LPE	C	2488	-	33,33,33	0.56	0	37,39,39	0.81	0
6	LPE	A	2483	-	33,33,33	0.55	0	37,39,39	0.82	0
5	PFS	C	2486	-	34,34,34	1.38	1 (2%)	39,41,41	2.50	3 (7%)
2	ACT	C	3324	-	3,3,3	1.27	1 (33%)	3,3,3	0.77	0
5	PFS	A	2482	-	34,34,34	1.40	1 (2%)	39,41,41	2.45	3 (7%)
6	LPE	B	2485	-	33,33,33	0.61	0	37,39,39	0.79	0
7	IPA	C	1511	-	3,3,3	0.60	0	3,3,3	0.92	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
6	LPE	C	2488	-	-	22/34/34/34	-
5	PFS	A	2482	-	-	24/36/36/36	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	A	900	-	-	0/9/19/19	0/1/1/1
6	LPE	A	2483	-	-	29/34/34/34	-
5	PFS	C	2486	-	-	28/36/36/36	-
6	LPE	B	2485	-	-	25/34/34/34	-
8	DAO	B	1364	-	-	2/11/11/11	-
4	EPE	C	901	-	-	3/9/19/19	0/1/1/1
5	PFS	B	2484	-	-	26/36/36/36	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2482	PFS	O2-C	-7.30	1.19	1.35
5	B	2484	PFS	O2-C	-7.18	1.19	1.35
5	C	2486	PFS	O2-C	-7.13	1.19	1.35
8	B	1364	DAO	O1-C1	3.83	1.34	1.22
8	B	1364	DAO	O2-C1	-2.84	1.21	1.30
4	A	900	EPE	C6-N1	2.51	1.53	1.46
4	A	900	EPE	C2-N1	2.46	1.53	1.46
4	C	901	EPE	C10-S	2.37	1.80	1.77
4	C	901	EPE	C6-N1	2.29	1.53	1.46
2	A	3321	ACT	O-C	2.22	1.32	1.22
4	A	900	EPE	C10-S	2.22	1.80	1.77
2	B	3323	ACT	O-C	2.19	1.31	1.22
2	A	3320	ACT	O-C	2.16	1.31	1.22
2	B	3322	ACT	O-C	2.15	1.31	1.22
2	C	3324	ACT	O-C	2.13	1.31	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2484	PFS	C2-O2-C	13.99	142.56	117.85
5	C	2486	PFS	C2-O2-C	13.58	141.83	117.85
5	A	2482	PFS	C2-O2-C	13.19	141.14	117.85
5	C	2486	PFS	O2-C-CH3	4.26	118.68	111.09
5	B	2484	PFS	O2-C-CH3	4.13	118.46	111.09
5	A	2482	PFS	O2-C-CH3	4.02	118.26	111.09
8	B	1364	DAO	O1-C1-C2	-3.96	110.55	123.09
8	B	1364	DAO	O2-C1-C2	3.40	124.75	114.00
5	C	2486	PFS	OXT-C-CH3	-2.45	116.09	124.77
5	A	2482	PFS	OXT-C-CH3	-2.44	116.12	124.77
5	B	2484	PFS	OXT-C-CH3	-2.42	116.20	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2484	PFS	C3-C2-C1	-2.03	107.05	111.78

There are no chirality outliers.

All (159) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2482	PFS	O1-C1-C2-O2
5	A	2482	PFS	C31-O33-P-O32
5	B	2484	PFS	O1-C1-C2-O2
5	B	2484	PFS	CH3-C-O2-C2
5	B	2484	PFS	C2-C3-O3-P
5	B	2484	PFS	C31-O33-P-O32
5	C	2486	PFS	O1-C1-C2-O2
5	C	2486	PFS	OXT-C-O2-C2
5	C	2486	PFS	CH3-C-O2-C2
5	C	2486	PFS	C31-O33-P-O3
5	C	2486	PFS	C31-O33-P-O31
5	C	2486	PFS	C31-O33-P-O32
6	A	2483	LPE	O1-C1-C2-O2H
6	A	2483	LPE	O1-C1-C2-C3
6	A	2483	LPE	O2H-C2-C3-O3
6	A	2483	LPE	C2-C3-O3-P
6	A	2483	LPE	C3-O3-P-O31
6	A	2483	LPE	C3-O3-P-O32
6	A	2483	LPE	C3-O3-P-O33
6	A	2483	LPE	C31-O33-P-O3
6	A	2483	LPE	C31-O33-P-O31
6	A	2483	LPE	C31-O33-P-O32
6	B	2485	LPE	O1-C1-C2-O2H
6	B	2485	LPE	O1-C1-C2-C3
6	B	2485	LPE	C2-C3-O3-P
6	B	2485	LPE	C3-O3-P-O31
6	B	2485	LPE	C3-O3-P-O33
6	B	2485	LPE	C31-O33-P-O3
6	B	2485	LPE	C31-O33-P-O31
6	B	2485	LPE	C31-O33-P-O32
6	C	2488	LPE	O1-C1-C2-O2H
6	C	2488	LPE	C3-O3-P-O33
6	C	2488	LPE	C31-O33-P-O3
6	C	2488	LPE	C31-O33-P-O31
6	C	2488	LPE	C31-O33-P-O32
5	B	2484	PFS	OXT-C-O2-C2

