



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:31 PM UTC

PDB ID : 8DH6 / pdb_00008dh6
EMDB ID : EMD-27430
Title : Cryo-EM structure of *Saccharomyces cerevisiae* cytochrome c oxidase (Complex IV) extracted in lipid nanodiscs
Authors : Godoy, A.S.; Song, Y.; Cheruvara, H.; Quigley, A.; Oliva, G.
Deposited on : 2022-06-25
Resolution : 2.94 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

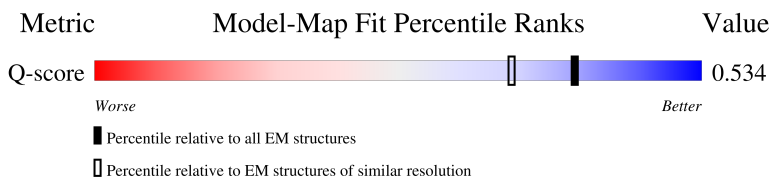
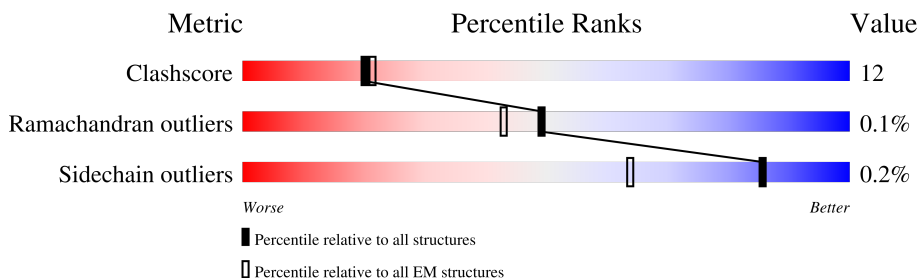
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.94 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13068 (2.44 - 3.44)

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 $\leq 5\%$. 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	534	
2	b	236	
3	c	269	
4	d	130	

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Mol	Chain	Length	Quality of chain
5	e	133	10% 74% 26%
6	f	108	5% 78% 17% 6%
7	g	59	5% 86% 14%
8	h	51	6% 80% 16%
9	i	55	6% 78% 22%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 12901 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
1	a	534	Total	C	N	O	S	0	0
			4162	2778	649	713	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	236	Total	C	N	O	S	0	0
			1889	1242	286	351	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	269	Total	C	N	O	S	0	0
			2146	1430	344	357	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	121	Total	C	N	O	S	0	0
			913	576	151	181	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	133	Total	C	N	O	S	0	0
			1049	663	184	198	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	102	Total	C	N	O	S	0	0
			851	545	137	168	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	59	Total	C	N	O	0	0
			484	328	83	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	51	Total	C	N	O	S	0	0
			408	278	66	63	1		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	55	Total	C	N	O	S	0	0
			456	300	79	74	3		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	a	1	Total	Ca	0
			1	1	

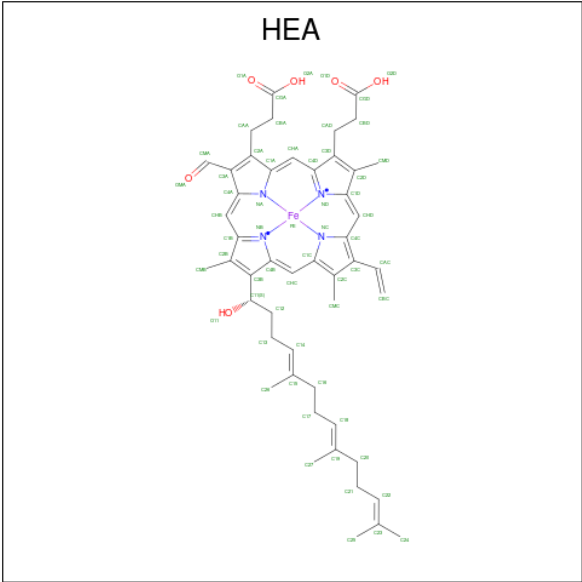
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	a	1	Total	Mg	0
			1	1	

- Molecule 12 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

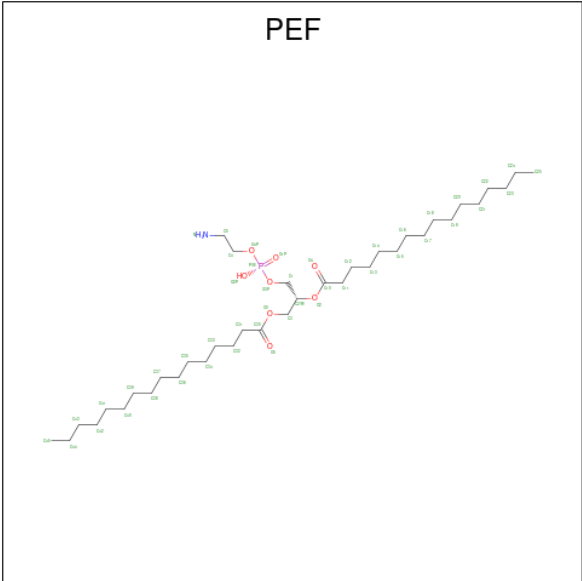
Mol	Chain	Residues	Atoms		AltConf
12	a	1	Total	Cu	0
			1	1	
12	b	1	Total	Cu	0
			1	1	

- Molecule 13 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
13	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 14 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	N	O	P	0
			33	23	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	b	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	b	1	Total	C	N	O	P	0
			33	23	1	8	1	
14	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
14	c	1	Total	C	N	O	P	0
			36	26	1	8	1	
14	c	1	Total	C	N	O	P	0
			41	31	1	8	1	
14	e	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	g	1	Total	C	N	O	P	0
			47	37	1	8	1	
14	h	1	Total	C	N	O	P	0
			47	37	1	8	1	

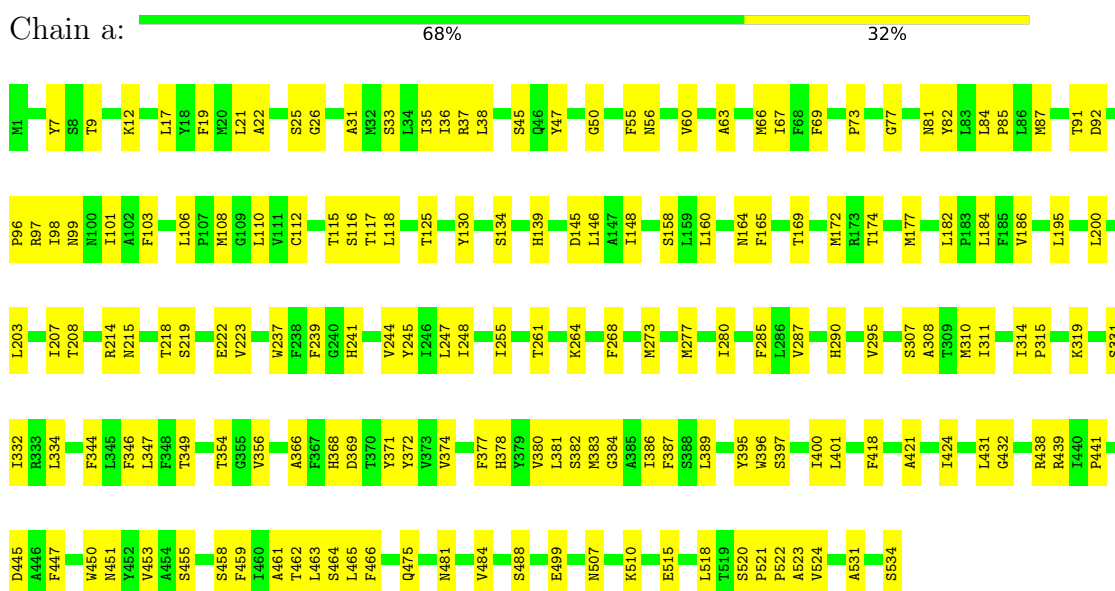
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	d	1	Total	Zn	0
			1	1	

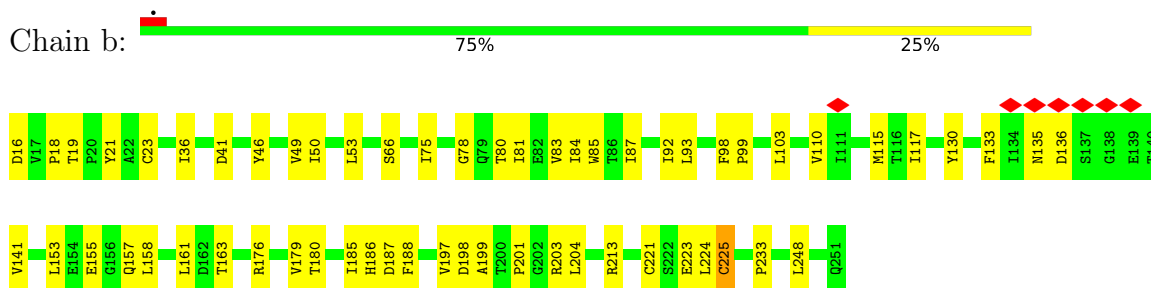
3 Residue-property plots

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.

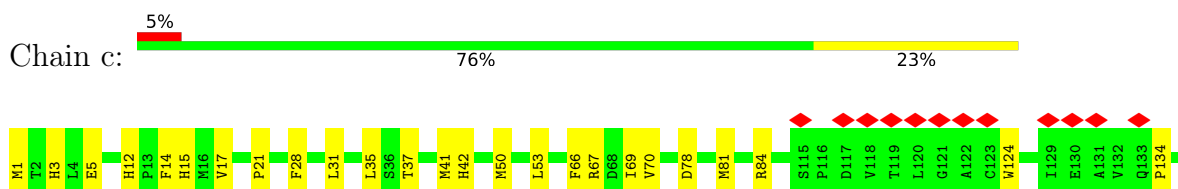
• Molecule 1: Cytochrome c oxidase subunit 1

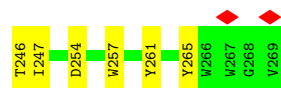


• Molecule 2: Cytochrome c oxidase subunit 2

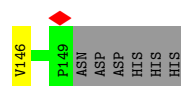
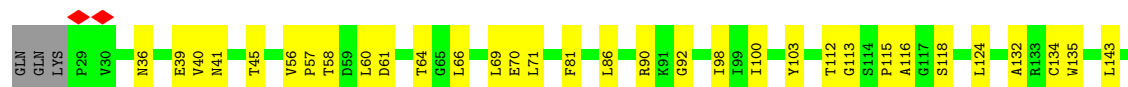


• Molecule 3: Cytochrome c oxidase subunit 3

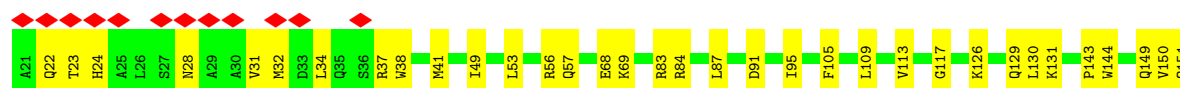
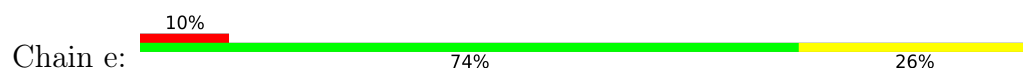




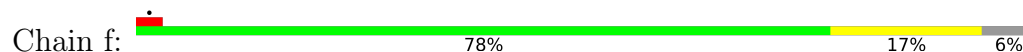
- Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial



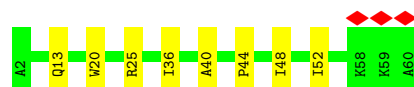
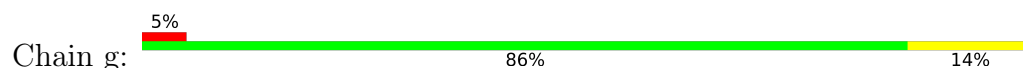
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



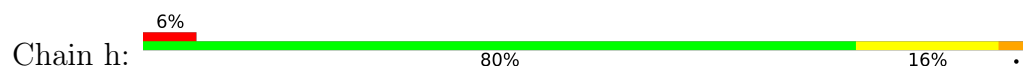
- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial



- Molecule 7: Cytochrome c oxidase subunit 7, mitochondrial

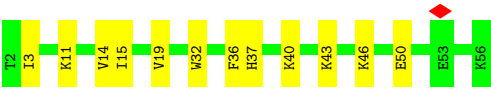
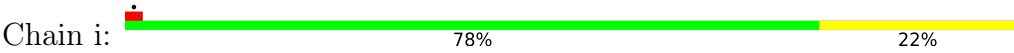


- Molecule 8: Cytochrome c oxidase subunit 8, mitochondrial





• Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247631	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 ($e^-/\text{\AA}^2$)	1.011775103	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.983	Depositor
Minimum map value	-1.684	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.46	Depositor
Map size ($\text{\AA}$)	331.6, 331.6, 331.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, CU, PEF, CA, HEA

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	0.19	0/4290	0.43	0/5857
2	b	0.22	0/1941	0.43	0/2653
3	c	0.27	0/2218	0.44	0/3036
4	d	0.18	0/932	0.44	0/1269
5	e	0.18	0/1074	0.39	0/1451
6	f	0.15	0/868	0.35	0/1174
7	g	0.24	0/500	0.52	0/681
8	h	0.34	0/423	0.66	1/569 (0.2%)
9	i	0.14	0/468	0.31	0/626
All	All	0.21	0/12714	0.43	1/17316 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	76	GLY	CA-C-O	-8.66	114.04	121.57

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	520	SER	Peptide

5.2 Too-close contacts

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	4162	0	4192	141	0
2	b	1889	0	1868	49	0
3	c	2146	0	2137	64	0
4	d	913	0	909	23	0
5	e	1049	0	1030	32	0
6	f	851	0	822	10	0
7	g	484	0	517	9	0
8	h	408	0	408	9	0
9	i	456	0	469	11	0
10	a	1	0	0	0	0
11	a	1	0	0	0	0
12	a	1	0	0	0	0
12	b	1	0	0	1	0
13	a	120	0	108	25	0
14	a	80	0	112	9	0
14	b	120	0	168	21	0
14	c	77	0	100	18	0
14	e	47	0	73	5	0
14	g	47	0	73	10	0
14	h	47	0	73	5	0
15	d	1	0	0	0	0
All	All	12901	0	13059	318	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 12.

