



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2020 – 02:58 PM EST

PDB ID : 6W1B
Title : N-terminal domain of mouse surfactant protein B with bound lipid,
Y59A/H79A mutant
Authors : Rapoport, T.A.; Bodnar, N.O.
Deposited on : 2020-03-04
Resolution : 2.31 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
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) : 2.14.6

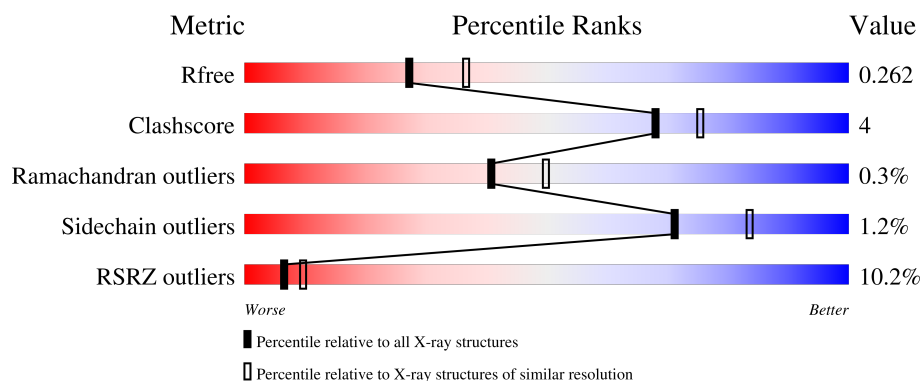
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on 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	87	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	87	<div> <div>9%</div> <div> <div></div> <div>77%</div> <div>11%</div> <div>11%</div> </div> </div>
1	C	87	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>8%</div> </div> </div>
1	D	87	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>9%</div> </div> </div>
1	E	87	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	87	
1	G	87	
1	H	87	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEE	A	101	-	-	-	X
2	PEE	A	102	-	-	-	X
2	PEE	B	102	-	-	-	X
2	PEE	B	103	-	-	-	X
2	PEE	D	102	-	-	-	X
2	PEE	E	101	-	-	-	X
2	PEE	E	102	-	-	-	X
2	PEE	F	101	-	-	-	X
2	PEE	H	101	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11653 atoms, of which 6027 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 Pulmonary surfactant-associated protein B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	78	Total	C	H	N	O	S	0	0	0
			1252	396	633	102	114	7			
1	E	81	Total	C	H	N	O	S	0	0	0
			1300	409	657	109	118	7			
1	B	77	Total	C	H	N	O	S	0	0	0
			1241	392	630	101	111	7			
1	C	80	Total	C	H	N	O	S	0	0	0
			1284	404	650	107	116	7			
1	D	79	Total	C	H	N	O	S	0	0	0
			1266	400	639	104	116	7			
1	F	78	Total	C	H	N	O	S	0	0	0
			1252	396	633	102	114	7			
1	G	78	Total	C	H	N	O	S	0	0	0
			1252	395	632	103	115	7			
1	H	78	Total	C	H	N	O	S	0	0	0
			1252	396	633	102	114	7			

There are 24 discrepancies between the modelled and reference sequences:

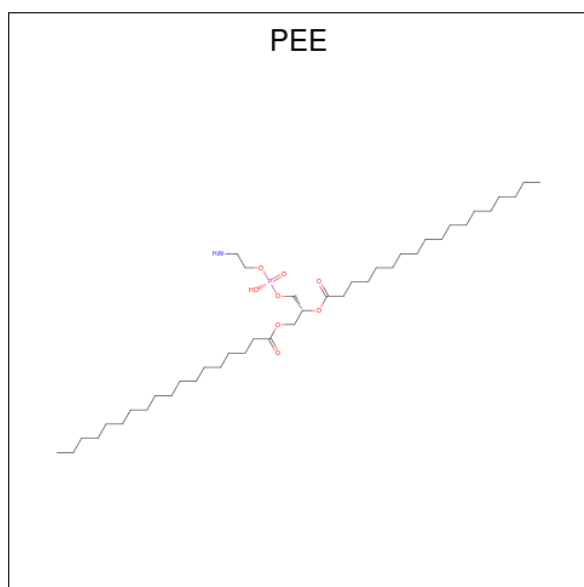
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P50405
A	59	ALA	TYR	engineered mutation	UNP P50405
A	79	ALA	HIS	engineered mutation	UNP P50405
E	1	SER	-	expression tag	UNP P50405
E	59	ALA	TYR	engineered mutation	UNP P50405
E	79	ALA	HIS	engineered mutation	UNP P50405
B	1	SER	-	expression tag	UNP P50405
B	59	ALA	TYR	engineered mutation	UNP P50405
B	79	ALA	HIS	engineered mutation	UNP P50405
C	1	SER	-	expression tag	UNP P50405
C	59	ALA	TYR	engineered mutation	UNP P50405
C	79	ALA	HIS	engineered mutation	UNP P50405
D	1	SER	-	expression tag	UNP P50405

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Chain	Residue	Modelled	Actual	Comment	Reference
D	59	ALA	TYR	engineered mutation	UNP P50405
D	79	ALA	HIS	engineered mutation	UNP P50405
F	1	SER	-	expression tag	UNP P50405
F	59	ALA	TYR	engineered mutation	UNP P50405
F	79	ALA	HIS	engineered mutation	UNP P50405
G	1	SER	-	expression tag	UNP P50405
G	59	ALA	TYR	engineered mutation	UNP P50405
G	79	ALA	HIS	engineered mutation	UNP P50405
H	1	SER	-	expression tag	UNP P50405
H	59	ALA	TYR	engineered mutation	UNP P50405
H	79	ALA	HIS	engineered mutation	UNP P50405

- Molecule 2 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			123	38	75	1	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			133	41	82	1	8	1		
2	E	1	Total	C	H	N	O	P	0	0
			133	41	82	1	8	1		
2	E	1	Total	C	H	O			0	0
			25	20	3	2				
2	B	1	Total	C	H	N	O	P	0	0
			133	41	82	1	8	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 133	C 41	H 82	N 1	O 8	P 1	0	0
2	B	1	Total 95	C 29	H 56	N 1	O 8	P 1	0	0
2	C	1	Total 133	C 41	H 82	N 1	O 8	P 1	0	0
2	C	1	Total 93	C 28	H 55	N 1	O 8	P 1	0	0
2	D	1	Total 133	C 41	H 82	N 1	O 8	P 1	0	0
2	D	1	Total 133	C 41	H 82	N 1	O 8	P 1	0	0
2	F	1	Total 123	C 38	H 75	N 1	O 8	P 1	0	0
2	H	1	Total 133	C 41	H 82	N 1	O 8	P 1	0	0

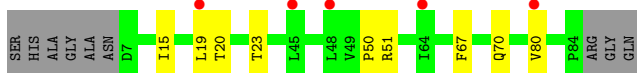
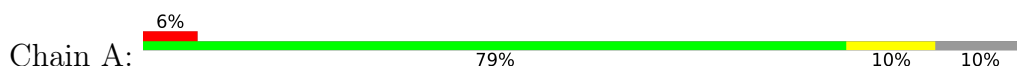
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	E	4	Total 4	O 4	0	0
3	B	6	Total 6	O 6	0	0
3	C	6	Total 6	O 6	0	0
3	D	5	Total 5	O 5	0	0
3	G	1	Total 1	O 1	0	0
3	H	3	Total 3	O 3	0	0

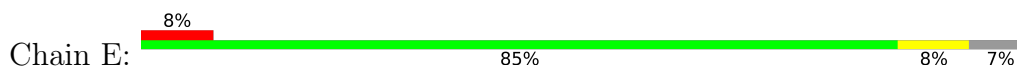
3 Residue-property plots [i](#)

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.

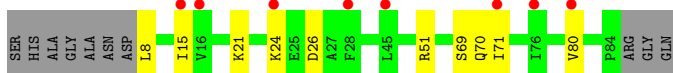
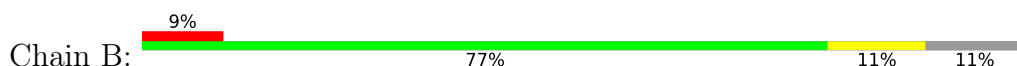
- Molecule 1: Pulmonary surfactant-associated protein B



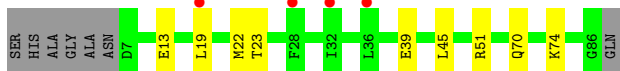
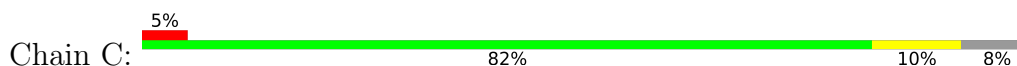
- Molecule 1: Pulmonary surfactant-associated protein B



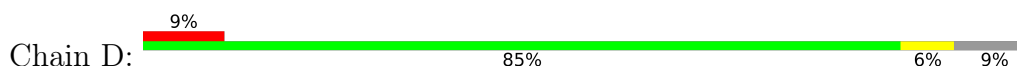
- Molecule 1: Pulmonary surfactant-associated protein B



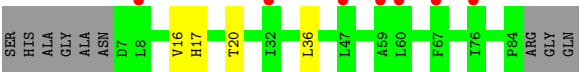
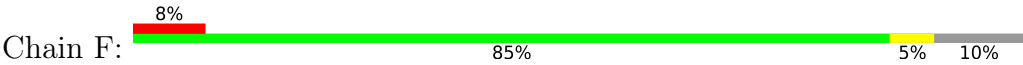
- Molecule 1: Pulmonary surfactant-associated protein B



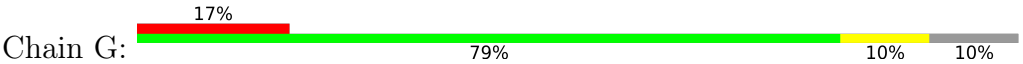
- Molecule 1: Pulmonary surfactant-associated protein B



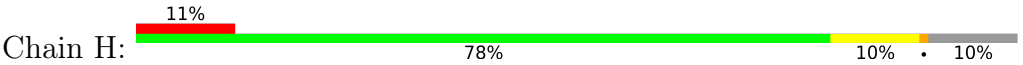
- Molecule 1: Pulmonary surfactant-associated protein B



• Molecule 1: Pulmonary surfactant-associated protein B



• Molecule 1: Pulmonary surfactant-associated protein B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.33Å 169.53Å 73.71Å 90.00° 126.90° 90.00°	Depositor
Resolution (Å)	84.76 – 2.31 84.76 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.5 (84.76-2.31) 97.5 (84.76-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.241 , 0.262 0.241 , 0.262	Depositor DCC
R_{free} test set	1831 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	77.1	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 78.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11653	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: PEE

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	0.26	0/628	0.41	0/851
1	B	0.24	0/620	0.40	0/840
1	C	0.25	0/643	0.42	0/870
1	D	0.24	0/636	0.43	0/862
1	E	0.25	0/652	0.42	0/882
1	F	0.25	0/628	0.40	0/851
1	G	0.26	0/628	0.46	0/850
1	H	0.25	0/628	0.43	0/851
All	All	0.25	0/5063	0.42	0/6857

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	619	633	633	7	0
1	B	611	630	629	5	0
1	C	634	650	649	5	0
1	D	627	639	639	4	0
1	E	643	657	657	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	619	633	633	2	0
1	G	620	632	632	8	0
1	H	619	633	633	7	0
2	A	99	157	155	3	0
2	B	141	220	216	1	0
2	C	89	137	135	0	0
2	D	102	164	164	2	0
2	E	73	85	119	5	0
2	F	48	75	73	1	0
2	H	51	82	82	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	5	0	0	0	0
3	E	4	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	0	0
All	All	5626	6027	6049	44	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 4.

