Full wwPDB EM Validation Report (i)

Dec 7, 2022 – 10:17 AM JST

PDB ID	:	5Z62
EMDB ID	:	EMD-6896
Title	:	Structure of human cytochrome c oxidase
Authors	:	Gu, J.; Zong, S.; Wu, M.; Yang, M.
Deposited on	:	2018-01-22
Resolution	:	3.60 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:

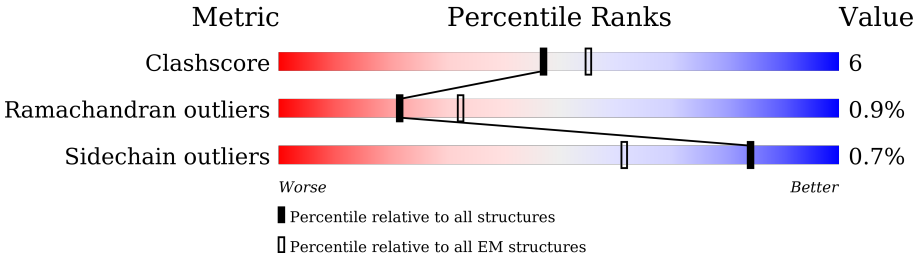
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.60 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	513	89% 10%
2	B	227	7% 91% 9%
3	C	260	87% 13%
4	D	144	10% 97%
5	E	109	7% 94% 6%
6	F	98	10% 82% 18%
7	G	75	15% 72% 20% 7%
8	H	82	5% 89% 5% 5%

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Mol	Chain	Length	Quality of chain
9	I	73	8% 97%
10	J	56	14% 88% 12%
11	K	49	6% 100%
12	L	47	13% 81% 11% 6%
13	M	43	30% 98%
14	N	79	35% 90% 6%

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
17	HEA	A	603	X	-	-	-
17	HEA	A	604	X	-	-	-
18	PEE	A	605	X	-	-	-
18	PEE	C	301	X	-	-	-
18	PEE	C	302	X	-	-	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 15037 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	513	4028	2699	622	674	33	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	227	1798	1180	279	326	13	0	0

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	260	2119	1417	339	352	11	0	0

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1189	768	201	213	7	0	0

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	109	882	560	149	171	2	0	0

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	98	744	462	135	142	5	0	0

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	75	616	402	110	102	2	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	82	662	415	118	124	5	0	0

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	73	604	389	113	98	4	0	0

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	56	436	286	68	81	1	0	0

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	49	388	252	65	70	1	0	0

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	47	378	250	62	64	2	0	0

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	43	335	222	55	56	2	0	0

- Molecule 14 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	N	79	480	309	86	85	0	0

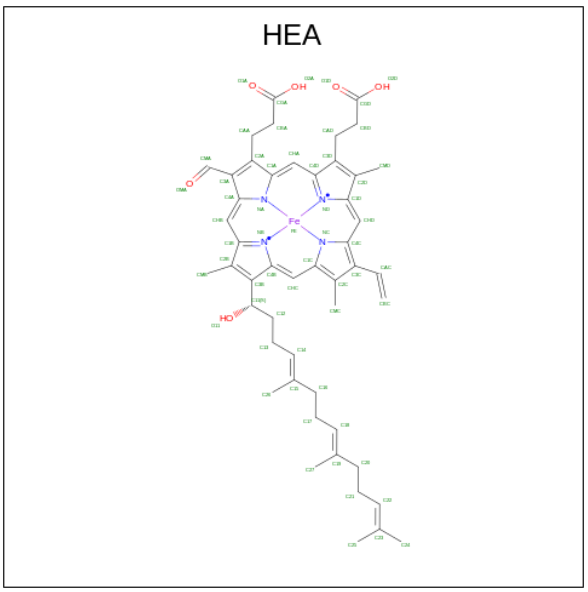
- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
15	A	1	1	1	0
15	B	2	2	2	0

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

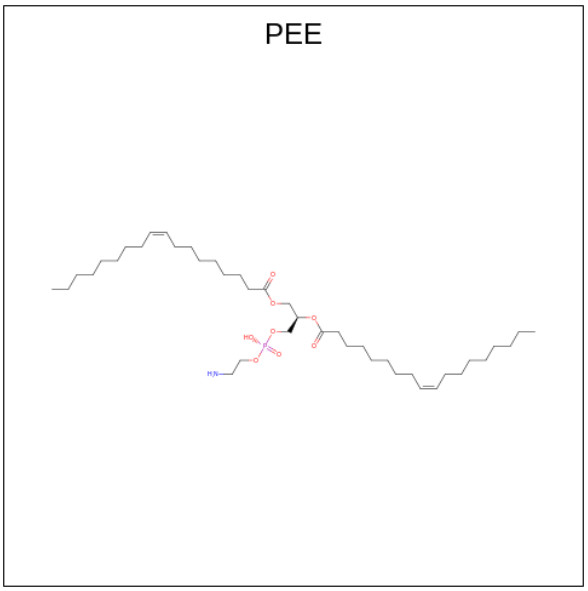
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
16	A	1	1	1	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



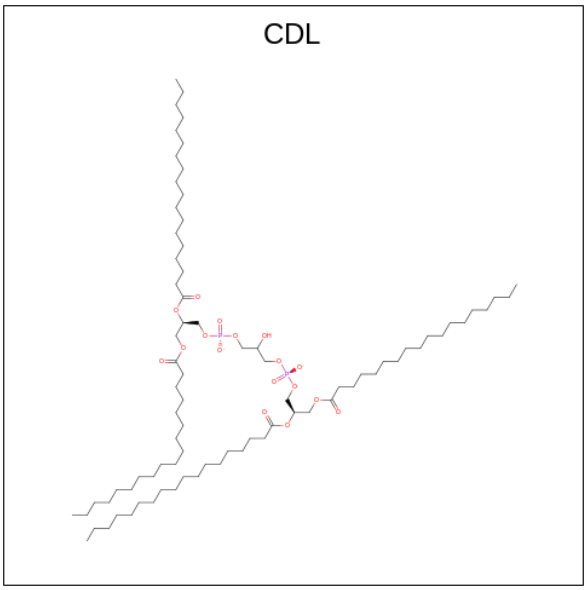
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
17	A	1	120	98	2	8	12	0
17	A	1	Total 120	C 98	Fe 2	N 8	O 12	0

- Molecule 18 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
18	C	1	Total	C	N	O	P	0
			102	82	2	16	2	
18	C	1	Total	C	N	O	P	0
			102	82	2	16	2	

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
19	C	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

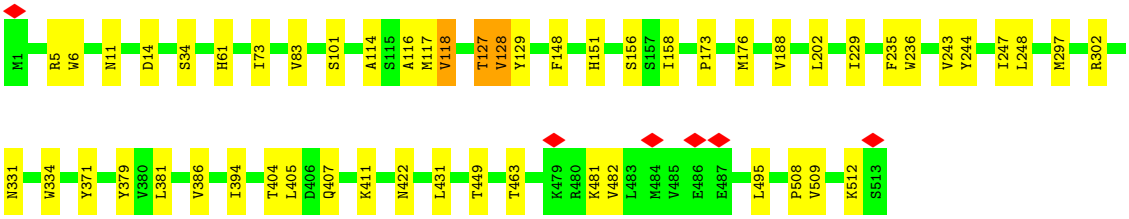
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
20	F	1	1	1	0

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.

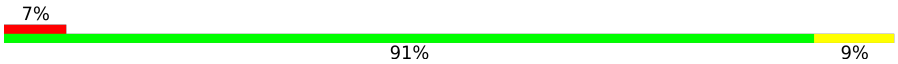
• Molecule 1: Cytochrome c oxidase subunit 1

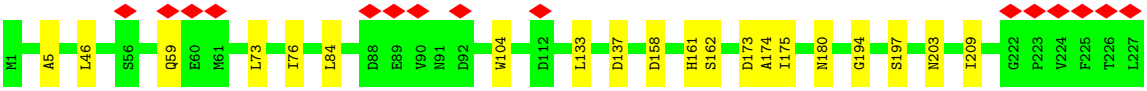
Chain A:



• Molecule 2: Cytochrome c oxidase subunit 2

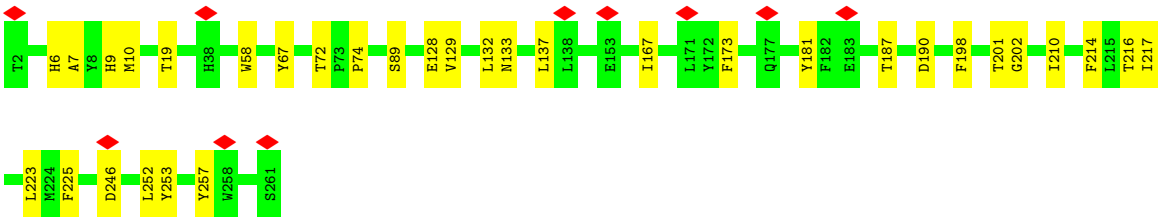
Chain B:





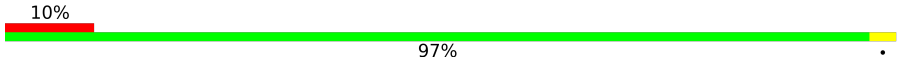
• Molecule 3: Cytochrome c oxidase subunit 3

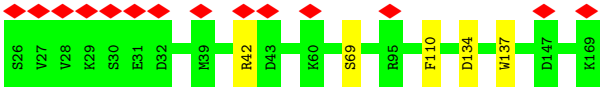
Chain C:



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

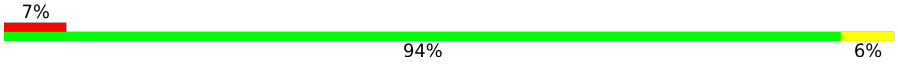
Chain D:

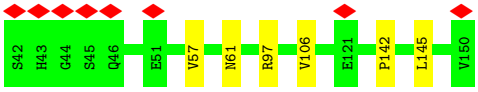




• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

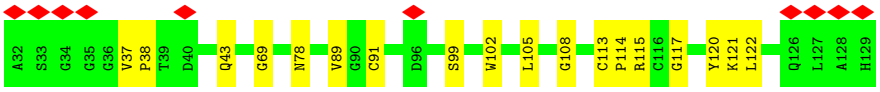
Chain E:





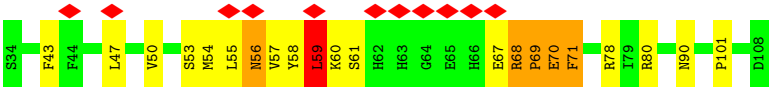
• Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



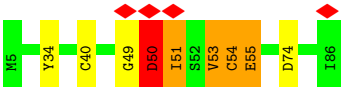
• Molecule 7: Cytochrome c oxidase subunit 6A1, mitochondrial

Chain G:



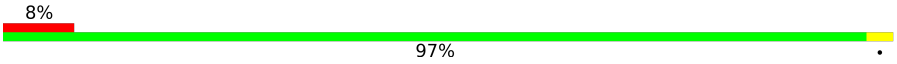
• Molecule 8: Cytochrome c oxidase subunit 6B1