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:206:TYR:CE2	14:c:302:PEF:O1P	1.93	1.21
3:c:192:ALA:HB3	14:c:302:PEF:HN2	0.92	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:95:ILE:HD11	14:e:201:PEF:O5	1.61	1.00
3:c:192:ALA:HB3	14:c:302:PEF:N	1.75	0.99
2:b:225:CYS:SG	12:b:303:CU:CU	1.55	0.95
5:e:95:ILE:HD11	14:e:201:PEF:C30	1.97	0.93
1:a:381:LEU:HD23	13:a:605:HEA:HBC2	1.49	0.93
1:a:66:MET:HB3	13:a:604:HEA:CBC	2.00	0.91
1:a:381:LEU:HD23	13:a:605:HEA:CBC	2.02	0.89
3:c:206:TYR:CD2	14:c:302:PEF:H11	2.09	0.87
1:a:273:MET:HE1	1:a:319:LYS:HA	1.57	0.84
3:c:192:ALA:CB	14:c:302:PEF:HN2	1.86	0.83
1:a:389:LEU:HB3	13:a:604:HEA:H242	1.60	0.82
14:b:301:PEF:H141	9:i:15:ILE:HG22	1.61	0.82
14:a:606:PEF:H362	14:c:301:PEF:H191	1.62	0.81
1:a:244:VAL:HB	13:a:605:HEA:HAC	1.65	0.78
3:c:67:ARG:HE	14:g:101:PEF:H122	1.50	0.75
3:c:195:THR:HG23	14:c:302:PEF:O2P	1.87	0.75
1:a:19:PHE:CZ	13:a:604:HEA:H241	2.24	0.73
5:e:22:GLN:HG2	5:e:23:THR:H	1.55	0.71
4:d:115:PRO:HD2	4:d:118:SER:HB2	1.73	0.71
3:c:1:MET:HE1	4:d:69:LEU:HD11	1.73	0.71
1:a:117:THR:O	8:h:71:GLN:NE2	2.24	0.70
3:c:134:PRO:HB3	3:c:265:TYR:HB3	1.73	0.70
1:a:130:TYR:OH	1:a:237:TRP:NE1	2.25	0.70
3:c:239:HIS:CD2	14:c:301:PEF:H41	2.27	0.70
3:c:81:MET:SD	3:c:84:ARG:NH2	2.66	0.69
3:c:206:TYR:HE2	14:c:302:PEF:O1P	1.71	0.68
3:c:164:ARG:NH2	3:c:231:ARG:O	2.27	0.68
3:c:156:HIS:NE2	3:c:244:GLU:OE2	2.27	0.67
3:c:179:VAL:HG22	14:g:101:PEF:H451	1.77	0.67
1:a:182:LEU:HD22	1:a:186:VAL:HG11	1.76	0.67
1:a:67:ILE:HD11	13:a:604:HEA:HMD3	1.75	0.67
3:c:206:TYR:CZ	14:c:302:PEF:O1P	2.48	0.66
2:b:41:ASP:OD2	9:i:37:HIS:ND1	2.27	0.66
1:a:499:GLU:O	5:e:83:ARG:NH2	2.28	0.66
2:b:21:TYR:HB3	14:b:302:PEF:O4	1.95	0.66
5:e:56:ARG:NH2	5:e:68:GLU:OE1	2.29	0.65
4:d:41:ASN:H	4:d:45:THR:HG21	1.62	0.64
1:a:507:ASN:O	1:a:510:LYS:NZ	2.30	0.64
7:g:25:ARG:HH22	14:g:101:PEF:H11	1.61	0.64
1:a:447:PHE:O	1:a:451:ASN:ND2	2.27	0.64
14:b:302:PEF:H51	5:e:151:GLN:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:52:SER:OG	14:h:101:PEF:H111	1.98	0.63
1:a:66:MET:HB3	13:a:604:HEA:HBC1	1.81	0.63
5:e:129:GLN:HB3	5:e:149:GLN:O	1.99	0.63
3:c:145:LEU:HD13	3:c:216:MET:HE1	1.81	0.62
1:a:524:VAL:HG21	8:h:30:PHE:HD2	1.65	0.62
13:a:605:HEA:H211	2:b:50:ILE:HG21	1.82	0.62
1:a:445:ASP:O	5:e:151:GLN:NE2	2.30	0.62
1:a:366:ALA:HB2	2:b:36:ILE:HD12	1.81	0.62
1:a:139:HIS:O	1:a:214:ARG:NH2	2.33	0.61
2:b:18:PRO:O	5:e:149:GLN:NE2	2.33	0.61
1:a:377:PHE:HA	1:a:380:VAL:HG22	1.82	0.61
1:a:66:MET:HB3	13:a:604:HEA:CAC	2.29	0.61
1:a:397:SER:OG	1:a:475:GLN:NE2	2.32	0.60
14:b:301:PEF:C10	9:i:11:LYS:HG3	2.32	0.60
3:c:239:HIS:HD2	14:c:301:PEF:H41	1.65	0.60
4:d:113:GLY:HA3	4:d:118:SER:HB3	1.83	0.60
1:a:82:TYR:CE2	1:a:400:ILE:HG12	2.36	0.60
2:b:186:HIS:O	2:b:199:ALA:HB3	2.02	0.60
9:i:46:LYS:NZ	9:i:50:GLU:OE2	2.34	0.60
2:b:23:CYS:HB2	14:b:304:PEF:H21	1.82	0.60
3:c:239:HIS:HD2	14:c:301:PEF:HN1	1.49	0.60
1:a:396:TRP:NE1	1:a:515:GLU:OE1	2.35	0.60
1:a:400:ILE:HD13	14:h:101:PEF:H241	1.84	0.60
1:a:97:ARG:NE	14:a:606:PEF:O1P	2.32	0.59
2:b:21:TYR:CD1	14:b:302:PEF:H21	2.38	0.59
1:a:374:VAL:HA	1:a:377:PHE:CE2	2.38	0.59
1:a:67:ILE:HD11	13:a:604:HEA:CMD	2.32	0.59
1:a:356:VAL:HG23	13:a:605:HEA:H263	1.85	0.59
5:e:28:ASN:HB3	5:e:32:MET:HE3	1.86	0.58
1:a:12:LYS:NZ	1:a:523:ALA:O	2.37	0.58
2:b:179:VAL:HG22	2:b:199:ALA:HB2	1.85	0.58
3:c:66:PHE:HA	3:c:69:ILE:HG22	1.86	0.58
8:h:45:ARG:HG2	14:h:101:PEF:H352	1.86	0.58
1:a:174:THR:OG1	1:a:531:ALA:O	2.19	0.58
1:a:37:ARG:HG3	1:a:455:SER:HA	1.87	0.57
2:b:78:GLY:HA2	14:b:301:PEF:N	2.19	0.57
1:a:115:THR:HG23	1:a:146:LEU:HD13	1.85	0.57
1:a:223:VAL:HG11	2:b:201:PRO:HB2	1.87	0.57
1:a:244:VAL:HB	13:a:605:HEA:CAC	2.34	0.57
3:c:239:HIS:CD2	14:c:301:PEF:HN1	2.22	0.57
1:a:22:ALA:HB2	1:a:73:PRO:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:261:THR:HG21	1:a:395:TYR:CE1	2.40	0.57
1:a:439:ARG:HD3	2:b:224:LEU:HD22	1.87	0.56
14:g:101:PEF:H111	14:g:101:PEF:N	2.20	0.56
1:a:466:PHE:HD2	14:a:607:PEF:H212	1.70	0.56
8:h:76:GLY:O	8:h:77:ALA:CB	2.53	0.56
3:c:236:THR:HG22	4:d:57:PRO:HB2	1.88	0.55
3:c:151:THR:HG21	3:c:173:ILE:HG23	1.88	0.55
14:a:607:PEF:H402	5:e:117:GLY:O	2.07	0.55
1:a:112:CYS:HA	1:a:115:THR:HG22	1.88	0.55
6:f:139:LEU:HB2	6:f:142:GLU:HG2	1.88	0.55
1:a:344:PHE:CD1	1:a:384:GLY:HA2	2.42	0.55
2:b:221:CYS:SG	2:b:225:CYS:SG	3.05	0.55
2:b:16:ASP:OD1	2:b:213:ARG:NH2	2.40	0.55
1:a:218:THR:OG1	3:c:203:SER:OG	2.22	0.54
6:f:132:ARG:HG3	6:f:137:VAL:HG13	1.88	0.54
14:a:607:PEF:H202	5:e:109:LEU:CD1	2.37	0.54
5:e:41:MET:HE1	5:e:49:ILE:HD12	1.89	0.54
3:c:3:HIS:HB3	4:d:146:VAL:HG13	1.89	0.54
3:c:137:LEU:HD23	3:c:188:GLU:HB2	1.88	0.54
1:a:19:PHE:HZ	13:a:604:HEA:H241	1.72	0.53
1:a:354:THR:HG22	14:b:304:PEF:H212	1.89	0.53
1:a:518:LEU:HD23	1:a:522:PRO:HB3	1.89	0.53
1:a:67:ILE:CD1	13:a:604:HEA:HMD3	2.38	0.53
6:f:53:THR:O	6:f:57:GLU:HG3	2.08	0.53
1:a:344:PHE:HD1	1:a:384:GLY:HA2	1.74	0.53
3:c:218:MET:HG2	14:c:301:PEF:H371	1.91	0.53
1:a:31:ALA:HB3	8:h:64:PRO:HG2	1.91	0.53
1:a:310:MET:HB3	2:b:93:LEU:HD22	1.90	0.53
2:b:81:ILE:HB	2:b:85:TRP:CZ3	2.43	0.53
1:a:488:SER:O	5:e:84:ARG:NH2	2.31	0.53
1:a:461:ALA:O	1:a:464:SER:OG	2.22	0.53
1:a:98:ILE:HG23	1:a:160:LEU:HB3	1.92	0.52
2:b:180:THR:HB	2:b:204:LEU:HD23	1.90	0.52
4:d:100:ILE:HG13	4:d:143:LEU:HD12	1.92	0.52
1:a:25:SER:OG	1:a:69:PHE:O	2.23	0.52
1:a:334:LEU:HD13	14:e:201:PEF:H111	1.92	0.52
6:f:115:VAL:HG11	6:f:121:TYR:HB2	1.91	0.52
1:a:400:ILE:CD1	14:h:101:PEF:H241	2.39	0.52
1:a:56:ASN:O	1:a:60:VAL:HG23	2.09	0.52
14:b:301:PEF:H211	9:i:19:VAL:HG12	1.92	0.52
4:d:58:THR:OG1	4:d:61:ASP:OD2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:70:VAL:HG12	14:c:301:PEF:H32	1.92	0.52
5:e:69:LYS:HD3	6:f:138:PRO:HG3	1.92	0.51
1:a:125:THR:HG21	1:a:134:SER:HB2	1.91	0.51
3:c:67:ARG:HB2	14:g:101:PEF:H172	1.91	0.51
1:a:77:GLY:O	1:a:81:ASN:HB2	2.10	0.51
2:b:36:ILE:HG22	2:b:103:LEU:HD21	1.93	0.51
5:e:28:ASN:HA	5:e:31:VAL:HG12	1.92	0.51
3:c:50:MET:HE1	7:g:40:ALA:HA	1.92	0.51
3:c:50:MET:HE2	7:g:44:PRO:HG3	1.92	0.50
1:a:145:ASP:OD1	1:a:214:ARG:NH1	2.44	0.50
1:a:208:THR:HG21	14:c:302:PEF:H372	1.93	0.50
1:a:346:PHE:O	1:a:349:THR:OG1	2.25	0.50
2:b:80:THR:O	2:b:84:ILE:HG12	2.11	0.50
2:b:158:LEU:HD22	2:b:161:LEU:HD23	1.94	0.50
2:b:179:VAL:HG11	2:b:197:VAL:HG23	1.93	0.50
1:a:21:LEU:HD11	1:a:110:LEU:HD12	1.93	0.50
1:a:463:LEU:HG	14:a:607:PEF:H211	1.94	0.50
1:a:97:ARG:NH2	14:a:606:PEF:O1P	2.44	0.49
1:a:241:HIS:CD2	1:a:245:TYR:HE2	2.30	0.49
4:d:70:GLU:HB2	4:d:81:PHE:HE2	1.76	0.49
1:a:287:VAL:O	1:a:290:HIS:ND1	2.45	0.49
14:b:304:PEF:H121	14:b:304:PEF:C30	2.43	0.49
3:c:196:ILE:HG13	3:c:206:TYR:HB2	1.95	0.49
5:e:23:THR:OG1	5:e:24:HIS:N	2.45	0.49
1:a:386:ILE:HG21	13:a:604:HEA:H162	1.94	0.49
4:d:36:ASN:OD1	4:d:39:GLU:HG3	2.12	0.49
14:b:304:PEF:H142	9:i:32:TRP:CH2	2.47	0.49
5:e:143:PRO:HG2	5:e:144:TRP:CE3	2.48	0.49
1:a:245:TYR:HA	1:a:248:ILE:HG22	1.94	0.49
2:b:78:GLY:HA2	14:b:301:PEF:HN1	1.77	0.49
14:a:607:PEF:H222	5:e:105:PHE:HE2	1.77	0.48
1:a:108:MET:HE1	3:c:28:PHE:CD2	2.48	0.48
2:b:135:ASN:HB3	2:b:141:VAL:HG22	1.94	0.48
5:e:95:ILE:CD1	14:e:201:PEF:C30	2.83	0.48
1:a:203:LEU:HB2	1:a:239:PHE:CG	2.48	0.48
1:a:347:LEU:HD11	1:a:418:PHE:CE1	2.48	0.48
14:g:101:PEF:H31	14:g:101:PEF:H132	1.94	0.48
1:a:314:ILE:HB	1:a:315:PRO:HD3	1.96	0.48
14:g:101:PEF:H161	14:g:101:PEF:H322	1.95	0.48
3:c:235:LEU:HD21	3:c:243:TYR:HB2	1.95	0.48
3:c:84:ARG:HD3	3:c:239:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:138:PRO:HB2	3:c:261:TYR:HE1	1.79	0.48
5:e:53:LEU:O	5:e:57:GLN:HG2	2.14	0.48
1:a:241:HIS:NE2	1:a:245:TYR:HE2	2.12	0.48
1:a:534:SER:HB3	4:d:86:LEU:HB3	1.96	0.48
1:a:383:MET:O	1:a:387:PHE:HB2	2.14	0.47
2:b:187:ASP:HB2	2:b:223:GLU:HB2	1.96	0.47
1:a:219:SER:HB2	1:a:222:GLU:HB2	1.94	0.47
5:e:95:ILE:CD1	14:e:201:PEF:O5	2.47	0.47
1:a:241:HIS:O	1:a:244:VAL:HG22	2.15	0.47
1:a:372:TYR:N	1:a:432:GLY:HA3	2.29	0.47
1:a:7:TYR:CE1	3:c:21:PRO:HB3	2.50	0.47
1:a:33:SER:HB2	13:a:604:HEA:C1B	2.43	0.47
1:a:421:ALA:HA	1:a:424:ILE:HG22	1.95	0.47
13:a:604:HEA:H202	13:a:604:HEA:H171	1.72	0.47
3:c:222:MET:HG2	14:c:301:PEF:H351	1.96	0.47
1:a:84:LEU:HD12	1:a:186:VAL:HG22	1.95	0.47
1:a:98:ILE:HA	1:a:101:ILE:HG22	1.96	0.47
1:a:172:MET:HE3	3:c:14:PHE:CG	2.49	0.47
2:b:163:THR:HG22	2:b:233:PRO:HG2	1.95	0.47
1:a:369:ASP:OD1	1:a:438:ARG:HB3	2.14	0.47
1:a:84:LEU:HB3	1:a:85:PRO:HD3	1.96	0.47
13:a:604:HEA:H172	13:a:604:HEA:H261	1.64	0.47
9:i:36:PHE:O	9:i:40:LYS:HG2	2.15	0.47
1:a:108:MET:HB3	3:c:31:LEU:HB2	1.97	0.46
2:b:19:THR:HG21	14:b:304:PEF:HN2	1.81	0.46
2:b:110:VAL:HG11	2:b:176:ARG:HH21	1.81	0.46
1:a:280:ILE:HG13	1:a:315:PRO:HB2	1.97	0.46
1:a:255:ILE:HG13	1:a:344:PHE:CD2	2.51	0.46
1:a:67:ILE:HG23	1:a:247:LEU:HD11	1.97	0.46
1:a:45:SER:HB2	1:a:50:GLY:H	1.80	0.46
1:a:307:SER:O	1:a:311:ILE:HG12	2.16	0.46
4:d:103:TYR:CZ	4:d:146:VAL:HG21	2.51	0.46
1:a:91:THR:HG21	3:c:12:HIS:CD2	2.51	0.46
2:b:115:MET:HG3	2:b:133:PHE:HE2	1.80	0.46
2:b:187:ASP:HA	2:b:198:ASP:HA	1.98	0.46
5:e:144:TRP:HB2	9:i:43:LYS:HB3	1.97	0.46
1:a:63:ALA:HB1	13:a:604:HEA:HMD1	1.98	0.46
4:d:124:LEU:HB3	4:d:132:ALA:HB1	1.98	0.46
5:e:87:LEU:HB3	5:e:91:ASP:HB2	1.98	0.45
6:f:55:ARG:HH21	6:f:56:TYR:HE2	1.64	0.45
1:a:47:TYR:OH	5:e:113:VAL:O	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:481:ASN:HA	1:a:484:VAL:HG12	1.98	0.45
3:c:162:GLY:HA2	4:d:56:VAL:HG21	1.98	0.45
3:c:35:LEU:HD21	7:g:48:ILE:HD11	1.98	0.45