All (44) 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)
2:A:101:PEE:H77	2:E:102:PEE:H66	1.79	0.65
1:A:20:THR:HG21	1:A:70:GLN:HE21	1.62	0.65
1:D:63:VAL:HG21	2:D:101:PEE:H80	1.79	0.64
2:B:101:PEE:H29	1:C:45:LEU:HD11	1.80	0.63
1:E:66:TYR:OH	2:E:102:PEE:H50	1.97	0.63
1:G:23:THR:HG21	1:G:67:PHE:CB	2.30	0.62
1:G:19:LEU:O	1:G:23:THR:HG23	2.01	0.60
1:H:20:THR:HG22	1:H:24:LYS:HE2	1.84	0.59
1:H:39:GLU:HB3	1:H:45:LEU:HD12	1.83	0.59
1:B:15:ILE:HD12	1:C:22:MET:HE1	1.85	0.58
1:A:20:THR:HG22	1:A:67:PHE:O	2.04	0.57
1:E:76:ILE:H	1:E:76:ILE:HD12	1.70	0.57
1:C:19:LEU:O	1:C:23:THR:HG23	2.06	0.56
1:C:39:GLU:HB3	1:C:45:LEU:HD12	1.90	0.54
1:E:70:GLN:CD	1:E:76:ILE:HD11	2.28	0.54
2:A:101:PEE:H82	2:E:102:PEE:H62	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:VAL:O	1:F:20:THR:HG23	2.07	0.53
1:D:62:LEU:HD23	1:H:47:LEU:HD23	1.91	0.53
1:E:70:GLN:NE2	1:E:76:ILE:HD11	2.23	0.53
1:B:69:SER:O	1:B:71:ILE:HG23	2.09	0.52
1:G:23:THR:HG21	1:G:67:PHE:HB2	1.93	0.51
2:A:102:PEE:H82	1:E:36:LEU:HD21	1.93	0.50
1:G:80:VAL:HG23	1:G:82:LEU:HG	1.92	0.50
1:A:15:ILE:HD12	1:E:22:MET:CE	2.42	0.49
1:G:62:LEU:HD23	1:G:62:LEU:C	2.33	0.48
1:A:15:ILE:HD12	1:E:22:MET:HE1	1.97	0.47
1:B:8:LEU:O	1:B:8:LEU:HD12	2.15	0.47
1:G:8:LEU:HD12	1:G:8:LEU:O	2.15	0.47
1:H:30:GLU:OE2	1:H:33:ARG:NH1	2.47	0.46
1:G:60:LEU:HB3	1:G:61:PRO:HD3	1.98	0.45
1:A:19:LEU:O	1:A:23:THR:HG23	2.17	0.44
1:C:13:GLU:OE2	1:C:74:LYS:NZ	2.27	0.44
1:B:80:VAL:O	1:B:80:VAL:HG12	2.18	0.43
2:E:101:PEE:C10	2:E:101:PEE:O3	2.66	0.43
1:G:23:THR:HG21	1:G:67:PHE:HB3	2.01	0.42
1:A:50:PRO:O	1:A:51:ARG:C	2.58	0.42
1:D:50:PRO:O	1:D:51:ARG:C	2.58	0.42
2:E:101:PEE:H72	1:F:36:LEU:HD13	2.02	0.42
1:H:20:THR:O	1:H:24:LYS:HG3	2.20	0.41
1:A:80:VAL:HG12	1:A:80:VAL:O	2.20	0.41
1:B:21:LYS:O	1:B:24:LYS:HG2	2.21	0.41
1:D:45:LEU:HD11	2:F:101:PEE:H55	2.03	0.40
2:D:101:PEE:H2	1:H:43:LEU:HD12	2.04	0.40
1:H:65:ASP:HA	1:H:68:GLN:HG2	2.03	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	76/87 (87%)	71 (93%)	5 (7%)	0	100	100
1	B	75/87 (86%)	71 (95%)	3 (4%)	1 (1%)	12	12
1	C	78/87 (90%)	71 (91%)	6 (8%)	1 (1%)	12	12
1	D	77/87 (88%)	74 (96%)	3 (4%)	0	100	100
1	E	79/87 (91%)	78 (99%)	1 (1%)	0	100	100
1	F	76/87 (87%)	75 (99%)	1 (1%)	0	100	100
1	G	76/87 (87%)	71 (93%)	5 (7%)	0	100	100
1	H	76/87 (87%)	74 (97%)	2 (3%)	0	100	100
All	All	613/696 (88%)	585 (95%)	26 (4%)	2 (0%)	41	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	GLN
1	C	51	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	72/77 (94%)	72 (100%)	0	100	100
1	B	71/77 (92%)	69 (97%)	2 (3%)	43	59
1	C	73/77 (95%)	72 (99%)	1 (1%)	67	80
1	D	73/77 (95%)	73 (100%)	0	100	100
1	E	74/77 (96%)	72 (97%)	2 (3%)	44	60
1	F	72/77 (94%)	71 (99%)	1 (1%)	67	80
1	G	72/77 (94%)	72 (100%)	0	100	100
1	H	72/77 (94%)	71 (99%)	1 (1%)	67	80
All	All	579/616 (94%)	572 (99%)	7 (1%)	71	83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	74	LYS
1	E	85	ARG
1	B	26	ASP
1	B	51	ARG
1	C	70	GLN
1	F	17	HIS
1	H	33	ARG

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

Mol	Chain	Res	Type
1	E	70	GLN

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](#)

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PEE	F	101	-	47,47,50	0.90	4 (8%)	50,52,55	0.98	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEE	D	101	-	50,50,50	0.88	4 (8%)	53,55,55	1.03	2 (3%)
2	PEE	B	101	-	50,50,50	0.87	4 (8%)	53,55,55	1.06	2 (3%)
2	PEE	D	102	-	50,50,50	0.88	4 (8%)	53,55,55	1.08	2 (3%)
2	PEE	B	103	-	38,38,50	1.00	4 (10%)	41,43,55	1.06	2 (4%)
2	PEE	E	102	-	21,21,50	0.82	1 (4%)	21,21,55	1.07	1 (4%)
2	PEE	B	102	-	50,50,50	0.87	4 (8%)	53,55,55	1.04	2 (3%)
2	PEE	A	102	-	50,50,50	0.88	4 (8%)	53,55,55	1.04	2 (3%)
2	PEE	E	101	-	50,50,50	0.89	4 (8%)	53,55,55	1.11	2 (3%)
2	PEE	C	101	-	50,50,50	0.87	4 (8%)	53,55,55	1.01	2 (3%)
2	PEE	A	101	-	47,47,50	0.91	4 (8%)	50,52,55	1.10	2 (4%)
2	PEE	H	101	-	50,50,50	0.88	4 (8%)	53,55,55	1.01	2 (3%)
2	PEE	C	102	-	37,37,50	0.99	4 (10%)	40,42,55	1.11	2 (5%)

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	PEE	F	101	-	-	26/51/51/54	-
2	PEE	D	101	-	-	24/54/54/54	-
2	PEE	B	101	-	-	29/54/54/54	-
2	PEE	D	102	-	-	27/54/54/54	-
2	PEE	B	103	-	-	19/42/42/54	-
2	PEE	E	102	-	-	11/20/20/54	-
2	PEE	B	102	-	-	31/54/54/54	-
2	PEE	A	102	-	-	20/54/54/54	-
2	PEE	E	101	-	-	26/54/54/54	-
2	PEE	C	101	-	-	32/54/54/54	-
2	PEE	A	101	-	-	24/51/51/54	-
2	PEE	H	101	-	-	24/54/54/54	-
2	PEE	C	102	-	-	21/41/41/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	103	PEE	O2-C2	-2.56	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	PEE	O3-C30	2.50	1.40	1.33
2	D	101	PEE	O2-C2	-2.50	1.40	1.46
2	C	101	PEE	O3-C30	2.50	1.40	1.33
2	H	101	PEE	O3-C30	2.48	1.40	1.33
2	H	101	PEE	O2-C2	-2.48	1.40	1.46
2	B	103	PEE	O3-C30	2.48	1.40	1.33
2	D	102	PEE	O2-C2	-2.48	1.40	1.46
2	F	101	PEE	O2-C2	-2.47	1.40	1.46
2	E	101	PEE	O3-C30	2.47	1.40	1.33
2	A	102	PEE	O2-C2	-2.46	1.40	1.46
2	D	102	PEE	O3-C30	2.45	1.40	1.33
2	A	101	PEE	O2-C2	-2.45	1.40	1.46
2	E	102	PEE	O3-C30	2.44	1.40	1.33
2	C	102	PEE	O2-C2	-2.44	1.40	1.46
2	C	102	PEE	O3-C30	2.44	1.40	1.33
2	A	101	PEE	O3-C30	2.44	1.40	1.33
2	D	101	PEE	O3-C30	2.43	1.40	1.33
2	B	102	PEE	O3-C30	2.41	1.40	1.33
2	C	101	PEE	O2-C2	-2.41	1.40	1.46
2	B	102	PEE	O2-C2	-2.41	1.40	1.46
2	A	102	PEE	O3-C30	2.41	1.40	1.33
2	E	101	PEE	O2-C2	-2.39	1.40	1.46
2	F	101	PEE	O3-C30	2.37	1.40	1.33
2	D	101	PEE	O2-C10	2.25	1.40	1.34
2	A	101	PEE	O2-C10	2.24	1.40	1.34
2	A	102	PEE	O2-C10	2.24	1.40	1.34
2	B	101	PEE	O2-C10	2.23	1.40	1.34
2	E	101	PEE	O2-C10	2.22	1.40	1.34
2	B	102	PEE	O2-C10	2.18	1.40	1.34
2	C	102	PEE	O2-C10	2.17	1.40	1.34
2	H	101	PEE	O2-C10	2.17	1.40	1.34
2	D	102	PEE	O2-C10	2.17	1.40	1.34
2	B	103	PEE	O2-C10	2.15	1.40	1.34
2	F	101	PEE	O2-C10	2.15	1.40	1.34
2	A	101	PEE	O3-C3	-2.12	1.40	1.45
2	D	102	PEE	O3-C3	-2.11	1.40	1.45
2	A	102	PEE	O3-C3	-2.10	1.40	1.45
2	B	101	PEE	O2-C2	-2.10	1.41	1.46
2	F	101	PEE	O3-C3	-2.09	1.40	1.45
2	B	102	PEE	O3-C3	-2.09	1.40	1.45
2	E	101	PEE	O3-C3	-2.09	1.40	1.45
2	C	101	PEE	O2-C10	2.09	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	101	PEE	O3-C3	-2.09	1.40	1.45
2	B	103	PEE	O3-C3	-2.08	1.40	1.45
2	H	101	PEE	O3-C3	-2.07	1.40	1.45
2	C	101	PEE	O3-C3	-2.02	1.40	1.45
2	B	101	PEE	O3-C3	-2.01	1.40	1.45
2	C	102	PEE	O3-C3	-2.00	1.40	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	101	PEE	O2-C10-C11	4.58	121.36	111.50
2	D	102	PEE	O2-C10-C11	4.39	120.96	111.50
2	A	101	PEE	O2-C10-C11	4.29	120.75	111.50
2	A	102	PEE	O2-C10-C11	4.15	120.45	111.50
2	B	101	PEE	O2-C10-C11	4.13	120.39	111.50
2	B	103	PEE	O2-C10-C11	3.89	119.89	111.50
2	B	102	PEE	O2-C10-C11	3.88	119.85	111.50
2	C	102	PEE	O2-C10-C11	3.83	119.75	111.50
2	C	101	PEE	O2-C10-C11	3.79	119.66	111.50
2	H	101	PEE	O2-C10-C11	3.74	119.56	111.50
2	F	101	PEE	O2-C10-C11	3.73	119.54	111.50
2	D	101	PEE	O2-C10-C11	3.62	119.31	111.50
2	C	102	PEE	O3-C30-C31	2.76	120.57	111.91
2	D	101	PEE	O3-C30-C31	2.72	120.44	111.91
2	E	102	PEE	O3-C30-C31	2.61	120.08	111.91
2	A	101	PEE	O3-C30-C31	2.59	120.02	111.91
2	B	102	PEE	O3-C30-C31	2.56	119.94	111.91
2	C	101	PEE	O3-C30-C31	2.52	119.82	111.91
2	B	103	PEE	O3-C30-C31	2.49	119.72	111.91
2	E	101	PEE	O3-C30-C31	2.46	119.64	111.91
2	B	101	PEE	O3-C30-C31	2.46	119.62	111.91
2	D	102	PEE	O3-C30-C31	2.42	119.51	111.91
2	A	102	PEE	O3-C30-C31	2.41	119.47	111.91
2	H	101	PEE	O3-C30-C31	2.34	119.26	111.91
2	F	101	PEE	O3-C30-C31	2.22	118.89	111.91