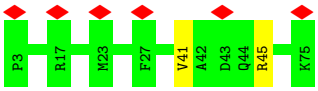
Chain H:



• Molecule 9: Cytochrome c oxidase subunit 6C

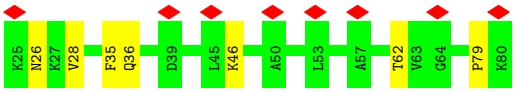
Chain I:





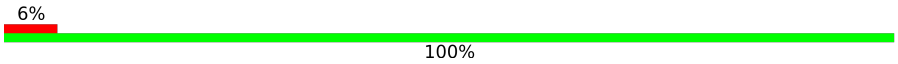
• Molecule 10: Cytochrome c oxidase subunit 7A2, mitochondrial

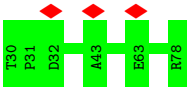
Chain J:



• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

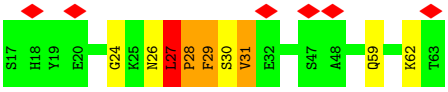
Chain K:





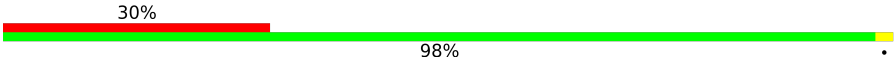
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

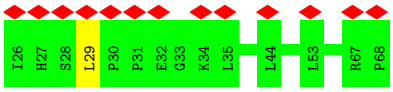
Chain L:



• Molecule 13: Cytochrome c oxidase subunit 8A, mitochondrial

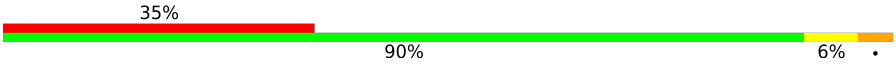
Chain M:

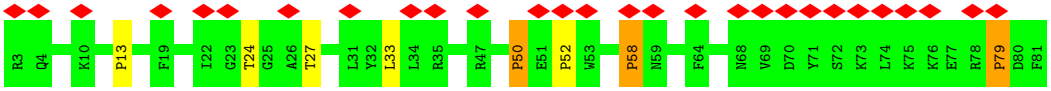




• Molecule 14: Cytochrome c oxidase subunit NDUFA4

Chain N:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1010000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	523.68, 523.68, 523.68	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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, CU, HEA, ZN, CDL, MG

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	0.40	0/4169	0.58	0/5695
2	B	0.34	0/1845	0.57	0/2525
3	C	0.35	0/2206	0.53	0/3018
4	D	0.31	0/1222	0.45	0/1641
5	E	0.31	0/901	0.45	0/1223
6	F	0.35	0/760	0.54	0/1029
7	G	0.31	0/642	0.50	0/877
8	H	0.34	0/682	0.48	0/926
9	I	0.29	0/616	0.41	0/820
10	J	0.31	0/444	0.56	0/600
11	K	0.29	0/401	0.48	0/551
12	L	0.33	0/390	0.59	1/527 (0.2%)
13	M	0.29	0/345	0.59	0/470
14	N	0.30	0/489	0.76	4/677 (0.6%)
All	All	0.35	0/15112	0.54	5/20579 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	27	LEU	C-N-CD	-7.74	103.57	120.60
14	N	79	PRO	N-CA-CB	6.79	111.45	103.30
14	N	58	PRO	N-CA-CB	6.19	110.73	103.30
14	N	50	PRO	N-CA-CB	6.05	110.56	103.30
14	N	52	PRO	N-CA-CB	5.79	110.25	103.30

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	4028	0	4015	40	0
2	B	1798	0	1823	14	0
3	C	2119	0	2046	27	0
4	D	1189	0	1183	5	0
5	E	882	0	872	4	0
6	F	744	0	729	15	0
7	G	616	0	590	62	0
8	H	662	0	586	12	0
9	I	604	0	630	1	0
10	J	436	0	451	7	0
11	K	388	0	372	0	0
12	L	378	0	377	18	0
13	M	335	0	346	1	0
14	N	480	0	347	3	0
15	A	1	0	0	0	0
15	B	2	0	0	0	0
16	A	1	0	0	0	0
17	A	120	0	108	5	0
18	A	51	0	82	4	0
18	C	102	0	164	12	0
19	C	100	0	156	3	0
20	F	1	0	0	0	0
All	All	15037	0	14877	190	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 6.

