Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 01:00 PM EST

PDB ID	:	7SFJ
EMDB ID	:	EMD-25079
Title	:	ChRmine in MSP1E3D1 lipid nanodisc
Authors	:	Tucker, K.; Brohawn, S.
Deposited on	:	2021-10-04
Resolution	:	2.74 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

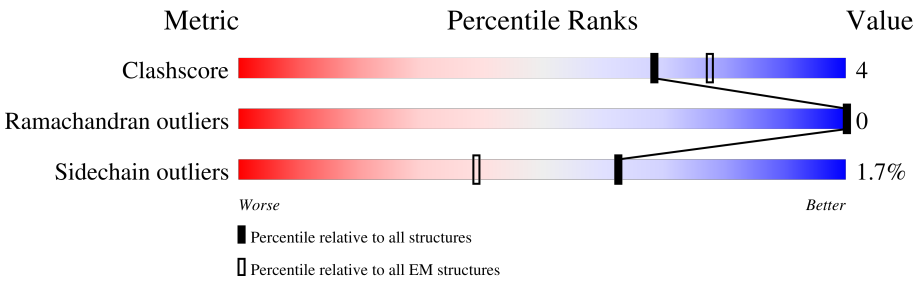
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	318	81% 8% 11%
1	B	318	80% 9% 11%
1	C	318	80% 9% 11%

2 Entry composition (i)

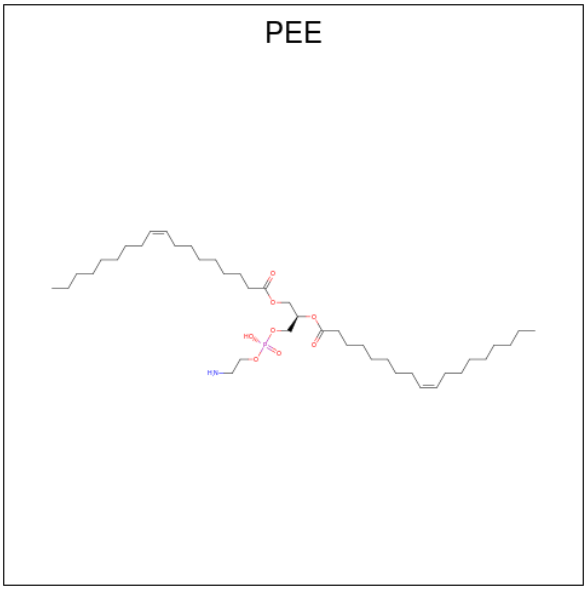
There are 4 unique types of molecules in this entry. The entry contains 7377 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ChRmine.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	284	2299	1520	365	398	16	0	0
1	B	284	2299	1520	365	398	16	0	0
1	C	284	2299	1520	365	398	16	0	0

- Molecule 2 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	148	130	1	16	1	0
2	A	1	148	130	1	16	1	0
2	A	1	148	130	1	16	1	0

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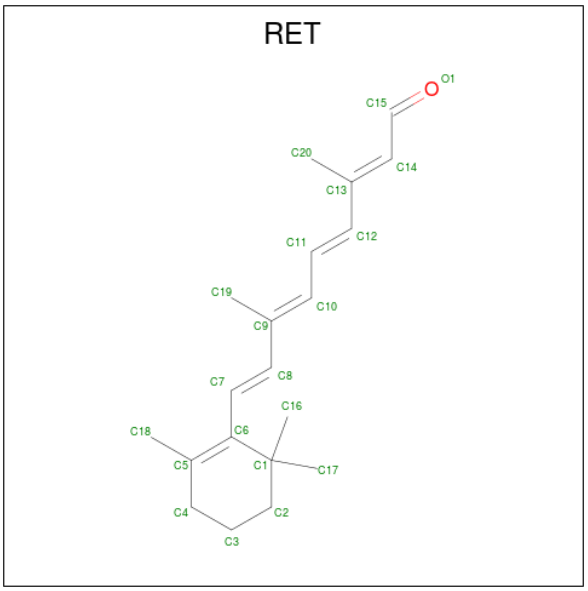
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	148	130	1	16	1	0
			Total	C	N	O	P	
2	A	1	148	130	1	16	1	0
			Total	C	N	O	P	
2	A	1	148	130	1	16	1	0
			Total	C	N	O	P	
2	A	1	148	130	1	16	1	0
			Total	C	N	O	P	
2	A	1	148	130	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	B	1	139	121	1	16	1	0
			Total	C	N	O	P	
2	C	1	130	112	1	16	1	0
			Total	C	N	O	P	
2	C	1	130	112	1	16	1	0
			Total	C	N	O	P	
2	C	1	130	112	1	16	1	0
			Total	C	N	O	P	
2	C	1	130	112	1	16	1	0
			Total	C	N	O	P	
2	C	1	130	112	1	16	1	0
			Total	C	N	O	P	
2	C	1	130	112	1	16	1	0

- Molecule 3 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
3	A	1	20	20	0
			Total	C	
3	B	1	20	20	0
			Total	C	
3	C	1	20	20	0

- Molecule 4 is water.

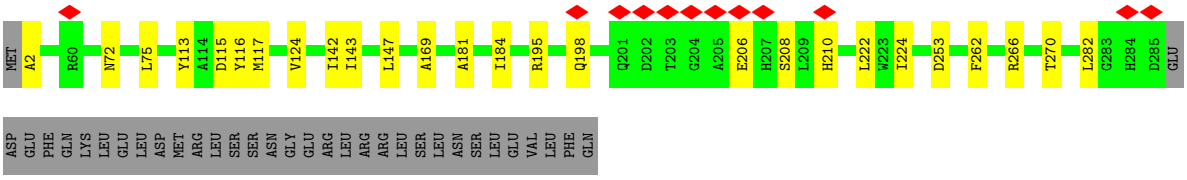
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
4	A	1	1	1	0
			Total	O	
4	B	1	1	1	0
			Total	O	
4	C	1	1	1	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

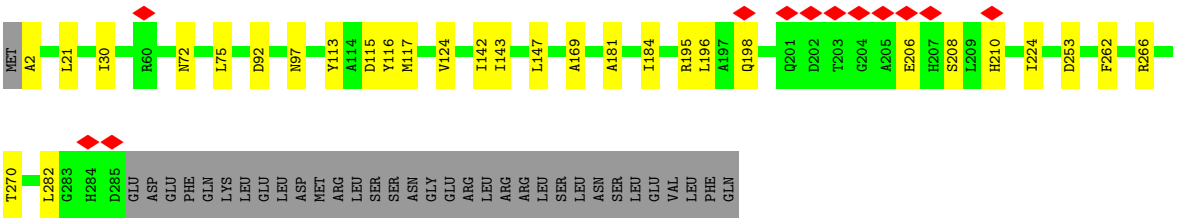
- Molecule 1: ChRmine

Chain A:



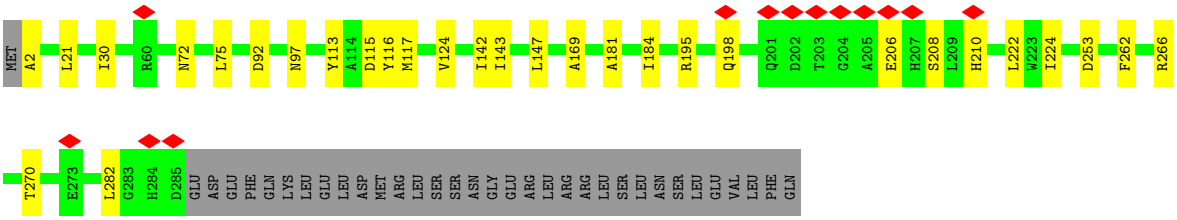
- Molecule 1: ChRmine

Chain B:



- Molecule 1: ChRmine

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	81839	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.465	Depositor
Minimum map value	-4.622	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	250.14, 250.14, 250.14	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.137, 1.137, 1.137	Depositor

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, RET, AYA

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	0.27	0/2368	0.44	0/3220
1	B	0.27	0/2368	0.44	0/3220
1	C	0.27	0/2368	0.44	0/3220
All	All	0.27	0/7104	0.44	0/9660

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	2299	0	2201	13	0
1	B	2299	0	2201	15	0
1	C	2299	0	2201	15	0
2	A	148	0	244	5	0
2	B	139	0	227	5	0
2	C	130	0	210	3	0
3	A	20	0	27	2	0
3	B	20	0	27	2	0
3	C	20	0	27	2	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	7377	0	7365	56	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 (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG21	1:A:143:ILE:HG13	1.78	0.65
1:B:124:VAL:HG21	1:B:143:ILE:HG13	1.78	0.65
1:C:124:VAL:HG21	1:C:143:ILE:HG13	1.78	0.65
1:A:195:ARG:NH1	1:A:282:LEU:O	2.31	0.64
1:B:195:ARG:NH1	1:B:282:LEU:O	2.31	0.64
1:C:195:ARG:NH1	1:C:282:LEU:O	2.31	0.64
1:A:169:ALA:HA	2:A:401:PEE:H28	1.82	0.62
1:B:169:ALA:HA	2:B:401:PEE:H28	1.81	0.61
1:C:169:ALA:HA	2:C:403:PEE:H28	1.82	0.61
2:A:405:PEE:H37	2:A:405:PEE:H66	1.89	0.55
2:B:404:PEE:H37	2:B:404:PEE:H66	1.89	0.53
2:C:406:PEE:H66	2:C:406:PEE:H37	1.89	0.53
1:A:142:ILE:HG21	1:A:181:ALA:HB2	1.91	0.53
1:B:142:ILE:HG21	1:B:181:ALA:HB2	1.91	0.52
1:C:142:ILE:HG21	1:C:181:ALA:HB2	1.91	0.52
1:A:115:ASP:N	1:A:115:ASP:OD1	2.43	0.49
1:C:115:ASP:OD1	1:C:115:ASP:N	2.42	0.47
1:B:116:TYR:OH	1:B:253:ASP:OD2	2.32	0.47
1:B:115:ASP:OD1	1:B:115:ASP:N	2.42	0.47
1:C:116:TYR:OH	1:C:253:ASP:OD2	2.32	0.47
1:A:116:TYR:OH	1:A:253:ASP:OD2	2.32	0.46
1:B:195:ARG:O	1:B:198:GLN:HG3	2.16	0.46
1:A:195:ARG:O	1:A:198:GLN:HG3	2.16	0.46
1:C:195:ARG:O	1:C:198:GLN:HG3	2.16	0.45
3:B:405:RET:H7	3:B:405:RET:H181	1.70	0.44
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.89	0.43
1:C:113:TYR:HB3	1:C:147:LEU:HD12	2.00	0.43
1:C:72:ASN:O	1:C:75:LEU:HB3	2.19	0.43
1:A:113:TYR:HB3	1:A:147:LEU:HD12	2.00	0.43
1:B:113:TYR:HB3	1:B:147:LEU:HD12	2.00	0.43
2:B:404:PEE:H52	2:B:404:PEE:H59	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:406:PEE:H52	2:C:406:PEE:H59	1.83	0.43
1:B:72:ASN:O	1:B:75:LEU:HB3	2.19	0.43
3:C:407:RET:H181	3:C:407:RET:H7	1.70	0.42
1:A:72:ASN:O	1:A:75:LEU:HB3	2.19	0.42
3:A:406:RET:H161	3:A:406:RET:H8	2.01	0.42
3:B:405:RET:H161	3:B:405:RET:H8	2.01	0.42
1:B:206:GLU:OE2	1:B:210:HIS:NE2	2.53	0.42
1:A:206:GLU:OE2	1:A:210:HIS:NE2	2.53	0.41
3:A:406:RET:H181	3:A:406:RET:H7	1.70	0.41
3:C:407:RET:H161	3:C:407:RET:H8	2.01	0.41
1:C:206:GLU:OE2	1:C:210:HIS:NE2	2.53	0.41
2:A:409:PEE:H69	1:B:184:ILE:HD12	2.03	0.41
2:B:408:PEE:H69	1:C:184:ILE:HD12	2.03	0.41
1:B:196:LEU:HD13	1:B:282:LEU:HD11	2.03	0.41
2:B:404:PEE:H17	2:B:404:PEE:H8	2.03	0.41
1:C:208:SER:HB3	1:C:270:THR:HG23	2.03	0.41
1:C:21:LEU:O	1:C:97:ASN:N	2.49	0.40
2:A:405:PEE:H31	2:A:405:PEE:H38	1.91	0.40
1:B:30:ILE:HG12	1:B:92:ASP:OD1	2.22	0.40
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.89	0.40
1:A:184:ILE:HD12	2:A:404:PEE:H69	2.03	0.40
1:A:208:SER:HB3	1:A:270:THR:HG23	2.04	0.40
1:B:21:LEU:O	1:B:97:ASN:N	2.49	0.40
1:B:208:SER:HB3	1:B:270:THR:HG23	2.04	0.40
1:C:30:ILE:HG12	1:C:92:ASP:OD1	2.22	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 PDB entries followed by that with respect to all EM entries.