There are no chirality outliers.

All (314) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	101	PEE	C2-C1-O3P-P
2	F	101	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
2	F	101	PEE	C1-O3P-P-O1P
2	F	101	PEE	C1-O3P-P-O2P
2	F	101	PEE	C4-O4P-P-O1P
2	F	101	PEE	C4-O4P-P-O3P
2	B	101	PEE	O4P-C4-C5-N
2	B	101	PEE	C11-C10-O2-C2
2	B	101	PEE	C4-O4P-P-O2P
2	D	102	PEE	C4-O4P-P-O1P
2	D	102	PEE	C4-O4P-P-O2P
2	D	102	PEE	C4-O4P-P-O3P
2	B	103	PEE	O4-C10-O2-C2
2	B	103	PEE	C1-O3P-P-O2P
2	B	103	PEE	C4-O4P-P-O1P
2	B	102	PEE	C1-O3P-P-O4P
2	B	102	PEE	C4-O4P-P-O1P
2	A	102	PEE	O4P-C4-C5-N
2	A	102	PEE	C4-O4P-P-O1P
2	E	101	PEE	O4P-C4-C5-N
2	E	101	PEE	C11-C10-O2-C2
2	E	101	PEE	C4-O4P-P-O1P
2	C	101	PEE	O4P-C4-C5-N
2	C	101	PEE	C11-C10-O2-C2
2	C	101	PEE	C1-O3P-P-O1P
2	C	101	PEE	C1-O3P-P-O2P
2	A	101	PEE	C1-O3P-P-O1P
2	A	101	PEE	C4-O4P-P-O1P
2	H	101	PEE	O4P-C4-C5-N
2	H	101	PEE	C5-C4-O4P-P
2	H	101	PEE	C1-O3P-P-O1P
2	H	101	PEE	C1-O3P-P-O4P
2	H	101	PEE	C4-O4P-P-O1P
2	H	101	PEE	C4-O4P-P-O2P
2	H	101	PEE	C4-O4P-P-O3P
2	C	102	PEE	O4P-C4-C5-N
2	C	102	PEE	C11-C10-O2-C2
2	C	102	PEE	C4-O4P-P-O1P
2	C	102	PEE	C4-O4P-P-O2P
2	D	101	PEE	O5-C30-O3-C3
2	A	102	PEE	O5-C30-O3-C3
2	F	101	PEE	O4-C10-O2-C2
2	B	101	PEE	O4-C10-O2-C2
2	E	101	PEE	O4-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
2	C	101	PEE	O4-C10-O2-C2
2	C	102	PEE	O4-C10-O2-C2
2	D	101	PEE	C31-C30-O3-C3
2	A	102	PEE	C31-C30-O3-C3
2	A	101	PEE	C31-C30-O3-C3
2	B	103	PEE	C11-C10-O2-C2
2	B	102	PEE	C31-C30-O3-C3
2	A	101	PEE	O5-C30-O3-C3
2	E	102	PEE	C31-C30-O3-C3
2	D	102	PEE	C11-C10-O2-C2
2	E	102	PEE	O5-C30-O3-C3
2	B	102	PEE	O5-C30-O3-C3
2	D	102	PEE	O4-C10-O2-C2
2	D	101	PEE	O3P-C1-C2-O2
2	B	102	PEE	C10-C11-C12-C13
2	B	101	PEE	C10-C11-C12-C13
2	F	101	PEE	C10-C11-C12-C13
2	F	101	PEE	C30-C31-C32-C33
2	D	101	PEE	C10-C11-C12-C13
2	F	101	PEE	C1-O3P-P-O4P
2	D	101	PEE	C4-O4P-P-O3P
2	B	101	PEE	C1-O3P-P-O4P
2	B	103	PEE	C1-O3P-P-O4P
2	B	103	PEE	C4-O4P-P-O3P
2	B	102	PEE	C4-O4P-P-O3P
2	C	101	PEE	C1-O3P-P-O4P
2	C	102	PEE	C4-O4P-P-O3P
2	E	101	PEE	C31-C30-O3-C3
2	A	101	PEE	C12-C13-C14-C15
2	B	101	PEE	C14-C15-C16-C17
2	B	101	PEE	C19-C20-C21-C22
2	D	101	PEE	C18-C19-C20-C21
2	C	101	PEE	C32-C33-C34-C35
2	B	103	PEE	C18-C19-C20-C21
2	C	101	PEE	C19-C20-C21-C22
2	C	101	PEE	C37-C38-C39-C40
2	H	101	PEE	C34-C35-C36-C37
2	B	102	PEE	C41-C42-C43-C44
2	C	101	PEE	C39-C40-C41-C42
2	E	101	PEE	C33-C34-C35-C36
2	E	101	PEE	O5-C30-O3-C3
2	B	102	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	D	102	PEE	C12-C13-C14-C15
2	B	103	PEE	C20-C21-C22-C23
2	H	101	PEE	C35-C36-C37-C38
2	B	102	PEE	C20-C21-C22-C23
2	H	101	PEE	C19-C20-C21-C22
2	D	102	PEE	C43-C44-C45-C46
2	C	101	PEE	C35-C36-C37-C38
2	A	101	PEE	C40-C41-C42-C43
2	A	101	PEE	C41-C42-C43-C44
2	D	102	PEE	C10-C11-C12-C13
2	D	102	PEE	C18-C19-C20-C21
2	D	102	PEE	C21-C22-C23-C24
2	A	102	PEE	C21-C22-C23-C24
2	E	101	PEE	C14-C15-C16-C17
2	C	101	PEE	C12-C13-C14-C15
2	B	101	PEE	C39-C40-C41-C42
2	H	101	PEE	C20-C21-C22-C23
2	D	102	PEE	O4P-C4-C5-N
2	D	101	PEE	C35-C36-C37-C38
2	D	102	PEE	C17-C18-C19-C20
2	D	102	PEE	C33-C34-C35-C36
2	B	102	PEE	C37-C38-C39-C40
2	E	101	PEE	C40-C41-C42-C43
2	C	101	PEE	C23-C24-C25-C26
2	H	101	PEE	C31-C30-O3-C3
2	F	101	PEE	C18-C19-C20-C21
2	D	102	PEE	C38-C39-C40-C41
2	D	101	PEE	C39-C40-C41-C42
2	B	102	PEE	C31-C32-C33-C34
2	D	102	PEE	C1-C2-C3-O3
2	B	101	PEE	C17-C18-C19-C20
2	D	101	PEE	C16-C17-C18-C19
2	H	101	PEE	C11-C10-O2-C2
2	H	101	PEE	C14-C15-C16-C17
2	B	103	PEE	C33-C34-C35-C36
2	E	102	PEE	C33-C34-C35-C36
2	A	102	PEE	C34-C35-C36-C37
2	E	101	PEE	C43-C44-C45-C46
2	D	101	PEE	C30-C31-C32-C33
2	H	101	PEE	O4-C10-O2-C2
2	F	101	PEE	C41-C42-C43-C44
2	C	102	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	H	101	PEE	O5-C30-O3-C3
2	B	102	PEE	C39-C40-C41-C42
2	C	101	PEE	C17-C18-C19-C20
2	E	101	PEE	C19-C20-C21-C22
2	F	101	PEE	C31-C32-C33-C34
2	H	101	PEE	C22-C23-C24-C25
2	C	102	PEE	C21-C22-C23-C24
2	C	102	PEE	C19-C20-C21-C22
2	F	101	PEE	C31-C30-O3-C3
2	C	101	PEE	C42-C43-C44-C45
2	B	102	PEE	C19-C20-C21-C22
2	D	102	PEE	C22-C23-C24-C25
2	A	102	PEE	C12-C13-C14-C15
2	C	101	PEE	C13-C14-C15-C16
2	C	101	PEE	O3P-C1-C2-O2
2	E	101	PEE	C18-C19-C20-C21
2	A	101	PEE	C13-C14-C15-C16
2	D	102	PEE	C13-C14-C15-C16
2	B	102	PEE	C42-C43-C44-C45
2	F	101	PEE	C19-C20-C21-C22
2	B	101	PEE	C40-C41-C42-C43
2	D	102	PEE	C40-C41-C42-C43
2	A	102	PEE	C4-O4P-P-O3P
2	A	101	PEE	C4-O4P-P-O3P
2	H	101	PEE	C11-C12-C13-C14
2	F	101	PEE	O5-C30-O3-C3
2	C	102	PEE	O3P-C1-C2-C3
2	B	101	PEE	C36-C37-C38-C39
2	C	101	PEE	C22-C23-C24-C25
2	A	101	PEE	C14-C15-C16-C17
2	D	101	PEE	C34-C35-C36-C37
2	B	101	PEE	C23-C24-C25-C26
2	B	102	PEE	C40-C41-C42-C43
2	B	103	PEE	C17-C18-C19-C20
2	C	101	PEE	C1-C2-C3-O3
2	A	102	PEE	C31-C32-C33-C34
2	H	101	PEE	C42-C43-C44-C45
2	D	101	PEE	C44-C45-C46-C47
2	E	101	PEE	C37-C38-C39-C40
2	D	101	PEE	C17-C18-C19-C20
2	C	101	PEE	C41-C42-C43-C44
2	C	101	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
2	D	101	PEE	C19-C20-C21-C22
2	B	101	PEE	C1-C2-O2-C10
2	B	101	PEE	C16-C17-C18-C19
2	C	102	PEE	C15-C16-C17-C18
2	D	101	PEE	C32-C33-C34-C35
2	B	103	PEE	C16-C17-C18-C19
2	A	101	PEE	C21-C22-C23-C24
2	D	102	PEE	C31-C30-O3-C3
2	D	102	PEE	C30-C31-C32-C33
2	B	101	PEE	C11-C12-C13-C14
2	F	101	PEE	O3P-C1-C2-C3
2	D	101	PEE	O3P-C1-C2-C3
2	A	101	PEE	C19-C20-C21-C22
2	B	101	PEE	C42-C43-C44-C45
2	F	101	PEE	C37-C38-C39-C40
2	B	102	PEE	C17-C18-C19-C20
2	H	101	PEE	C1-C2-C3-O3
2	E	101	PEE	C24-C25-C26-C27
2	F	101	PEE	C34-C35-C36-C37
2	B	101	PEE	C4-O4P-P-O3P
2	A	101	PEE	C1-O3P-P-O4P
2	D	101	PEE	C31-C32-C33-C34
2	A	101	PEE	C36-C37-C38-C39
2	B	102	PEE	O3P-C1-C2-O2
2	D	102	PEE	O2-C10-C11-C12
2	A	101	PEE	C39-C40-C41-C42
2	B	102	PEE	O2-C2-C3-O3
2	B	101	PEE	C24-C25-C26-C27
2	B	101	PEE	C2-C1-O3P-P
2	B	102	PEE	C18-C19-C20-C21
2	E	102	PEE	C34-C35-C36-C37
2	D	102	PEE	C24-C25-C26-C27
2	D	102	PEE	O5-C30-O3-C3
2	C	101	PEE	O3P-C1-C2-C3
2	A	101	PEE	C33-C34-C35-C36
2	F	101	PEE	C13-C14-C15-C16
2	B	103	PEE	C14-C15-C16-C17
2	B	102	PEE	C11-C10-O2-C2
2	B	101	PEE	C21-C22-C23-C24
2	A	101	PEE	C11-C12-C13-C14
2	F	101	PEE	O3P-C1-C2-O2
2	A	102	PEE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
2	D	102	PEE	O2-C2-C3-O3
2	H	101	PEE	O2-C2-C3-O3
2	D	102	PEE	C36-C37-C38-C39
2	C	101	PEE	C15-C16-C17-C18
2	B	102	PEE	O4-C10-O2-C2
2	D	101	PEE	C43-C44-C45-C46
2	F	101	PEE	C36-C37-C38-C39
2	E	102	PEE	C35-C36-C37-C38
2	E	101	PEE	C41-C42-C43-C44
2	H	101	PEE	C15-C16-C17-C18
2	E	101	PEE	C4-O4P-P-O3P
2	D	101	PEE	C42-C43-C44-C45
2	B	102	PEE	C11-C12-C13-C14
2	D	101	PEE	C4-O4P-P-O2P
2	B	101	PEE	C1-O3P-P-O1P
2	B	101	PEE	C1-O3P-P-O2P
2	B	101	PEE	C4-O4P-P-O1P
2	B	103	PEE	C1-O3P-P-O1P
2	A	102	PEE	C1-O3P-P-O2P
2	A	102	PEE	C4-O4P-P-O2P
2	C	102	PEE	C1-O3P-P-O2P
2	B	101	PEE	C43-C44-C45-C46
2	E	101	PEE	C5-C4-O4P-P
2	C	102	PEE	O3P-C1-C2-O2
2	A	102	PEE	C39-C40-C41-C42
2	A	101	PEE	C15-C16-C17-C18
2	D	101	PEE	O2-C2-C3-O3
2	C	101	PEE	O2-C2-C3-O3
2	A	101	PEE	C42-C43-C44-C45
2	B	102	PEE	C2-C1-O3P-P
2	A	101	PEE	C32-C33-C34-C35
2	A	101	PEE	C10-C11-C12-C13
2	D	101	PEE	C23-C24-C25-C26
2	F	101	PEE	C14-C15-C16-C17
2	E	101	PEE	C21-C22-C23-C24
2	H	101	PEE	C17-C18-C19-C20
2	B	103	PEE	C34-C35-C36-C37
2	E	101	PEE	C12-C13-C14-C15
2	C	102	PEE	C1-O3P-P-O4P
2	B	102	PEE	C1-C2-C3-O3
2	C	101	PEE	C21-C22-C23-C24
2	E	101	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
2	E	101	PEE	C39-C40-C41-C42
2	B	103	PEE	C31-C32-C33-C34
2	D	101	PEE	C22-C23-C24-C25
2	H	101	PEE	C38-C39-C40-C41
2	B	101	PEE	C37-C38-C39-C40
2	A	102	PEE	C19-C20-C21-C22
2	A	102	PEE	C18-C19-C20-C21
2	B	102	PEE	C14-C15-C16-C17
2	C	102	PEE	C13-C14-C15-C16
2	B	102	PEE	C43-C44-C45-C46
2	B	102	PEE	C44-C45-C46-C47
2	E	102	PEE	C38-C39-C40-C41
2	C	102	PEE	O2-C10-C11-C12
2	C	101	PEE	C44-C45-C46-C47
2	B	103	PEE	C11-C12-C13-C14
2	E	102	PEE	C37-C38-C39-C40
2	B	103	PEE	C22-C23-C24-C25
2	D	101	PEE	C1-C2-C3-O3
2	B	102	PEE	C34-C35-C36-C37
2	F	101	PEE	C35-C36-C37-C38
2	E	101	PEE	C31-C32-C33-C34
2	C	101	PEE	C33-C34-C35-C36
2	B	102	PEE	O3P-C1-C2-C3
2	C	102	PEE	O3-C30-C31-C32
2	E	101	PEE	O2-C2-C3-O3
2	D	102	PEE	C34-C35-C36-C37
2	E	101	PEE	C11-C12-C13-C14
2	E	101	PEE	C17-C18-C19-C20
2	B	103	PEE	C15-C16-C17-C18
2	A	102	PEE	C44-C45-C46-C47
2	A	102	PEE	C43-C44-C45-C46
2	B	101	PEE	O2-C2-C3-O3
2	E	102	PEE	C2-C3-O3-C30
2	B	102	PEE	C21-C22-C23-C24
2	E	102	PEE	O3-C30-C31-C32
2	C	101	PEE	O2-C10-C11-C12
2	A	102	PEE	C33-C34-C35-C36
2	B	102	PEE	C24-C25-C26-C27
2	C	102	PEE	C22-C23-C24-C25
2	C	102	PEE	C17-C18-C19-C20
2	A	101	PEE	C31-C32-C33-C34
2	D	102	PEE	O4-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	102	PEE	C1-O3P-P-O4P
2	C	101	PEE	C2-C3-O3-C30
2	C	101	PEE	O4-C10-C11-C12
2	F	101	PEE	C16-C17-C18-C19
2	C	102	PEE	C24-C25-C26-C27
2	A	101	PEE	O4P-C4-C5-N
2	B	103	PEE	C5-C4-O4P-P
2	A	101	PEE	C5-C4-O4P-P
2	C	102	PEE	C5-C4-O4P-P
2	F	101	PEE	C38-C39-C40-C41
2	C	101	PEE	C20-C21-C22-C23
2	A	102	PEE	C40-C41-C42-C43
2	E	102	PEE	O5-C30-C31-C32
2	B	101	PEE	C38-C39-C40-C41
2	B	101	PEE	C41-C42-C43-C44
2	C	101	PEE	C14-C15-C16-C17
2	E	102	PEE	C30-C31-C32-C33
2	E	101	PEE	O2-C10-C11-C12