All (190) 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)
7:G:57:VAL:HG23	7:G:61:SER:CB	1.38	1.51
1:A:6:TRP:CZ2	12:L:27:LEU:O	1.64	1.48
7:G:54:MET:HG3	7:G:58:TYR:CD2	1.54	1.41
7:G:57:VAL:CG2	7:G:61:SER:CB	2.07	1.30
7:G:57:VAL:CA	7:G:61:SER:HB2	1.63	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:ASN:O	7:G:60:LYS:NZ	1.65	1.28
7:G:68:ARG:HB2	7:G:69:PRO:CD	1.64	1.26
7:G:57:VAL:CG2	7:G:61:SER:HB2	1.62	1.24
7:G:54:MET:CG	7:G:58:TYR:CD2	2.29	1.15
7:G:54:MET:HG3	7:G:58:TYR:CG	1.83	1.12
7:G:57:VAL:CG2	7:G:61:SER:HB3	1.76	1.11
12:L:27:LEU:HB2	12:L:28:PRO:HD2	1.35	1.04
7:G:57:VAL:CB	7:G:61:SER:HB2	1.88	1.03
7:G:56:ASN:O	7:G:60:LYS:CE	2.08	1.02
7:G:57:VAL:HA	7:G:61:SER:CB	1.89	1.01
7:G:68:ARG:CB	7:G:69:PRO:HD2	1.89	1.01
7:G:57:VAL:HA	7:G:61:SER:HB2	1.39	1.01
7:G:68:ARG:HB2	7:G:69:PRO:HD2	1.02	1.00
1:A:129:TYR:OH	1:A:236:TRP:NE1	1.96	0.97
7:G:54:MET:SD	7:G:58:TYR:CE2	2.61	0.94
1:A:129:TYR:HH	1:A:236:TRP:HE1	1.14	0.93
7:G:54:MET:SD	7:G:58:TYR:CD2	2.64	0.90
7:G:57:VAL:CA	7:G:61:SER:CB	2.46	0.90
1:A:6:TRP:HZ2	12:L:27:LEU:O	1.26	0.90
7:G:57:VAL:O	7:G:61:SER:N	2.06	0.87
1:A:127:THR:HG22	1:A:235:PHE:CE2	2.10	0.87
12:L:27:LEU:HB2	12:L:28:PRO:CD	1.96	0.87
7:G:56:ASN:C	7:G:60:LYS:HZ2	1.78	0.86
1:A:6:TRP:CH2	12:L:27:LEU:O	2.28	0.86
7:G:56:ASN:C	7:G:60:LYS:NZ	2.28	0.86
7:G:50:VAL:O	7:G:53:SER:OG	1.94	0.85
12:L:24:GLY:C	12:L:27:LEU:HD21	1.96	0.85
7:G:57:VAL:HA	7:G:61:SER:OG	1.81	0.80
12:L:27:LEU:HD23	12:L:27:LEU:H	1.47	0.79
7:G:57:VAL:C	7:G:61:SER:HB2	2.03	0.79
7:G:55:LEU:O	7:G:60:LYS:HE3	1.81	0.79
7:G:57:VAL:HG23	7:G:61:SER:HB3	0.82	0.78
8:H:40:CYS:HG	8:H:54:CYS:HG	1.26	0.76
12:L:27:LEU:CB	12:L:28:PRO:HD2	2.15	0.75
12:L:27:LEU:HD23	12:L:27:LEU:N	2.03	0.74
12:L:27:LEU:CB	12:L:28:PRO:CD	2.64	0.74
7:G:57:VAL:O	7:G:61:SER:CA	2.36	0.73
7:G:58:TYR:O	7:G:60:LYS:N	2.24	0.70
3:C:132:LEU:CD1	7:G:58:TYR:CE1	2.75	0.69
8:H:50:ASP:N	8:H:50:ASP:OD1	2.23	0.69
1:A:229:ILE:HD11	2:B:175:ILE:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:ASN:O	7:G:60:LYS:CG	2.41	0.68
3:C:132:LEU:HD13	7:G:58:TYR:CE1	2.29	0.68
7:G:58:TYR:C	7:G:60:LYS:H	1.94	0.68
7:G:56:ASN:O	7:G:60:LYS:HE3	1.96	0.66
8:H:49:GLY:C	8:H:50:ASP:OD1	2.34	0.65
7:G:57:VAL:O	7:G:61:SER:HB2	1.96	0.65
7:G:57:VAL:HG22	7:G:61:SER:CB	2.24	0.64
7:G:57:VAL:HG22	7:G:61:SER:HB2	1.71	0.64
3:C:132:LEU:HD13	7:G:58:TYR:CZ	2.32	0.63
2:B:59:GLN:HG2	14:N:13:PRO:HD2	1.81	0.63
7:G:56:ASN:OD1	7:G:56:ASN:N	2.30	0.63
18:A:605:PEE:H38	18:C:301:PEE:H72	1.81	0.62
8:H:53:VAL:O	8:H:53:VAL:HG23	2.00	0.62
6:F:78:ASN:HD22	6:F:120:TYR:HE1	1.48	0.61
1:A:381:LEU:HD13	17:A:603:HEA:HAC	1.82	0.61
1:A:243:VAL:HB	17:A:604:HEA:HAC	1.83	0.60
3:C:132:LEU:CD1	7:G:58:TYR:CZ	2.84	0.60
1:A:114:ALA:O	1:A:118:VAL:HG13	2.00	0.60
8:H:53:VAL:C	8:H:55:GLU:H	2.04	0.60
7:G:56:ASN:HA	7:G:60:LYS:HZ1	1.66	0.59
18:A:605:PEE:H25	18:C:301:PEE:H60	1.83	0.59
18:A:605:PEE:H30	18:A:605:PEE:H58	1.84	0.58
1:A:331:ASN:HD21	4:D:42:ARG:HB2	1.68	0.58
6:F:105:LEU:HD22	6:F:122:LEU:HB2	1.86	0.58
3:C:217:ILE:HG21	18:C:301:PEE:H20	1.85	0.58
6:F:43:GLN:HE21	10:J:28:VAL:HG21	1.68	0.58
7:G:56:ASN:O	7:G:60:LYS:HG3	2.02	0.58
7:G:56:ASN:CA	7:G:60:LYS:HZ1	2.17	0.58
17:A:604:HEA:H251	2:B:73:LEU:HD21	1.85	0.58
6:F:91:CYS:HG	6:F:120:TYR:HH	1.52	0.57
1:A:449:THR:HG21	2:B:5:ALA:HB2	1.87	0.57
3:C:225:PHE:HE1	10:J:26:ASN:HB3	1.70	0.57
7:G:68:ARG:HB2	7:G:69:PRO:HD3	1.77	0.57
7:G:80:ARG:NH1	7:G:90:ASN:OD1	2.37	0.57
1:A:128:VAL:HG13	1:A:128:VAL:O	2.05	0.57
7:G:68:ARG:CB	7:G:69:PRO:CD	2.43	0.57
7:G:57:VAL:O	7:G:61:SER:CB	2.53	0.56
1:A:509:VAL:HG11	6:F:102:TRP:HZ3	1.70	0.56
1:A:508:PRO:HG3	3:C:6:HIS:HB3	1.88	0.56
7:G:59:LEU:HG	7:G:59:LEU:O	2.05	0.56
3:C:19:THR:HG23	10:J:62:THR:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:51:ILE:O	8:H:51:ILE:HG22	2.05	0.55
3:C:132:LEU:HD13	7:G:58:TYR:OH	2.05	0.55
18:C:301:PEE:H71	18:C:302:PEE:H47	1.88	0.55
4:D:69:SER:HA	5:E:97:ARG:HH22	1.72	0.55
7:G:78:ARG:HE	7:G:101:PRO:HG2	1.71	0.55
12:L:24:GLY:HA3	12:L:31:VAL:HG11	1.87	0.55
1:A:116:ALA:O	12:L:59:GLN:NE2	2.40	0.54
1:A:394:ILE:HG23	1:A:405:LEU:HD11	1.88	0.54
6:F:99:SER:OG	6:F:115:ARG:NH2	2.40	0.54
1:A:379:TYR:OH	1:A:422:ASN:ND2	2.40	0.54
7:G:58:TYR:C	7:G:60:LYS:N	2.61	0.54
2:B:173:ASP:O	2:B:180:ASN:ND2	2.40	0.54
3:C:7:ALA:HB1	3:C:72:THR:HG21	1.89	0.54
1:A:297:MET:O	1:A:302:ARG:NH2	2.41	0.54
19:C:303:CDL:H602	19:C:303:CDL:H821	1.89	0.54
7:G:56:ASN:CA	7:G:60:LYS:NZ	2.71	0.53
1:A:404:THR:HG23	1:A:482:VAL:HG22	1.89	0.52
6:F:99:SER:O	6:F:115:ARG:NH2	2.41	0.52
6:F:113:CYS:N	6:F:117:GLY:O	2.40	0.52
1:A:148:PHE:HA	1:A:151:HIS:HD2	1.73	0.52
1:A:244:TYR:HA	1:A:247:ILE:HG22	1.92	0.52
7:G:56:ASN:HA	7:G:60:LYS:NZ	2.25	0.52
8:H:51:ILE:N	8:H:51:ILE:CD1	2.73	0.52
1:A:371:TYR:HD2	1:A:431:LEU:HD22	1.74	0.52
3:C:223:LEU:O	10:J:26:ASN:ND2	2.44	0.51
12:L:24:GLY:CA	12:L:27:LEU:HD21	2.40	0.51
1:A:495:LEU:HD11	6:F:102:TRP:HB3	1.92	0.51
12:L:29:PHE:HD1	12:L:30:SER:H	1.59	0.51
8:H:51:ILE:N	8:H:51:ILE:HD12	2.26	0.50
10:J:35:PHE:O	10:J:46:LYS:NZ	2.42	0.50
1:A:386:VAL:HG11	17:A:603:HEA:H261	1.93	0.50
7:G:54:MET:SD	7:G:58:TYR:HE2	2.31	0.50
3:C:67:TYR:O	10:J:36:GLN:NE2	2.45	0.50
7:G:57:VAL:CB	7:G:61:SER:CB	2.67	0.49
3:C:181:TYR:O	18:C:302:PEE:N	2.43	0.49
8:H:53:VAL:C	8:H:55:GLU:N	2.65	0.49
3:C:9:HIS:ND1	3:C:10:MET:O	2.43	0.49
3:C:214:PHE:HD1	18:C:301:PEE:H27	1.77	0.49
7:G:70:GLU:O	7:G:71:PHE:C	2.50	0.49
7:G:56:ASN:HA	7:G:60:LYS:CE	2.43	0.48
6:F:108:GLY:O	6:F:121:LYS:NZ	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:C:301:PEE:H78	18:C:302:PEE:H41	1.95	0.48
7:G:58:TYR:O	7:G:60:LYS:HG2	2.13	0.48
5:E:142:PRO:HA	5:E:145:LEU:HB2	1.95	0.48
1:A:481:LYS:HB2	13:M:29:LEU:HD12	1.94	0.48
7:G:54:MET:CG	7:G:58:TYR:HD2	2.17	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.47
8:H:34:TYR:OH	8:H:74:ASP:OD1	2.27	0.47
6:F:105:LEU:HD11	6:F:120:TYR:HB3	1.95	0.47
3:C:137:LEU:HD23	3:C:246:ASP:HA	1.95	0.47
1:A:512:LYS:HE2	6:F:69:GLY:H	1.80	0.47
19:C:303:CDL:H761	19:C:303:CDL:H611	1.97	0.47
18:A:605:PEE:H39	18:A:605:PEE:H68	1.96	0.46
3:C:253:TYR:HA	3:C:257:TYR:HD2	1.80	0.46
1:A:173:PRO:HD2	1:A:176:MET:HE1	1.97	0.46
2:B:73:LEU:HD23	2:B:76:ILE:HD12	1.98	0.46
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.79	0.46
7:G:57:VAL:O	7:G:61:SER:C	2.53	0.46
18:C:302:PEE:H69	18:C:302:PEE:H63	1.65	0.46
1:A:83:VAL:HG21	1:A:188:VAL:HG11	1.99	0.45
5:E:57:VAL:HG12	5:E:61:ASN:HD21	1.80	0.45
1:A:463:THR:HG21	4:D:110:PHE:HB3	1.99	0.45
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.52	0.45
3:C:201:THR:HG22	3:C:252:LEU:HD21	1.98	0.45
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.99	0.44
1:A:407:GLN:HE21	1:A:411:LYS:HE3	1.82	0.44
1:A:244:TYR:O	1:A:248:LEU:N	2.40	0.44
1:A:5:ARG:HH21	12:L:26:ASN:HA	1.83	0.44
9:I:41:VAL:HG12	9:I:45:ARG:HH12	1.82	0.44
6:F:37:VAL:HA	6:F:38:PRO:HD3	1.85	0.43
1:A:101:SER:O	1:A:156:SER:OG	2.32	0.43
18:C:301:PEE:H25	18:C:301:PEE:H32	1.91	0.43
8:H:51:ILE:CD1	8:H:51:ILE:H	2.30	0.43
12:L:24:GLY:HA2	12:L:27:LEU:HD21	2.00	0.43
14:N:24:THR:HA	14:N:27:THR:HG22	2.01	0.43
2:B:194:GLY:N	2:B:209:ILE:O	2.52	0.43
1:A:158:ILE:HD11	3:C:89:SER:HB2	2.00	0.43
3:C:167:ILE:HD13	3:C:216:THR:HG22	2.01	0.43
7:G:43:PHE:HA	7:G:47:LEU:HD12	2.00	0.43
3:C:210:ILE:HG12	18:C:301:PEE:H39	2.00	0.42
1:A:73:ILE:HD13	17:A:603:HEA:H253	2.02	0.42
18:C:302:PEE:H33	18:C:302:PEE:H39	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ARG:HD2	2:B:84:LEU:HD11	2.02	0.42
19:C:303:CDL:H552	14:N:33:LEU:HD11	2.02	0.42
3:C:187:THR:HB	3:C:190:ASP:HB2	2.02	0.42
4:D:134:ASP:HB2	4:D:137:TRP:CD1	2.55	0.42
10:J:79:PRO:HD3	12:L:62:LYS:HE3	2.00	0.42
8:H:53:VAL:O	8:H:55:GLU:N	2.53	0.41
3:C:72:THR:HG22	3:C:74:PRO:HD2	2.03	0.41
2:B:162:SER:HB3	2:B:197:SER:HB2	2.03	0.41
1:A:11:ASN:HB3	1:A:14:ASP:HB2	2.02	0.41
2:B:158:ASP:OD1	2:B:158:ASP:N	2.54	0.41
5:E:106:VAL:HG13	5:E:142:PRO:HG3	2.03	0.41
6:F:89:VAL:HG21	6:F:105:LEU:HD12	2.01	0.41
3:C:198:PHE:O	3:C:202:GLY:N	2.54	0.41
4:D:134:ASP:HB2	4:D:137:TRP:HD1	1.86	0.41
3:C:58:TRP:CE2	18:C:301:PEE:H23	2.55	0.41
12:L:31:VAL:HG22	12:L:31:VAL:O	2.21	0.41
3:C:133:ASN:HB3	3:C:173:PHE:HE1	1.84	0.41
6:F:113:CYS:HA	6:F:114:PRO:HD3	1.96	0.40
2:B:133:LEU:N	2:B:137:ASP:OD2	2.53	0.40
3:C:128:GLU:HB3	3:C:129:VAL:H	1.62	0.40
7:G:68:ARG:CG	7:G:69:PRO:HD2	2.49	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	511/513 (100%)	489 (96%)	21 (4%)	1 (0%)	47 79
2	B	225/227 (99%)	212 (94%)	13 (6%)	0	100 100
3	C	258/260 (99%)	246 (95%)	12 (5%)	0	100 100
4	D	142/144 (99%)	139 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
7	G	73/75 (97%)	58 (80%)	11 (15%)	4 (6%)	2	19
8	H	80/82 (98%)	72 (90%)	3 (4%)	5 (6%)	1	17
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
11	K	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	0	3 (7%)	1	15
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
14	N	77/79 (98%)	58 (75%)	16 (21%)	3 (4%)	3	27
All	All	1827/1855 (98%)	1717 (94%)	94 (5%)	16 (1%)	21	57

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	59	LEU
7	G	68	ARG
7	G	69	PRO
8	H	51	ILE
8	H	55	GLU
12	L	27	LEU
12	L	28	PRO
14	N	58	PRO
14	N	79	PRO
8	H	53	VAL
7	G	71	PHE
8	H	50	ASP
8	H	54	CYS
14	N	50	PRO
1	A	128	VAL
12	L	31	VAL

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	427/427 (100%)	423 (99%)	4 (1%)	78	90
2	B	202/202 (100%)	202 (100%)	0	100	100
3	C	226/226 (100%)	226 (100%)	0	100	100
4	D	128/128 (100%)	128 (100%)	0	100	100
5	E	97/97 (100%)	97 (100%)	0	100	100
6	F	79/79 (100%)	79 (100%)	0	100	100
7	G	66/66 (100%)	62 (94%)	4 (6%)	18	53
8	H	67/74 (90%)	66 (98%)	1 (2%)	65	84
9	I	61/61 (100%)	61 (100%)	0	100	100
10	J	45/45 (100%)	45 (100%)	0	100	100
11	K	41/41 (100%)	41 (100%)	0	100	100
12	L	41/41 (100%)	39 (95%)	2 (5%)	25	59
13	M	37/37 (100%)	37 (100%)	0	100	100
14	N	25/70 (36%)	25 (100%)	0	100	100
All	All	1542/1594 (97%)	1531 (99%)	11 (1%)	84	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	MET
1	A	118	VAL
1	A	127	THR
1	A	202	LEU
7	G	56	ASN
7	G	59	LEU
7	G	67	GLU
7	G	70	GLU
8	H	50	ASP
12	L	27	LEU
12	L	29	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	413	HIS
1	A	422	ASN
2	B	54	ASN
2	B	102	HIS
3	C	148	HIS
3	C	207	HIS
5	E	61	ASN
5	E	75	ASN
5	E	128	GLN
6	F	63	ASN
6	F	106	HIS
7	G	95	HIS
8	H	26	GLN
10	J	26	ASN
13	M	61	HIS