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	282/318 (89%)	275 (98%)	7 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	282/318 (89%)	275 (98%)	7 (2%)	0	100	100
1	C	282/318 (89%)	275 (98%)	7 (2%)	0	100	100
All	All	846/954 (89%)	825 (98%)	21 (2%)	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 PDB entries followed by that with respect to all EM entries.

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	234/267 (88%)	230 (98%)	4 (2%)	60	76
1	B	234/267 (88%)	230 (98%)	4 (2%)	60	76
1	C	234/267 (88%)	230 (98%)	4 (2%)	60	76
All	All	702/801 (88%)	690 (98%)	12 (2%)	62	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	MET
1	A	224	ILE
1	A	262	PHE
1	A	266	ARG
1	B	117	MET
1	B	224	ILE
1	B	262	PHE
1	B	266	ARG
1	C	117	MET
1	C	224	ILE
1	C	262	PHE
1	C	266	ARG

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)

3 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	AYA	C	2	1	6,7,8	1.27	1 (16%)	5,8,10	1.21	1 (20%)
1	AYA	A	2	1	6,7,8	1.28	1 (16%)	5,8,10	1.23	1 (20%)
1	AYA	B	2	1	6,7,8	1.28	1 (16%)	5,8,10	1.23	1 (20%)

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
1	AYA	C	2	1	-	0/4/6/8	-
1	AYA	A	2	1	-	0/4/6/8	-
1	AYA	B	2	1	-	0/4/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	AYA	CA-N	-2.51	1.43	1.46
1	B	2	AYA	CA-N	-2.51	1.43	1.46
1	C	2	AYA	CA-N	-2.47	1.44	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	AYA	CB-CA-N	2.54	112.43	109.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2	AYA	CB-CA-N	2.52	112.41	109.61
1	C	2	AYA	CB-CA-N	2.49	112.38	109.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	B	407	-	11,11,50	1.11	1 (9%)	9,10,55	0.87	0
2	PEE	A	401	-	19,19,50	1.37	3 (15%)	19,19,55	1.36	3 (15%)
2	PEE	C	402	-	11,11,50	1.11	1 (9%)	9,10,55	0.88	0
2	PEE	A	408	-	11,11,50	1.11	1 (9%)	9,10,55	0.88	0
2	PEE	C	405	-	15,15,50	1.56	3 (20%)	15,15,55	1.45	3 (20%)
2	PEE	A	402	-	14,14,50	1.07	1 (7%)	14,14,55	1.11	1 (7%)
2	PEE	B	401	-	19,19,50	1.36	3 (15%)	19,19,55	1.36	3 (15%)
2	PEE	B	403	-	15,15,50	1.57	3 (20%)	15,15,55	1.46	3 (20%)
2	PEE	A	404	-	8,8,50	0.19	0	7,7,55	0.63	0
2	PEE	A	403	-	15,15,50	1.56	3 (20%)	15,15,55	1.46	3 (20%)
2	PEE	B	404	-	50,50,50	1.16	3 (6%)	53,55,55	1.10	3 (5%)
2	PEE	B	408	-	8,8,50	0.19	0	7,7,55	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PEE	C	404	-	14,14,50	1.07	1 (7%)	14,14,55	1.11	1 (7%)
2	PEE	C	406	-	50,50,50	1.16	3 (6%)	53,55,55	1.10	3 (5%)
3	RET	C	407	1	20,20,21	0.76	0	27,27,28	1.66	8 (29%)
2	PEE	C	403	-	19,19,50	1.37	3 (15%)	19,19,55	1.37	3 (15%)
2	PEE	B	406	-	15,15,50	1.01	1 (6%)	15,15,55	1.13	1 (6%)
2	PEE	C	401	-	15,15,50	1.01	1 (6%)	15,15,55	1.13	1 (6%)
2	PEE	B	402	-	14,14,50	1.07	1 (7%)	14,14,55	1.11	1 (7%)
2	PEE	A	407	-	15,15,50	1.01	1 (6%)	15,15,55	1.13	1 (6%)
3	RET	B	405	1	20,20,21	0.76	0	27,27,28	1.66	8 (29%)
2	PEE	A	409	-	8,8,50	0.19	0	7,7,55	0.63	0
3	RET	A	406	1	20,20,21	0.76	0	27,27,28	1.66	8 (29%)
2	PEE	A	405	-	50,50,50	1.16	3 (6%)	53,55,55	1.10	3 (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	B	407	-	-	3/9/9/54	-
2	PEE	A	401	-	-	2/17/17/54	-
2	PEE	C	402	-	-	3/9/9/54	-
2	PEE	A	408	-	-	3/9/9/54	-
2	PEE	C	405	-	-	4/13/13/54	-
2	PEE	A	402	-	-	2/12/12/54	-
2	PEE	B	401	-	-	2/17/17/54	-
2	PEE	B	403	-	-	4/13/13/54	-
2	PEE	A	404	-	-	0/6/6/54	-
2	PEE	A	403	-	-	4/13/13/54	-
2	PEE	B	404	-	-	20/54/54/54	-
2	PEE	B	408	-	-	0/6/6/54	-
2	PEE	C	404	-	-	2/12/12/54	-
2	PEE	C	406	-	-	20/54/54/54	-
3	RET	C	407	1	-	0/13/30/31	0/1/1/1
2	PEE	C	403	-	-	2/17/17/54	-
2	PEE	B	406	-	-	3/13/13/54	-
2	PEE	C	401	-	-	3/13/13/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEE	B	402	-	-	2/12/12/54	-
2	PEE	A	407	-	-	3/13/13/54	-
3	RET	B	405	1	-	0/13/30/31	0/1/1/1
2	PEE	A	409	-	-	0/6/6/54	-
3	RET	A	406	1	-	0/13/30/31	0/1/1/1
2	PEE	A	405	-	-	20/54/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	405	PEE	P-O4P	4.47	1.77	1.59
2	B	404	PEE	P-O4P	4.47	1.77	1.59
2	C	406	PEE	P-O4P	4.46	1.77	1.59
2	B	403	PEE	O5-C30	4.09	1.35	1.22
2	A	403	PEE	O5-C30	4.08	1.35	1.22
2	A	401	PEE	O4-C10	4.07	1.35	1.22
2	C	403	PEE	O4-C10	4.07	1.35	1.22
2	C	405	PEE	O5-C30	4.07	1.35	1.22
2	B	401	PEE	O4-C10	4.06	1.35	1.22
2	C	405	PEE	C39-C38	3.63	1.52	1.31
2	B	403	PEE	C39-C38	3.63	1.52	1.31
2	A	403	PEE	C39-C38	3.63	1.52	1.31
2	B	402	PEE	C39-C38	3.62	1.52	1.31
2	A	402	PEE	C39-C38	3.61	1.52	1.31
2	C	406	PEE	C39-C38	3.61	1.52	1.31
2	B	404	PEE	C39-C38	3.61	1.52	1.31
2	C	406	PEE	C18-C19	3.61	1.52	1.31
2	A	405	PEE	C39-C38	3.61	1.52	1.31
2	C	404	PEE	C39-C38	3.61	1.52	1.31
2	A	405	PEE	C18-C19	3.61	1.52	1.31
2	B	404	PEE	C18-C19	3.60	1.52	1.31
2	C	402	PEE	C39-C38	3.58	1.52	1.31
2	B	407	PEE	C39-C38	3.58	1.52	1.31
2	A	408	PEE	C39-C38	3.57	1.52	1.31
2	B	401	PEE	C18-C19	3.54	1.52	1.31
2	C	401	PEE	C39-C38	3.54	1.52	1.31
2	A	407	PEE	C39-C38	3.54	1.52	1.31
2	C	403	PEE	C18-C19	3.54	1.52	1.31
2	A	401	PEE	C18-C19	3.54	1.52	1.31
2	B	406	PEE	C39-C38	3.53	1.52	1.31
2	C	405	PEE	O3-C30	-2.45	1.22	1.30
2	B	403	PEE	O3-C30	-2.44	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	403	PEE	O3-C30	-2.43	1.22	1.30
2	A	401	PEE	O2-C10	-2.38	1.22	1.30
2	C	403	PEE	O2-C10	-2.38	1.22	1.30
2	B	401	PEE	O2-C10	-2.37	1.22	1.30