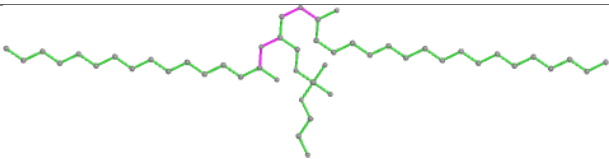
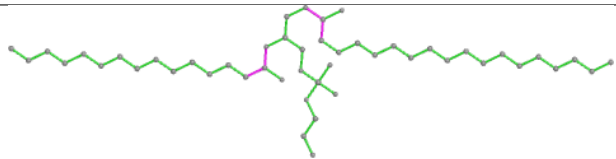
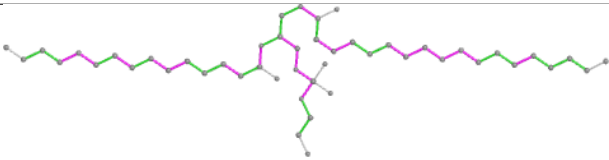
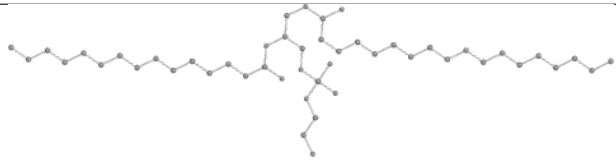
There are no ring outliers.

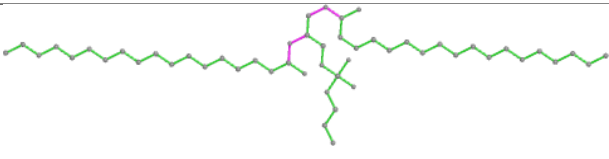
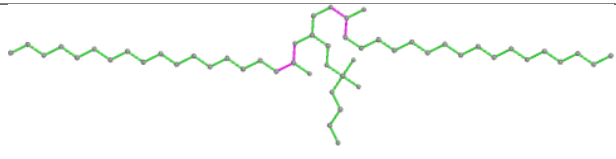
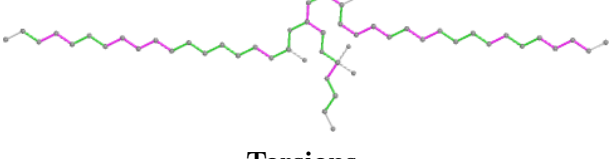
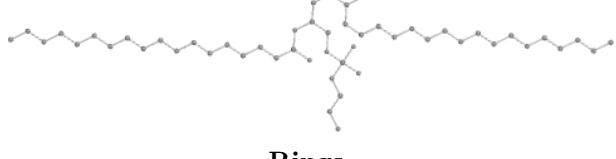
7 monomers are involved in 10 short contacts:

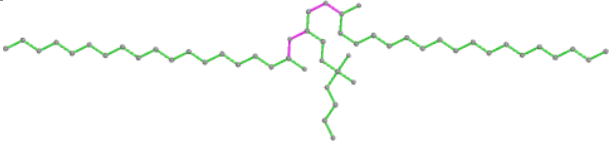
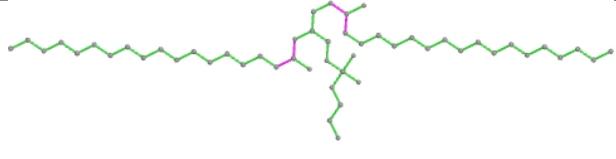
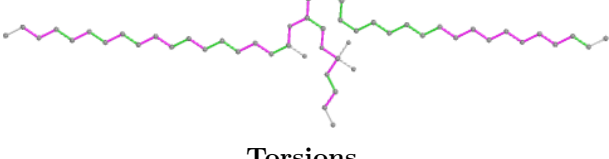
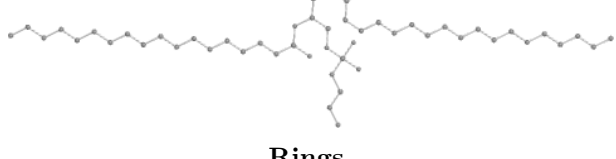
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	101	PEE	1	0
2	D	101	PEE	2	0
2	B	101	PEE	1	0
2	E	102	PEE	3	0
2	A	102	PEE	1	0
2	E	101	PEE	2	0
2	A	101	PEE	2	0