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)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	PEE	C	302	-	50,50,50	1.16	4 (8%)	53,55,55	1.11	4 (7%)
19	CDL	C	303	-	99,99,99	0.92	4 (4%)	105,111,111	1.08	7 (6%)
18	PEE	A	605	-	50,50,50	1.14	4 (8%)	53,55,55	1.21	3 (5%)
18	PEE	C	301	-	50,50,50	1.19	4 (8%)	53,55,55	1.18	3 (5%)
17	HEA	A	603	1	57,67,67	1.96	14 (24%)	61,103,103	2.52	25 (40%)
17	HEA	A	604	1	57,67,67	1.96	16 (28%)	61,103,103	2.47	28 (45%)

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
18	PEE	C	302	-	1/1/4/8	24/54/54/54	-
19	CDL	C	303	-	-	48/110/110/110	-
18	PEE	A	605	-	1/1/4/8	14/54/54/54	-
18	PEE	C	301	-	1/1/4/8	17/54/54/54	-
17	HEA	A	603	1	2/2/7/16	11/32/76/76	-
17	HEA	A	604	1	2/2/7/16	4/32/76/76	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	603	HEA	C3B-C2B	5.24	1.46	1.34
17	A	604	HEA	C3B-C2B	5.17	1.46	1.34
17	A	604	HEA	CHD-C1D	4.67	1.46	1.35
17	A	603	HEA	C3A-C2A	4.62	1.46	1.40
17	A	604	HEA	C3D-C2D	4.60	1.46	1.36
17	A	603	HEA	CHC-C4B	4.58	1.46	1.35
17	A	604	HEA	C3A-C2A	4.55	1.46	1.40
18	C	301	PEE	O3-C30	4.51	1.46	1.33
17	A	603	HEA	CHD-C1D	4.46	1.46	1.35
17	A	604	HEA	CHC-C4B	4.39	1.46	1.35
17	A	603	HEA	C3D-C2D	4.34	1.45	1.36
19	C	303	CDL	OB8-CB7	4.28	1.45	1.33
17	A	604	HEA	C3C-C2C	4.23	1.46	1.40
19	C	303	CDL	OA8-CA7	4.20	1.45	1.33
19	C	303	CDL	OA6-CA5	4.12	1.45	1.34
17	A	603	HEA	C3C-C2C	4.12	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	303	CDL	OB6-CB5	4.09	1.45	1.34
18	C	302	PEE	O2-C10	3.92	1.45	1.34
18	C	301	PEE	O2-C10	3.89	1.45	1.34
18	C	302	PEE	O3-C30	3.87	1.44	1.33
18	A	605	PEE	O2-C10	3.83	1.45	1.34
18	A	605	PEE	O3-C30	3.77	1.44	1.33
18	C	301	PEE	C39-C38	3.70	1.53	1.31
18	C	302	PEE	C39-C38	3.69	1.53	1.31
18	A	605	PEE	C19-C18	3.64	1.52	1.31
18	A	605	PEE	C39-C38	3.63	1.52	1.31
18	C	302	PEE	C19-C18	3.61	1.52	1.31
18	C	301	PEE	C19-C18	3.57	1.52	1.31
17	A	603	HEA	C1D-ND	-3.29	1.34	1.40
17	A	604	HEA	C1D-ND	-3.13	1.34	1.40
17	A	604	HEA	FE-NB	2.94	2.11	1.96
17	A	603	HEA	C4B-NB	-2.89	1.35	1.40
17	A	604	HEA	FE-ND	2.88	2.11	1.96
17	A	603	HEA	FE-ND	2.87	2.11	1.96
17	A	603	HEA	FE-NB	2.85	2.11	1.96
17	A	604	HEA	C4B-NB	-2.79	1.35	1.40
17	A	604	HEA	C4B-C3B	2.74	1.49	1.44
17	A	603	HEA	C4B-C3B	2.53	1.48	1.44
17	A	603	HEA	C2A-C1A	2.50	1.48	1.42
17	A	604	HEA	C2A-C1A	2.40	1.48	1.42
17	A	603	HEA	C4D-C3D	2.21	1.48	1.45
17	A	604	HEA	C4C-CHD	2.13	1.46	1.41
17	A	604	HEA	C1B-NB	-2.13	1.34	1.38
17	A	604	HEA	C1D-C2D	2.10	1.48	1.44
17	A	603	HEA	C1B-NB	-2.03	1.34	1.38
17	A	604	HEA	C4D-ND	-2.01	1.34	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	604	HEA	C3D-C4D-ND	7.02	117.16	110.36
17	A	603	HEA	C3D-C4D-ND	6.34	116.50	110.36
17	A	604	HEA	C3B-C4B-NB	6.03	116.98	109.84
17	A	603	HEA	C2B-C1B-NB	5.67	116.67	109.88
17	A	604	HEA	C2B-C1B-NB	5.62	116.61	109.88
17	A	603	HEA	C3B-C4B-NB	5.35	116.18	109.84
17	A	604	HEA	C2D-C1D-ND	5.33	116.16	109.84
17	A	603	HEA	C2D-C1D-ND	5.19	115.99	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	603	HEA	CAD-C3D-C4D	4.74	132.94	124.66
17	A	603	HEA	CBA-CAA-C2A	-4.41	105.17	112.60
17	A	603	HEA	C3C-C4C-NC	4.33	114.81	109.21
19	C	303	CDL	OA6-CA5-C11	4.33	120.84	111.50
17	A	604	HEA	C1D-C2D-C3D	-4.20	102.54	106.96
18	A	605	PEE	O2-C10-C11	4.17	120.50	111.50
19	C	303	CDL	OB6-CB5-C51	3.95	120.01	111.50
18	C	301	PEE	O2-C10-C11	3.90	119.92	111.50
17	A	603	HEA	CAD-CBD-CGD	-3.77	105.50	113.60
17	A	603	HEA	CHA-C4D-ND	-3.76	120.35	124.43
17	A	604	HEA	CMC-C2C-C3C	3.67	131.55	124.68
18	C	302	PEE	O2-C10-C11	3.67	119.41	111.50
17	A	603	HEA	C4D-C3D-C2D	-3.62	101.62	106.90
17	A	604	HEA	C4B-C3B-C2B	-3.59	101.28	107.41
17	A	603	HEA	C1B-C2B-C3B	-3.55	102.55	106.80
18	C	301	PEE	O3-C30-C31	3.55	123.06	111.91
18	C	302	PEE	C2-O2-C10	-3.51	109.14	117.79
17	A	604	HEA	C3C-C4C-NC	3.48	113.71	109.21
17	A	603	HEA	C13-C12-C11	-3.44	109.18	114.35
17	A	603	HEA	CMC-C2C-C3C	3.42	131.08	124.68
18	A	605	PEE	C2-O2-C10	-3.35	109.53	117.79
17	A	603	HEA	C1D-C2D-C3D	-3.34	103.45	106.96
17	A	604	HEA	C4D-C3D-C2D	-3.32	102.05	106.90
19	C	303	CDL	OB8-CB7-C71	3.16	121.83	111.91
17	A	604	HEA	C4B-NB-C1B	-3.11	101.86	105.07
17	A	603	HEA	C4B-C3B-C2B	-3.02	102.25	107.41
17	A	604	HEA	CAD-CBD-CGD	-2.97	107.21	113.60
17	A	604	HEA	C1B-C2B-C3B	-2.96	103.26	106.80
17	A	604	HEA	CBA-CAA-C2A	-2.94	107.65	112.60
17	A	604	HEA	C1D-ND-C4D	-2.89	102.09	105.07
17	A	604	HEA	C27-C19-C20	2.83	120.03	115.27
17	A	603	HEA	C13-C14-C15	-2.75	121.04	127.66
17	A	604	HEA	CHA-C4D-C3D	-2.70	120.87	124.84
19	C	303	CDL	OA8-CA7-C31	2.69	120.36	111.91
18	C	302	PEE	O3-C30-C31	2.68	120.31	111.91
17	A	603	HEA	C4B-NB-C1B	-2.64	102.34	105.07
17	A	603	HEA	C27-C19-C20	2.60	119.65	115.27
17	A	603	HEA	C17-C18-C19	-2.58	121.44	127.66
17	A	603	HEA	C1D-ND-C4D	-2.56	102.43	105.07
17	A	604	HEA	CMD-C2D-C1D	2.54	128.91	125.04
17	A	604	HEA	C26-C15-C14	-2.49	117.30	123.68
17	A	604	HEA	CHB-C1B-NB	-2.48	121.74	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	603	HEA	CHD-C1D-C2D	-2.45	119.96	126.72
17	A	603	HEA	CMD-C2D-C1D	2.44	128.76	125.04
18	A	605	PEE	O3-C30-C31	2.43	119.52	111.91
17	A	604	HEA	C12-C13-C14	-2.41	105.86	112.23
19	C	303	CDL	CA4-OA6-CA5	-2.37	111.96	117.79
17	A	603	HEA	CMB-C2B-C1B	2.37	128.64	125.04
17	A	604	HEA	CHC-C4B-NB	-2.33	121.51	124.38
17	A	603	HEA	CHB-C1B-C2B	-2.31	121.37	124.98
17	A	603	HEA	CHB-C1B-NB	-2.29	121.94	124.43
17	A	604	HEA	CHA-C4D-ND	-2.26	121.97	124.43
17	A	604	HEA	C25-C23-C24	2.24	119.55	114.60
17	A	604	HEA	C26-C15-C16	2.22	119.01	115.27
19	C	303	CDL	CB4-OB6-CB5	-2.19	112.40	117.79
17	A	604	HEA	C17-C18-C19	-2.18	122.41	127.66
17	A	604	HEA	CHB-C1B-C2B	-2.14	121.64	124.98
17	A	604	HEA	CMB-C2B-C1B	2.12	128.26	125.04
17	A	604	HEA	CHD-C1D-C2D	-2.09	120.94	126.72
19	C	303	CDL	OA6-CA5-OA7	-2.08	118.69	123.70
18	C	301	PEE	O3-C30-O5	-2.04	118.45	123.59
18	C	302	PEE	O3-C30-O5	-2.02	118.48	123.59

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	603	HEA	NB
17	A	603	HEA	ND
17	A	604	HEA	NB
17	A	604	HEA	ND
18	A	605	PEE	C2
18	C	301	PEE	C2
18	C	302	PEE	C2