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Mol	Chain	Res	Type	Atoms
6	A	2483	LPE	C1-C2-C3-O3
6	C	2488	LPE	O1-C1-C2-C3
5	B	2484	PFS	C31-C32-N-C3N
5	C	2486	PFS	O1-C11-C12-C13
5	A	2482	PFS	CH3-C-O2-C2
5	A	2482	PFS	C31-C32-N-C3N
5	C	2486	PFS	C31-C32-N-C3N
6	A	2483	LPE	C31-C32-N-C3N
6	B	2485	LPE	C31-C32-N-C3N
6	C	2488	LPE	C31-C32-N-C3N
6	C	2488	LPE	O1-C11-C12-C13
5	B	2484	PFS	C3-C2-O2-C
6	C	2488	LPE	C11-C12-C13-C14
6	B	2485	LPE	C11-C12-C13-C14
5	C	2486	PFS	C31-C32-N-C2N
6	B	2485	LPE	C31-C32-N-C2N
5	C	2486	PFS	C13-C14-C15-C16
6	B	2485	LPE	C20-C21-C22-C23
5	B	2484	PFS	C20-C21-C22-C23
6	A	2483	LPE	C21-C22-C23-C24
5	A	2482	PFS	C16-C17-C18-C19
6	A	2483	LPE	C18-C19-C20-C21
6	A	2483	LPE	O1-C11-C12-C13
5	B	2484	PFS	C12-C13-C14-C15
5	B	2484	PFS	C17-C18-C19-C20
5	C	2486	PFS	C14-C15-C16-C17
6	A	2483	LPE	C15-C16-C17-C18
5	C	2486	PFS	C11-C12-C13-C14
6	B	2485	LPE	C24-C25-C26-C27
5	A	2482	PFS	C11-C12-C13-C14
5	C	2486	PFS	C21-C22-C23-C24
5	B	2484	PFS	C22-C23-C24-C25
5	C	2486	PFS	C17-C18-C19-C20
5	A	2482	PFS	C31-C32-N-C1N
5	A	2482	PFS	C31-C32-N-C2N
5	B	2484	PFS	C31-C32-N-C1N
5	B	2484	PFS	C31-C32-N-C2N
5	C	2486	PFS	C31-C32-N-C1N
6	A	2483	LPE	C31-C32-N-C1N
6	A	2483	LPE	C31-C32-N-C2N
6	B	2485	LPE	C31-C32-N-C1N
6	C	2488	LPE	C31-C32-N-C1N

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Mol	Chain	Res	Type	Atoms
6	C	2488	LPE	C31-C32-N-C2N
5	A	2482	PFS	C18-C19-C20-C21
5	B	2484	PFS	C16-C17-C18-C19
6	C	2488	LPE	C18-C19-C20-C21
5	B	2484	PFS	C19-C20-C21-C22
5	B	2484	PFS	C21-C22-C23-C24
6	A	2483	LPE	C20-C21-C22-C23
6	C	2488	LPE	C16-C17-C18-C19
4	C	901	EPE	N4-C7-C8-O8
6	C	2488	LPE	C13-C14-C15-C16
5	C	2486	PFS	C18-C19-C20-C21
6	B	2485	LPE	C18-C19-C20-C21
5	B	2484	PFS	C11-C12-C13-C14
6	C	2488	LPE	C23-C24-C25-C26
6	B	2485	LPE	C17-C18-C19-C20
5	B	2484	PFS	O1-C11-C12-C13
6	B	2485	LPE	C19-C20-C21-C22
6	B	2485	LPE	C15-C16-C17-C18
5	A	2482	PFS	C20-C21-C22-C23
6	A	2483	LPE	C16-C17-C18-C19
6	A	2483	LPE	C13-C14-C15-C16
6	C	2488	LPE	C15-C16-C17-C18
5	C	2486	PFS	C23-C24-C25-C26
6	C	2488	LPE	C19-C20-C21-C22
8	B	1364	DAO	C4-C5-C6-C7
5	A	2482	PFS	OXT-C-O2-C2
5	A	2482	PFS	C23-C24-C25-C26
6	A	2483	LPE	C25-C26-C27-C28
8	B	1364	DAO	C6-C7-C8-C9
6	A	2483	LPE	C19-C20-C21-C22
5	C	2486	PFS	C2-C3-O3-P
5	B	2484	PFS	C14-C15-C16-C17
5	C	2486	PFS	C1-C2-C3-O3
5	C	2486	PFS	C22-C23-C24-C25
6	A	2483	LPE	C2-C1-O1-C11
5	A	2482	PFS	O1-C1-C2-C3
5	B	2484	PFS	O1-C1-C2-C3
5	C	2486	PFS	O1-C1-C2-C3
6	B	2485	LPE	C32-C31-O33-P
6	B	2485	LPE	C12-C13-C14-C15
6	C	2488	LPE	C2-C3-O3-P
5	A	2482	PFS	O1-C11-C12-C13