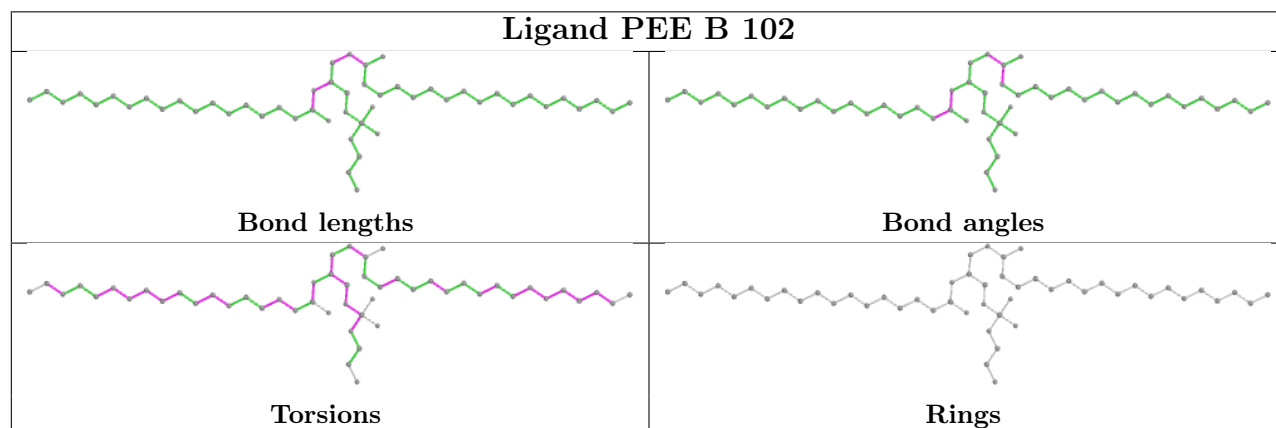
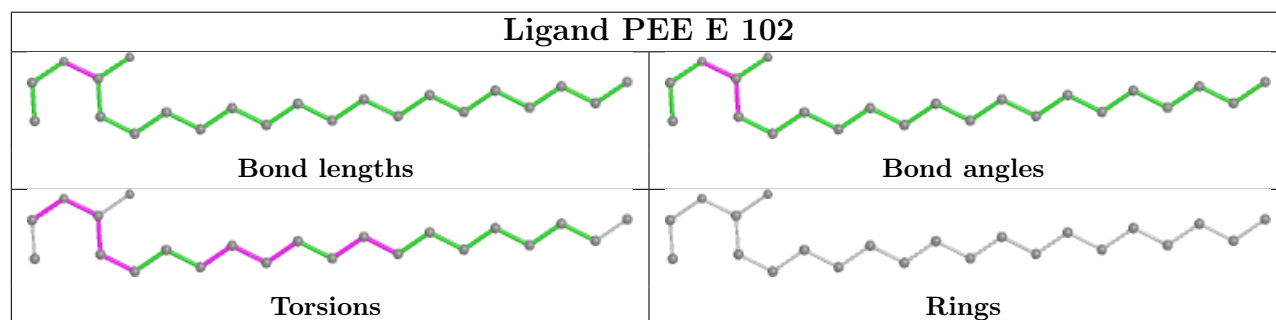
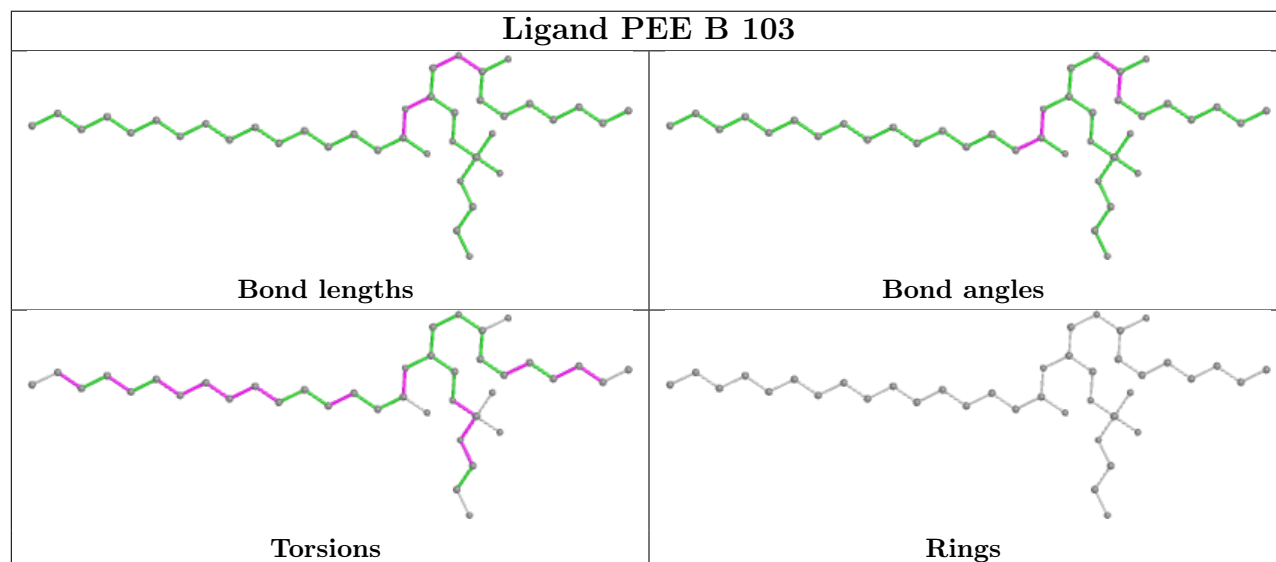
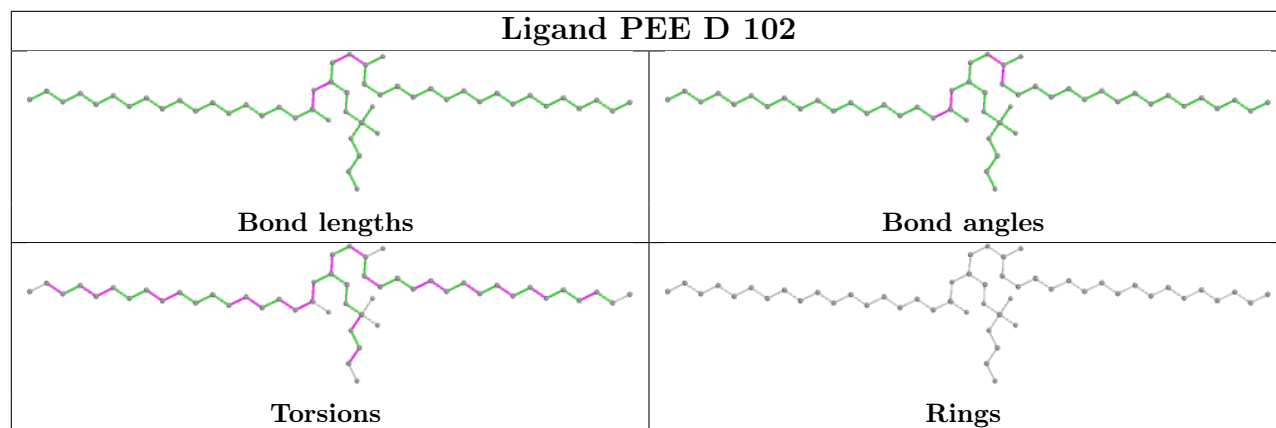
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

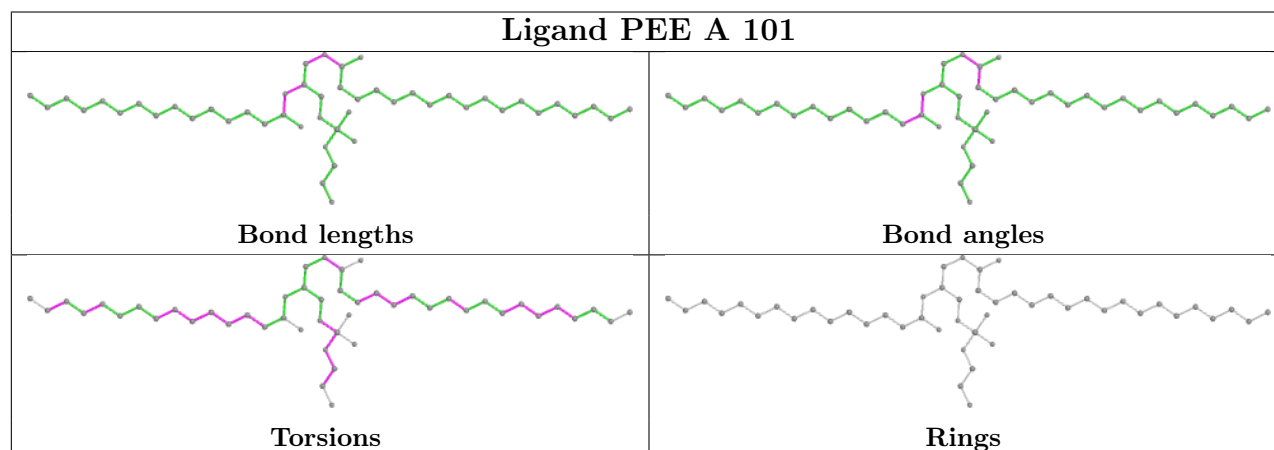
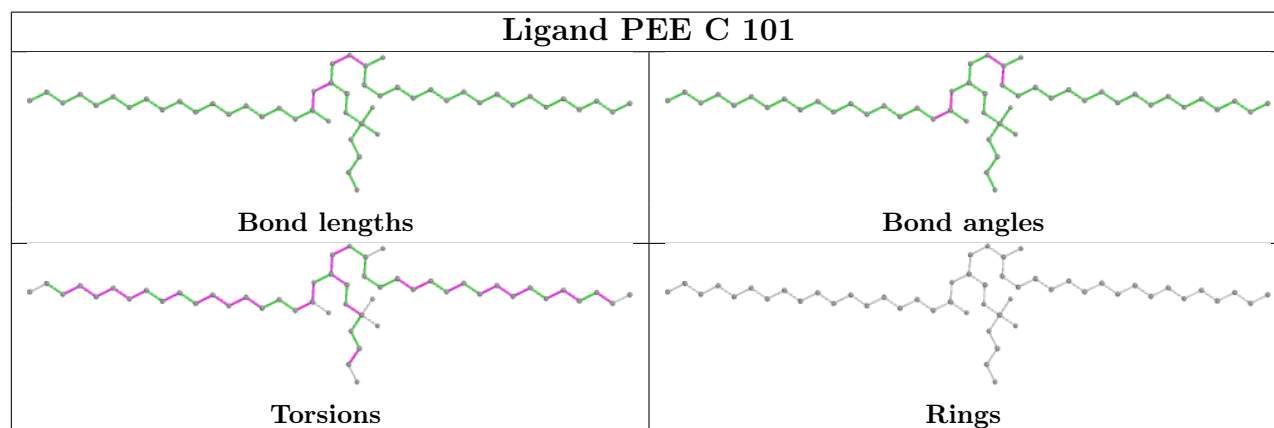
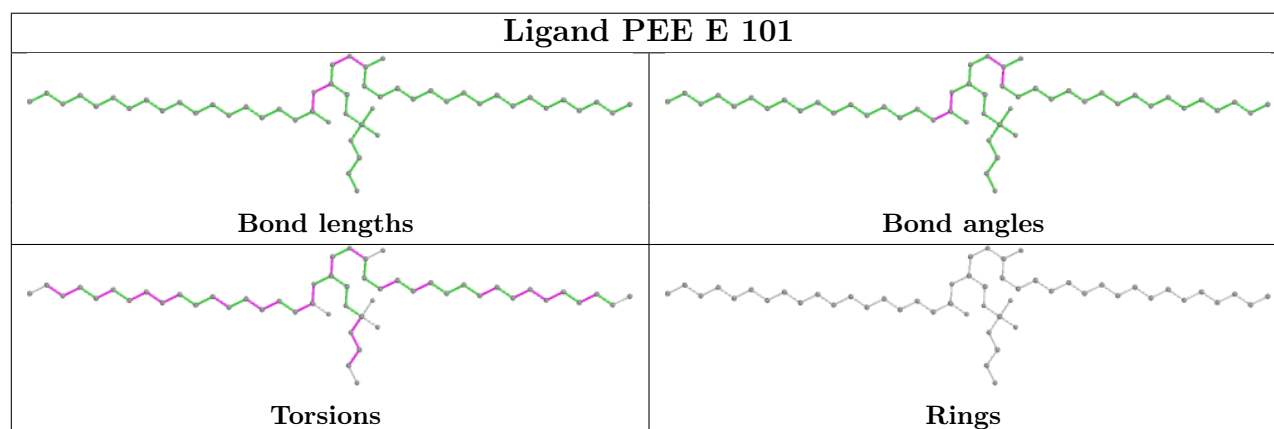
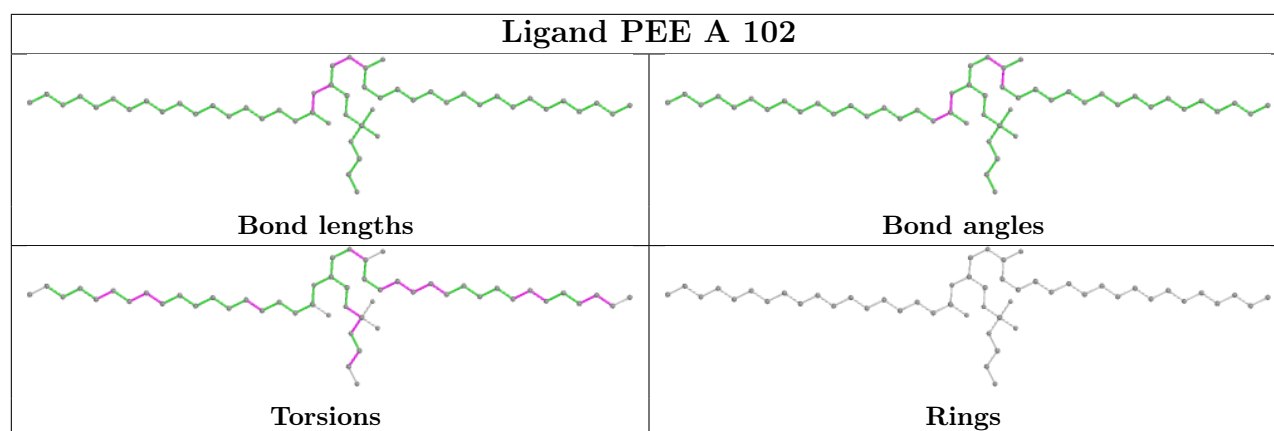
equivalents in the CSD to analyse the geometry.