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	605	PEE	O4P-C4-C5-N
18	A	605	PEE	C1-O3P-P-O1P
18	A	605	PEE	C1-O3P-P-O2P
18	C	301	PEE	C4-O4P-P-O1P
18	C	301	PEE	C4-O4P-P-O2P
18	C	302	PEE	O4P-C4-C5-N
18	C	302	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
18	C	302	PEE	C4-O4P-P-O2P
19	C	303	CDL	CA2-C1-CB2-OB2
19	C	303	CDL	CA2-OA2-PA1-OA3
19	C	303	CDL	CA2-OA2-PA1-OA5
19	C	303	CDL	CA3-OA5-PA1-OA3
18	A	605	PEE	O5-C30-O3-C3
18	C	302	PEE	O4-C10-O2-C2
18	A	605	PEE	C31-C30-O3-C3
19	C	303	CDL	C71-CB7-OB8-CB6
18	C	302	PEE	C11-C10-O2-C2
18	A	605	PEE	C37-C38-C39-C40
18	C	301	PEE	C37-C38-C39-C40
18	C	302	PEE	C17-C18-C19-C20
19	C	303	CDL	OB9-CB7-OB8-CB6
19	C	303	CDL	O1-C1-CB2-OB2
18	C	301	PEE	C31-C30-O3-C3
19	C	303	CDL	C51-CB5-OB6-CB4
18	C	301	PEE	O5-C30-O3-C3
19	C	303	CDL	OB7-CB5-OB6-CB4
18	C	302	PEE	C31-C30-O3-C3
19	C	303	CDL	C31-CA7-OA8-CA6
19	C	303	CDL	C11-CA5-OA6-CA4
18	A	605	PEE	C10-C11-C12-C13
18	C	302	PEE	O5-C30-O3-C3
19	C	303	CDL	OA9-CA7-OA8-CA6
18	A	605	PEE	C1-O3P-P-O4P
18	C	301	PEE	C4-O4P-P-O3P
19	C	303	CDL	CB2-OB2-PB2-OB5
19	C	303	CDL	CB3-OB5-PB2-OB2
19	C	303	CDL	OA7-CA5-OA6-CA4
18	A	605	PEE	C11-C10-O2-C2
19	C	303	CDL	C40-C41-C42-C43
19	C	303	CDL	C57-C58-C59-C60
18	A	605	PEE	O4-C10-O2-C2
18	C	301	PEE	C17-C18-C19-C20
19	C	303	CDL	C52-C53-C54-C55
19	C	303	CDL	C22-C23-C24-C25
18	C	301	PEE	C12-C13-C14-C15
18	C	301	PEE	C10-C11-C12-C13
18	A	605	PEE	C14-C15-C16-C17
19	C	303	CDL	C31-C32-C33-C34
18	C	302	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
18	C	302	PEE	C35-C36-C37-C38
18	C	302	PEE	C33-C34-C35-C36
19	C	303	CDL	C14-C15-C16-C17
19	C	303	CDL	C58-C59-C60-C61
17	A	603	HEA	C26-C15-C16-C17
17	A	603	HEA	C14-C15-C16-C17
18	C	302	PEE	C39-C40-C41-C42
19	C	303	CDL	C36-C37-C38-C39
18	C	301	PEE	C11-C12-C13-C14
18	C	302	PEE	C38-C39-C40-C41
18	C	302	PEE	C19-C20-C21-C22
18	C	302	PEE	C1-O3P-P-O4P
18	C	302	PEE	C15-C16-C17-C18
18	C	301	PEE	C1-C2-C3-O3
19	C	303	CDL	CB7-C71-C72-C73
18	A	605	PEE	C34-C35-C36-C37
19	C	303	CDL	C20-C21-C22-C23
19	C	303	CDL	C19-C20-C21-C22
18	C	302	PEE	C4-O4P-P-O3P
18	C	301	PEE	C22-C23-C24-C25
19	C	303	CDL	C64-C65-C66-C67
17	A	603	HEA	C2D-C3D-CAD-CBD
19	C	303	CDL	OB5-CB3-CB4-CB6
18	C	302	PEE	C36-C37-C38-C39
19	C	303	CDL	C16-C17-C18-C19
19	C	303	CDL	CA7-C31-C32-C33
19	C	303	CDL	C75-C76-C77-C78
19	C	303	CDL	C38-C39-C40-C41
19	C	303	CDL	C23-C24-C25-C26
19	C	303	CDL	CA3-OA5-PA1-OA2
18	C	302	PEE	C4-O4P-P-O1P
19	C	303	CDL	CB2-OB2-PB2-OB3
19	C	303	CDL	CB3-OB5-PB2-OB3
18	C	302	PEE	C37-C38-C39-C40
19	C	303	CDL	C13-C14-C15-C16
19	C	303	CDL	C53-C54-C55-C56
17	A	604	HEA	C26-C15-C16-C17
19	C	303	CDL	OB5-CB3-CB4-OB6
18	C	301	PEE	O2-C2-C3-O3
17	A	603	HEA	C4D-C3D-CAD-CBD
18	C	301	PEE	C14-C15-C16-C17
18	C	301	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
19	C	303	CDL	C54-C55-C56-C57
17	A	603	HEA	CAD-CBD-CGD-O1D
17	A	604	HEA	CAA-CBA-CGA-O2A
19	C	303	CDL	CA3-CA4-OA6-CA5
17	A	604	HEA	CAA-CBA-CGA-O1A
18	C	302	PEE	C31-C32-C33-C34
18	C	302	PEE	C41-C42-C43-C44
17	A	603	HEA	CAD-CBD-CGD-O2D
19	C	303	CDL	C84-C85-C86-C87
17	A	603	HEA	C3D-CAD-CBD-CGD
18	A	605	PEE	C18-C19-C20-C21
18	C	301	PEE	C16-C17-C18-C19
18	C	301	PEE	C38-C39-C40-C41
19	C	303	CDL	C21-C22-C23-C24
19	C	303	CDL	C51-C52-C53-C54
18	A	605	PEE	C36-C37-C38-C39
17	A	603	HEA	CAA-CBA-CGA-O2A
18	C	302	PEE	C1-O3P-P-O2P
19	C	303	CDL	CB2-OB2-PB2-OB4
17	A	603	HEA	O11-C11-C12-C13
17	A	603	HEA	C27-C19-C20-C21
18	C	302	PEE	C5-C4-O4P-P
19	C	303	CDL	CA6-CA4-OA6-CA5
17	A	604	HEA	C14-C15-C16-C17
19	C	303	CDL	C12-C11-CA5-OA7
19	C	303	CDL	C12-C11-CA5-OA6
17	A	603	HEA	CAA-CBA-CGA-O1A

There are no ring outliers.

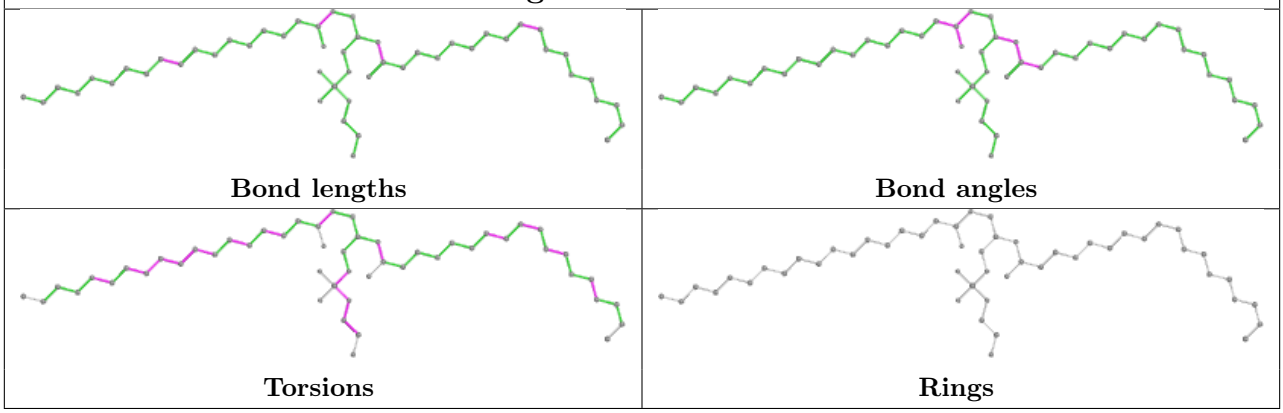
6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	302	PEE	5	0
19	C	303	CDL	3	0
18	A	605	PEE	4	0
18	C	301	PEE	9	0
17	A	603	HEA	3	0
17	A	604	HEA	2	0

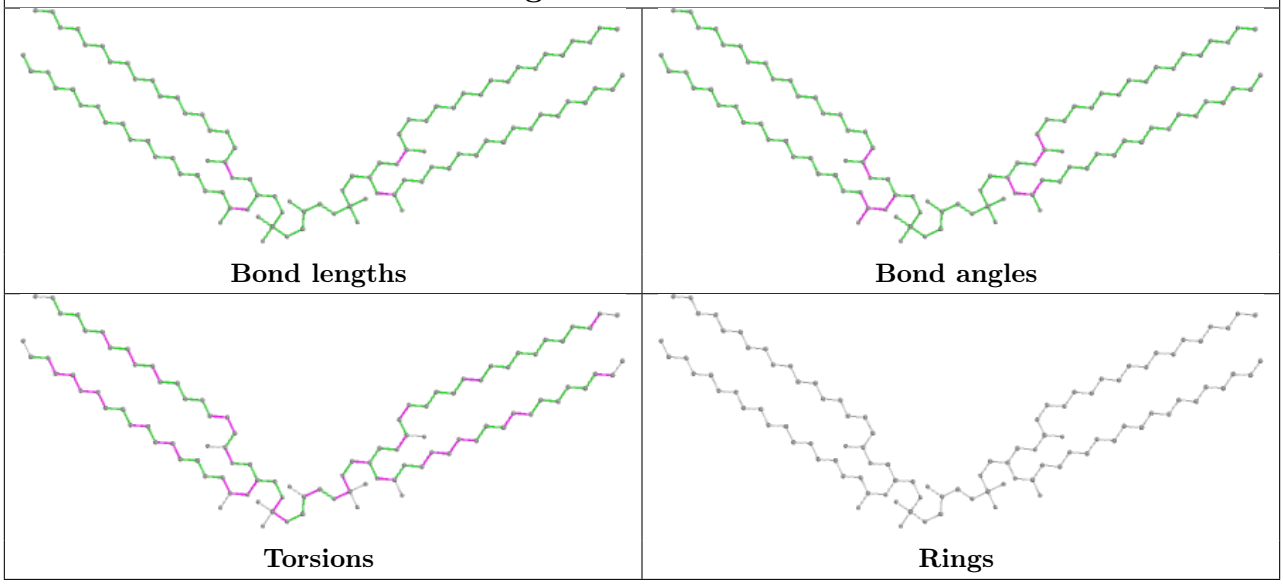
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