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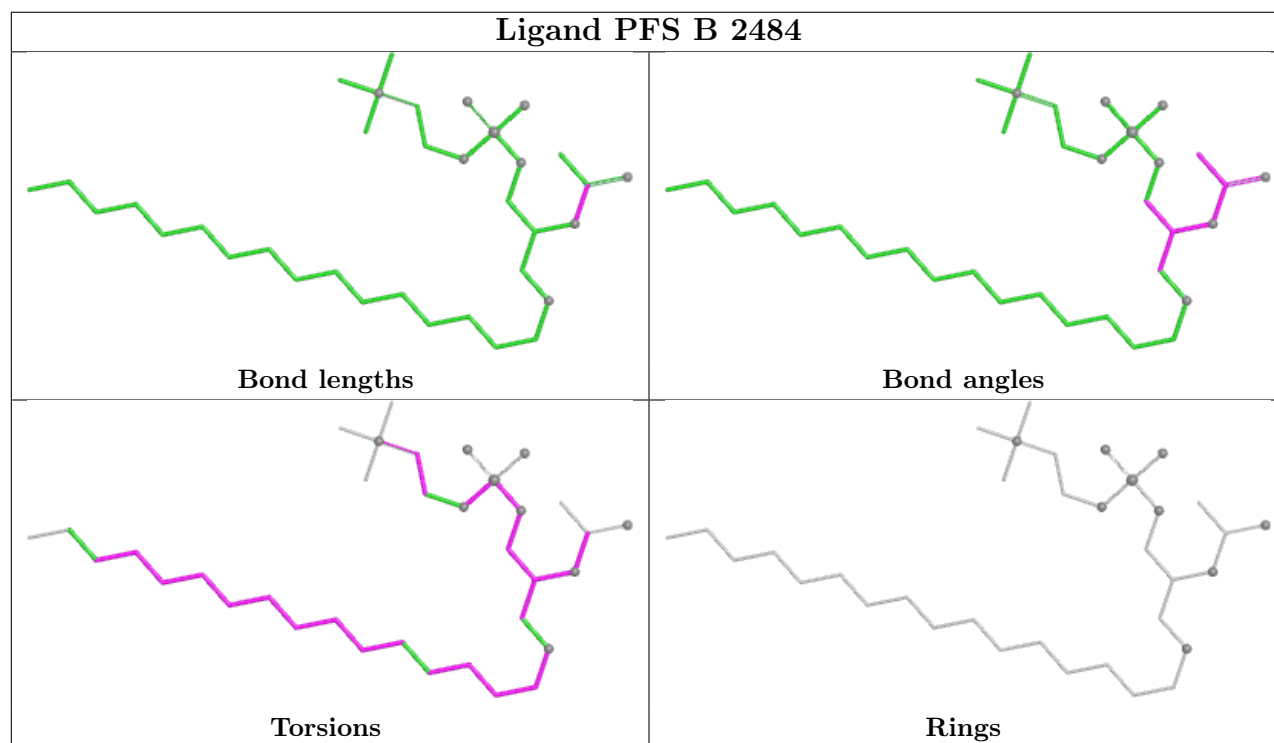
Mol	Chain	Res	Type	Atoms
6	B	2485	LPE	C25-C26-C27-C28
5	A	2482	PFS	O33-C31-C32-N
5	B	2484	PFS	O33-C31-C32-N
5	C	2486	PFS	O33-C31-C32-N
6	A	2483	LPE	O33-C31-C32-N
6	B	2485	LPE	O33-C31-C32-N
6	C	2488	LPE	O33-C31-C32-N
5	C	2486	PFS	C15-C16-C17-C18
5	A	2482	PFS	C12-C11-O1-C1
5	B	2484	PFS	C15-C16-C17-C18
6	B	2485	LPE	O1-C11-C12-C13
6	B	2485	LPE	C23-C24-C25-C26
5	A	2482	PFS	O2-C2-C3-O3
5	C	2486	PFS	O2-C2-C3-O3
5	A	2482	PFS	C13-C14-C15-C16
5	A	2482	PFS	C19-C20-C21-C22
6	A	2483	LPE	C11-C12-C13-C14
5	C	2486	PFS	C12-C11-O1-C1
5	B	2484	PFS	C3-O3-P-O32
5	C	2486	PFS	C3-O3-P-O32
6	C	2488	LPE	C3-O3-P-O31
5	A	2482	PFS	C2-C3-O3-P
4	C	901	EPE	C10-C9-N1-C2
4	C	901	EPE	C10-C9-N1-C6
5	B	2484	PFS	C1-C2-C3-O3
6	C	2488	LPE	C2-C1-O1-C11
5	B	2484	PFS	C12-C11-O1-C1
5	C	2486	PFS	C19-C20-C21-C22
5	C	2486	PFS	C12-C13-C14-C15
6	C	2488	LPE	O2H-C2-C3-O3
5	B	2484	PFS	C18-C19-C20-C21
5	A	2482	PFS	C22-C23-C24-C25
6	A	2483	LPE	C12-C13-C14-C15
5	A	2482	PFS	C14-C15-C16-C17
5	A	2482	PFS	C1-C2-C3-O3
6	A	2483	LPE	C22-C23-C24-C25
5	A	2482	PFS	C12-C13-C14-C15
6	A	2483	LPE	C24-C25-C26-C27
6	B	2485	LPE	O2H-C2-C3-O3