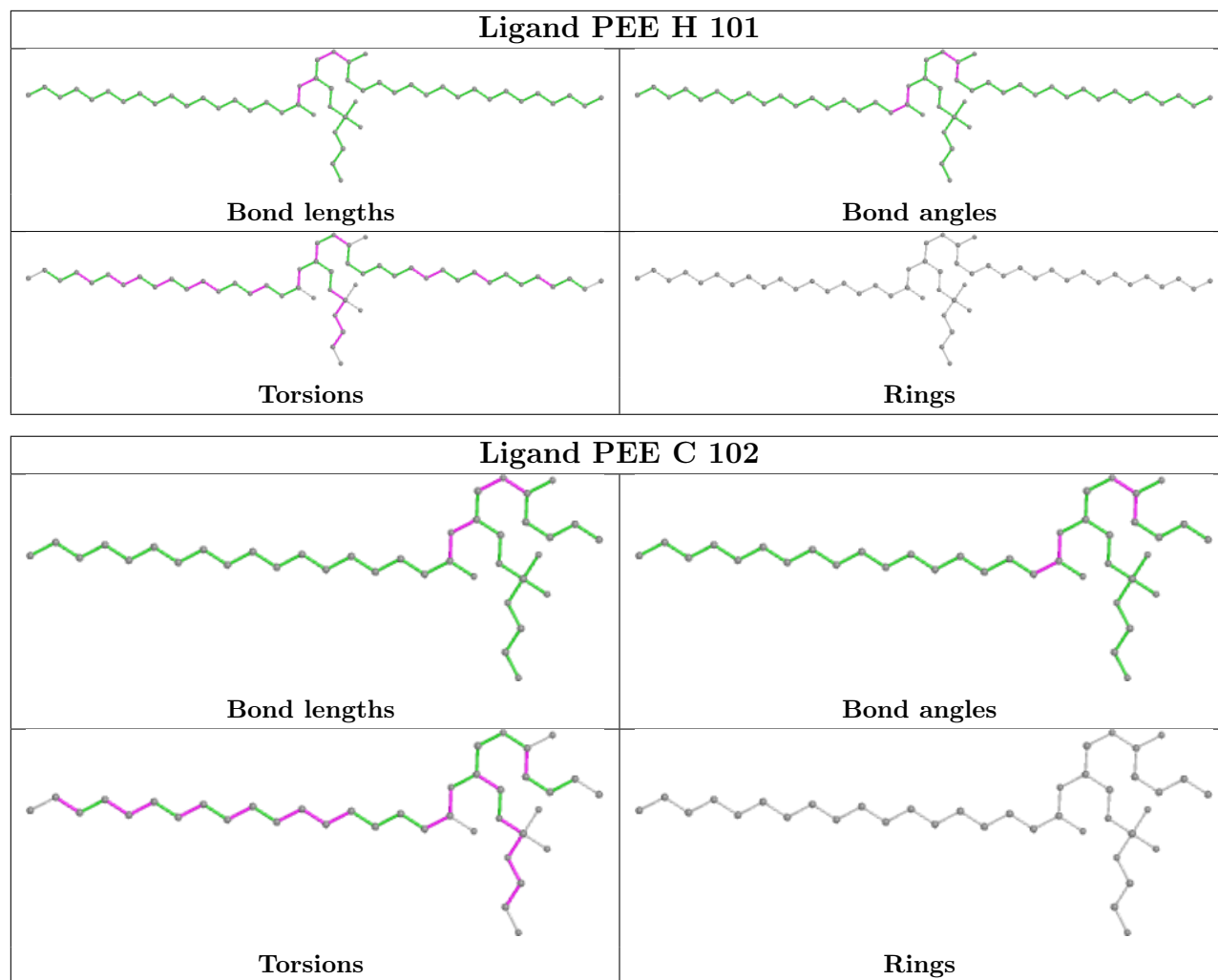
Ligand PEE F 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE D 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings







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	78/87 (89%)	0.81	5 (6%) 19 25	59, 91, 130, 145	0
1	B	77/87 (88%)	0.91	8 (10%) 6 9	59, 90, 133, 150	0
1	C	80/87 (91%)	0.80	4 (5%) 28 36	64, 86, 118, 161	0
1	D	79/87 (90%)	0.87	8 (10%) 7 10	76, 104, 146, 175	0
1	E	81/87 (93%)	0.90	7 (8%) 10 14	57, 83, 113, 144	0
1	F	78/87 (89%)	0.77	7 (8%) 9 13	73, 101, 134, 145	0
1	G	78/87 (89%)	1.23	15 (19%) 1 1	81, 135, 181, 272	0
1	H	78/87 (89%)	0.96	10 (12%) 3 5	73, 105, 175, 192	0
All	All	629/696 (90%)	0.91	64 (10%) 6 10	57, 97, 156, 272	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	67	PHE	7.7
1	G	71	ILE	5.9
1	H	8	LEU	5.3
1	G	60	LEU	4.5
1	G	62	LEU	4.3
1	H	71	ILE	4.1
1	G	72	ASN	4.1
1	F	76	ILE	4.0
1	G	58	VAL	3.8
1	G	64	ILE	3.7
1	G	75	ALA	3.3
1	B	24	LYS	3.3
1	D	58	VAL	3.2
1	B	28	PHE	3.2
1	H	80	VAL	3.1
1	H	79	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	28	PHE	3.0
1	D	55	VAL	2.9
1	F	8	LEU	2.9
1	A	80	VAL	2.9
1	C	36	LEU	2.8
1	F	60	LEU	2.8
1	D	56	LEU	2.8
1	E	49	VAL	2.7
1	G	29	GLN	2.7
1	G	19	LEU	2.7
1	B	80	VAL	2.7
1	G	63	VAL	2.7
1	D	62	LEU	2.6
1	H	11	GLU	2.6
1	G	45	LEU	2.6
1	G	77	CYS	2.6
1	A	48	LEU	2.6
1	E	23	THR	2.5
1	B	71	ILE	2.5
1	A	19	LEU	2.5
1	B	15	ILE	2.5
1	B	76	ILE	2.5
1	C	19	LEU	2.5
1	H	81	GLY	2.5
1	D	36	LEU	2.5
1	E	64	ILE	2.4
1	B	45	LEU	2.4
1	E	67	PHE	2.4
1	E	32	ILE	2.4
1	H	76	ILE	2.4
1	F	47	LEU	2.4
1	E	71	ILE	2.4
1	F	32	ILE	2.3
1	A	45	LEU	2.3
1	D	71	ILE	2.3
1	C	28	PHE	2.3
1	F	59	ALA	2.3
1	A	64	ILE	2.2
1	D	19	LEU	2.2
1	G	28	PHE	2.2
1	H	82	LEU	2.2
1	H	84	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	67	PHE	2.1
1	C	32	ILE	2.1
1	G	16	VAL	2.1
1	E	28	PHE	2.0
1	D	45	LEU	2.0
1	B	16	VAL	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, 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.