1:a:148:ILE:HG23	1:a:207:ILE:HG22	1.98	0.45
1:a:195:LEU:HD22	1:a:285:PHE:HE2	1.82	0.45
1:a:438:ARG:HH21	1:a:439:ARG:HH12	1.64	0.45
14:b:304:PEF:H331	14:b:304:PEF:H361	1.52	0.45
2:b:179:VAL:HG21	2:b:188:PHE:HB2	1.98	0.45
1:a:17:LEU:HB3	1:a:103:PHE:CZ	2.51	0.45
2:b:185:ILE:HA	2:b:199:ALA:O	2.17	0.45
1:a:431:LEU:HD21	1:a:450:TRP:HB2	1.99	0.45
14:b:301:PEF:H162	14:b:301:PEF:H192	1.62	0.45
14:b:301:PEF:H341	9:i:14:VAL:HG13	1.98	0.45
3:c:145:LEU:HD21	3:c:254:ASP:HA	1.99	0.45
1:a:424:ILE:HD13	13:a:604:HEA:HMB3	1.99	0.45
3:c:67:ARG:HG3	14:g:101:PEF:H121	1.99	0.45
3:c:212:HIS:NE2	3:c:257:TRP:HB2	2.31	0.45
1:a:264:LYS:HD3	1:a:331:SER:OG	2.18	0.44
2:b:135:ASN:OD1	2:b:136:ASP:N	2.40	0.44
1:a:9:THR:HG21	3:c:17:VAL:O	2.18	0.44
1:a:347:LEU:HD11	1:a:418:PHE:HE1	1.82	0.44
1:a:424:ILE:HD12	1:a:458:SER:HB3	1.98	0.44
2:b:155:GLU:HG2	5:e:131:LYS:HD2	2.00	0.44
14:b:304:PEF:H142	9:i:32:TRP:HH2	1.82	0.44
8:h:76:GLY:O	8:h:77:ALA:HB3	2.15	0.44
1:a:401:LEU:C	1:a:521:PRO:HG3	2.42	0.44
3:c:195:THR:CG2	14:c:302:PEF:O2P	2.63	0.44
5:e:22:GLN:HG2	5:e:23:THR:N	2.29	0.44
1:a:371:TYR:HA	1:a:374:VAL:HG22	2.00	0.44
2:b:83:VAL:O	2:b:87:ILE:HG12	2.17	0.44
2:b:19:THR:CG2	14:b:304:PEF:HN2	2.31	0.44
2:b:81:ILE:HG23	14:b:301:PEF:H131	1.99	0.44
4:d:90:ARG:NH1	4:d:92:GLY:HA2	2.33	0.44
2:b:50:ILE:HD11	2:b:92:ILE:HG21	2.00	0.43
2:b:46:TYR:HA	2:b:49:VAL:HG22	2.00	0.43
1:a:368:HIS:ND1	13:a:605:HEA:O1A	2.49	0.43
5:e:126:LYS:HE2	5:e:130:LEU:HD21	2.00	0.43
5:e:150:VAL:O	5:e:152:SER:N	2.52	0.43
3:c:53:LEU:HD11	7:g:36:ILE:HG23	2.00	0.43
3:c:124:TRP:CH2	3:c:200:VAL:HG23	2.53	0.43
6:f:89:GLU:OE1	6:f:131:VAL:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:106:LEU:HD23	1:a:106:LEU:HA	1.91	0.43
1:a:145:ASP:CG	1:a:215:ASN:HD21	2.25	0.43
2:b:53:LEU:HD21	14:b:301:PEF:H402	1.99	0.43
3:c:200:VAL:O	3:c:204:VAL:HG22	2.19	0.43
2:b:180:THR:C	2:b:199:ALA:HB1	2.44	0.43
1:a:381:LEU:CD2	13:a:605:HEA:CBC	2.86	0.43
4:d:92:GLY:HA3	4:d:98:ILE:HG13	2.00	0.43
4:d:134:CYS:O	4:d:135:TRP:HB3	2.18	0.43
2:b:98:PHE:HB2	2:b:99:PRO:HD3	2.01	0.43
6:f:82:VAL:HG22	6:f:114:LYS:HG3	2.01	0.43
1:a:148:ILE:HG23	1:a:207:ILE:CG2	2.49	0.42
1:a:184:LEU:HD22	1:a:277:MET:HE1	2.00	0.42
1:a:372:TYR:H	1:a:432:GLY:HA3	1.83	0.42
4:d:112:THR:OG1	4:d:116:ALA:O	2.25	0.42
1:a:378:HIS:O	1:a:382:SER:HB3	2.19	0.42
2:b:46:TYR:O	2:b:49:VAL:HG22	2.20	0.42
3:c:124:TRP:HH2	3:c:200:VAL:HG23	1.84	0.42
1:a:55:PHE:CG	1:a:441:PRO:HB3	2.54	0.42
3:c:5:GLU:HG2	4:d:40:VAL:O	2.19	0.42
3:c:37:THR:O	3:c:41:MET:HG3	2.19	0.42
1:a:36:ILE:HG23	1:a:55:PHE:CZ	2.55	0.42
1:a:165:PHE:O	1:a:169:THR:HG22	2.19	0.42
3:c:35:LEU:HD23	7:g:44:PRO:HB2	2.01	0.42
3:c:137:LEU:HD12	3:c:137:LEU:HA	1.86	0.42
1:a:9:THR:HG23	1:a:96:PRO:HB2	2.01	0.42
1:a:26:GLY:HA3	13:a:604:HEA:H273	2.01	0.42
1:a:35:ILE:HD11	8:h:65:PHE:CD1	2.55	0.42
1:a:462:THR:O	1:a:465:LEU:HB3	2.20	0.42
2:b:133:PHE:HB3	2:b:248:LEU:HD21	2.01	0.42
1:a:158:SER:HB2	1:a:200:LEU:HD11	2.02	0.42
4:d:60:LEU:HD22	4:d:71:LEU:HD21	2.00	0.42
4:d:64:THR:OG1	7:g:13:GLN:NE2	2.41	0.42
4:d:66:LEU:HG	4:d:81:PHE:HZ	1.84	0.42
6:f:124:TYR:CZ	9:i:3:ILE:HG21	2.55	0.42
8:h:38:ILE:HD12	8:h:40:PHE:CE2	2.55	0.42
1:a:9:THR:O	1:a:96:PRO:HB3	2.19	0.42
1:a:118:LEU:HB3	7:g:52:ILE:HG12	2.02	0.42
14:g:101:PEF:H132	14:g:101:PEF:H162	1.50	0.41
1:a:287:VAL:HG12	1:a:308:ALA:HB1	2.02	0.41
14:b:304:PEF:H172	14:b:304:PEF:H201	1.83	0.41
3:c:15:HIS:ND1	3:c:78:ASP:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:185:GLN:HE21	3:c:209:THR:HG23	1.85	0.41
1:a:466:PHE:CD2	14:a:607:PEF:H212	2.52	0.41
2:b:153:LEU:HD22	2:b:157:GLN:HB2	2.01	0.41
1:a:438:ARG:NH2	1:a:439:ARG:HH12	2.18	0.41
5:e:34:LEU:HD11	5:e:38:TRP:HE3	1.86	0.41
1:a:92:ASP:O	1:a:172:MET:HE1	2.21	0.41
1:a:268:PHE:HE1	2:b:75:ILE:HG22	1.85	0.41
3:c:243:TYR:CE2	3:c:247:ILE:HD11	2.55	0.41
5:e:37:ARG:NH1	5:e:41:MET:SD	2.94	0.41
6:f:122:LYS:HA	6:f:125:LEU:HG	2.03	0.41
1:a:63:ALA:HB1	13:a:604:HEA:CMD	2.51	0.41
1:a:295:VAL:O	2:b:203:ARG:NH2	2.36	0.41
4:d:103:TYR:CE2	4:d:146:VAL:HG11	2.56	0.41
14:h:101:PEF:H342	14:h:101:PEF:H372	1.82	0.41
3:c:243:TYR:O	3:c:246:THR:HG22	2.20	0.41
14:g:101:PEF:H132	14:g:101:PEF:C3	2.51	0.41
1:a:38:LEU:HD13	1:a:459:PHE:HE1	1.86	0.40
2:b:117:ILE:HG22	2:b:130:TYR:HA	2.03	0.40
3:c:228:TRP:CD1	3:c:232:ASN:OD1	2.74	0.40
1:a:99:ASN:HB2	1:a:164:ASN:ND2	2.35	0.40
1:a:145:ASP:OD2	3:c:42:HIS:NE2	2.33	0.40
3:c:21:PRO:HD3	7:g:20:TRP:CH2	2.56	0.40
1:a:332:ILE:HB	2:b:66:SER:HA	2.03	0.40
1:a:521:PRO:HA	1:a:522:PRO:HD3	1.87	0.40
5:e:126:LYS:O	5:e:130:LEU:HD23	2.21	0.40
1:a:87:MET:O	1:a:177:MET:HE1	2.21	0.40
1:a:116:SER:HB3	1:a:146:LEU:HB2	2.03	0.40
1:a:450:TRP:HA	1:a:453:VAL:HG12	2.03	0.40
3:c:140:LEU:HA	3:c:143:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	532/534 (100%)	508 (96%)	24 (4%)	0	100	100
2	b	234/236 (99%)	223 (95%)	11 (5%)	0	100	100
3	c	267/269 (99%)	264 (99%)	3 (1%)	0	100	100
4	d	119/130 (92%)	106 (89%)	13 (11%)	0	100	100
5	e	131/133 (98%)	120 (92%)	11 (8%)	0	100	100
6	f	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
7	g	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
8	h	49/51 (96%)	45 (92%)	3 (6%)	1 (2%)	6	17
9	i	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
All	All	1542/1575 (98%)	1466 (95%)	75 (5%)	1 (0%)	49	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	h	77	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	447/447 (100%)	447 (100%)	0	100	100
2	b	209/209 (100%)	208 (100%)	1 (0%)	81	90
3	c	228/228 (100%)	227 (100%)	1 (0%)	84	92
4	d	102/111 (92%)	102 (100%)	0	100	100
5	e	110/110 (100%)	110 (100%)	0	100	100
6	f	91/96 (95%)	91 (100%)	0	100	100
7	g	50/50 (100%)	50 (100%)	0	100	100
8	h	41/41 (100%)	41 (100%)	0	100	100
9	i	46/46 (100%)	46 (100%)	0	100	100
All	All	1324/1338 (99%)	1322 (100%)	2 (0%)	85	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	225	CYS
3	c	179	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	46	GLN
1	a	152	HIS
1	a	475	GLN
1	a	501	ASN
2	b	212	GLN
3	c	12	HIS
3	c	226	ASN
3	c	239	HIS
5	e	149	GLN
6	f	133	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	$\# Z > 2$
13	HEA	a	604	1	67,67,67	2.25	24 (35%)	81,103,103	2.63	39 (48%)
14	PEF	c	301	-	35,35,46	0.41	0	38,40,51	0.49	0
14	PEF	g	101	-	46,46,46	0.41	0	49,51,51	0.40	0
14	PEF	c	302	-	40,40,46	1.03	2 (5%)	43,45,51	1.21	3 (6%)
14	PEF	h	101	-	46,46,46	0.40	0	49,51,51	0.34	0
13	HEA	a	605	1	67,67,67	2.25	25 (37%)	81,103,103	2.47	30 (37%)
14	PEF	b	301	-	46,46,46	0.42	0	49,51,51	0.50	0
14	PEF	a	607	-	46,46,46	0.33	0	49,51,51	0.48	0
14	PEF	b	302	-	32,32,46	0.36	0	35,37,51	0.44	0
14	PEF	e	201	-	46,46,46	0.93	2 (4%)	49,51,51	1.12	4 (8%)
14	PEF	a	606	-	32,32,46	1.10	2 (6%)	35,37,51	1.27	4 (11%)
14	PEF	b	304	-	39,39,46	0.40	0	42,44,51	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEA	a	604	1	-	9/36/76/76	-
14	PEF	c	301	-	-	18/39/39/50	-
14	PEF	g	101	-	-	36/50/50/50	-
14	PEF	c	302	-	-	9/44/44/50	-
14	PEF	h	101	-	-	29/50/50/50	-
13	HEA	a	605	1	-	11/36/76/76	-
14	PEF	b	301	-	-	21/50/50/50	-
14	PEF	a	607	-	-	33/50/50/50	-
14	PEF	b	302	-	-	23/36/36/50	-
14	PEF	e	201	-	-	16/50/50/50	-
14	PEF	a	606	-	-	8/36/36/50	-
14	PEF	b	304	-	-	25/43/43/50	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	604	HEA	FE-ND	5.24	2.11	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	605	HEA	FE-NB	5.14	2.10	1.94
13	a	605	HEA	FE-ND	5.11	2.10	1.94
13	a	604	HEA	FE-NB	5.02	2.10	1.94
13	a	605	HEA	C3B-C2B	4.76	1.45	1.34
13	a	604	HEA	C3B-C2B	4.57	1.45	1.34
13	a	605	HEA	C3D-C2D	4.55	1.46	1.36
13	a	605	HEA	FE-NC	4.45	2.09	1.95
13	a	604	HEA	CHC-C4B	4.41	1.47	1.38
14	c	302	PEF	O3-C30	4.39	1.46	1.33
13	a	605	HEA	CHD-C1D	4.31	1.47	1.38
13	a	604	HEA	C3D-C2D	4.21	1.45	1.36
13	a	604	HEA	FE-NC	4.09	2.08	1.95
14	e	201	PEF	O3-C30	4.02	1.45	1.33
13	a	604	HEA	CHB-C4A	4.00	1.46	1.38
14	e	201	PEF	O2-C10	3.99	1.45	1.34
13	a	605	HEA	C3A-C2A	3.96	1.46	1.37
14	a	606	PEF	O3-C30	3.93	1.44	1.33
14	a	606	PEF	O2-C10	3.92	1.45	1.34
13	a	604	HEA	C1A-NA	3.91	1.47	1.39
14	c	302	PEF	O2-C10	3.89	1.45	1.34
13	a	605	HEA	C1A-NA	3.73	1.46	1.39
13	a	604	HEA	C3A-C2A	3.72	1.45	1.37
13	a	604	HEA	CHD-C1D	3.71	1.45	1.38
13	a	604	HEA	CHC-C1C	3.69	1.47	1.39
13	a	605	HEA	CHB-C4A	3.64	1.45	1.38
13	a	605	HEA	C4A-NA	3.55	1.46	1.39
13	a	605	HEA	CHC-C4B	3.55	1.45	1.38
13	a	604	HEA	C1D-ND	-3.55	1.34	1.40
13	a	605	HEA	CHD-C4C	3.50	1.47	1.39
13	a	605	HEA	CHA-C1A	3.49	1.45	1.38
13	a	604	HEA	C4A-NA	3.49	1.46	1.39
13	a	604	HEA	CHA-C1A	3.41	1.45	1.38
13	a	605	HEA	C4B-NB	-3.31	1.34	1.40
13	a	605	HEA	C1D-ND	-3.18	1.34	1.40
13	a	604	HEA	C11-C3B	-3.04	1.47	1.51
13	a	604	HEA	CHD-C4C	3.00	1.46	1.39
13	a	605	HEA	C11-C3B	-2.89	1.47	1.51
13	a	604	HEA	CHB-C1B	2.88	1.45	1.39
13	a	604	HEA	C4C-NC	-2.86	1.34	1.39
13	a	605	HEA	C1C-NC	-2.83	1.34	1.39
13	a	605	HEA	CHA-C4D	2.79	1.45	1.39
13	a	604	HEA	C4B-NB	-2.77	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	605	HEA	CHB-C1B	2.72	1.45	1.39
13	a	605	HEA	CHC-C1C	2.70	1.45	1.39
13	a	604	HEA	CHA-C4D	2.69	1.45	1.39
13	a	604	HEA	C1B-NB	-2.48	1.34	1.38
13	a	605	HEA	C4C-NC	-2.48	1.34	1.39
13	a	604	HEA	C1C-NC	-2.47	1.35	1.39
13	a	604	HEA	C4B-C3B	2.46	1.49	1.44
13	a	605	HEA	C4D-ND	-2.38	1.34	1.38
13	a	605	HEA	C1B-NB	-2.37	1.34	1.38
13	a	604	HEA	C1C-C2C	2.24	1.48	1.43
13	a	605	HEA	C4B-C3B	2.02	1.48	1.44
13	a	605	HEA	C1D-C2D	2.01	1.48	1.44