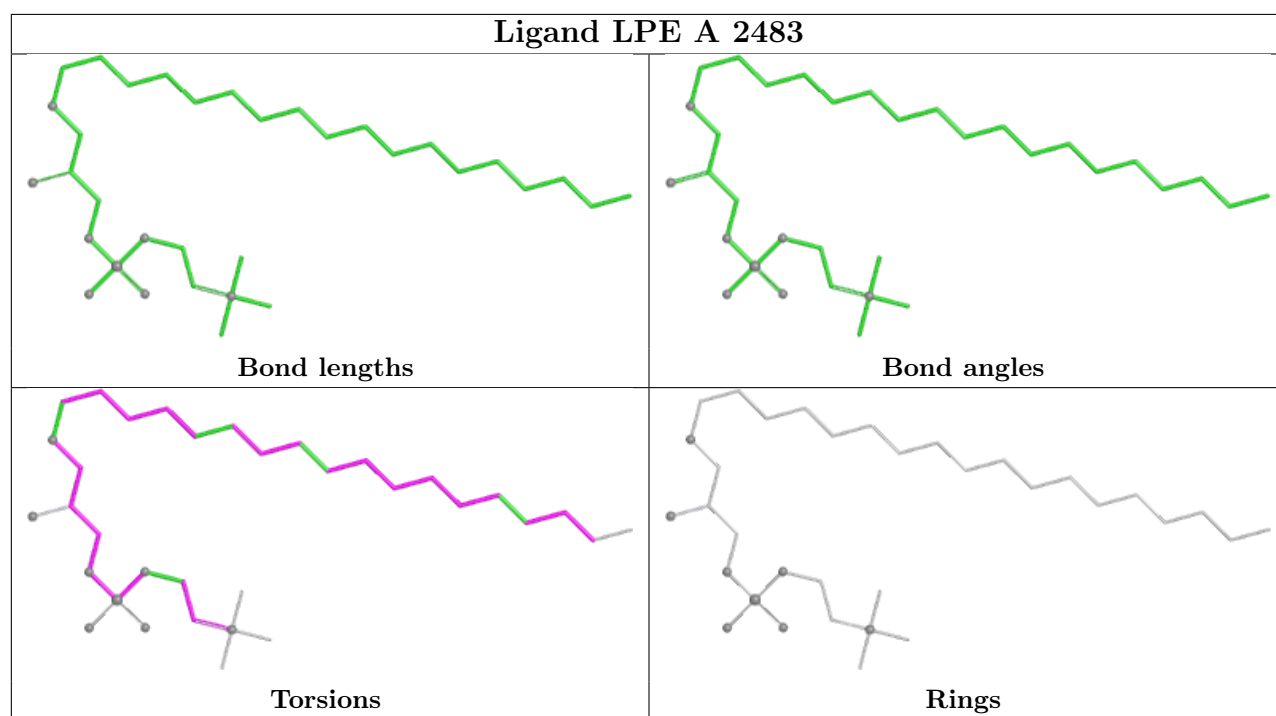
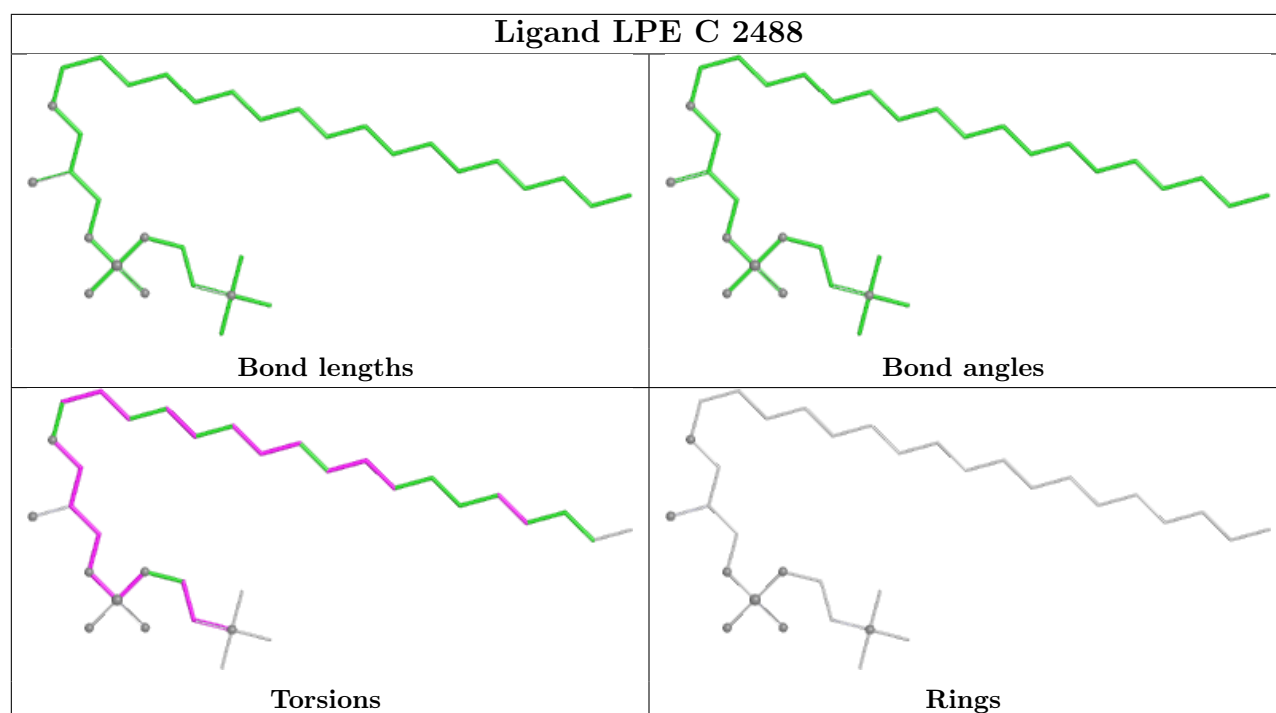
There are no ring outliers.