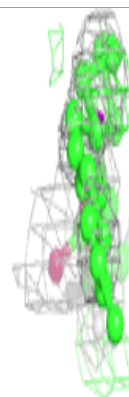
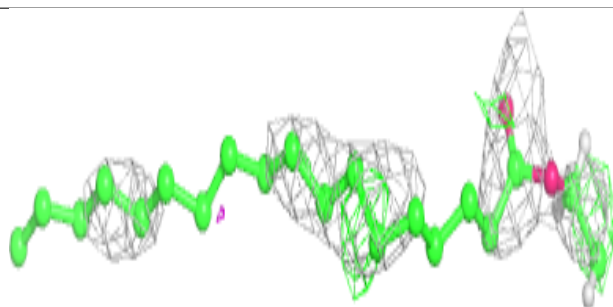
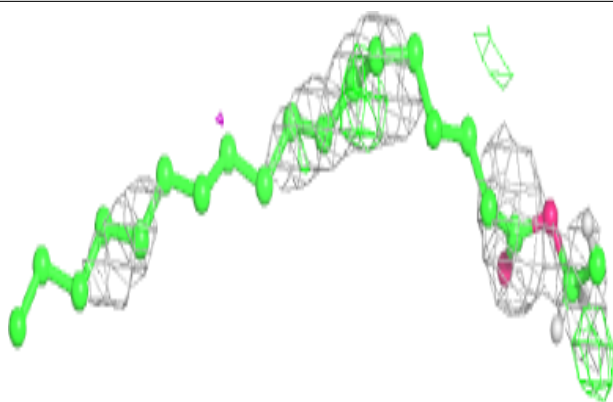
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEE	E	102	22/51	0.58	0.53	90,125,147,150	0
2	PEE	A	101	48/51	0.60	0.53	84,122,170,181	0
2	PEE	B	103	39/51	0.63	0.67	126,155,182,189	0
2	PEE	C	102	38/51	0.65	0.33	109,148,189,190	0
2	PEE	B	101	51/51	0.68	0.39	81,113,156,178	0
2	PEE	F	101	48/51	0.69	0.58	122,157,178,203	0
2	PEE	B	102	51/51	0.70	0.52	119,151,166,181	0
2	PEE	A	102	51/51	0.71	0.57	103,140,161,187	0
2	PEE	D	102	51/51	0.72	0.61	128,157,187,191	0
2	PEE	H	101	51/51	0.77	0.43	117,145,180,183	0
2	PEE	E	101	51/51	0.78	0.77	116,152,173,198	0
2	PEE	D	101	51/51	0.80	0.50	113,146,165,175	0
2	PEE	C	101	51/51	0.84	0.37	81,108,138,144	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.

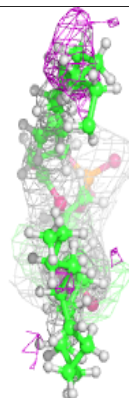
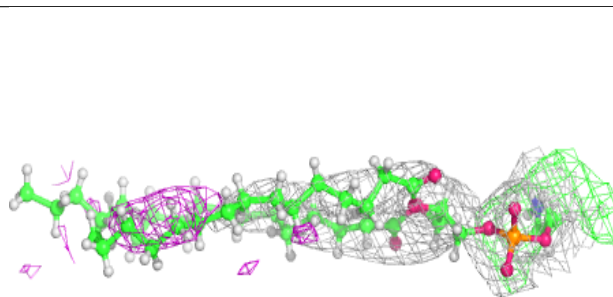
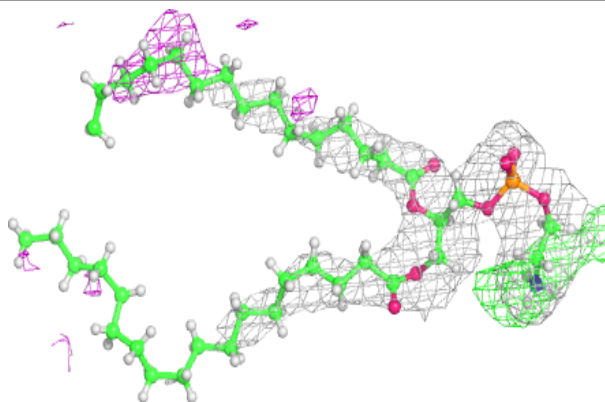
Electron density around PEE E 102:

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



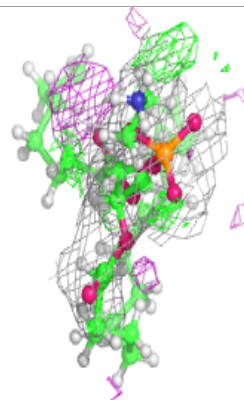
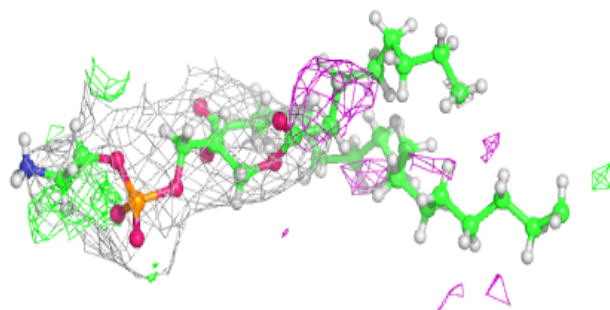
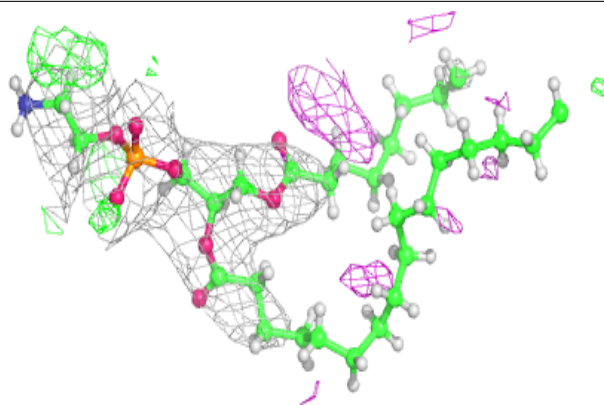
Electron density around PEE A 101:

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

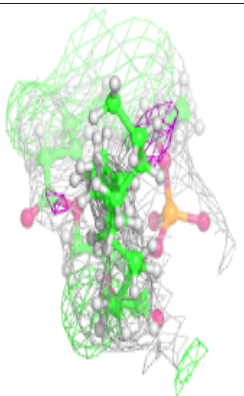
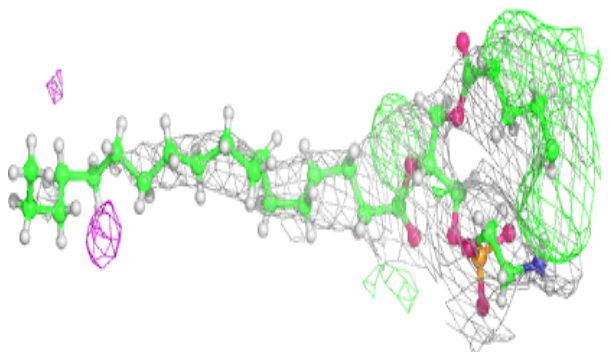
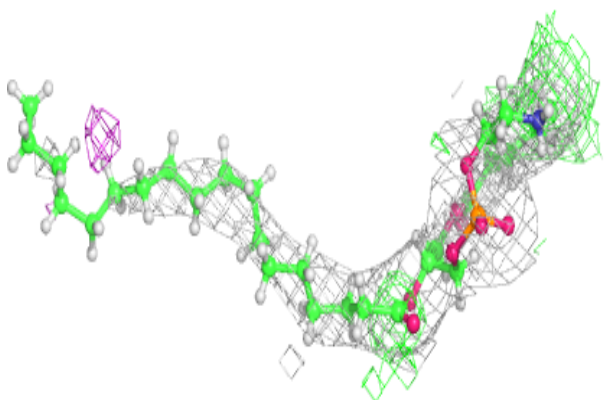


Electron density around PEE B 103:

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

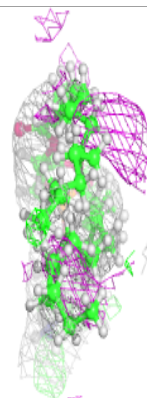
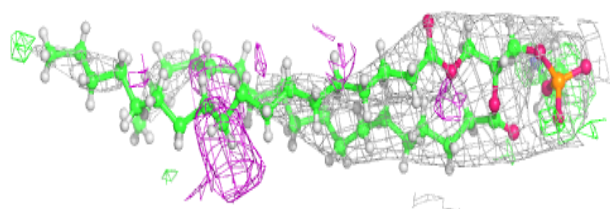
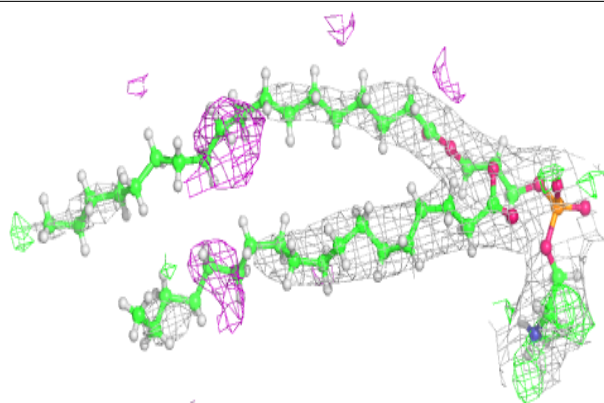
**Electron density around PEE C 102:**

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

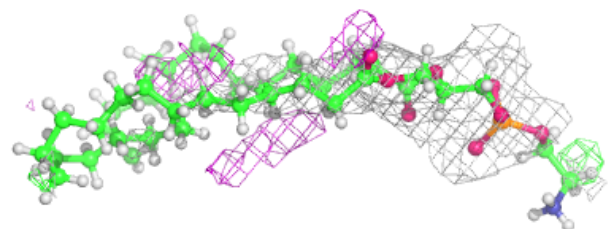
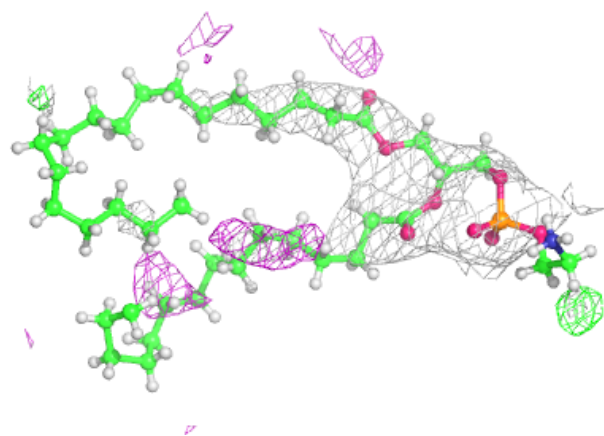


Electron density around PEE B 101:

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

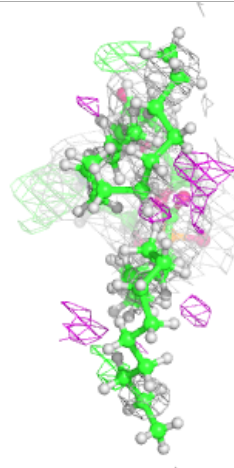
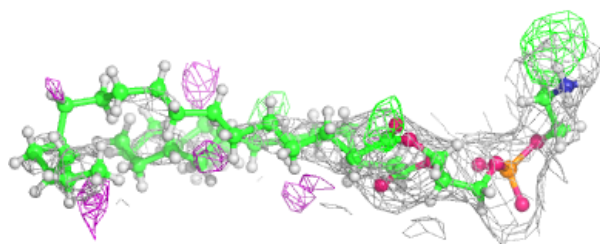
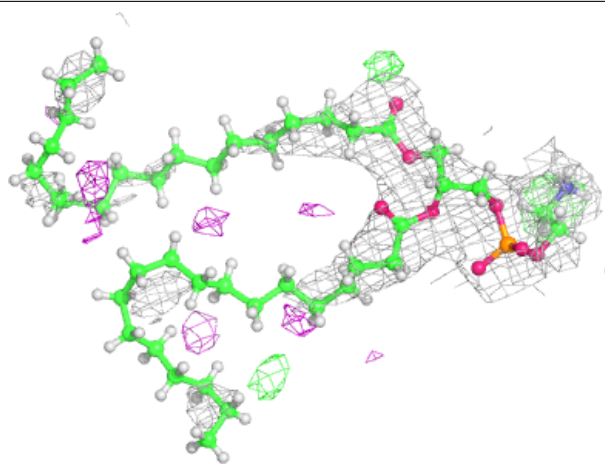
**Electron density around PEE F 101:**