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	604	HEA	C3D-C4D-ND	7.20	117.31	110.35
13	a	605	HEA	C3D-C4D-ND	7.17	117.28	110.35
13	a	604	HEA	C3C-C4C-NC	5.84	114.72	109.80
13	a	604	HEA	C2D-C1D-ND	5.81	116.52	109.84
13	a	605	HEA	C2B-C1B-NB	5.80	116.61	109.90
13	a	605	HEA	C3B-C4B-NB	5.73	116.43	109.84
13	a	605	HEA	C3C-C2C-C1C	-5.52	100.66	107.17
13	a	604	HEA	C2B-C1B-NB	5.36	116.10	109.90
13	a	604	HEA	C2A-C1A-NA	5.27	115.41	110.32
13	a	604	HEA	C13-C12-C11	-5.13	106.20	114.39
13	a	605	HEA	C2D-C1D-ND	5.10	115.70	109.84
13	a	604	HEA	C3C-C2C-C1C	-4.71	101.61	107.17
13	a	605	HEA	C2A-C1A-NA	4.68	114.84	110.32
13	a	604	HEA	C3B-C4B-NB	4.51	115.02	109.84
13	a	605	HEA	C2C-C1C-NC	4.51	117.37	110.14
13	a	604	HEA	C26-C15-C16	4.46	122.98	115.23
14	a	606	PEF	O2-C10-C11	4.29	120.76	111.48
13	a	605	HEA	C3C-C4C-NC	4.27	113.40	109.80
13	a	604	HEA	CBA-CAA-C2A	-4.03	101.40	112.53
14	e	201	PEF	O2-C10-C11	4.00	120.14	111.48
14	c	302	PEF	O2-C10-C11	3.96	120.05	111.48
13	a	605	HEA	C1D-C2D-C3D	-3.83	102.95	106.98
13	a	604	HEA	C4D-C3D-C2D	-3.74	101.45	106.89
13	a	605	HEA	C3A-C2A-C1A	-3.72	103.53	107.05
13	a	604	HEA	C1D-C2D-C3D	-3.72	103.07	106.98
13	a	605	HEA	C4D-C3D-C2D	-3.64	101.60	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	605	HEA	C1B-C2B-C3B	-3.61	102.61	106.80
13	a	605	HEA	C13-C12-C11	-3.55	108.72	114.39
13	a	604	HEA	C3A-C2A-C1A	-3.50	103.73	107.05
13	a	605	HEA	CMB-C2B-C1B	3.33	130.24	125.03
14	e	201	PEF	C2-O2-C10	-3.25	110.01	117.80
14	a	606	PEF	O3-C30-C31	3.24	121.72	111.83
13	a	604	HEA	C4A-NA-C1A	-3.17	100.65	105.82
13	a	604	HEA	CHB-C4A-NA	-3.14	121.03	124.45
13	a	605	HEA	CHC-C1C-C2C	-3.14	118.31	127.43
13	a	605	HEA	C4B-C3B-C2B	-3.13	102.17	107.44
14	c	302	PEF	C2-O2-C10	-3.07	110.44	117.80
13	a	604	HEA	C27-C19-C20	3.06	120.54	115.23
13	a	604	HEA	C2C-C1C-NC	3.05	115.04	110.14
13	a	604	HEA	CAD-C3D-C4D	3.05	130.01	124.70
13	a	604	HEA	C4B-C3B-C2B	-3.04	102.32	107.44
13	a	604	HEA	C1D-ND-C4D	-3.01	101.64	105.21
13	a	604	HEA	CHA-C1A-C2A	-2.97	120.17	124.86
13	a	605	HEA	C4A-NA-C1A	-2.97	100.98	105.82
13	a	604	HEA	C1B-C2B-C3B	-2.91	103.43	106.80
14	c	302	PEF	O3-C30-C31	2.88	120.61	111.83
13	a	604	HEA	C12-C13-C14	-2.87	104.61	112.16
13	a	604	HEA	OMA-CMA-C3A	-2.82	119.25	125.62
14	e	201	PEF	O3-C30-C31	2.81	120.41	111.83
13	a	604	HEA	CHA-C4D-ND	-2.77	121.45	124.42
13	a	604	HEA	C17-C18-C19	-2.76	121.31	127.62
13	a	605	HEA	C26-C15-C16	2.66	119.84	115.23
13	a	605	HEA	C13-C14-C15	-2.64	121.59	127.62
13	a	605	HEA	CHA-C4D-C3D	-2.61	120.97	124.77
13	a	605	HEA	C4B-NB-C1B	-2.56	102.18	105.21
13	a	605	HEA	CHA-C4D-ND	-2.51	121.72	124.42
13	a	605	HEA	C27-C19-C20	2.45	119.48	115.23
13	a	604	HEA	C4C-C3C-C2C	-2.44	104.27	107.30
13	a	604	HEA	C25-C23-C24	2.43	120.19	114.59
13	a	604	HEA	C4A-CHB-C1B	-2.43	120.86	126.02
13	a	604	HEA	CHA-C4D-C3D	-2.43	121.23	124.77
13	a	604	HEA	C21-C20-C19	-2.41	105.20	113.19
13	a	605	HEA	CHB-C1B-C2B	-2.41	121.22	125.03
13	a	605	HEA	C1D-ND-C4D	-2.32	102.46	105.21
13	a	604	HEA	C13-C14-C15	-2.31	122.33	127.62
14	a	606	PEF	C2-O2-C10	-2.28	112.33	117.80
13	a	605	HEA	CAA-CBA-CGA	-2.28	107.61	113.67
14	a	606	PEF	O3-C30-O5	-2.23	118.05	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	605	HEA	CAD-CBD-CGD	-2.20	107.84	113.67
13	a	604	HEA	CMD-C2D-C1D	2.16	128.40	125.03
13	a	605	HEA	CHB-C1B-NB	-2.14	122.12	124.42
13	a	604	HEA	C21-C22-C23	-2.13	120.56	127.64
13	a	604	HEA	CMB-C2B-C1B	2.12	128.35	125.03
14	e	201	PEF	O2-C10-O4	-2.12	118.75	123.70
13	a	605	HEA	CHD-C1D-C2D	-2.11	120.95	126.95
13	a	604	HEA	CHB-C1B-C2B	-2.11	121.70	125.03
13	a	604	HEA	CHB-C1B-NB	-2.09	122.17	124.42
13	a	604	HEA	O1A-CGA-CBA	-2.07	116.52	123.09
13	a	605	HEA	CMD-C2D-C1D	2.06	128.25	125.03
13	a	604	HEA	CHD-C1D-C2D	-2.04	121.16	126.95