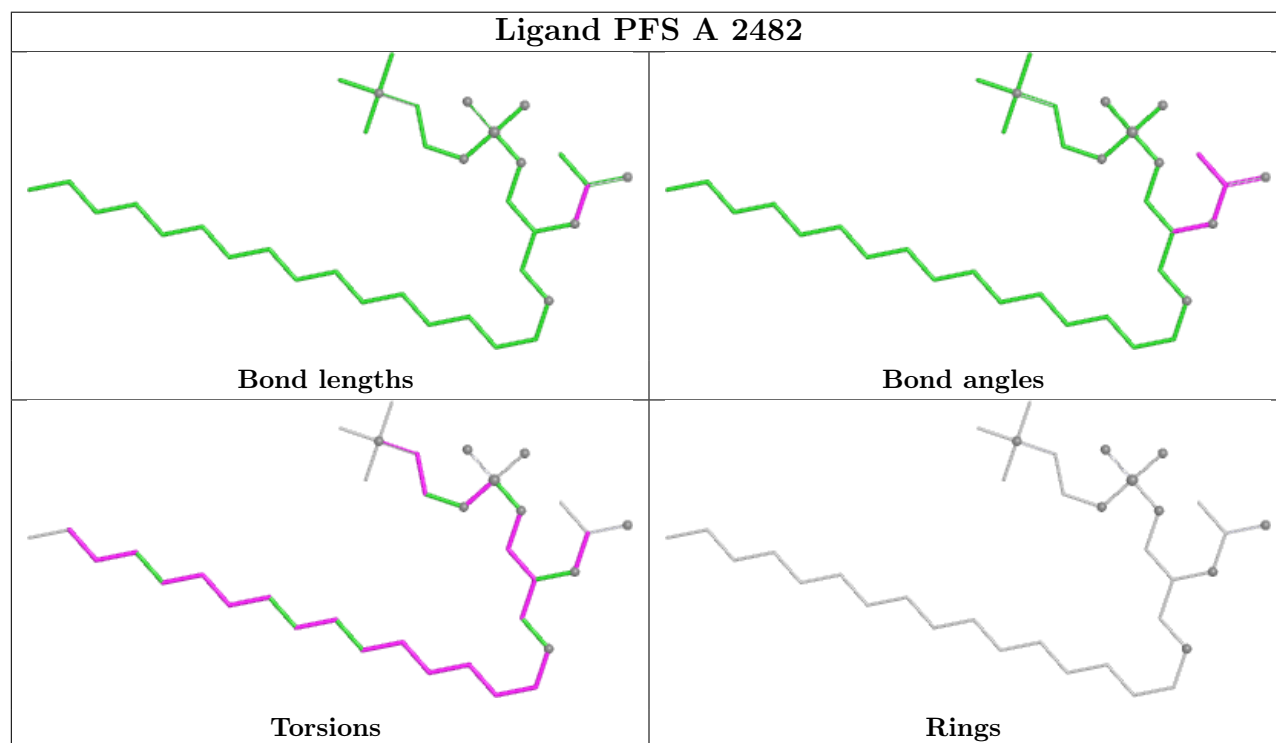
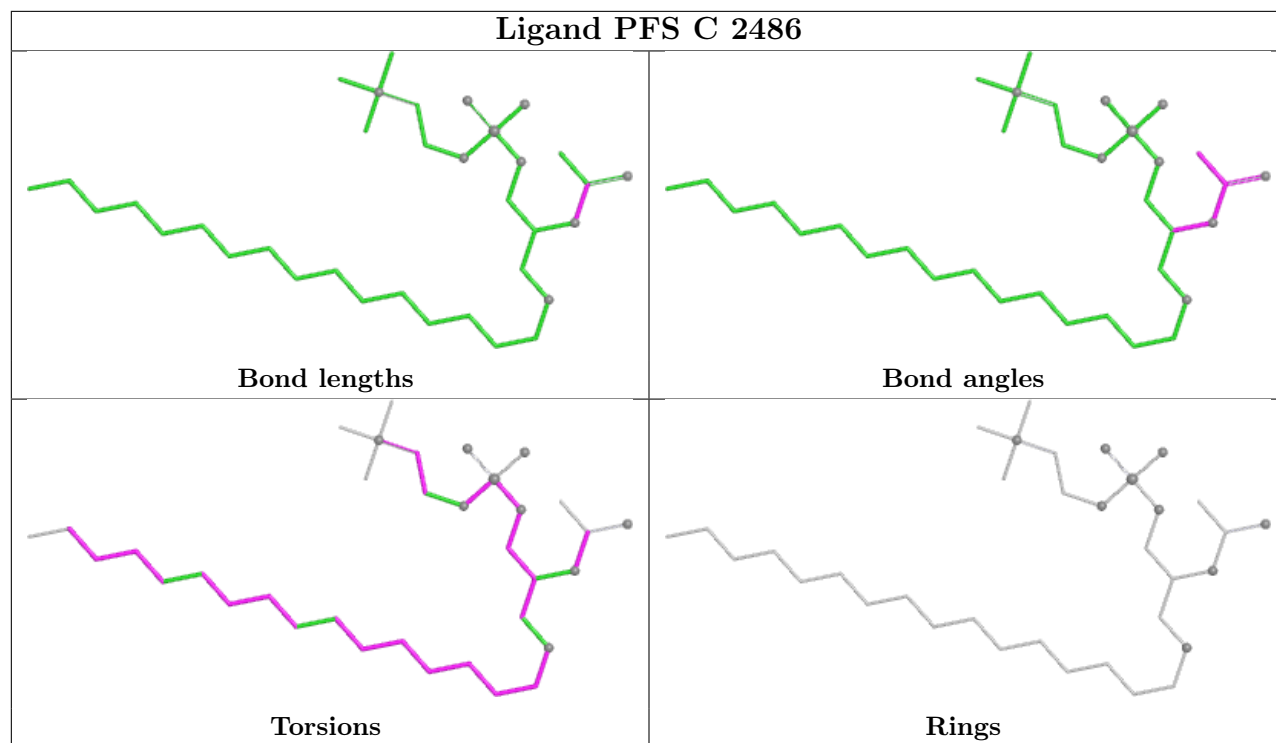
8 monomers are involved in 21 short contacts:

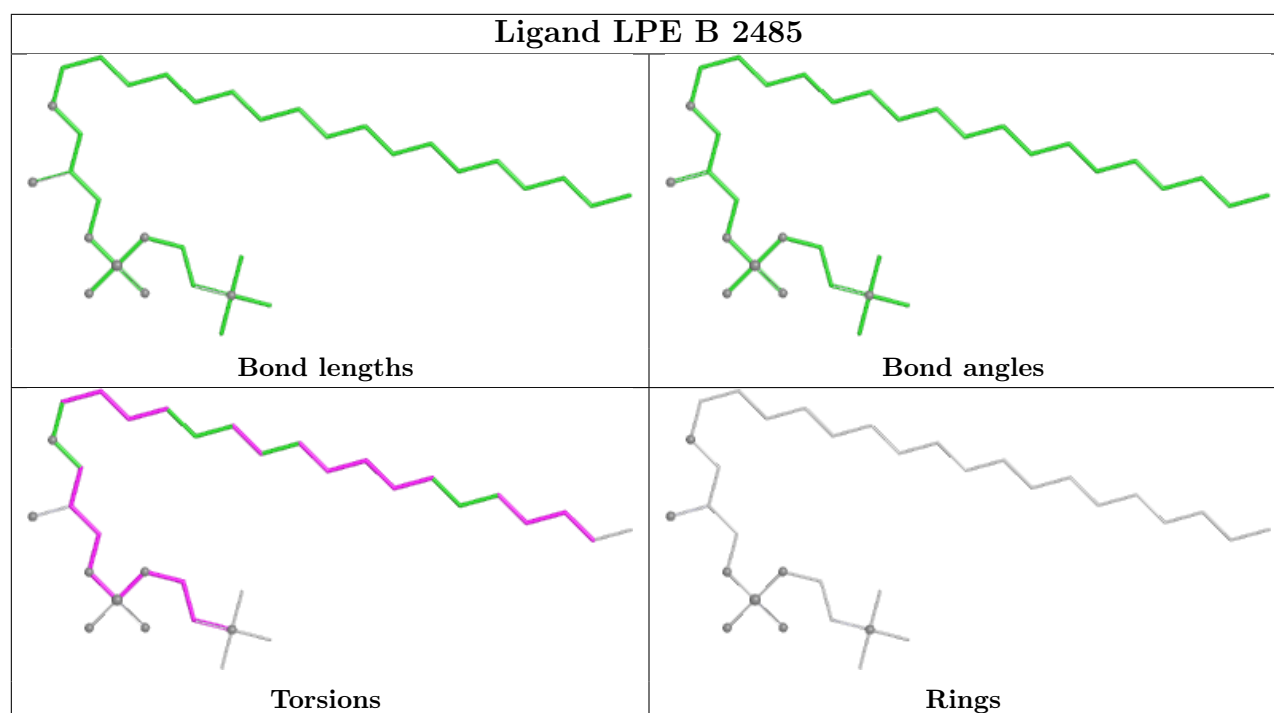
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1503	IPA	1	0
4	C	901	EPE	2	0
5	B	2484	PFS	2	0
6	C	2488	LPE	1	0
6	A	2483	LPE	5	0
5	C	2486	PFS	1	0
5	A	2482	PFS	6	0
6	B	2485	LPE	3	0

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 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-0.03	10 (6%) 27 26	11, 21, 52, 73	0
1	B	164/164 (100%)	-0.11	12 (7%) 21 19	11, 21, 49, 71	0
1	C	163/164 (99%)	0.09	8 (4%) 35 34	16, 25, 49, 67	0
All	All	491/492 (99%)	-0.02	30 (6%) 27 26	11, 23, 52, 73	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	ILE	5.4
1	C	164	ILE	5.3
1	C	13	GLY	4.0
1	A	164	ILE	3.9
1	B	128	LEU	3.6
1	C	2	MET	3.5
1	B	92	THR	3.4
1	B	126	PRO	2.9
1	B	132	SER	2.9
1	A	1	HIS	2.9
1	B	133	TRP	2.9
1	B	93	GLY	2.7
1	B	131	PRO	2.6
1	A	91	PRO	2.6
1	A	127	ASP	2.6
1	C	12	GLU	2.5
1	B	90	ILE	2.5
1	C	11	ASP	2.4
1	A	2	MET	2.4
1	B	127	ASP	2.4
1	A	129	GLU	2.4
1	A	126	PRO	2.4
1	C	133	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	10	CYS	2.3
1	C	4	SER	2.3
1	A	95	PRO	2.2
1	A	128	LEU	2.2
1	B	14	LYS	2.2
1	A	94	GLU	2.2
1	B	89	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