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



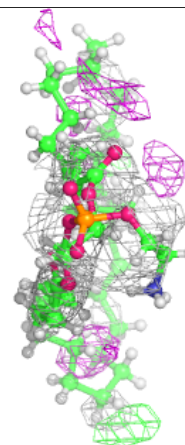
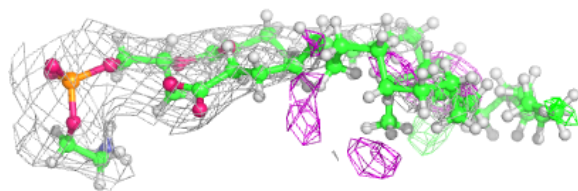
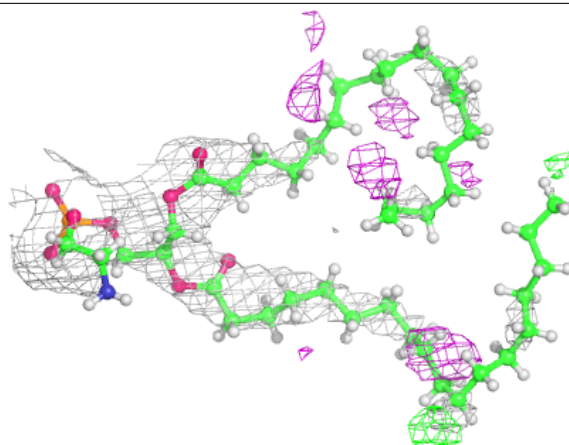
Electron density around PEE B 102:

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



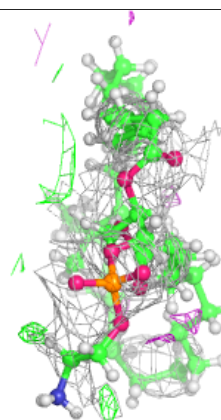
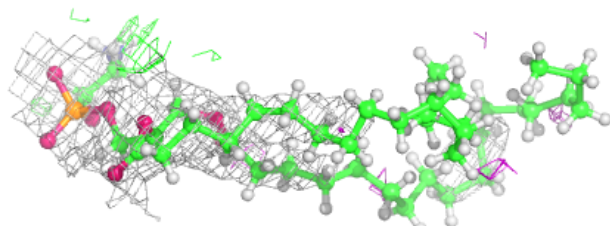
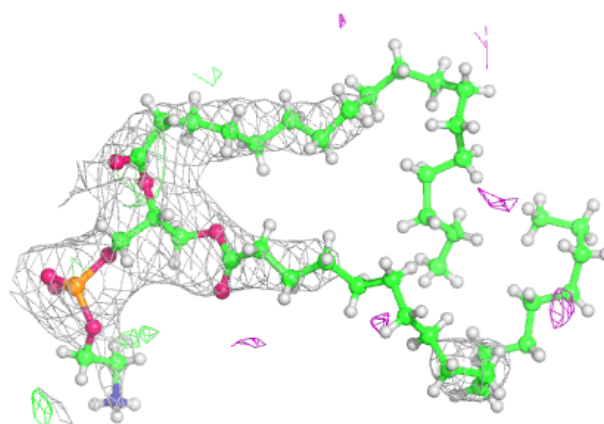
Electron density around PEE A 102:

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

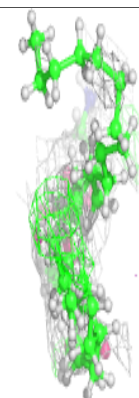
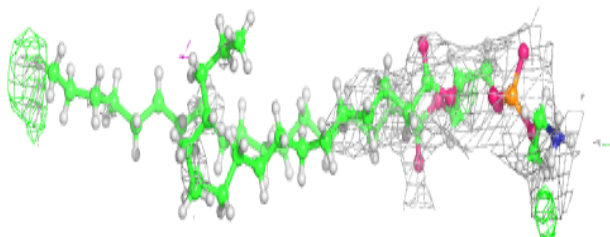
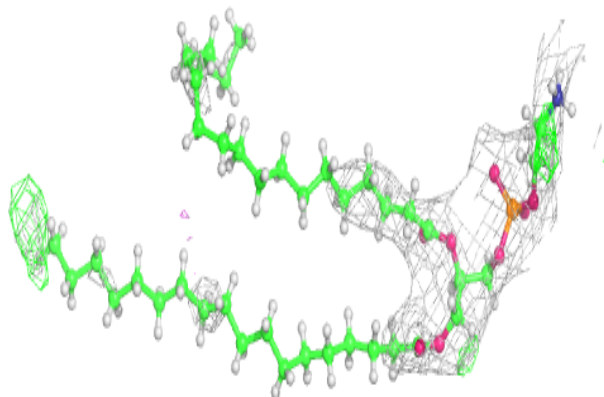


Electron density around PEE D 102:

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

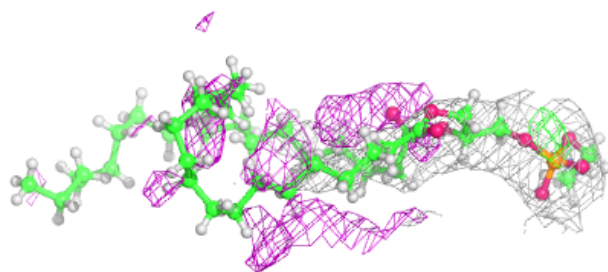
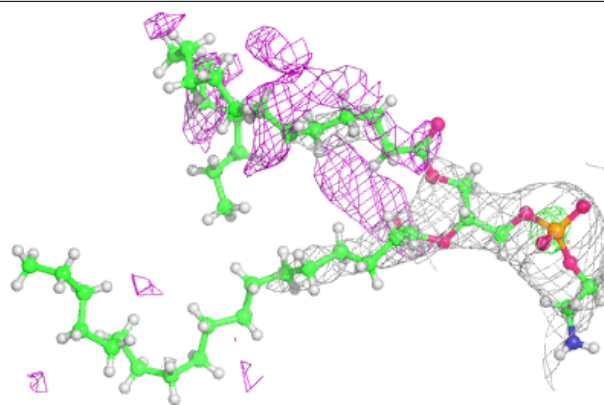
**Electron density around PEE H 101:**

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



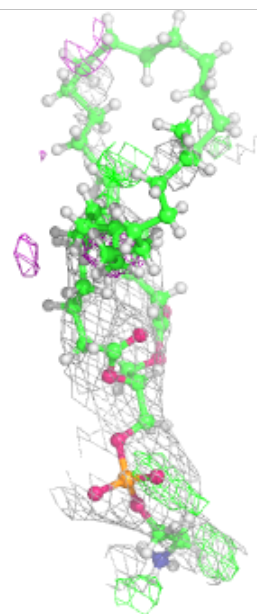
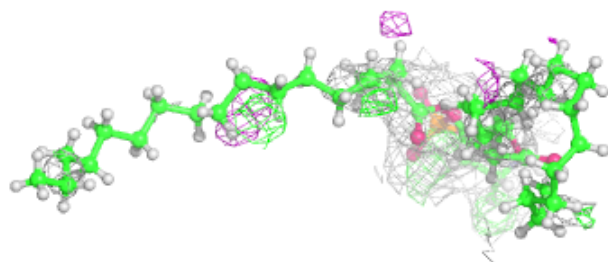
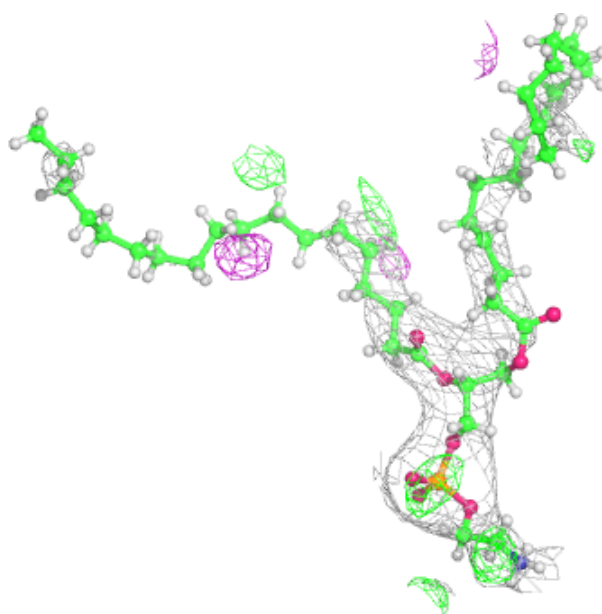
Electron density around PEE E 101:

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



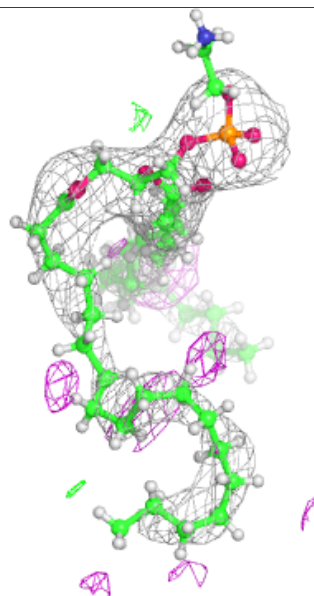
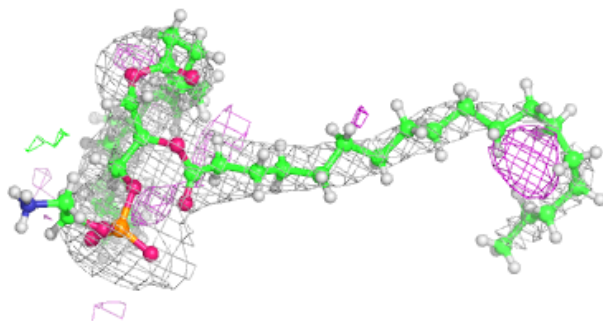
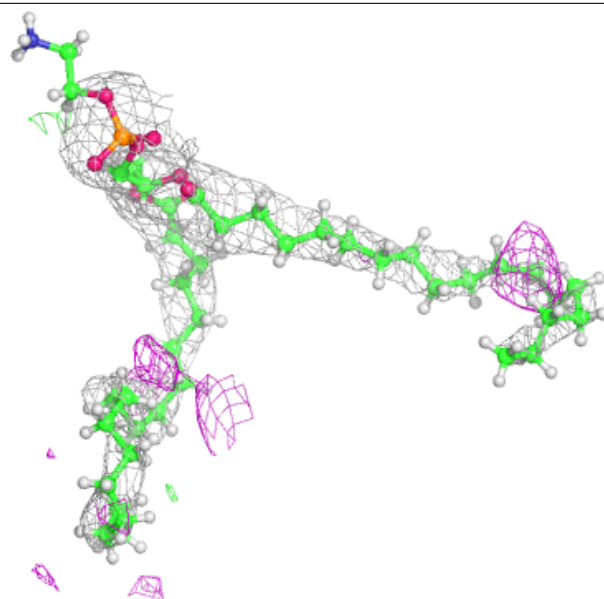
Electron density around PEE D 101:

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



Electron density around PEE C 101:

$2mF_o-DF_c$ (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.