There are no chirality outliers.

All (238) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	a	604	HEA	C2A-C3A-CMA-OMA
13	a	604	HEA	C11-C12-C13-C14
13	a	605	HEA	C2A-C3A-CMA-OMA
14	a	606	PEF	C1-O3P-P-O2P
14	a	606	PEF	C1-O3P-P-O4P
14	a	606	PEF	C4-O4P-P-O1P
14	a	606	PEF	C4-O4P-P-O2P
14	a	606	PEF	C4-O4P-P-O3P
14	a	607	PEF	O4P-C4-C5-N
14	a	607	PEF	C11-C10-O2-C2
14	a	607	PEF	O4-C10-O2-C2
14	a	607	PEF	C4-O4P-P-O3P
14	b	301	PEF	C11-C10-O2-C2
14	b	301	PEF	C1-O3P-P-O4P
14	b	302	PEF	O4P-C4-C5-N
14	b	302	PEF	C1-O3P-P-O2P
14	b	302	PEF	C4-O4P-P-O3P
14	b	304	PEF	C11-C10-O2-C2
14	b	304	PEF	C1-O3P-P-O1P
14	b	304	PEF	C1-O3P-P-O2P
14	b	304	PEF	C1-O3P-P-O4P
14	b	304	PEF	C4-O4P-P-O3P
14	c	301	PEF	O4P-C4-C5-N
14	c	301	PEF	C1-O3P-P-O1P
14	c	301	PEF	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
14	c	301	PEF	C1-O3P-P-O4P
14	c	301	PEF	C4-O4P-P-O1P
14	c	302	PEF	C1-O3P-P-O2P
14	c	302	PEF	C1-O3P-P-O4P
14	c	302	PEF	C4-O4P-P-O1P
14	c	302	PEF	C4-O4P-P-O3P
14	e	201	PEF	C11-C10-O2-C2
14	e	201	PEF	O4-C10-O2-C2
14	e	201	PEF	C1-O3P-P-O2P
14	e	201	PEF	C1-O3P-P-O4P
14	g	101	PEF	C1-O3P-P-O2P
14	g	101	PEF	C1-O3P-P-O4P
14	g	101	PEF	C4-O4P-P-O2P
14	g	101	PEF	C4-O4P-P-O3P
14	h	101	PEF	O2-C2-C3-O3
14	h	101	PEF	C1-O3P-P-O4P
14	h	101	PEF	C4-O4P-P-O1P
14	h	101	PEF	C4-O4P-P-O3P
14	a	607	PEF	O5-C30-O3-C3
14	b	302	PEF	O5-C30-O3-C3
14	a	607	PEF	C31-C30-O3-C3
14	b	302	PEF	C31-C30-O3-C3
14	b	301	PEF	O4-C10-O2-C2
14	b	304	PEF	O4-C10-O2-C2
14	h	101	PEF	C31-C30-O3-C3
14	h	101	PEF	O5-C30-O3-C3
13	a	604	HEA	C26-C15-C16-C17
13	a	604	HEA	C14-C15-C16-C17
13	a	604	HEA	C15-C16-C17-C18
14	g	101	PEF	C10-C11-C12-C13
14	b	301	PEF	C16-C17-C18-C19
14	b	304	PEF	C33-C34-C35-C36
14	g	101	PEF	C11-C10-O2-C2
14	b	302	PEF	C33-C34-C35-C36
14	b	304	PEF	C31-C30-O3-C3
14	a	607	PEF	C35-C36-C37-C38
14	g	101	PEF	C13-C14-C15-C16
14	g	101	PEF	O4-C10-O2-C2
14	b	304	PEF	C30-C31-C32-C33
14	a	607	PEF	C10-C11-C12-C13
14	a	607	PEF	C40-C41-C42-C43
14	b	301	PEF	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
14	b	301	PEF	C30-C31-C32-C33
14	c	302	PEF	C11-C10-O2-C2
14	b	301	PEF	C40-C41-C42-C43
14	b	304	PEF	O5-C30-O3-C3
14	c	301	PEF	C30-C31-C32-C33
14	a	607	PEF	C21-C22-C23-C24
14	a	607	PEF	C17-C18-C19-C20
14	c	302	PEF	O4-C10-O2-C2
14	g	101	PEF	C31-C30-O3-C3
14	c	301	PEF	C10-C11-C12-C13
14	g	101	PEF	O5-C30-O3-C3
14	g	101	PEF	C34-C35-C36-C37
14	b	304	PEF	C13-C14-C15-C16
14	b	304	PEF	C15-C16-C17-C18
14	g	101	PEF	C12-C13-C14-C15
14	h	101	PEF	C17-C18-C19-C20
14	a	607	PEF	C13-C14-C15-C16
14	b	301	PEF	C33-C34-C35-C36
14	g	101	PEF	C41-C42-C43-C44
14	a	607	PEF	C14-C15-C16-C17
14	a	607	PEF	C31-C32-C33-C34
14	a	607	PEF	C41-C42-C43-C44
13	a	605	HEA	C4C-C3C-CAC-CBC
14	e	201	PEF	C38-C39-C40-C41
14	a	607	PEF	C36-C37-C38-C39
14	a	607	PEF	C32-C33-C34-C35
14	g	101	PEF	C15-C16-C17-C18
14	b	302	PEF	C11-C10-O2-C2
14	a	607	PEF	C34-C35-C36-C37
14	h	101	PEF	C15-C16-C17-C18
14	h	101	PEF	C33-C34-C35-C36
14	h	101	PEF	C41-C42-C43-C44
14	g	101	PEF	C17-C18-C19-C20
14	a	607	PEF	C37-C38-C39-C40
14	b	302	PEF	C35-C36-C37-C38
14	h	101	PEF	C31-C32-C33-C34
14	a	607	PEF	C39-C40-C41-C42
14	a	607	PEF	C42-C43-C44-C45
14	b	302	PEF	O4-C10-O2-C2
14	h	101	PEF	C22-C23-C24-C25
14	b	301	PEF	C42-C43-C44-C45
14	b	304	PEF	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
14	c	301	PEF	C35-C36-C37-C38
14	c	301	PEF	C15-C16-C17-C18
14	h	101	PEF	C18-C19-C20-C21
14	b	301	PEF	C36-C37-C38-C39
14	b	301	PEF	C20-C21-C22-C23
14	g	101	PEF	C32-C33-C34-C35
14	b	302	PEF	C34-C35-C36-C37
14	g	101	PEF	C16-C17-C18-C19
14	e	201	PEF	C37-C38-C39-C40
14	b	304	PEF	C31-C32-C33-C34
14	e	201	PEF	C10-C11-C12-C13
14	b	302	PEF	C32-C33-C34-C35
14	b	301	PEF	C3-C2-O2-C10
14	a	607	PEF	O3P-C1-C2-O2
14	b	301	PEF	C37-C38-C39-C40
14	c	302	PEF	C31-C32-C33-C34
14	g	101	PEF	C38-C39-C40-C41
14	b	302	PEF	C11-C12-C13-C14
14	g	101	PEF	C40-C41-C42-C43
13	a	605	HEA	C3B-C11-C12-C13
14	h	101	PEF	C34-C35-C36-C37
14	b	301	PEF	C22-C23-C24-C25
14	b	304	PEF	O3P-C1-C2-C3
14	a	607	PEF	C22-C23-C24-C25
14	h	101	PEF	C42-C43-C44-C45
14	b	302	PEF	C15-C16-C17-C18
14	b	301	PEF	C32-C33-C34-C35
14	g	101	PEF	C1-C2-C3-O3
14	h	101	PEF	C1-C2-C3-O3
14	a	606	PEF	C31-C32-C33-C34
14	a	607	PEF	C15-C16-C17-C18
14	b	304	PEF	C18-C19-C20-C21
14	h	101	PEF	C12-C13-C14-C15
14	a	607	PEF	O2-C2-C3-O3
14	a	607	PEF	C18-C19-C20-C21
14	b	304	PEF	C22-C23-C24-C25
14	h	101	PEF	C37-C38-C39-C40
14	e	201	PEF	C42-C43-C44-C45
14	g	101	PEF	C21-C22-C23-C24
14	h	101	PEF	C35-C36-C37-C38
14	c	302	PEF	C32-C33-C34-C35
14	a	606	PEF	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
14	c	301	PEF	O3P-C1-C2-C3
14	b	301	PEF	C21-C22-C23-C24
14	c	301	PEF	C14-C15-C16-C17
14	g	101	PEF	C37-C38-C39-C40
14	b	302	PEF	C14-C15-C16-C17
14	c	301	PEF	C32-C33-C34-C35
14	c	301	PEF	O3P-C1-C2-O2
14	h	101	PEF	O3P-C1-C2-O2
14	e	201	PEF	C1-C2-C3-O3
13	a	604	HEA	O11-C11-C12-C13
14	e	201	PEF	C17-C18-C19-C20
14	b	301	PEF	C15-C16-C17-C18
14	b	304	PEF	C11-C12-C13-C14
14	g	101	PEF	C14-C15-C16-C17
14	g	101	PEF	O2-C2-C3-O3
14	h	101	PEF	C20-C21-C22-C23
14	c	301	PEF	C17-C18-C19-C20
14	a	607	PEF	O3P-C1-C2-C3
14	c	301	PEF	C12-C13-C14-C15
14	b	301	PEF	C2-C1-O3P-P
14	c	301	PEF	C36-C37-C38-C39
14	a	606	PEF	O3P-C1-C2-O2
14	b	304	PEF	O3P-C1-C2-O2
14	g	101	PEF	O3P-C1-C2-O2
14	g	101	PEF	C22-C23-C24-C25
13	a	604	HEA	C4A-C3A-CMA-OMA
13	a	605	HEA	C4A-C3A-CMA-OMA
14	b	304	PEF	C32-C33-C34-C35
14	b	302	PEF	O2-C2-C3-O3
14	g	101	PEF	C33-C34-C35-C36
14	b	302	PEF	C1-C2-C3-O3
14	b	302	PEF	C30-C31-C32-C33
14	a	607	PEF	C4-O4P-P-O1P
14	b	301	PEF	O4P-C4-C5-N
14	b	301	PEF	C1-O3P-P-O1P
14	b	302	PEF	C1-O3P-P-O1P
14	b	302	PEF	C1-O3P-P-O4P
14	b	302	PEF	C4-O4P-P-O1P
14	b	304	PEF	C4-O4P-P-O1P
14	e	201	PEF	C1-O3P-P-O1P
14	g	101	PEF	C1-O3P-P-O1P
14	g	101	PEF	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
14	h	101	PEF	C1-O3P-P-O1P
14	h	101	PEF	C4-O4P-P-O2P
13	a	605	HEA	C2C-C3C-CAC-CBC
14	b	304	PEF	C2-C1-O3P-P
14	g	101	PEF	C2-C1-O3P-P
14	e	201	PEF	C20-C21-C22-C23
14	h	101	PEF	O3P-C1-C2-C3
14	b	304	PEF	C35-C36-C37-C38
14	b	302	PEF	O3P-C1-C2-O2
14	a	607	PEF	C12-C13-C14-C15
14	b	301	PEF	C34-C35-C36-C37
14	c	301	PEF	C13-C14-C15-C16
14	a	607	PEF	C2-C1-O3P-P
14	h	101	PEF	C11-C12-C13-C14
14	g	101	PEF	C20-C21-C22-C23
14	b	304	PEF	C14-C15-C16-C17
14	a	607	PEF	C38-C39-C40-C41
14	g	101	PEF	C35-C36-C37-C38
14	c	302	PEF	C33-C34-C35-C36
14	a	607	PEF	C3-C2-O2-C10
14	h	101	PEF	C19-C20-C21-C22
14	g	101	PEF	C18-C19-C20-C21
13	a	605	HEA	CAA-CBA-CGA-O2A
13	a	605	HEA	CAA-CBA-CGA-O1A
14	g	101	PEF	C31-C32-C33-C34
13	a	605	HEA	C26-C15-C16-C17
13	a	605	HEA	CAD-CBD-CGD-O2D
14	g	101	PEF	O3-C30-C31-C32
13	a	605	HEA	C14-C15-C16-C17
13	a	605	HEA	CAD-CBD-CGD-O1D
14	h	101	PEF	C40-C41-C42-C43
14	a	607	PEF	C1-C2-C3-O3
14	g	101	PEF	O3P-C1-C2-C3
14	e	201	PEF	C13-C14-C15-C16
14	b	302	PEF	C13-C14-C15-C16
14	e	201	PEF	C21-C22-C23-C24
13	a	604	HEA	CAA-CBA-CGA-O1A
13	a	604	HEA	CAA-CBA-CGA-O2A
14	c	301	PEF	C31-C32-C33-C34
14	b	304	PEF	C21-C22-C23-C24
14	e	201	PEF	C31-C30-O3-C3
14	h	101	PEF	C38-C39-C40-C41