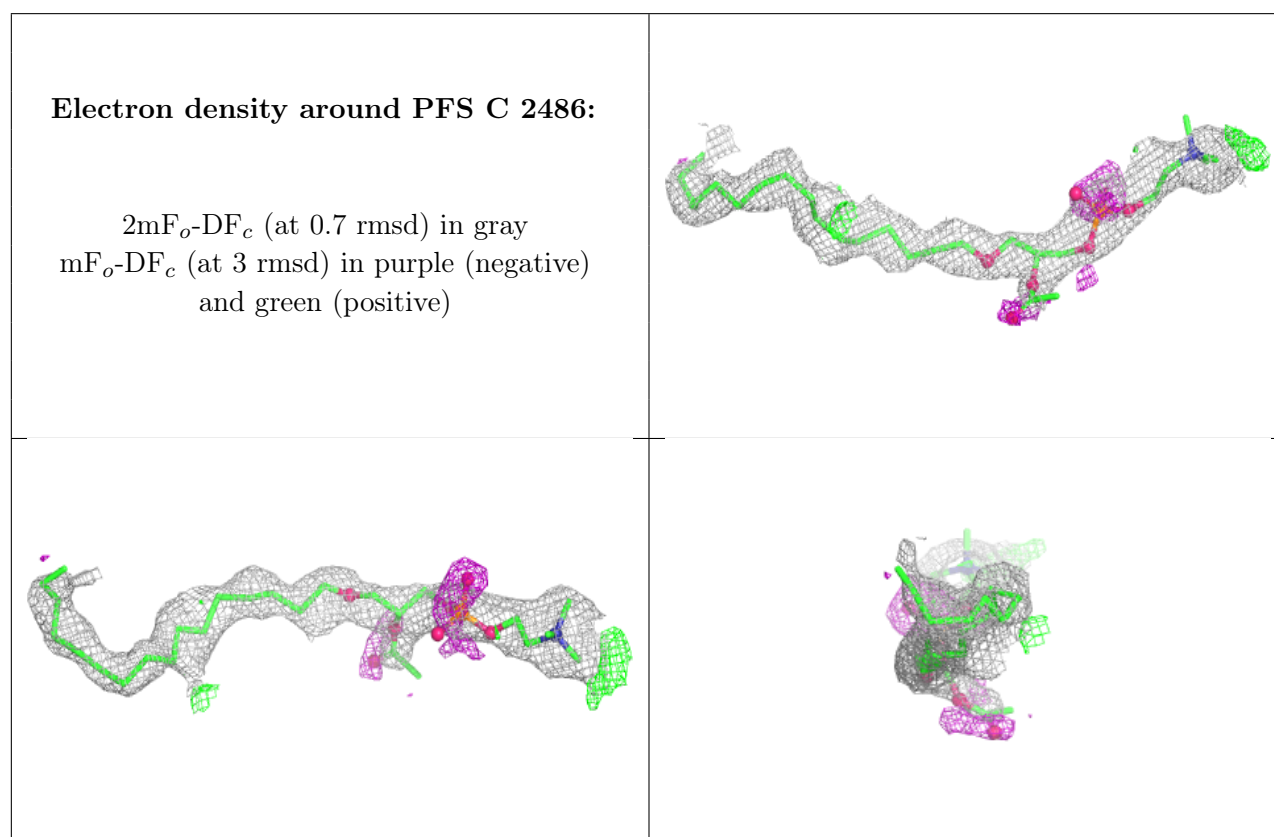
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	IPA	C	1513	4/4	0.65	0.19	59,60,61,61	0
7	IPA	B	1515	4/4	0.66	0.30	61,61,63,64	0
5	PFS	C	2486	35/35	0.68	0.18	59,66,74,76	0
8	DAO	B	1364	14/14	0.68	0.16	63,65,67,68	0
6	LPE	B	2485	34/34	0.71	0.18	51,64,74,76	0
2	ACT	B	3323	4/4	0.72	0.15	60,61,61,62	0
7	IPA	C	1511	4/4	0.74	0.18	53,55,55,56	0
6	LPE	C	2488	34/34	0.75	0.17	53,62,78,80	0
4	EPE	C	901	15/15	0.76	0.20	53,63,66,69	0
6	LPE	A	2483	34/34	0.76	0.18	51,60,75,78	0
5	PFS	A	2482	35/35	0.76	0.17	49,64,73,76	0
5	PFS	B	2484	35/35	0.76	0.18	57,63,74,77	0
7	IPA	C	1514	4/4	0.81	0.15	57,58,58,59	0
2	ACT	C	3324	4/4	0.82	0.13	62,63,63,65	0
7	IPA	A	1503	4/4	0.83	0.16	61,63,63,63	0
2	ACT	B	3322	4/4	0.83	0.11	61,61,61,61	0

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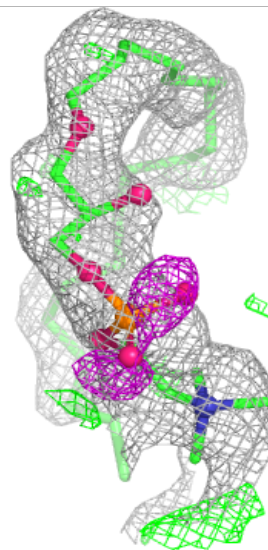
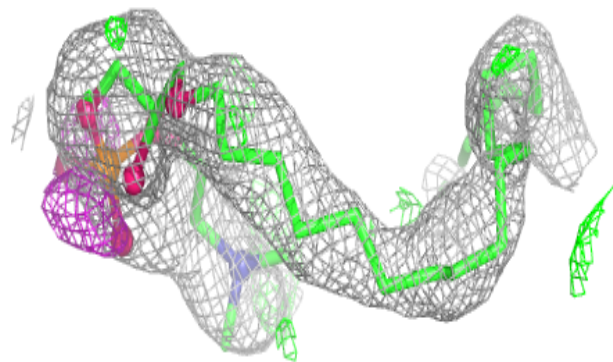
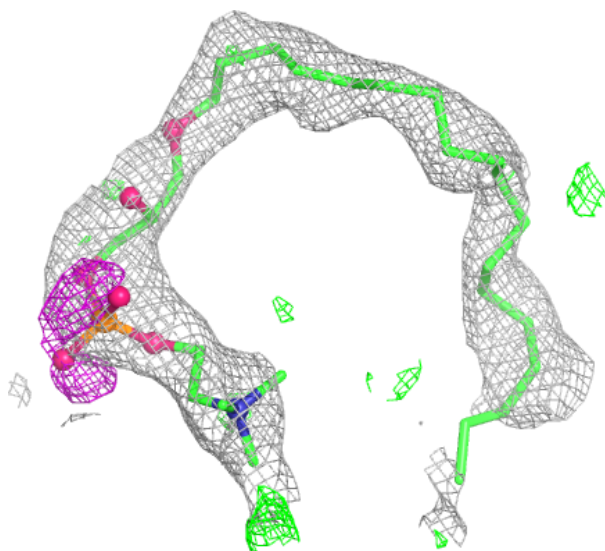
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	3321	4/4	0.84	0.12	58,61,61,64	0
2	ACT	A	3320	4/4	0.85	0.12	55,58,58,58	0
4	EPE	A	900	15/15	0.93	0.10	29,36,43,46	0
3	CL	C	803	1/1	0.97	0.07	26,26,26,26	0
3	CL	B	802	1/1	0.99	0.03	20,20,20,20	0
3	CL	A	801	1/1	0.99	0.02	17,17,17,17	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.