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	404	PEE	O2P-P-O1P	3.33	128.71	112.24
2	A	405	PEE	O2P-P-O1P	3.33	128.68	112.24
2	C	406	PEE	O2P-P-O1P	3.32	128.68	112.24
3	C	407	RET	C7-C8-C9	3.22	131.10	126.23
3	B	405	RET	C7-C8-C9	3.20	131.06	126.23
3	A	406	RET	C7-C8-C9	3.18	131.05	126.23
2	B	403	PEE	O3-C30-C31	3.08	123.93	114.03
2	C	403	PEE	O2-C10-C11	3.07	123.90	114.03
2	A	403	PEE	O3-C30-C31	3.07	123.88	114.03
2	B	401	PEE	O2-C10-C11	3.06	123.87	114.03
2	C	405	PEE	O3-C30-C31	3.06	123.86	114.03
2	A	401	PEE	O2-C10-C11	3.06	123.86	114.03
3	A	406	RET	C16-C1-C6	2.89	114.99	110.30
3	B	405	RET	C16-C1-C6	2.88	114.97	110.30
3	C	407	RET	C16-C1-C6	2.88	114.97	110.30
3	C	407	RET	C2-C1-C6	2.81	114.81	110.48
3	B	405	RET	C2-C1-C6	2.80	114.79	110.48
3	C	407	RET	C1-C6-C7	2.80	123.69	115.78
3	B	405	RET	C1-C6-C7	2.79	123.67	115.78
3	A	406	RET	C2-C1-C6	2.79	114.77	110.48
3	A	406	RET	C1-C6-C7	2.77	123.63	115.78
3	C	407	RET	C16-C1-C2	-2.55	98.72	108.91
3	B	405	RET	C16-C1-C2	-2.55	98.72	108.91
3	A	406	RET	C16-C1-C2	-2.54	98.74	108.91
2	B	406	PEE	C32-C31-C30	-2.51	108.16	114.47
2	A	407	PEE	C32-C31-C30	-2.50	108.16	114.47
2	C	401	PEE	C32-C31-C30	-2.50	108.16	114.47
2	C	406	PEE	O2-C10-C11	2.46	116.79	111.50
3	B	405	RET	C1-C6-C5	-2.45	119.16	122.61
3	C	407	RET	C1-C6-C5	-2.45	119.16	122.61
2	A	405	PEE	O2-C10-C11	2.45	116.79	111.50
2	B	404	PEE	O2-C10-C11	2.44	116.77	111.50
3	A	406	RET	C1-C6-C5	-2.44	119.18	122.61
2	C	403	PEE	C12-C11-C10	-2.40	108.42	114.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	PEE	C12-C11-C10	-2.40	108.43	114.47
2	A	401	PEE	C12-C11-C10	-2.39	108.44	114.47
2	A	403	PEE	C32-C31-C30	-2.34	108.56	114.47
2	B	403	PEE	C32-C31-C30	-2.34	108.57	114.47
2	C	405	PEE	C32-C31-C30	-2.33	108.61	114.47
3	B	405	RET	C18-C5-C4	-2.28	109.24	113.62
2	C	404	PEE	C32-C31-C30	-2.25	108.80	114.47
3	C	407	RET	C18-C5-C4	-2.25	109.30	113.62
3	A	406	RET	C18-C5-C4	-2.25	109.30	113.62
2	B	402	PEE	C32-C31-C30	-2.23	108.84	114.47
2	A	402	PEE	C32-C31-C30	-2.23	108.85	114.47
2	C	403	PEE	O4-C10-C11	-2.23	115.92	123.08
2	A	401	PEE	O4-C10-C11	-2.23	115.93	123.08
2	B	401	PEE	O4-C10-C11	-2.22	115.93	123.08
2	B	403	PEE	O5-C30-C31	-2.22	115.95	123.08
2	A	403	PEE	O5-C30-C31	-2.21	115.97	123.08
2	C	405	PEE	O5-C30-C31	-2.20	116.00	123.08
2	C	406	PEE	O4P-P-O1P	-2.19	100.49	109.07
2	A	405	PEE	O4P-P-O1P	-2.19	100.50	109.07
2	B	404	PEE	O4P-P-O1P	-2.19	100.51	109.07
3	C	407	RET	C7-C6-C5	-2.03	116.55	121.46
3	B	405	RET	C7-C6-C5	-2.02	116.56	121.46
3	A	406	RET	C7-C6-C5	-2.02	116.57	121.46

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	405	PEE	C11-C10-O2-C2
2	A	405	PEE	O4-C10-O2-C2
2	A	405	PEE	C1-O3P-P-O1P
2	A	405	PEE	C4-O4P-P-O1P
2	A	405	PEE	O4P-C4-C5-N
2	B	404	PEE	C11-C10-O2-C2
2	B	404	PEE	O4-C10-O2-C2
2	B	404	PEE	C1-O3P-P-O1P
2	B	404	PEE	C4-O4P-P-O1P
2	B	404	PEE	O4P-C4-C5-N
2	C	406	PEE	C11-C10-O2-C2
2	C	406	PEE	O4-C10-O2-C2
2	C	406	PEE	C1-O3P-P-O1P
2	C	406	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	C	406	PEE	O4P-C4-C5-N
2	A	405	PEE	O5-C30-O3-C3
2	B	404	PEE	O5-C30-O3-C3
2	C	406	PEE	O5-C30-O3-C3
2	A	405	PEE	C31-C30-O3-C3
2	B	404	PEE	C31-C30-O3-C3
2	C	406	PEE	C31-C30-O3-C3
2	A	403	PEE	C37-C38-C39-C40
2	B	403	PEE	C37-C38-C39-C40
2	C	405	PEE	C37-C38-C39-C40
2	A	403	PEE	C32-C33-C34-C35
2	B	403	PEE	C32-C33-C34-C35
2	C	405	PEE	C32-C33-C34-C35
2	A	405	PEE	O3P-C1-C2-O2
2	B	404	PEE	O3P-C1-C2-O2
2	C	406	PEE	O3P-C1-C2-O2
2	A	405	PEE	C31-C32-C33-C34
2	B	404	PEE	C31-C32-C33-C34
2	C	406	PEE	C31-C32-C33-C34
2	A	408	PEE	C36-C37-C38-C39
2	B	407	PEE	C36-C37-C38-C39
2	C	402	PEE	C36-C37-C38-C39
2	A	405	PEE	O3P-C1-C2-C3
2	B	404	PEE	O3P-C1-C2-C3
2	C	406	PEE	O3P-C1-C2-C3
2	C	406	PEE	C32-C33-C34-C35
2	B	404	PEE	C32-C33-C34-C35
2	A	405	PEE	C32-C33-C34-C35
2	B	407	PEE	C44-C45-C46-C47
2	A	405	PEE	C3-C2-O2-C10
2	B	404	PEE	C3-C2-O2-C10
2	C	406	PEE	C3-C2-O2-C10
2	A	408	PEE	C44-C45-C46-C47
2	C	402	PEE	C44-C45-C46-C47
2	A	408	PEE	C38-C39-C40-C41
2	C	402	PEE	C38-C39-C40-C41
2	A	405	PEE	C1-O3P-P-O4P
2	A	405	PEE	C4-O4P-P-O3P
2	B	404	PEE	C1-O3P-P-O4P
2	B	404	PEE	C4-O4P-P-O3P
2	C	406	PEE	C1-O3P-P-O4P
2	C	406	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	B	407	PEE	C38-C39-C40-C41
2	A	407	PEE	C36-C37-C38-C39
2	B	406	PEE	C36-C37-C38-C39
2	B	406	PEE	C38-C39-C40-C41
2	C	401	PEE	C36-C37-C38-C39
2	B	404	PEE	C10-C11-C12-C13
2	A	405	PEE	C10-C11-C12-C13
2	C	406	PEE	C10-C11-C12-C13
2	A	405	PEE	C18-C19-C20-C21
2	A	407	PEE	C38-C39-C40-C41
2	B	404	PEE	C18-C19-C20-C21
2	C	401	PEE	C38-C39-C40-C41
2	C	406	PEE	C18-C19-C20-C21
2	A	402	PEE	C38-C39-C40-C41
2	A	405	PEE	C38-C39-C40-C41
2	B	402	PEE	C38-C39-C40-C41
2	C	404	PEE	C38-C39-C40-C41
2	C	406	PEE	C38-C39-C40-C41
2	B	404	PEE	C38-C39-C40-C41
2	A	401	PEE	C16-C17-C18-C19
2	B	401	PEE	C16-C17-C18-C19
2	C	403	PEE	C16-C17-C18-C19
2	B	404	PEE	C11-C12-C13-C14
2	A	405	PEE	C11-C12-C13-C14
2	C	406	PEE	C11-C12-C13-C14
2	A	403	PEE	C36-C37-C38-C39
2	A	403	PEE	C38-C39-C40-C41
2	B	403	PEE	C36-C37-C38-C39
2	B	403	PEE	C38-C39-C40-C41
2	C	405	PEE	C36-C37-C38-C39
2	C	405	PEE	C38-C39-C40-C41
2	A	407	PEE	C35-C36-C37-C38
2	B	406	PEE	C35-C36-C37-C38
2	C	401	PEE	C35-C36-C37-C38
2	A	401	PEE	C18-C19-C20-C21
2	A	405	PEE	C16-C17-C18-C19
2	B	401	PEE	C18-C19-C20-C21
2	B	404	PEE	C16-C17-C18-C19
2	C	403	PEE	C18-C19-C20-C21
2	C	406	PEE	C16-C17-C18-C19
2	B	404	PEE	C36-C37-C38-C39
2	A	405	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
2	C	406	PEE	C36-C37-C38-C39
2	A	402	PEE	O3-C30-C31-C32
2	C	404	PEE	O3-C30-C31-C32
2	B	402	PEE	O3-C30-C31-C32

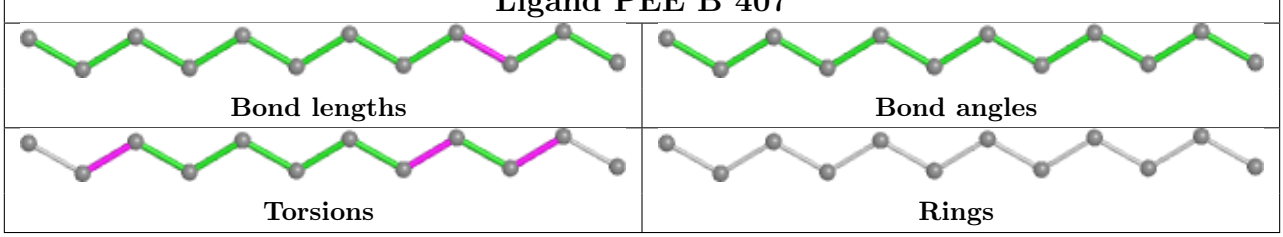
There are no ring outliers.