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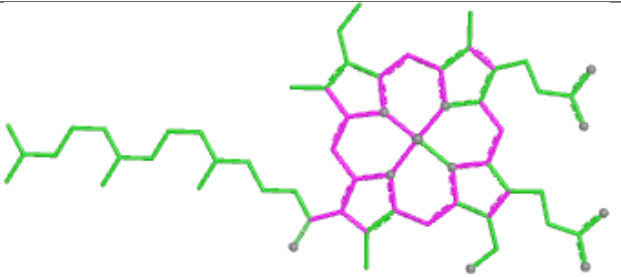
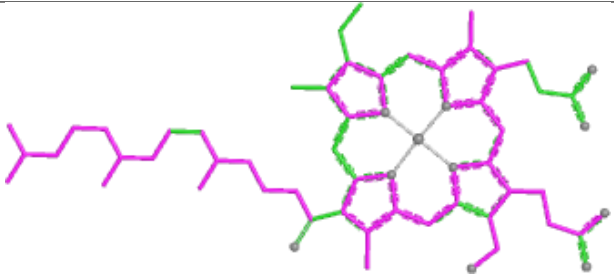
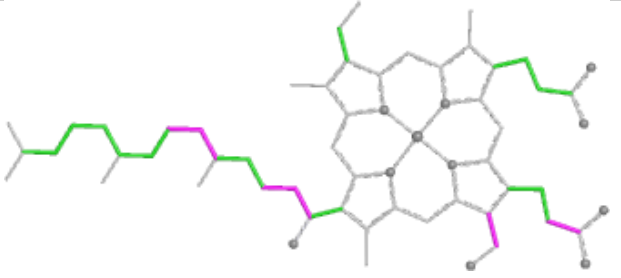
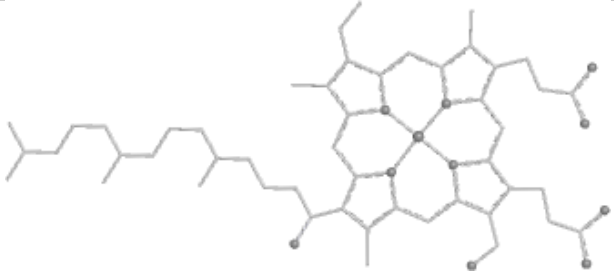
Mol	Chain	Res	Type	Atoms
14	h	101	PEF	C10-C11-C12-C13
14	e	201	PEF	O5-C30-O3-C3
14	b	302	PEF	O2-C10-C11-C12

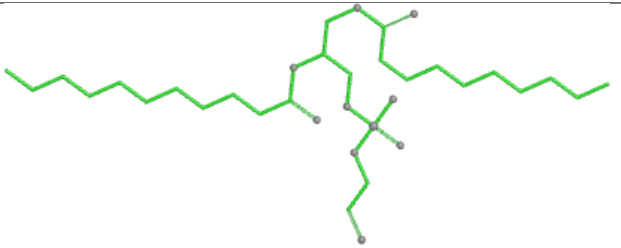
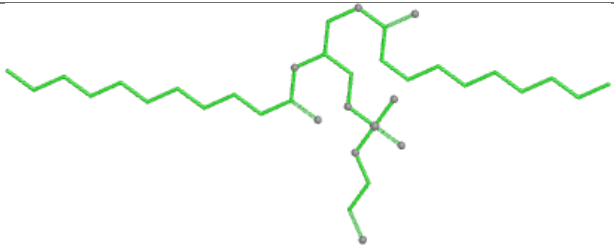
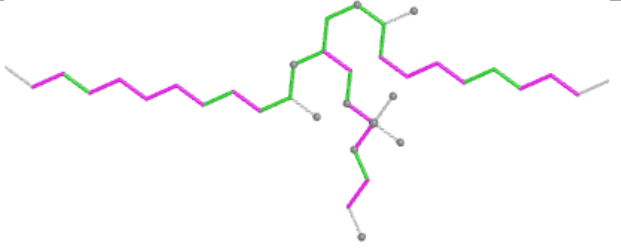
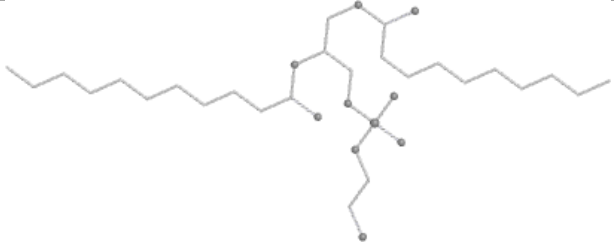
There are no ring outliers.

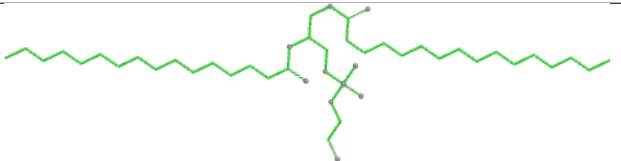
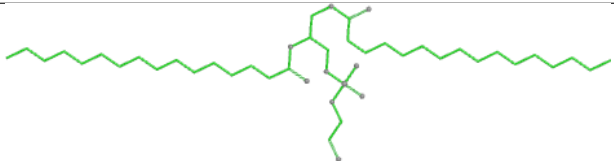
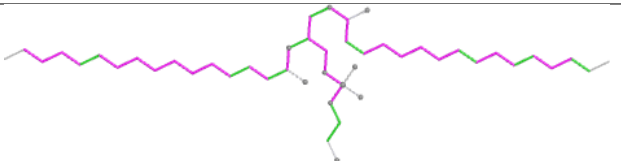
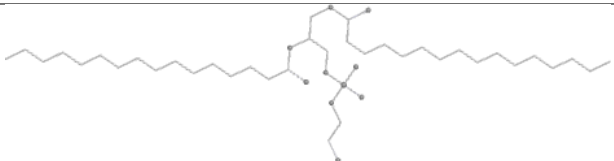
12 monomers are involved in 92 short contacts:

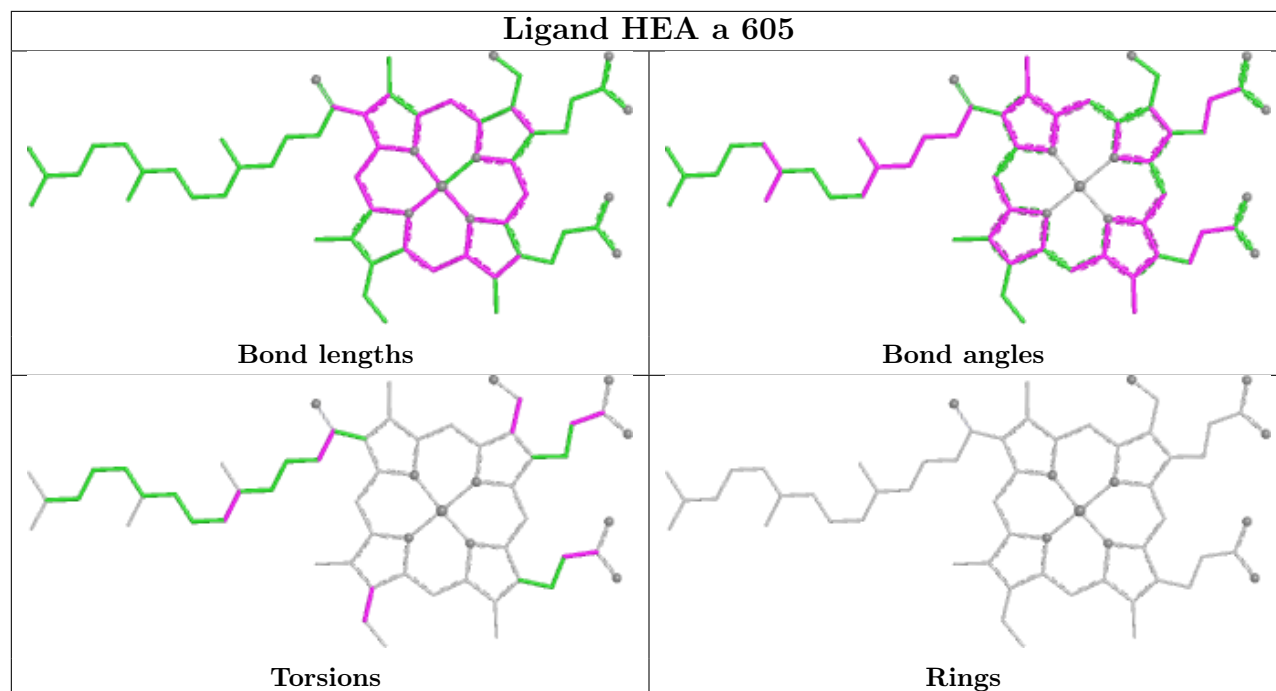
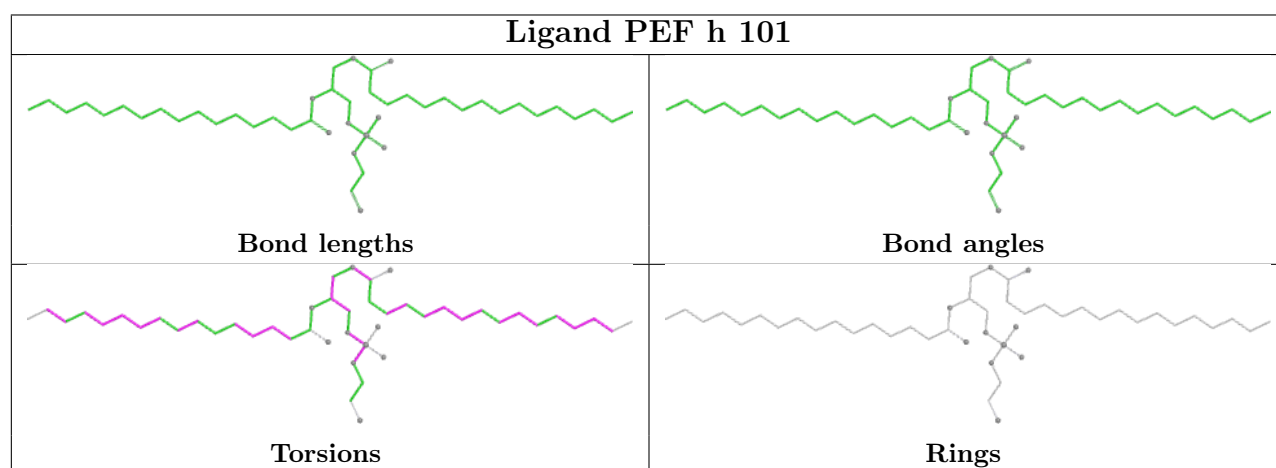
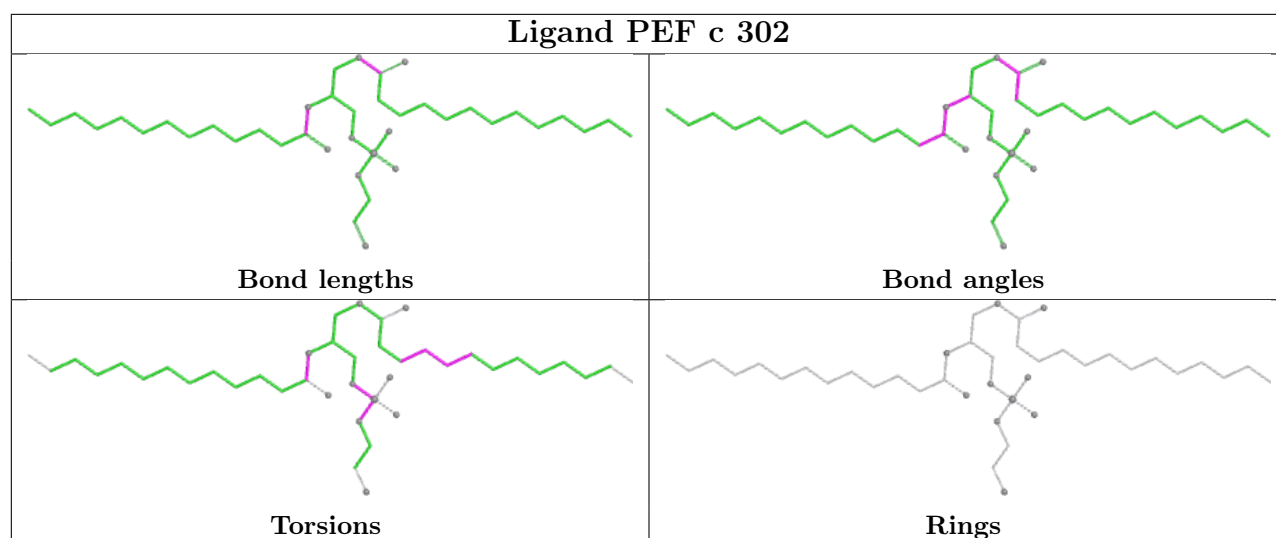
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	604	HEA	17	0
14	c	301	PEF	8	0
14	g	101	PEF	10	0
14	c	302	PEF	10	0
14	h	101	PEF	5	0
13	a	605	HEA	8	0
14	b	301	PEF	9	0
14	a	607	PEF	6	0
14	b	302	PEF	3	0
14	e	201	PEF	5	0
14	a	606	PEF	3	0
14	b	304	PEF	9	0