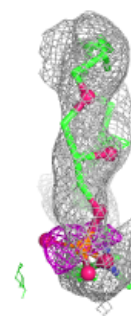
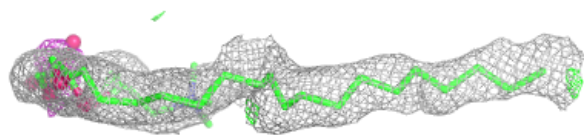
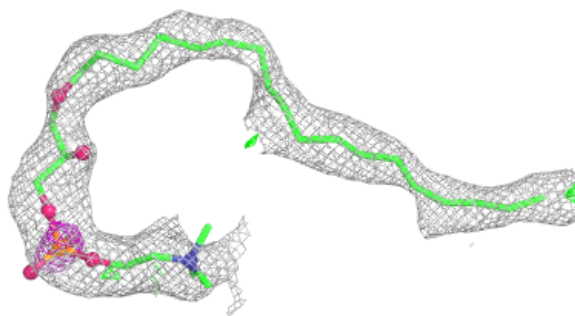
Electron density around LPE B 2485:

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



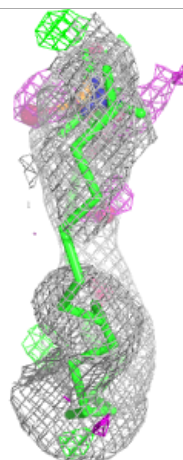
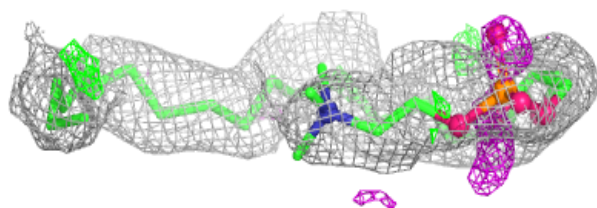
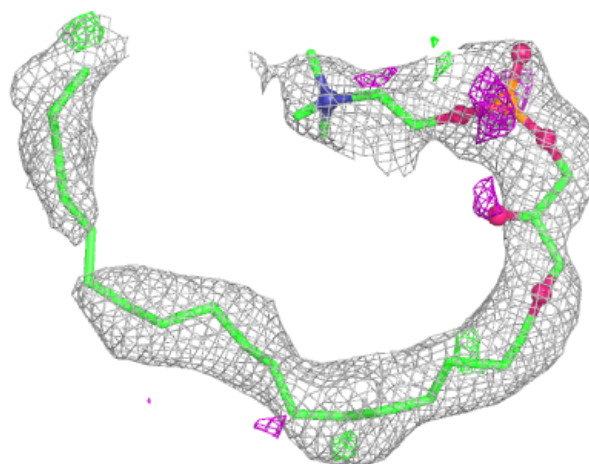
Electron density around LPE C 2488:

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



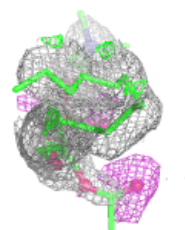
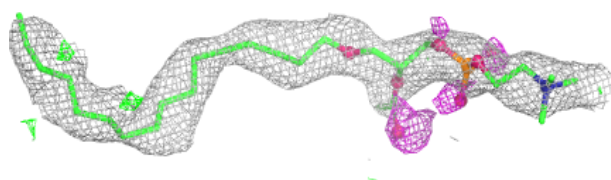
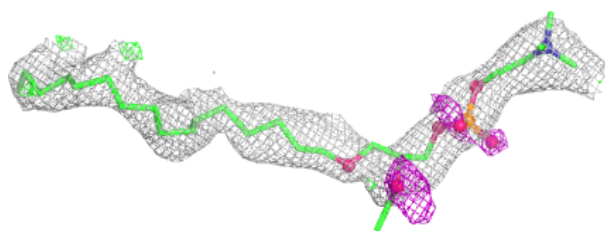
Electron density around LPE A 2483:

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

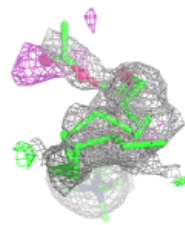
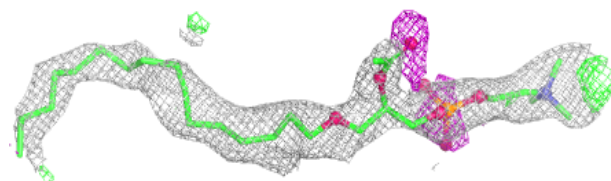
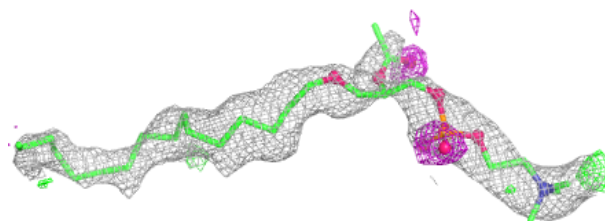


Electron density around PFS A 2482:

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

**Electron density around PFS B 2484:**

$2mF_o-DF_c$ (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.