12 monomers are involved in 19 short contacts:

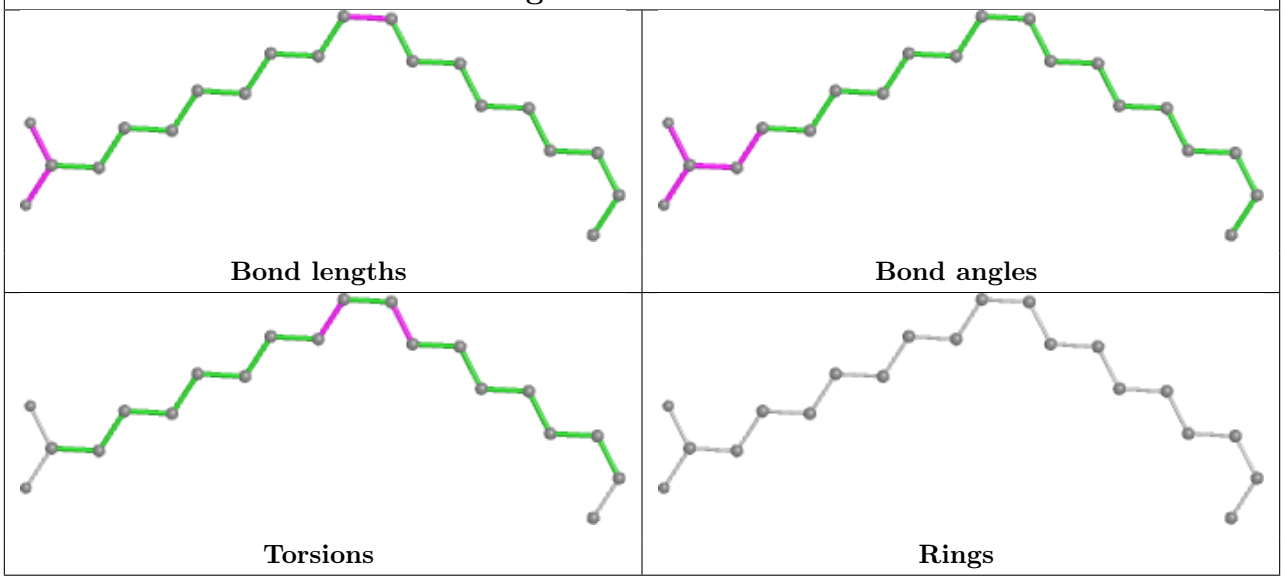
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PEE	1	0
2	B	401	PEE	1	0
2	A	404	PEE	1	0
2	B	404	PEE	3	0
2	B	408	PEE	1	0
2	C	406	PEE	2	0
3	C	407	RET	2	0
2	C	403	PEE	1	0
3	B	405	RET	2	0
2	A	409	PEE	1	0
3	A	406	RET	2	0
2	A	405	PEE	2	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PEE B 407



Ligand PEE A 401



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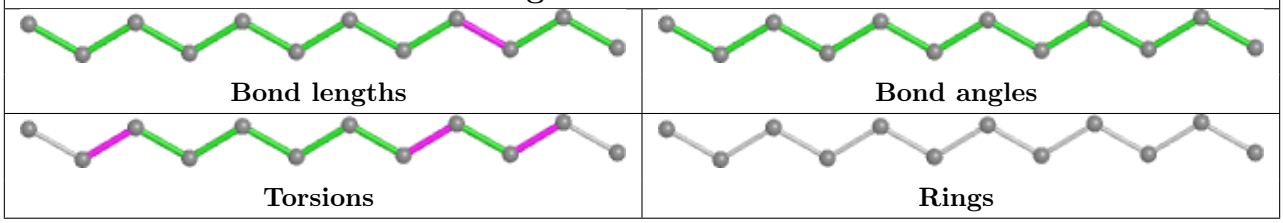

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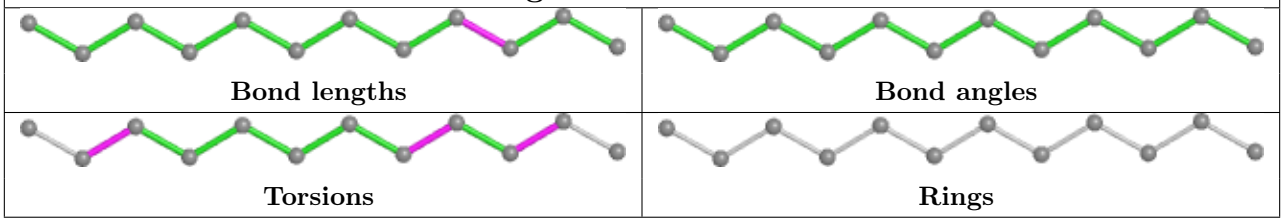

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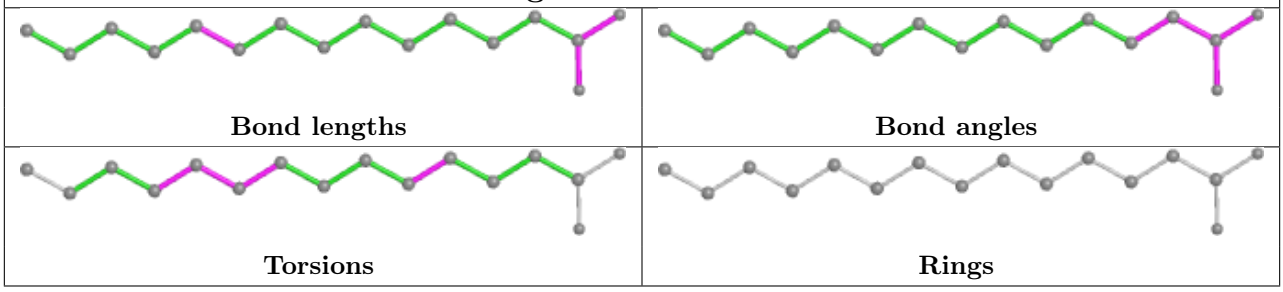

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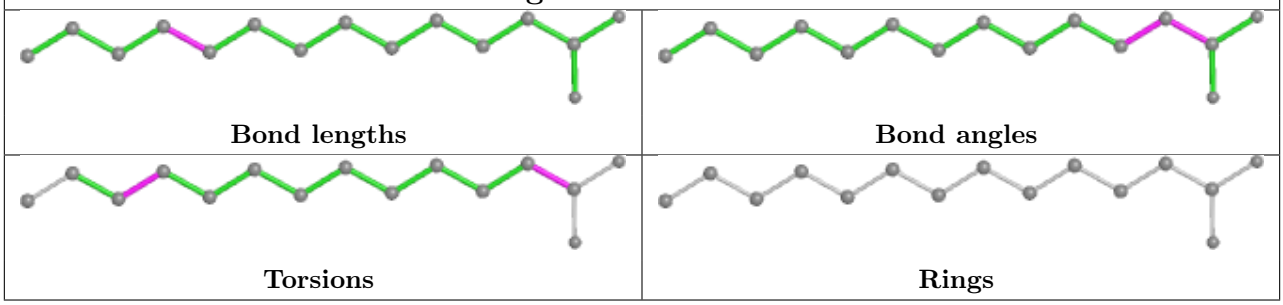
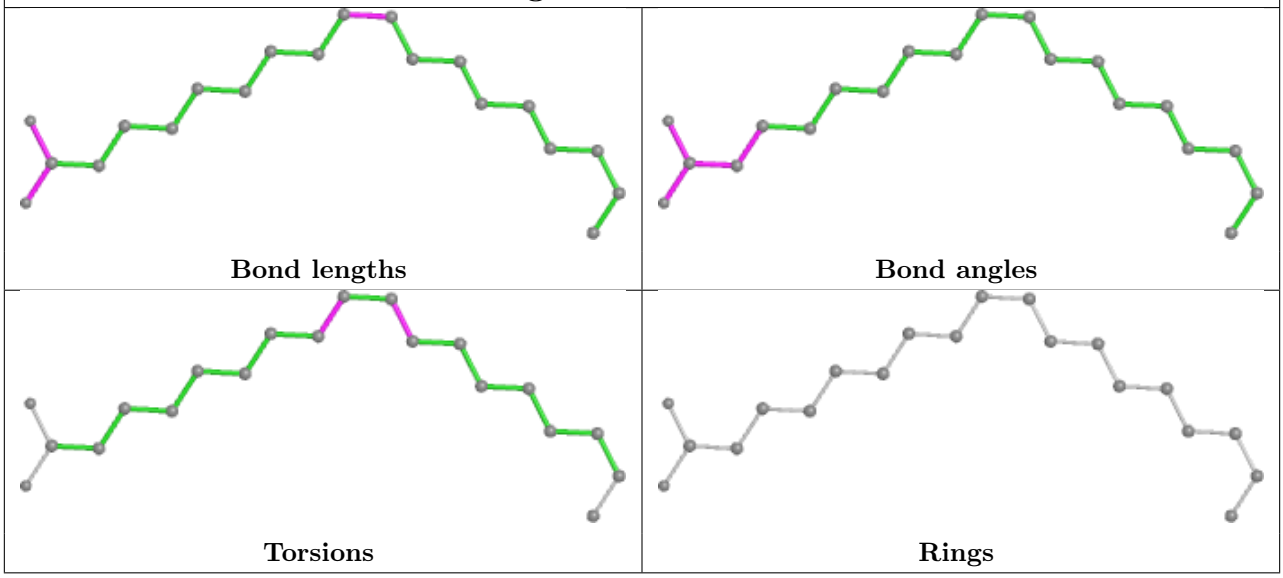
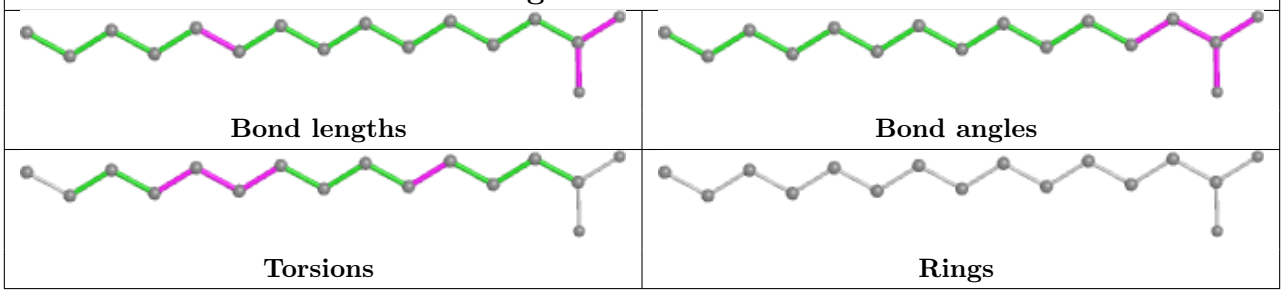


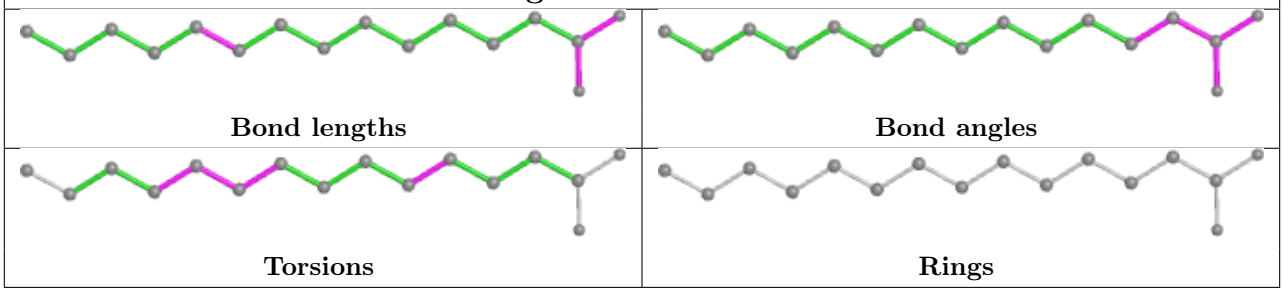
Ligand PEE B 401

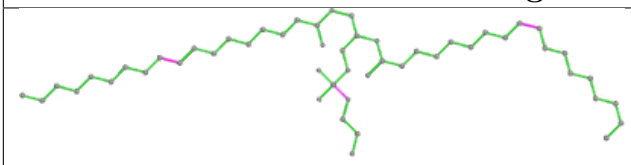
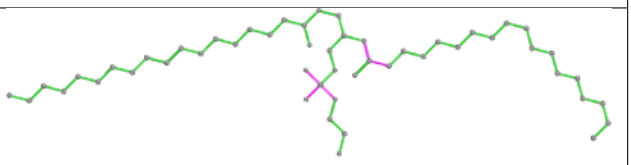
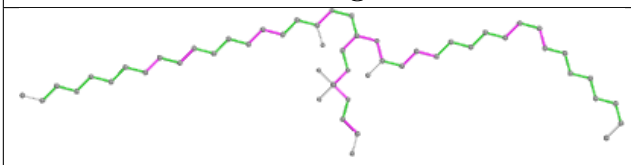
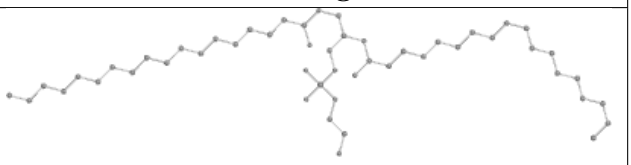