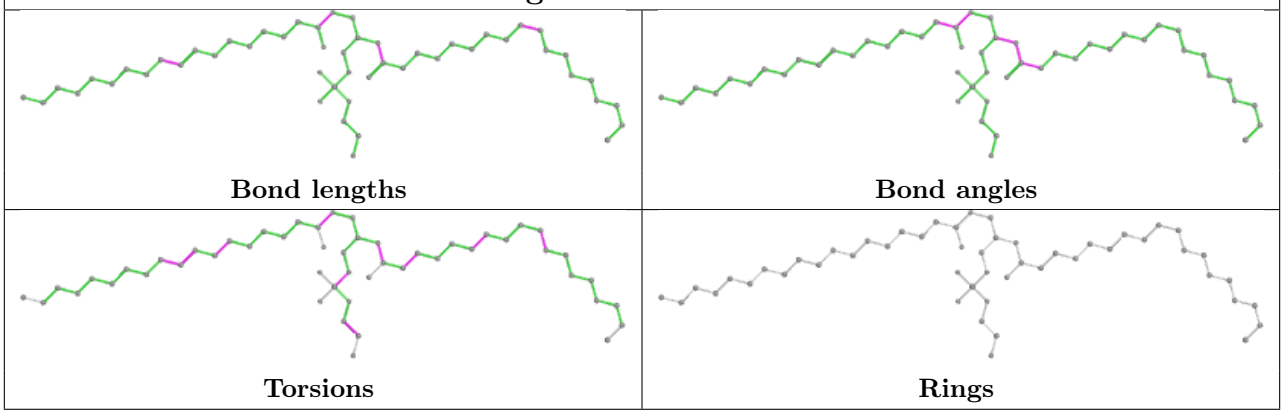
Ligand PEE C 302



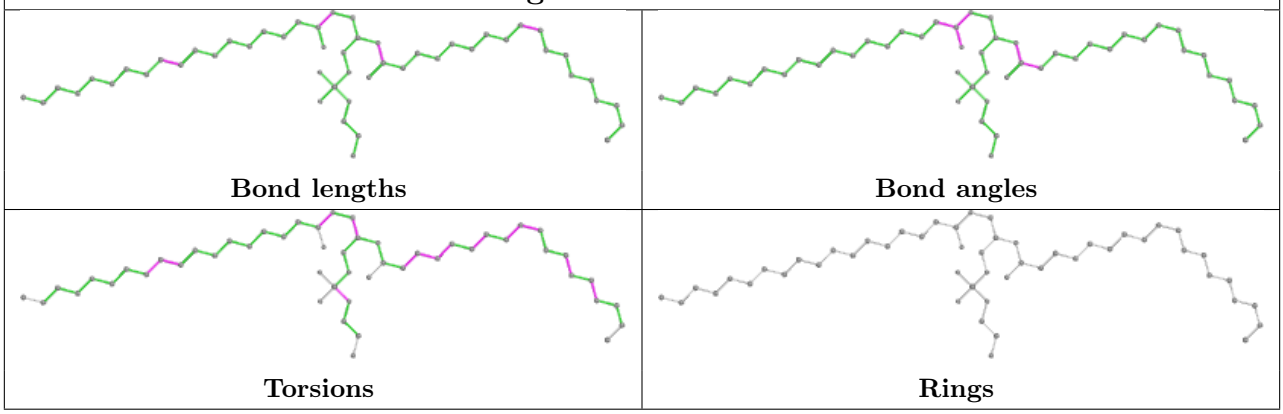
Ligand CDL C 303



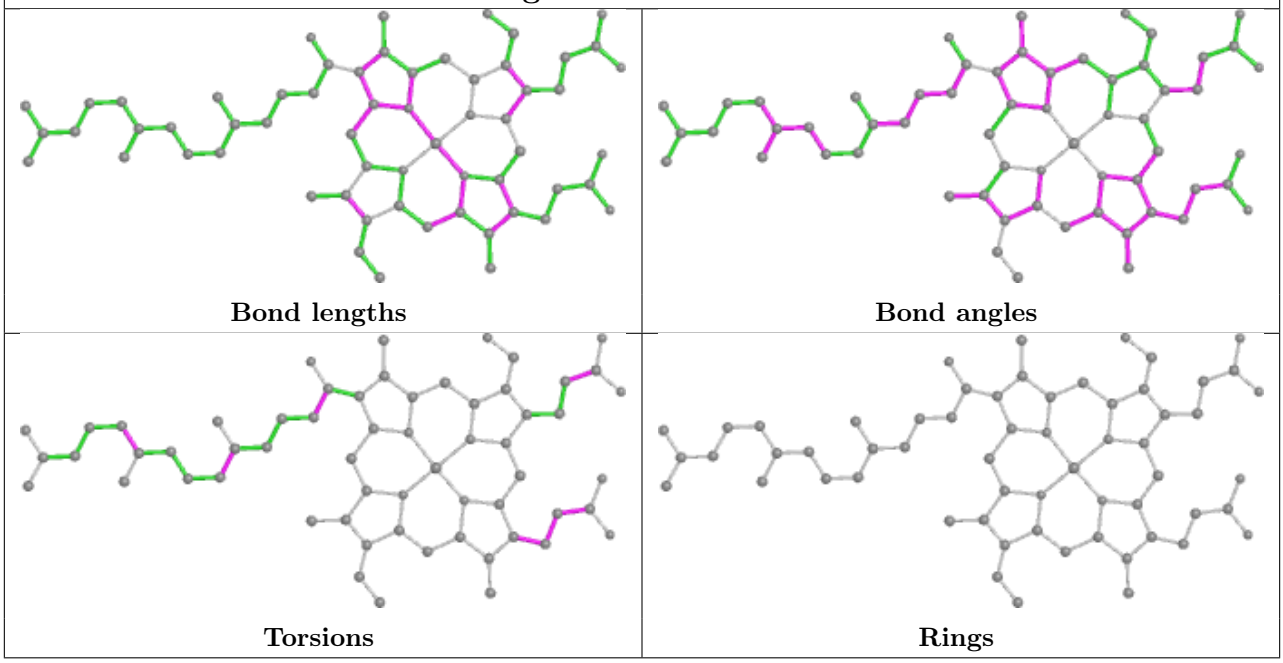
Ligand PEE A 605

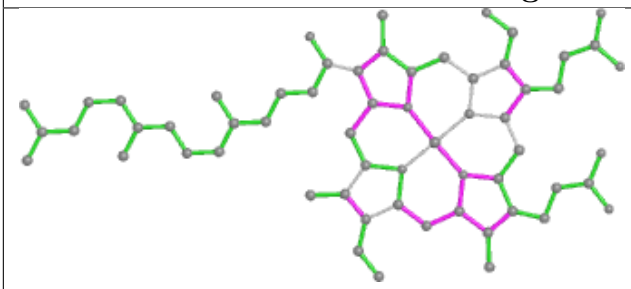
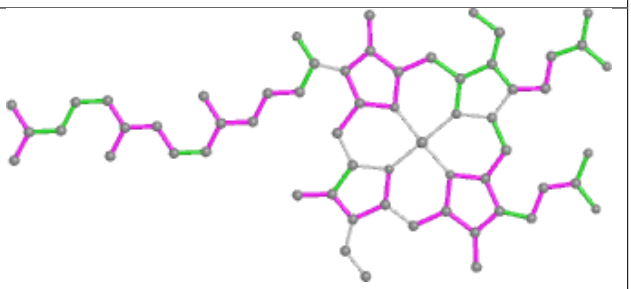
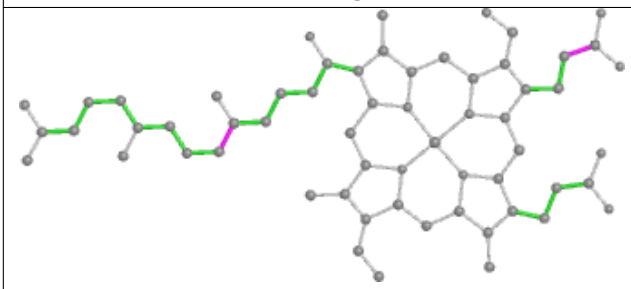
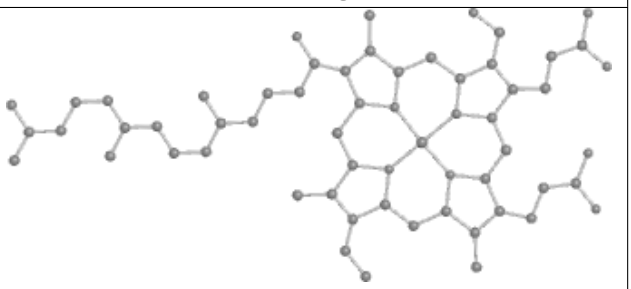


Ligand PEE C 301



Ligand HEA A 603



Ligand HEA A 604	
 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.

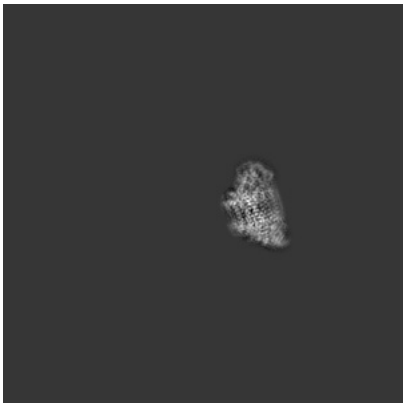
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-6896. 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.

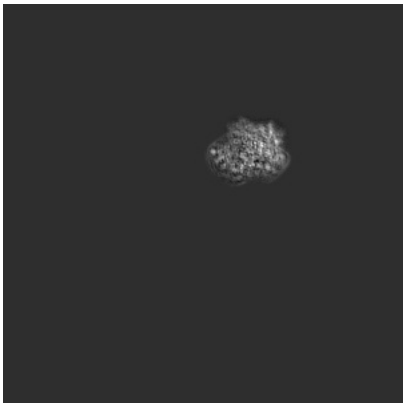
6.1 Orthogonal projections (i)

6.1.1 Primary map



X

Y

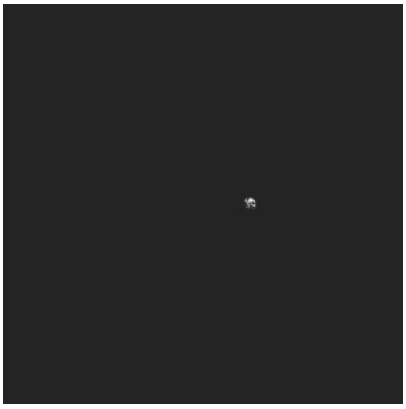


Z

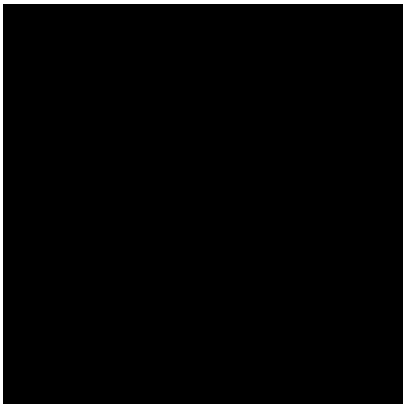
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 240



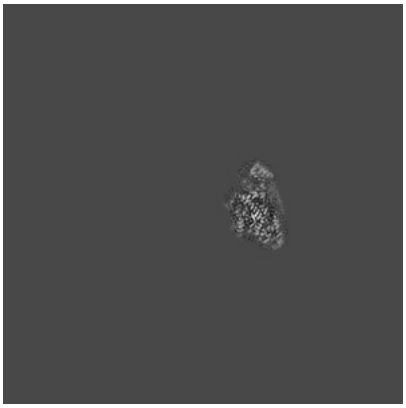
Y Index: 240

Z Index: 240

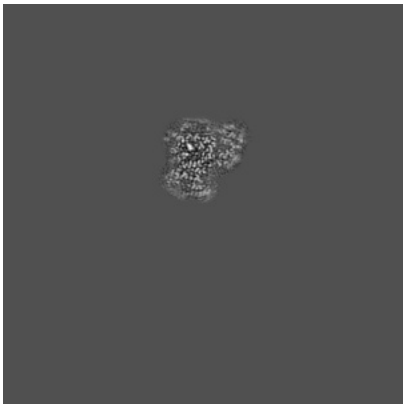
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