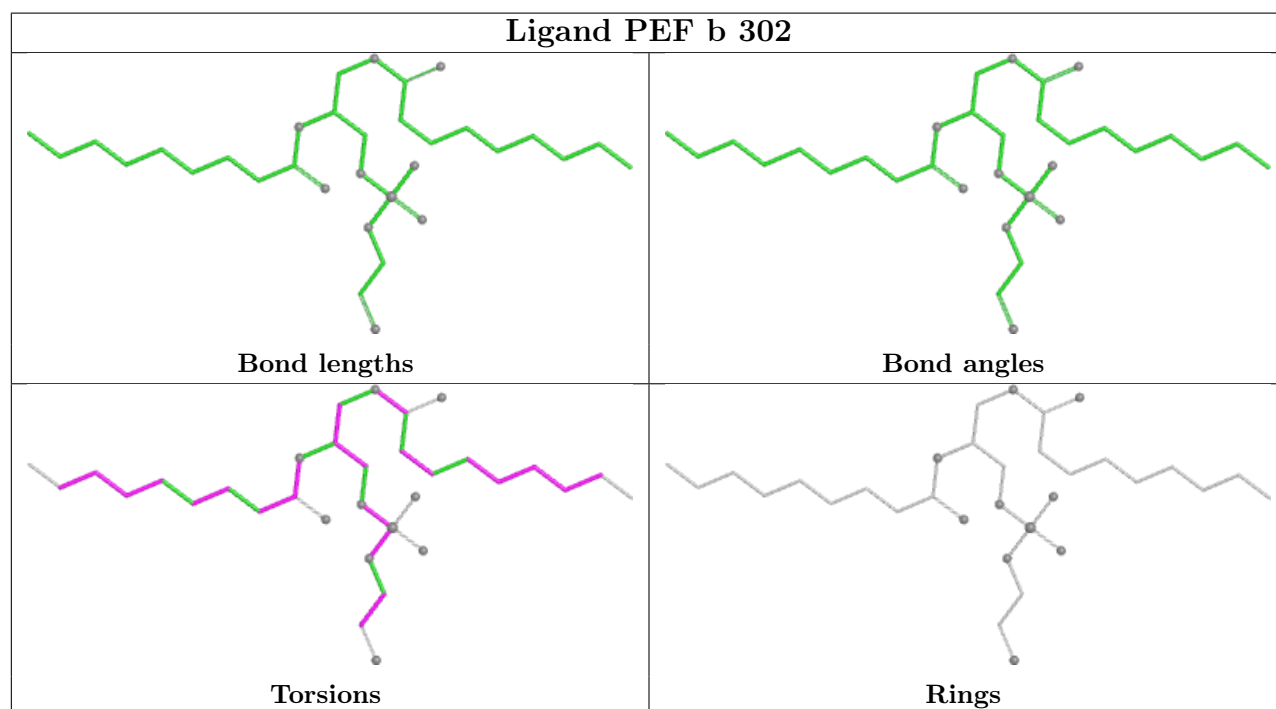
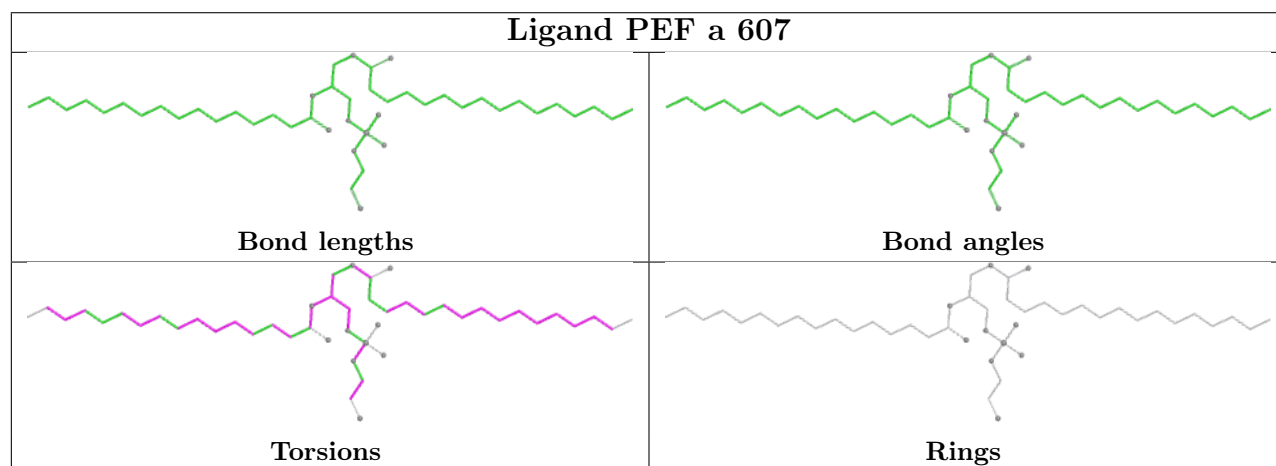
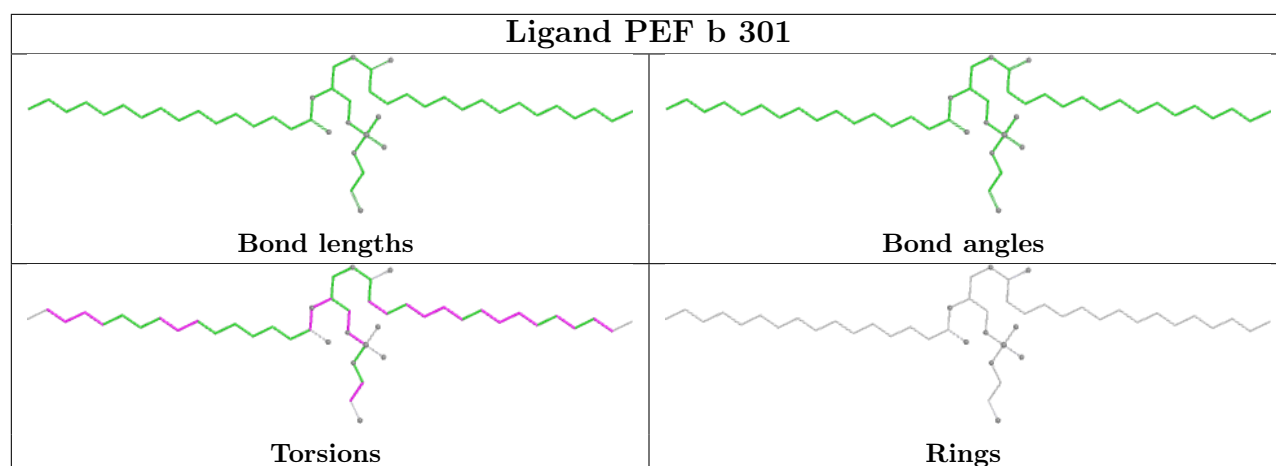
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEA a 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

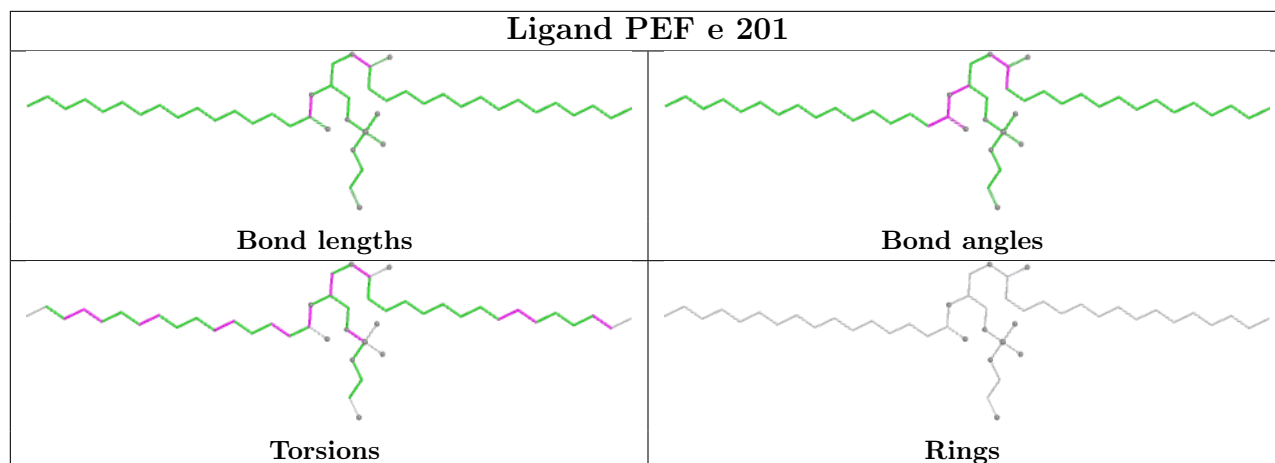
Ligand PEF c 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEF g 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

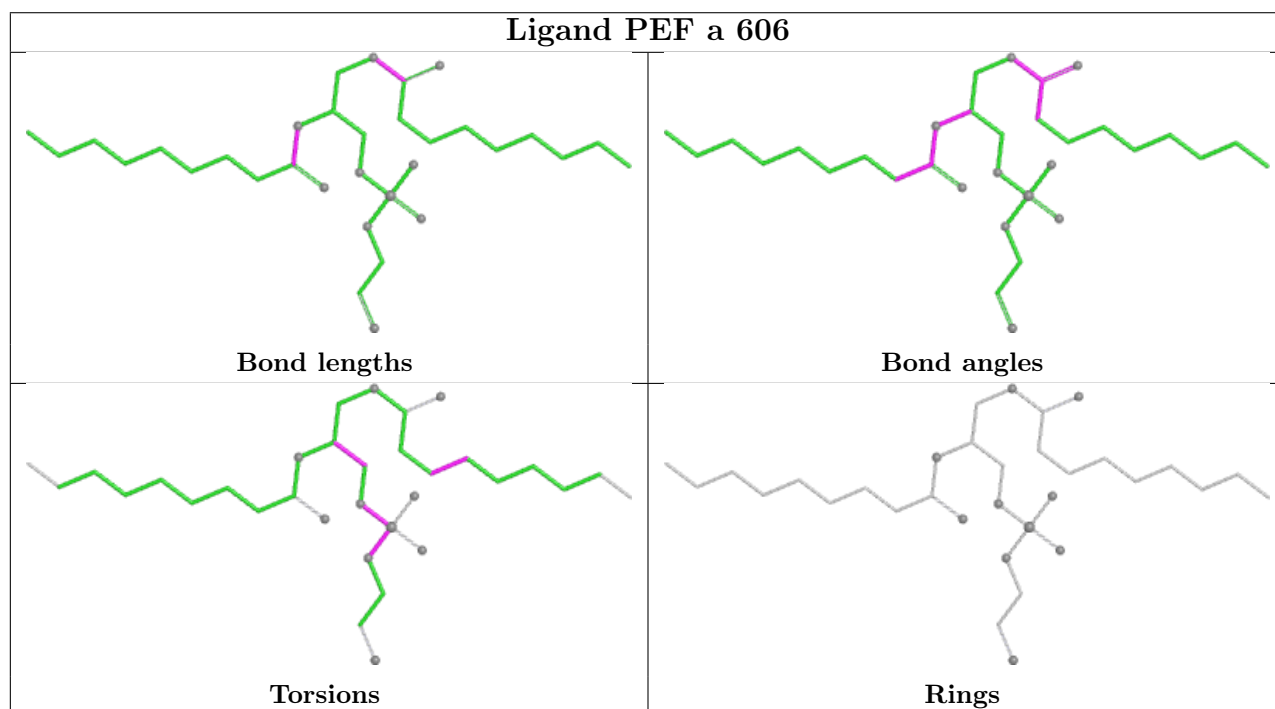




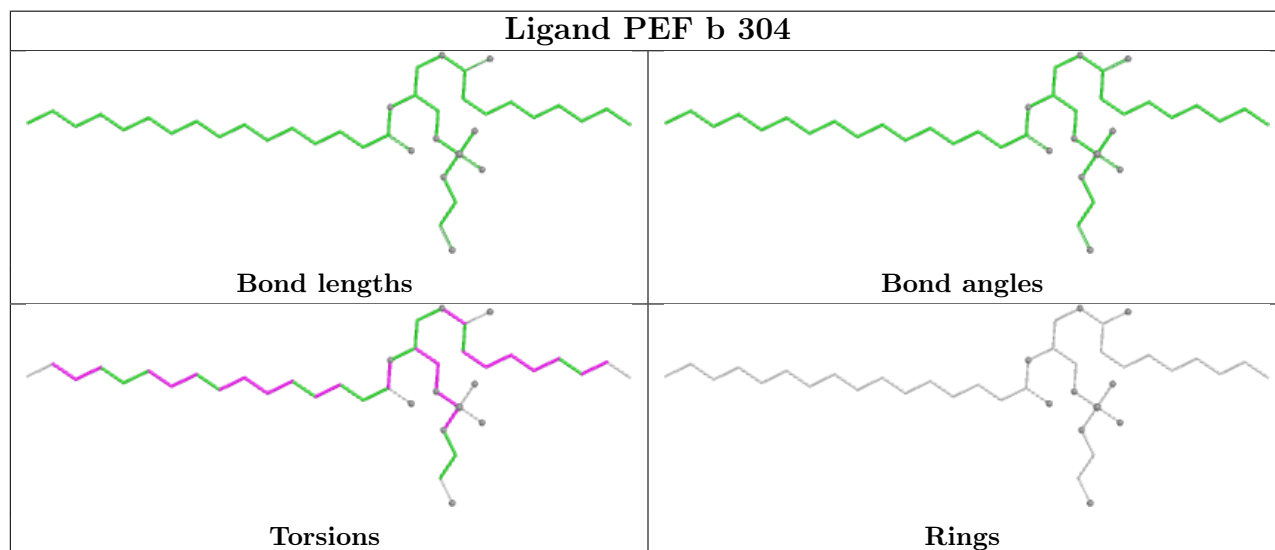
Ligand PEF e 201



Ligand PEF a 606



Ligand PEF b 304



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.