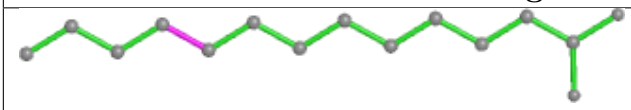
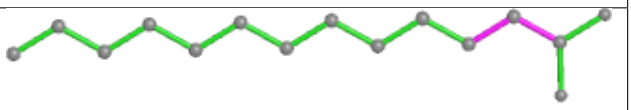
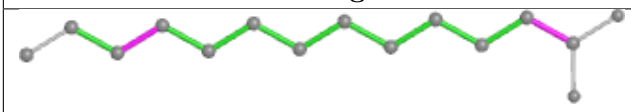
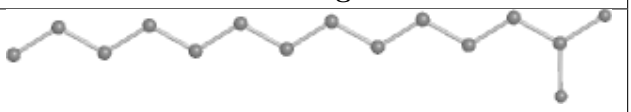
Ligand PEE B 403

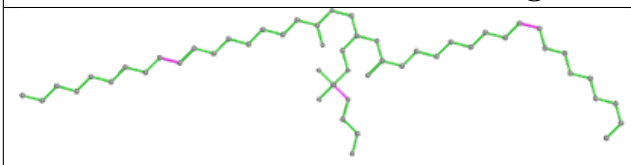
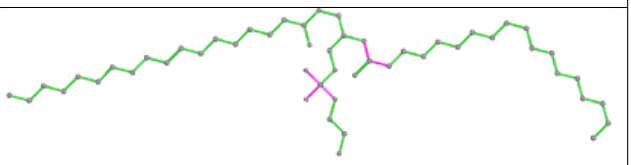
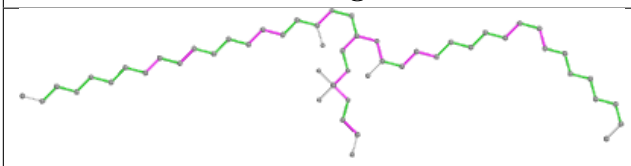
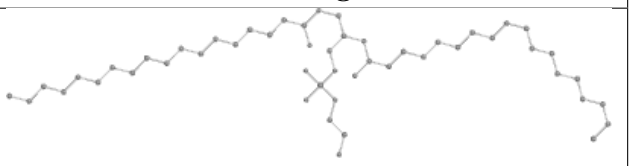


Ligand PEE A 403

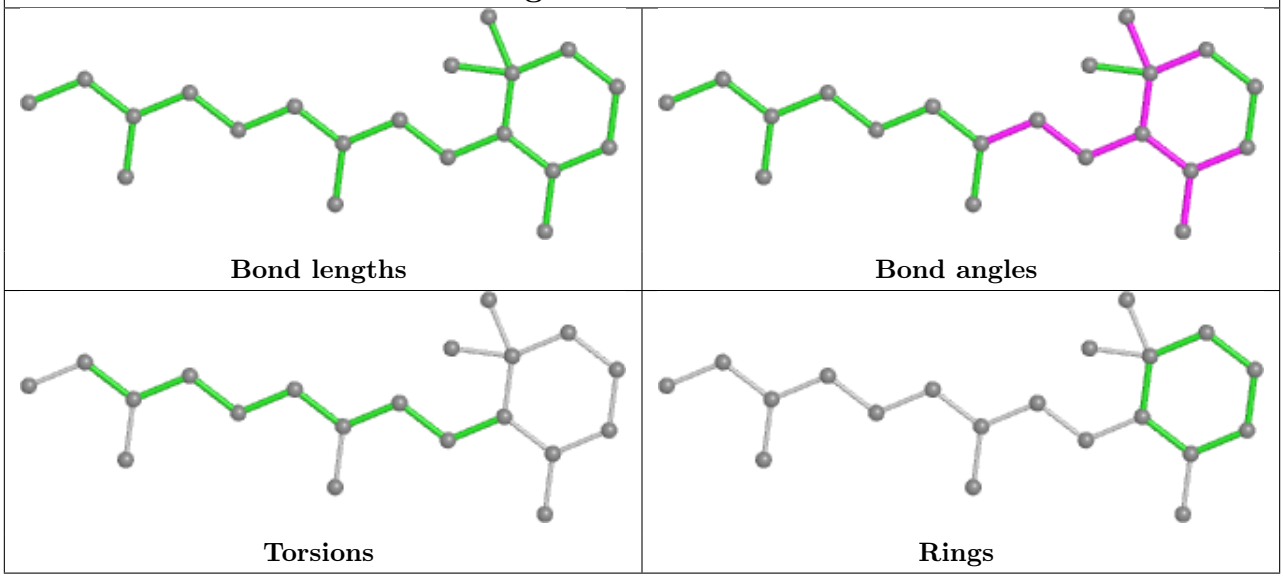


Ligand PEE B 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

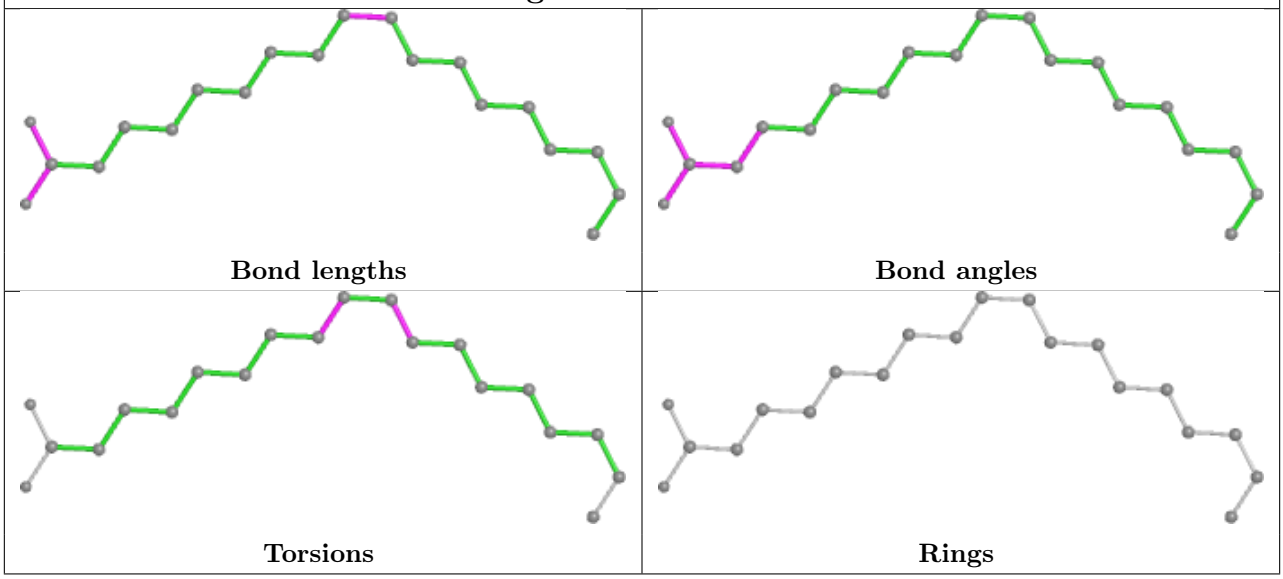
Ligand PEE C 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE C 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand RET C 407