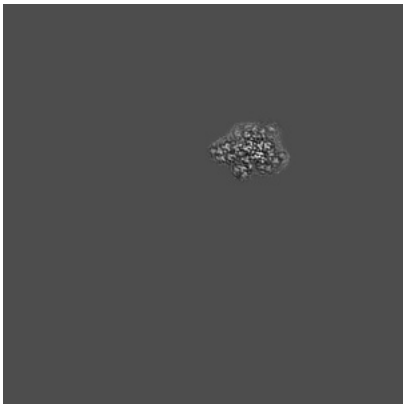
6.3.1 Primary map



X Index: 309



Y Index: 300

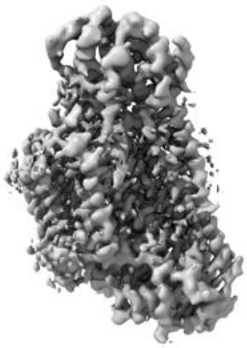


Z Index: 223

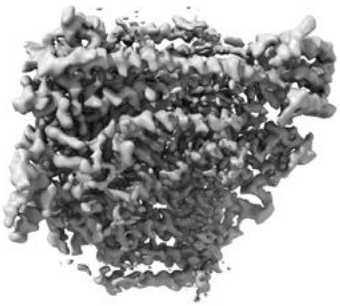
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

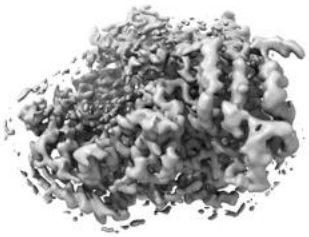
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

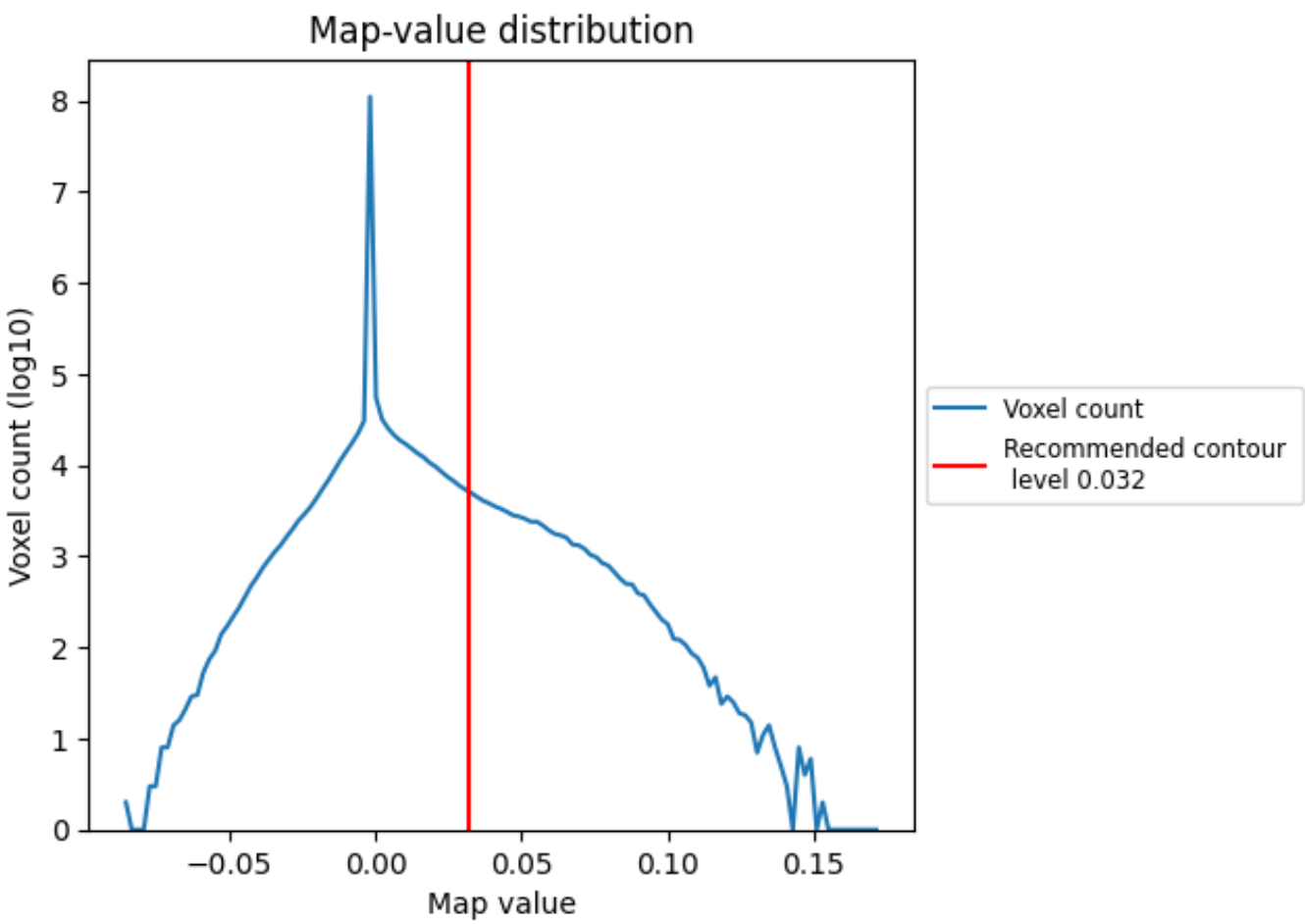
6.5 Mask visualisation (i)

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

7 Map analysis (i)

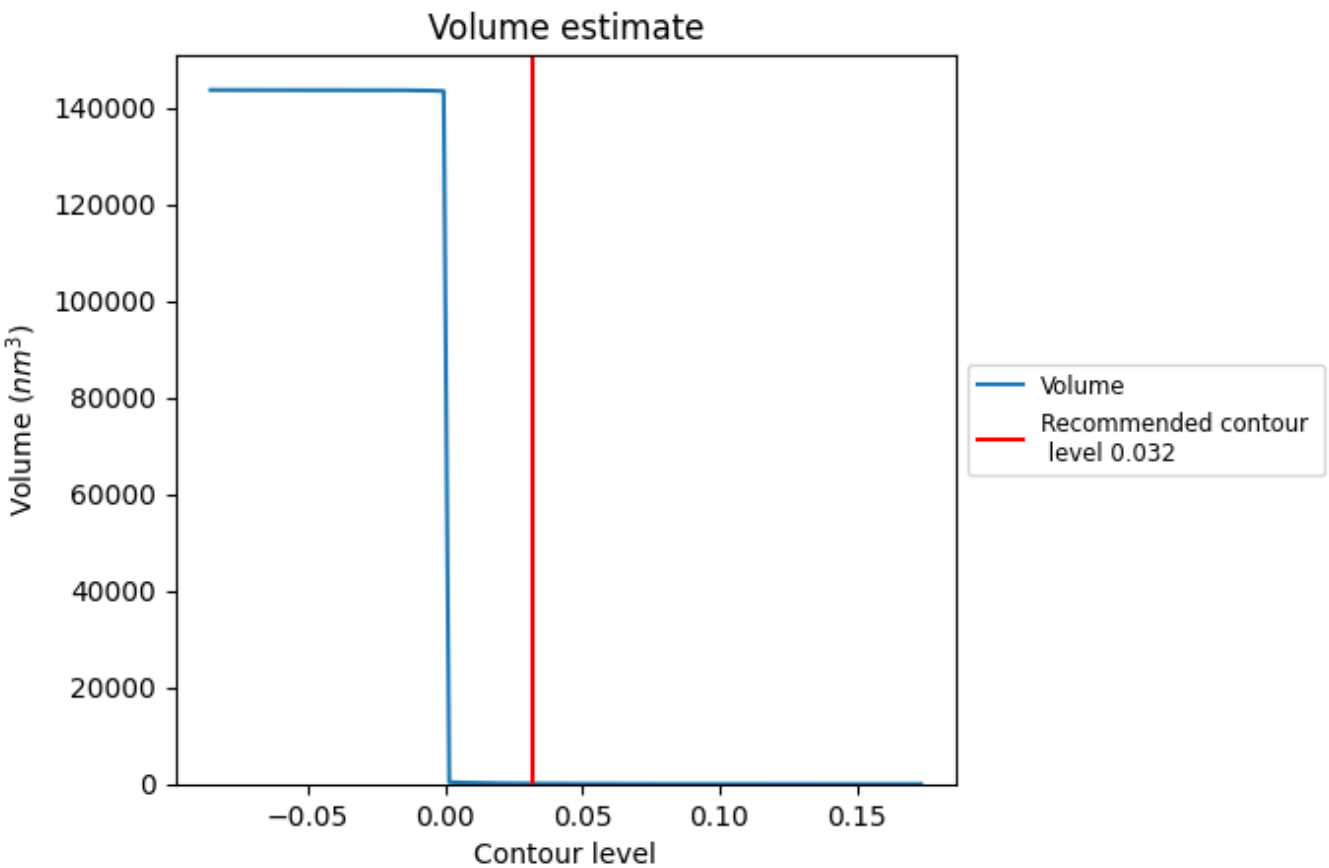
This section contains the results of statistical analysis of the map.

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.