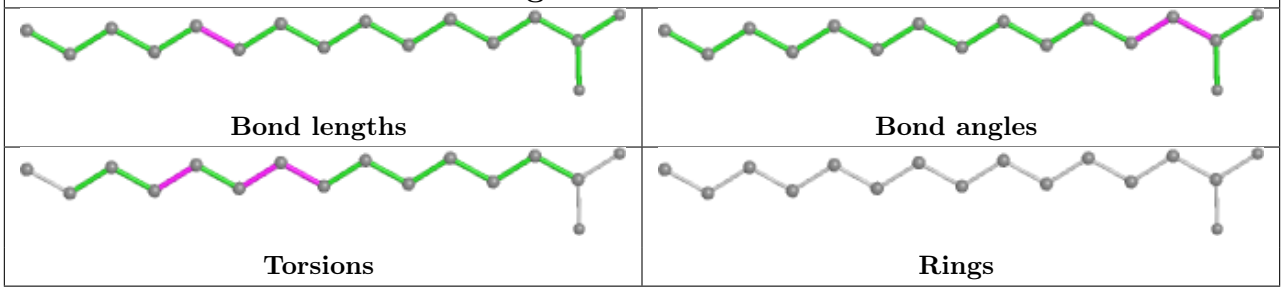


Ligand PEE C 403

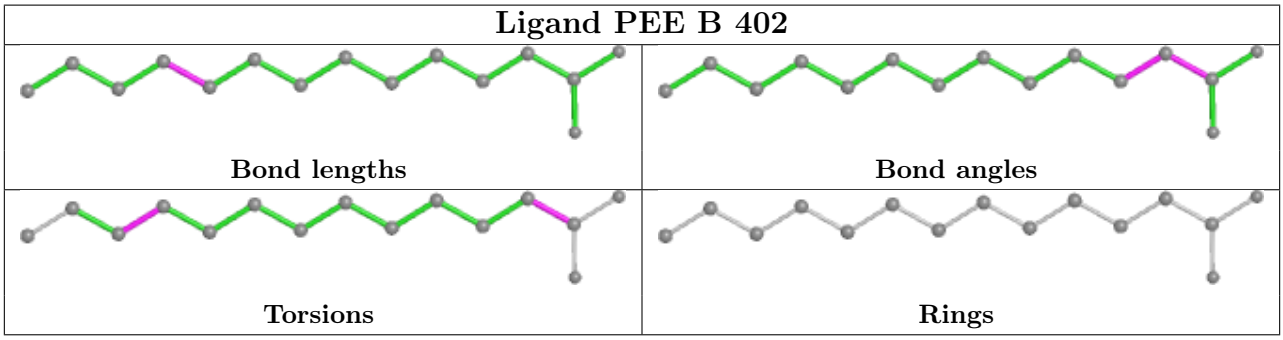


Ligand PEE B 406

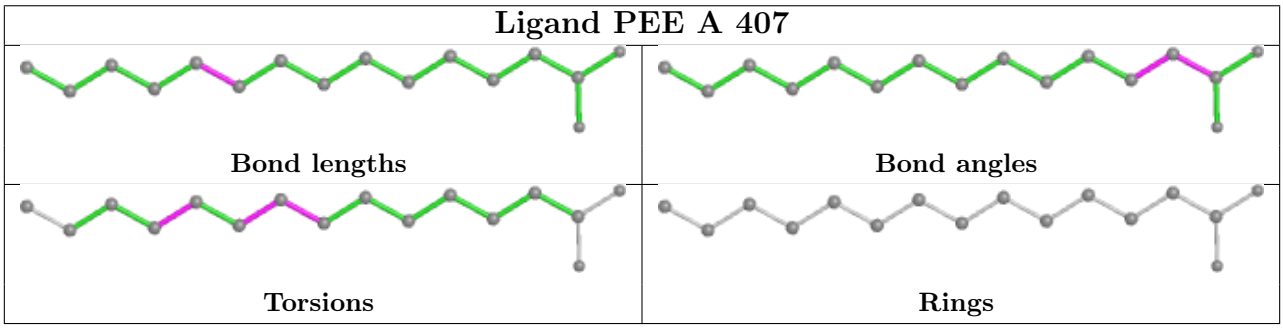
Ligand PEE C 401



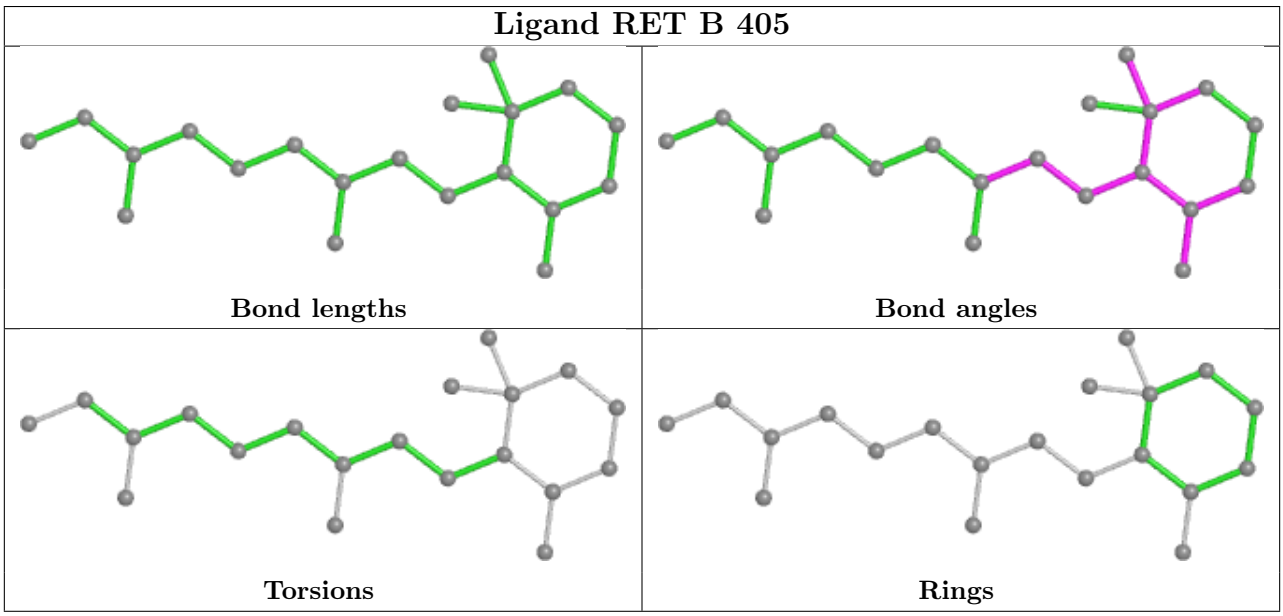
Ligand PEE B 402

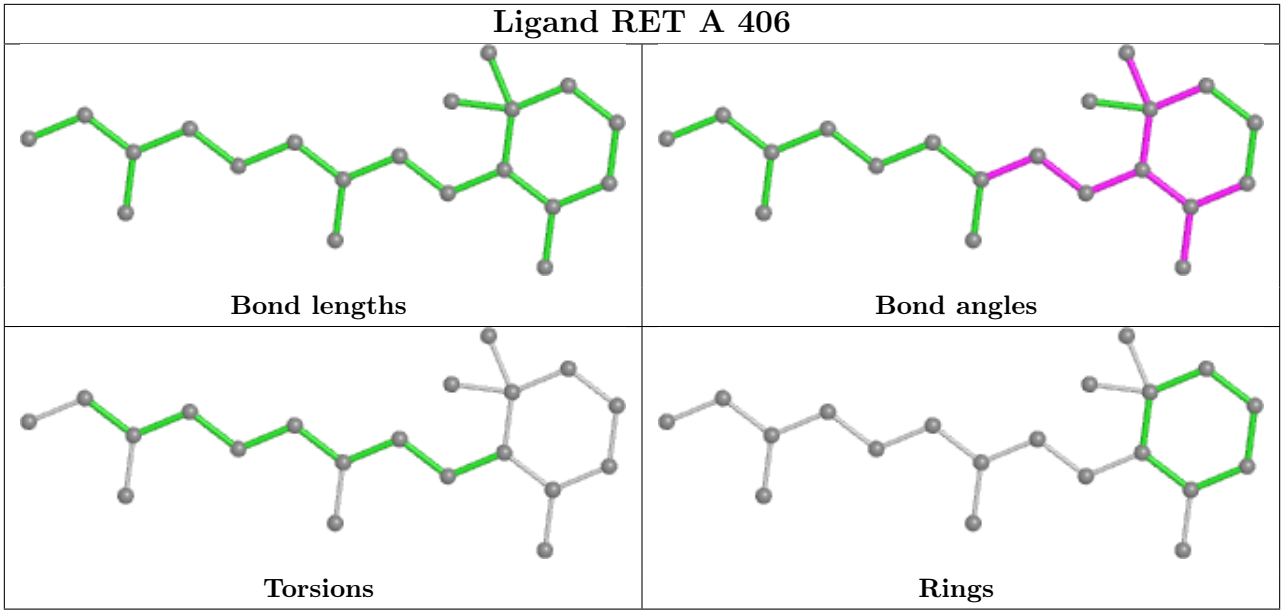


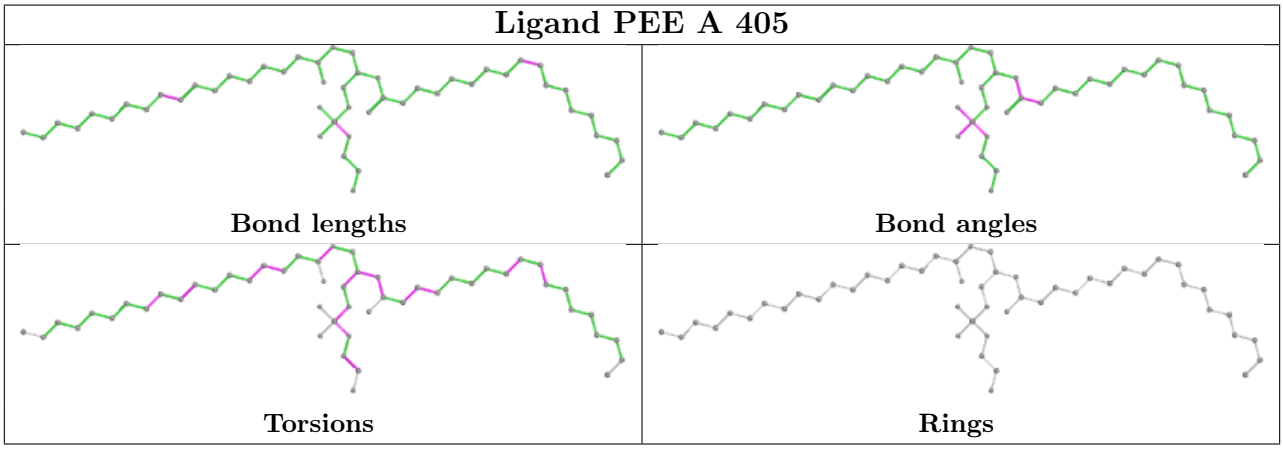
Ligand PEE A 407



Ligand RET B 405







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.

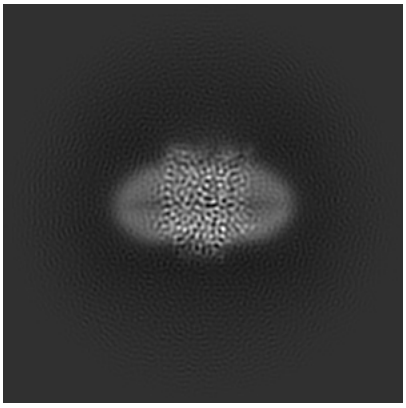
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25079. These allow visual inspection of the internal detail of the map and identification of artifacts.

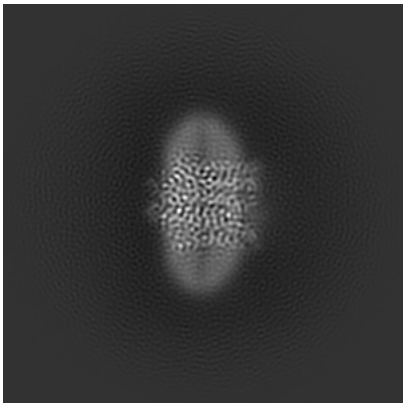
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

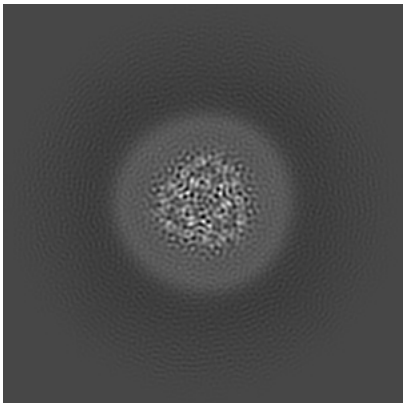
6.1.1 Primary map



X



Y

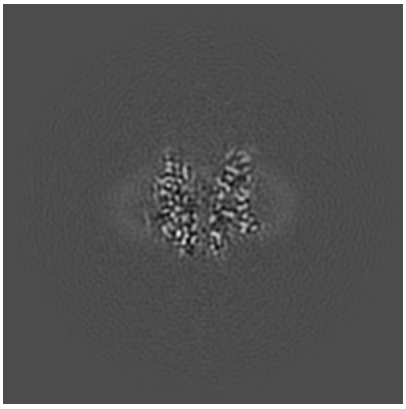


Z

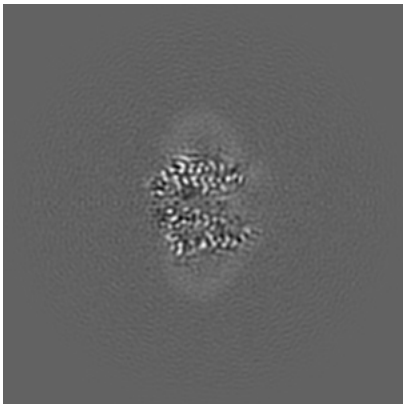
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

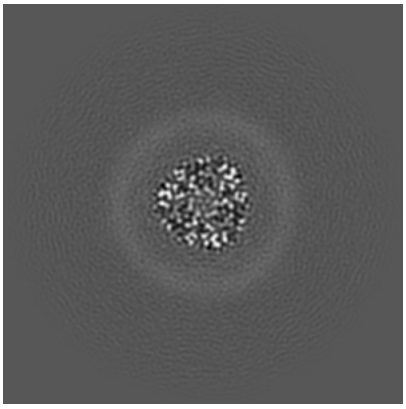
6.2.1 Primary map



X Index: 110



Y Index: 110

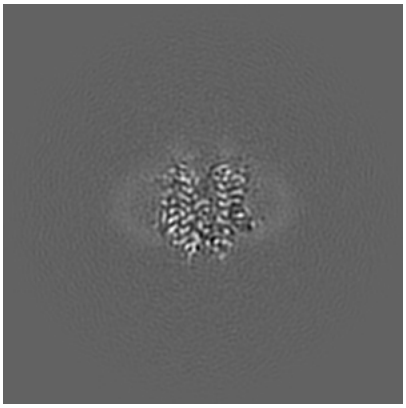


Z Index: 110

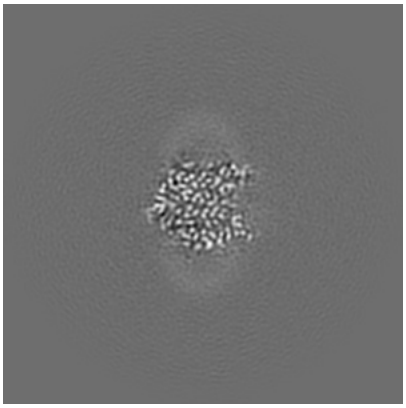
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

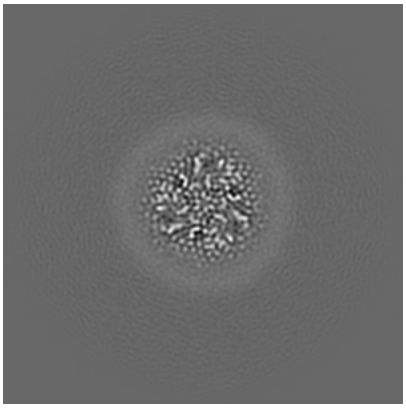
6.3.1 Primary map



X Index: 103



Y Index: 119

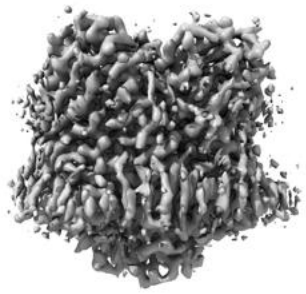


Z Index: 101

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

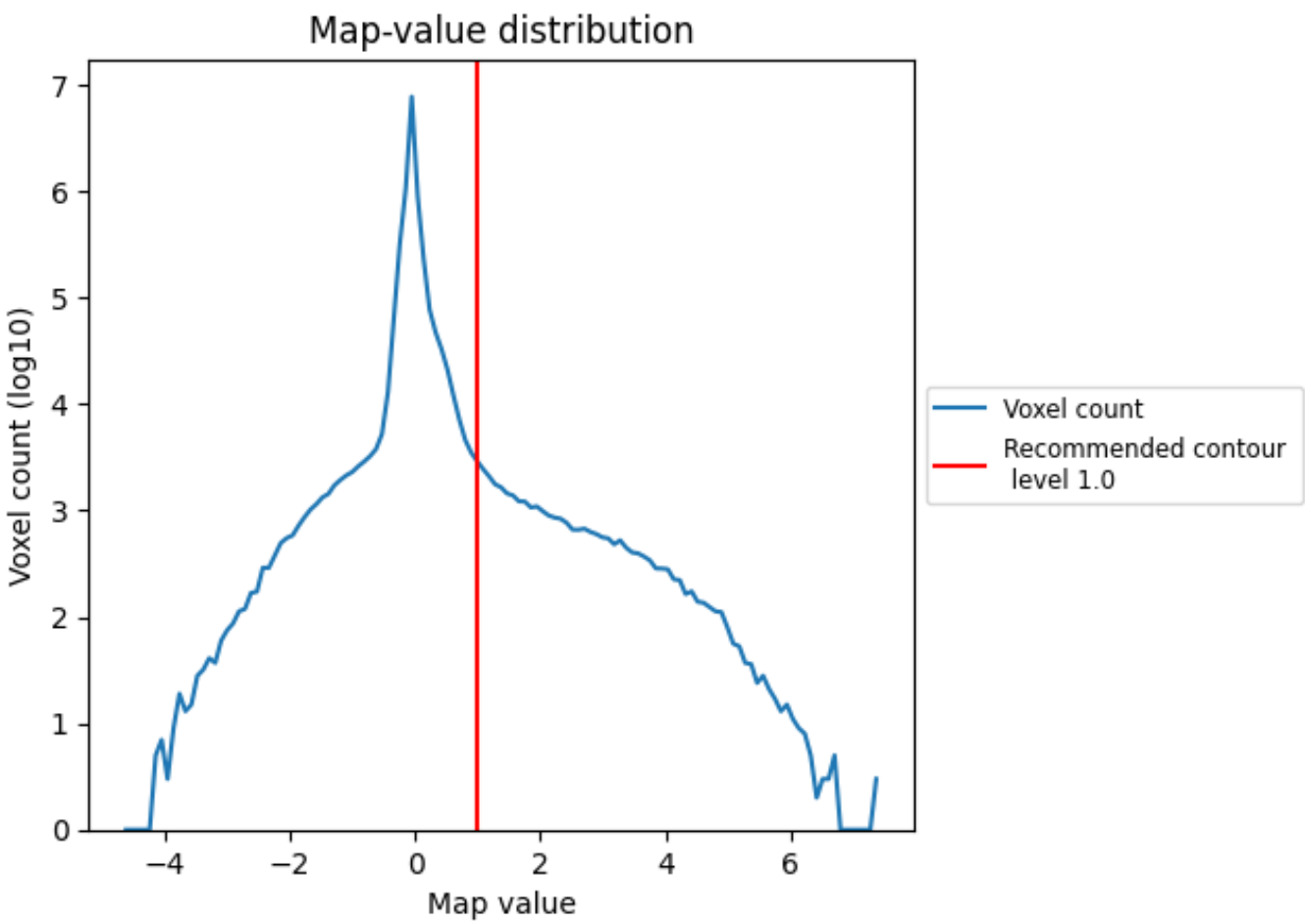
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

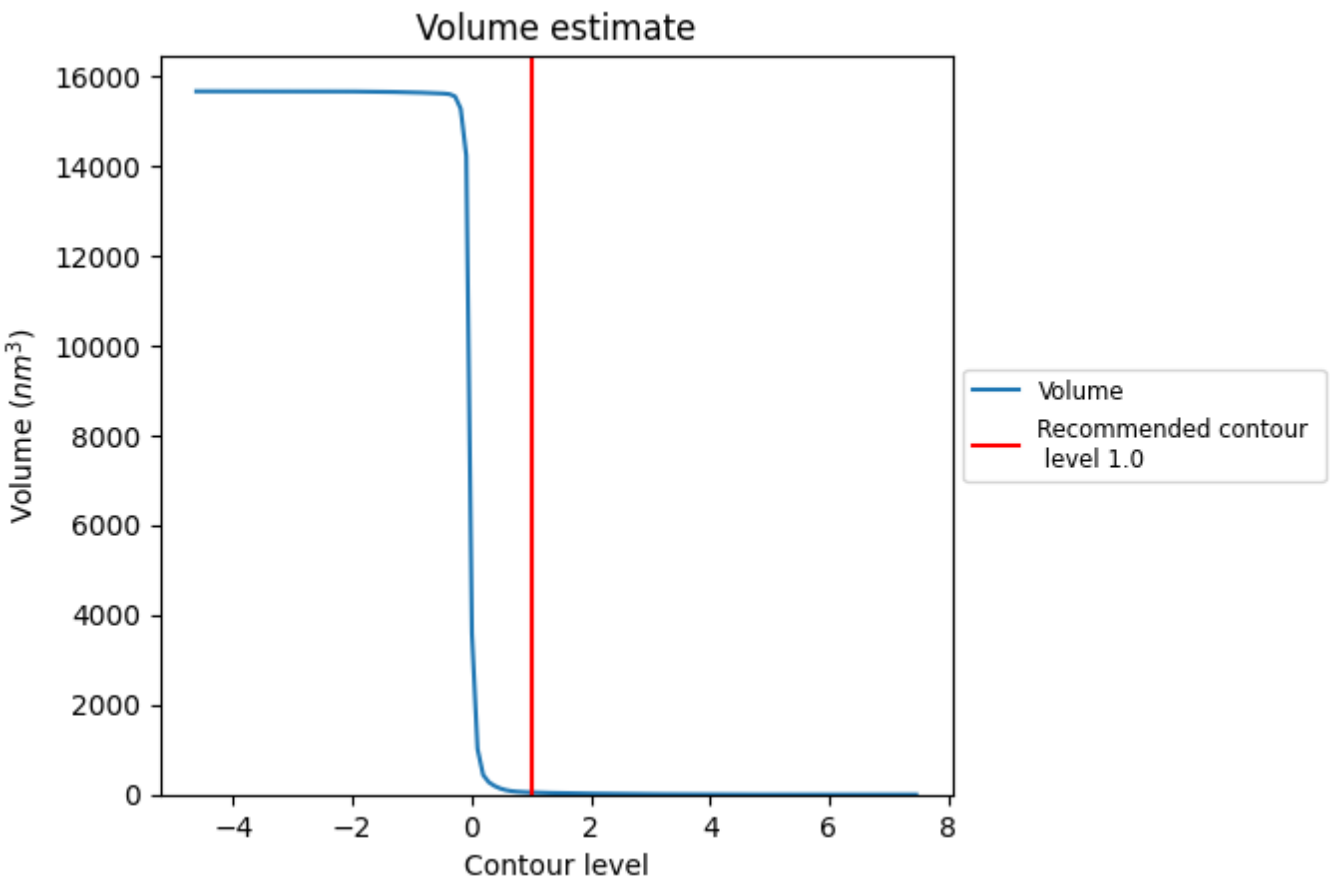
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