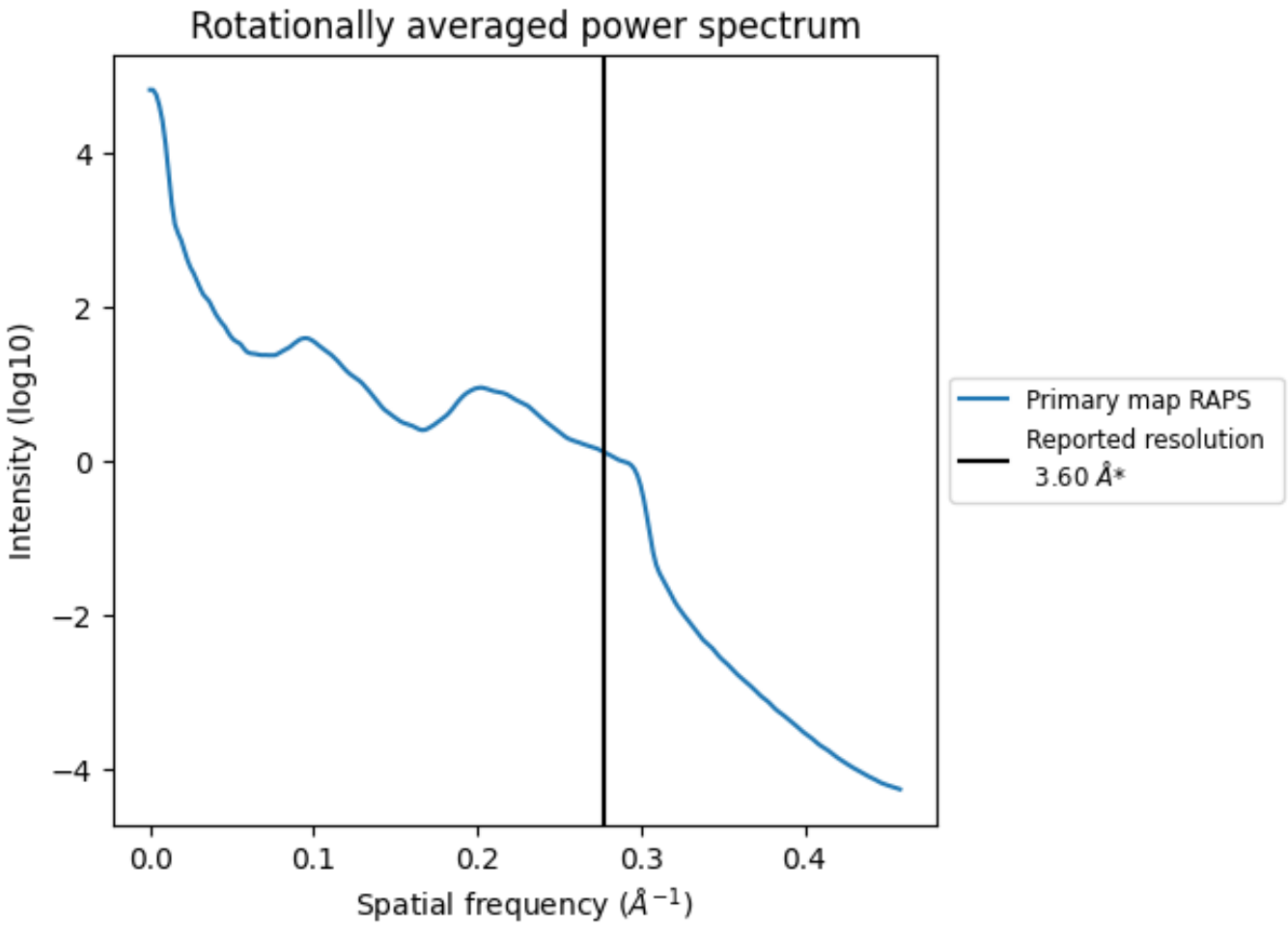
7.2 Volume estimate (i)



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 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 0.278 Å^{-1}

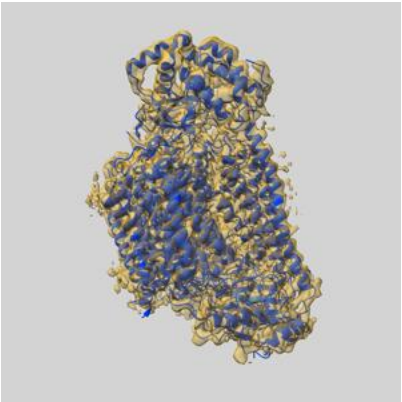
8 Fourier-Shell correlation (i)

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

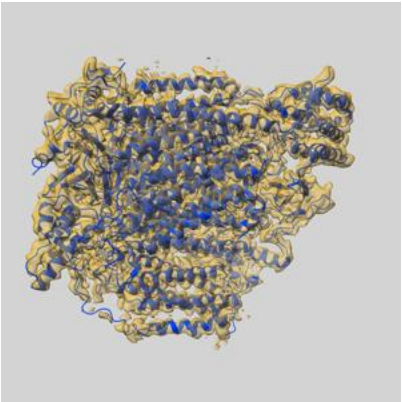
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6896 and PDB model 5Z62. Per-residue inclusion information can be found in section 3 on page 9.

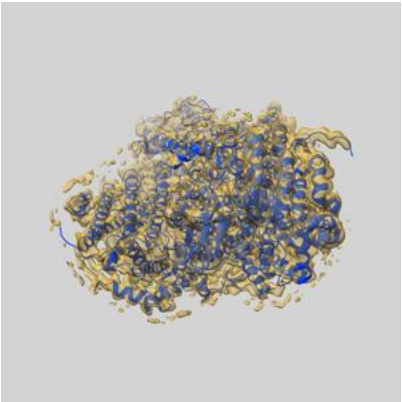
9.1 Map-model overlay (i)



X



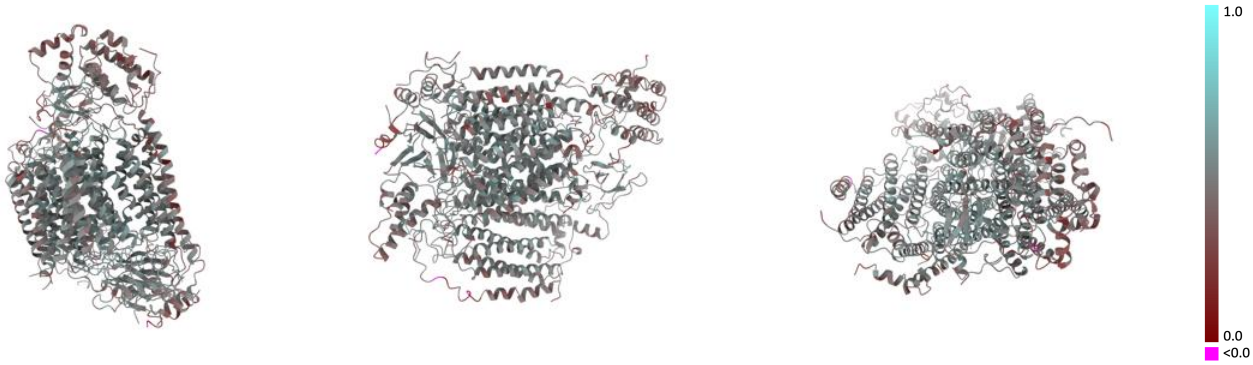
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

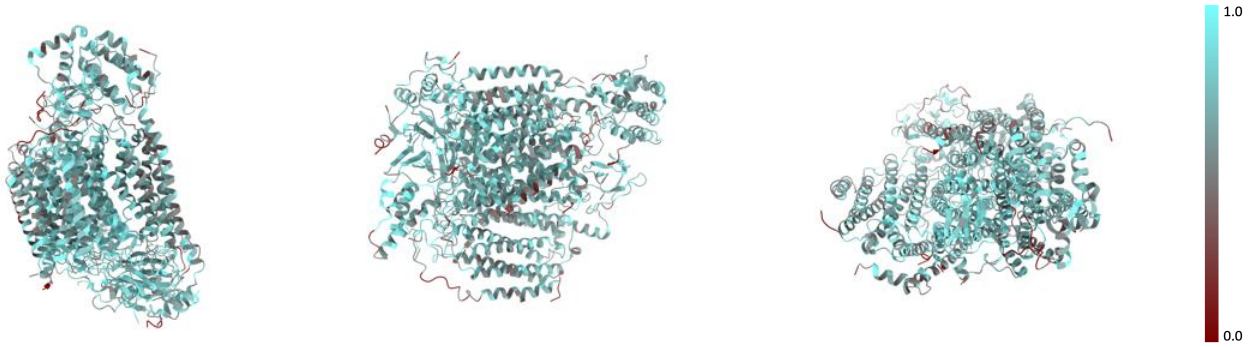
9.2 Q-score mapped to coordinate model (i)



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.

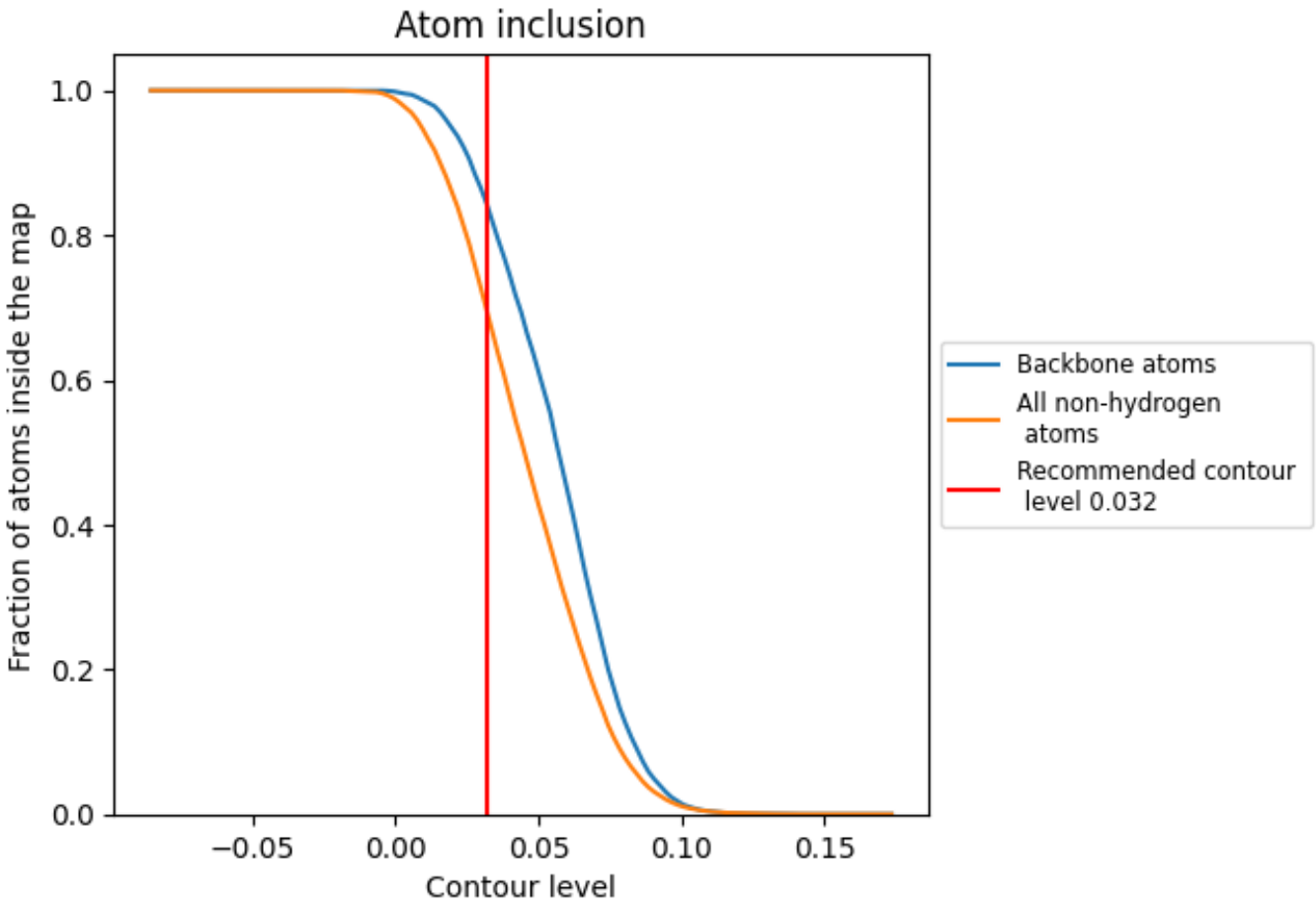
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6945	0.4740
A	0.7734	0.5270
B	0.6868	0.4800
C	0.6949	0.4900
D	0.6541	0.4340
E	0.6624	0.4080
F	0.6895	0.4620
G	0.6235	0.4180
H	0.7407	0.4520
I	0.6460	0.4190
J	0.6070	0.4350
K	0.7071	0.4580
L	0.6917	0.4820
M	0.4863	0.3780
N	0.5021	0.4240