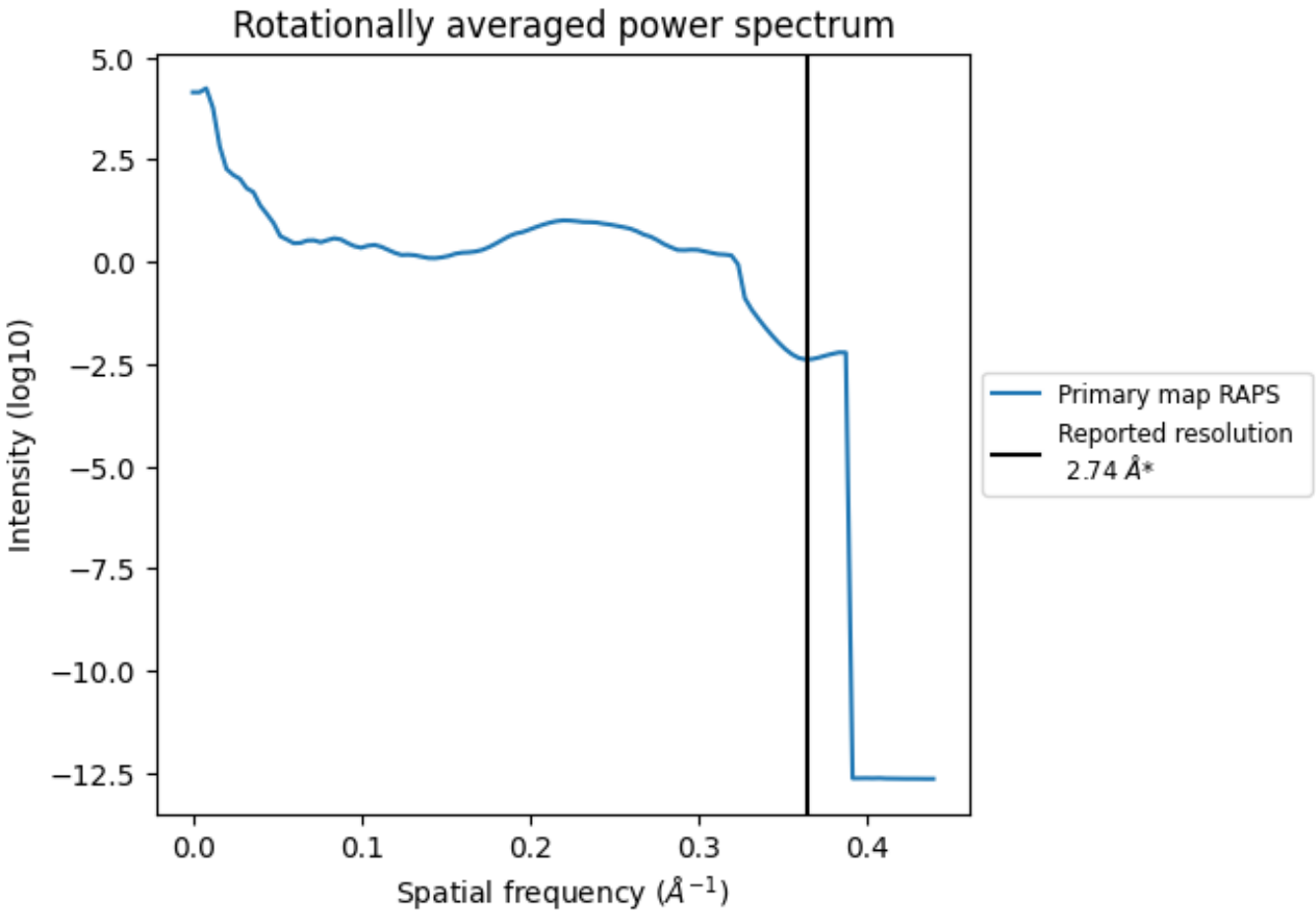
7.2 Volume estimate (i)



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 43 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.365 Å^{-1}

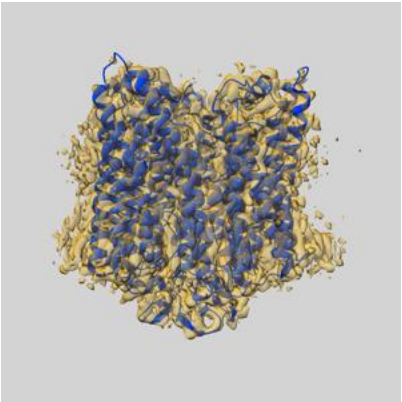
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

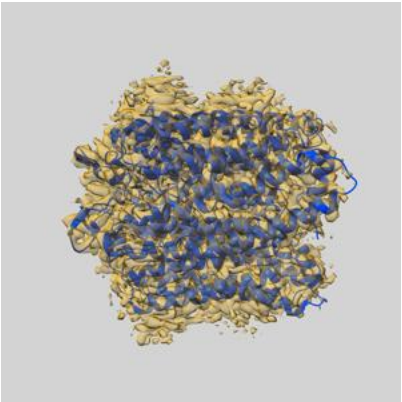
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25079 and PDB model 7SFJ. Per-residue inclusion information can be found in section 3 on page 6.

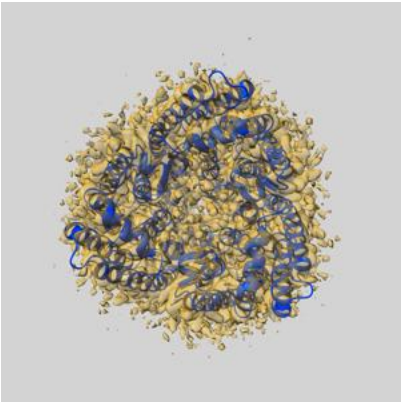
9.1 Map-model overlay (i)



X



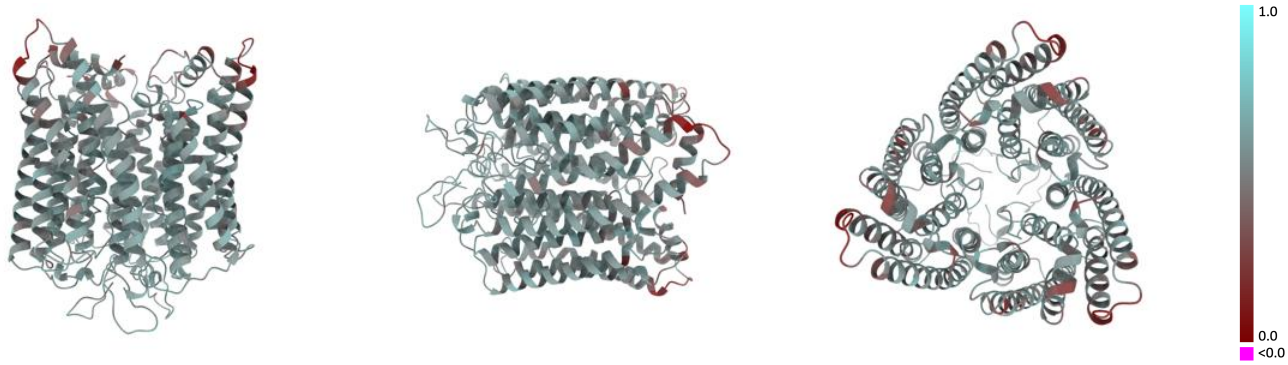
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

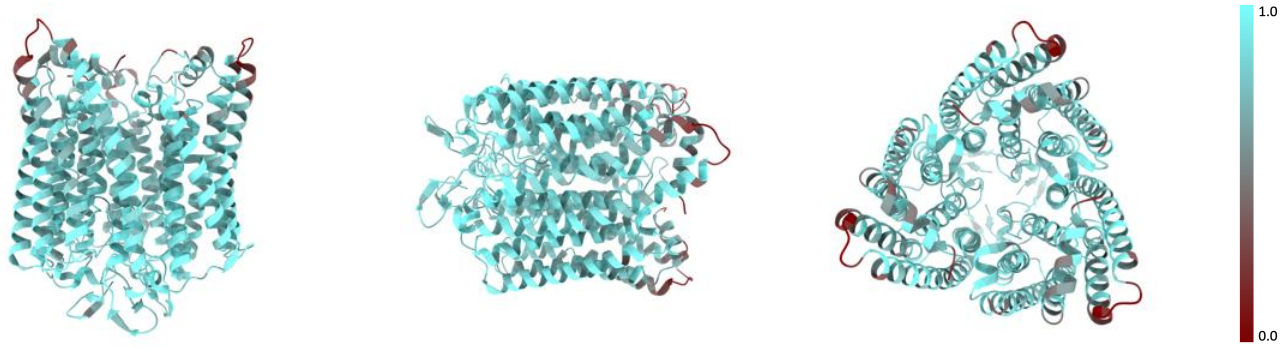
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

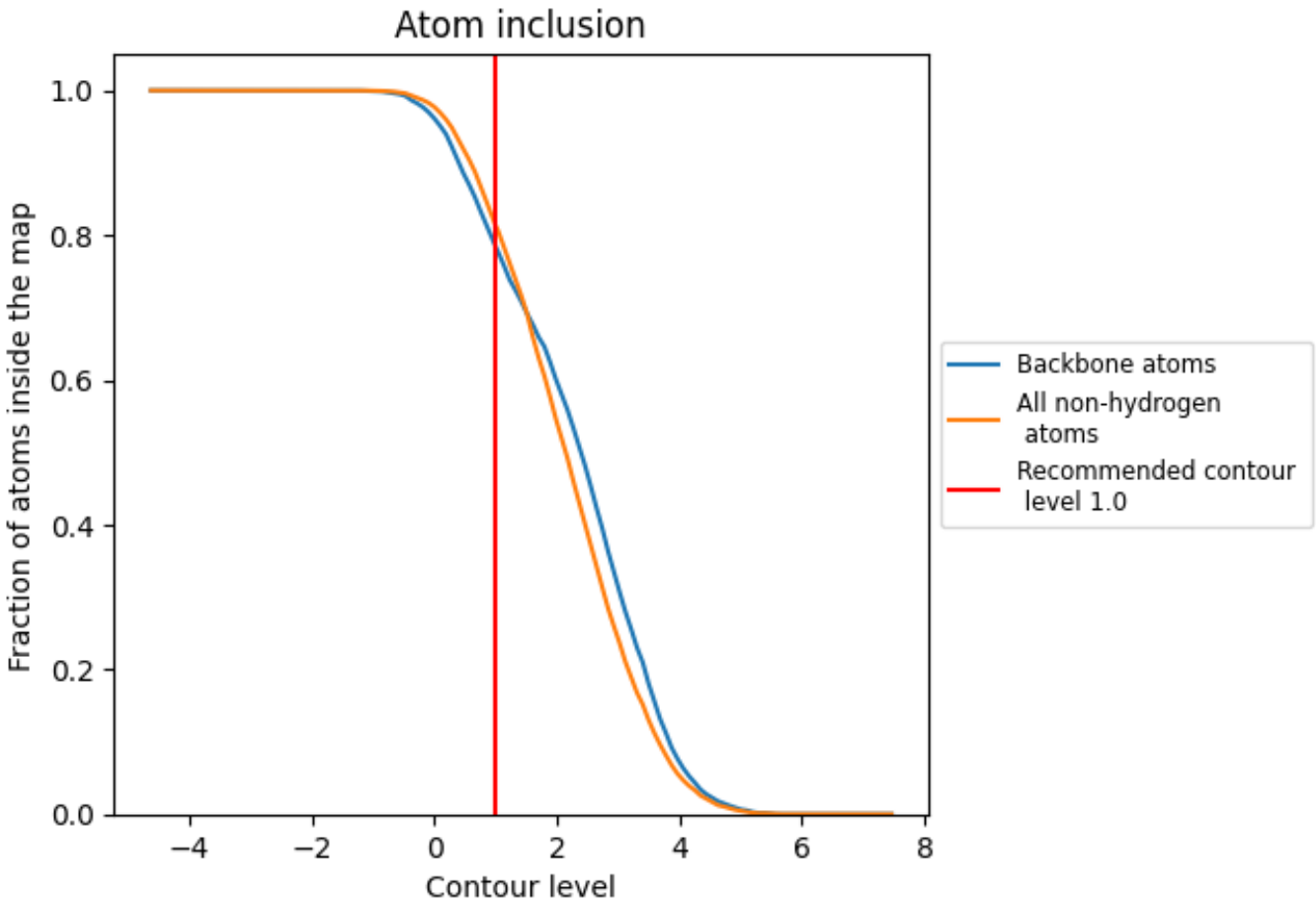
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8137	0.5390
A	0.8215	0.5410
B	0.8204	0.5370
C	0.8164	0.5390