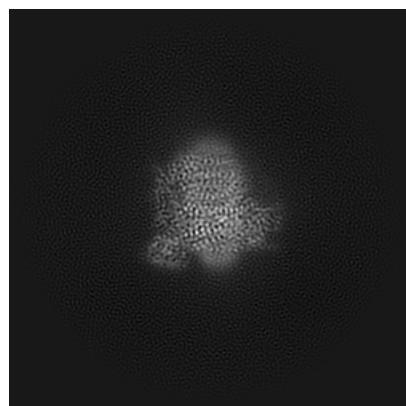
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27430. These allow visual inspection of the internal detail of the map and identification of artifacts.

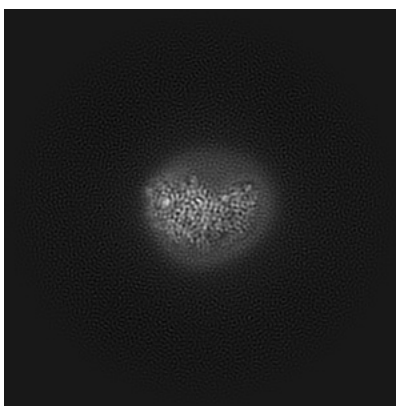
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

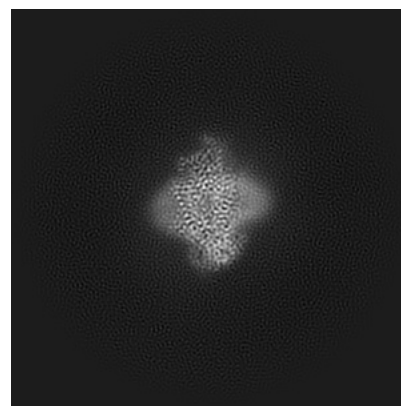
6.1.1 Primary map



X

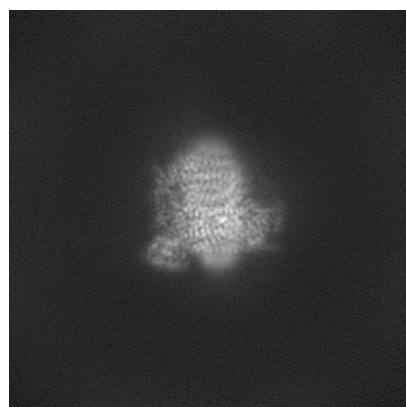


Y

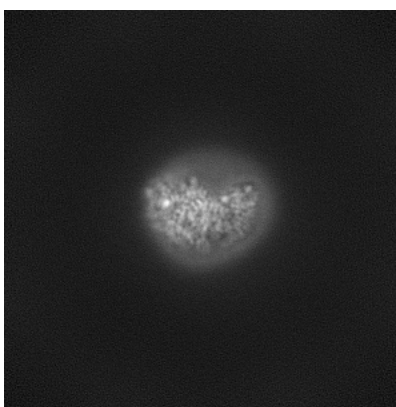


Z

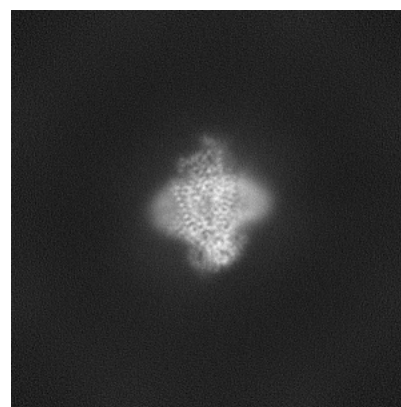
6.1.2 Raw map



X



Y

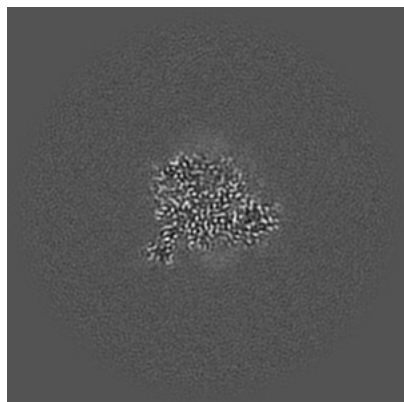


Z

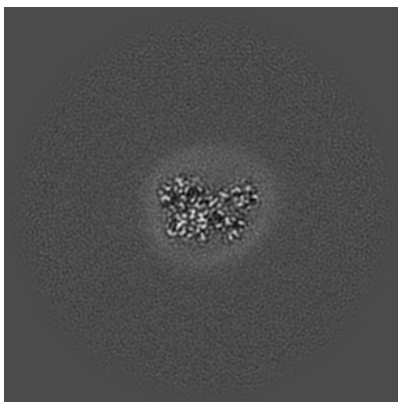
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

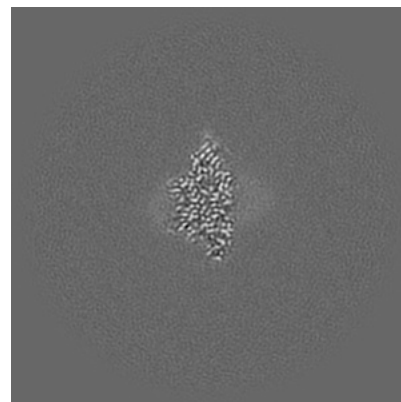
6.2.1 Primary map



X Index: 200

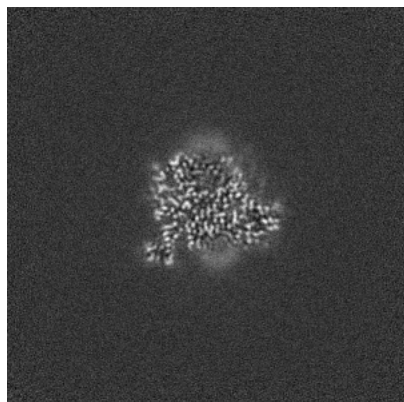


Y Index: 200

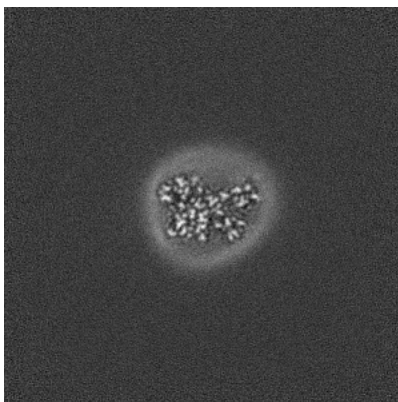


Z Index: 200

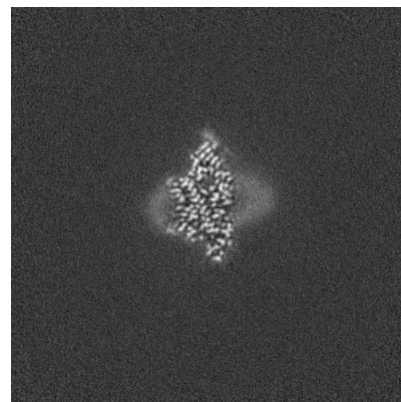
6.2.2 Raw map



X Index: 200



Y Index: 200

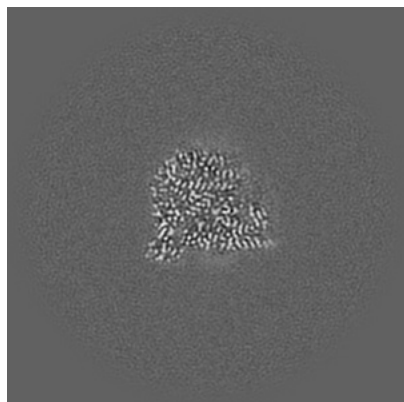


Z Index: 200

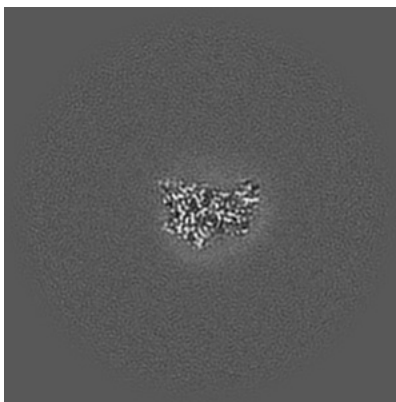
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

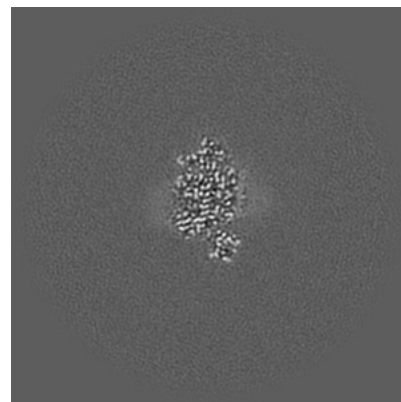
6.3.1 Primary map



X Index: 208

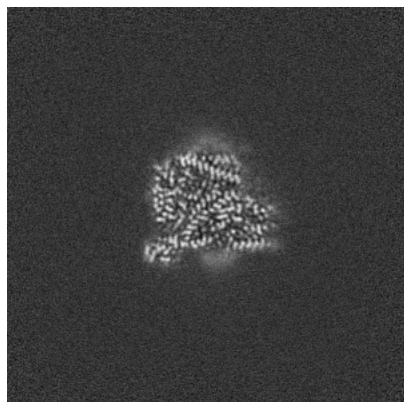


Y Index: 187

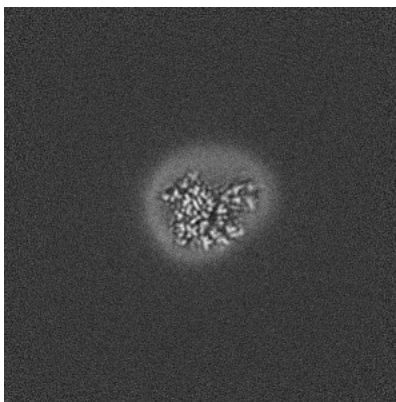


Z Index: 188

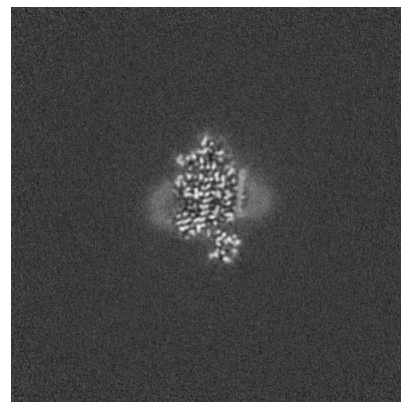
6.3.2 Raw map



X Index: 205



Y Index: 216

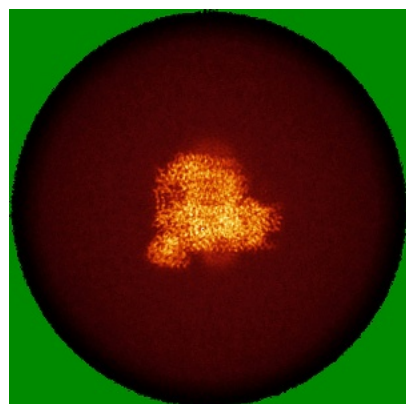


Z Index: 188

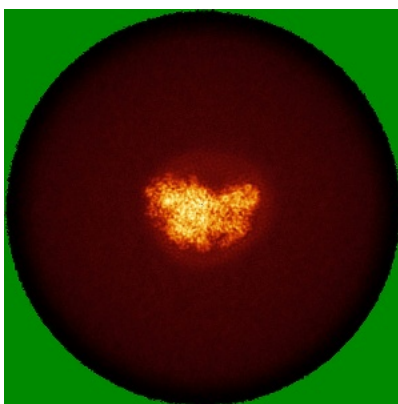
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

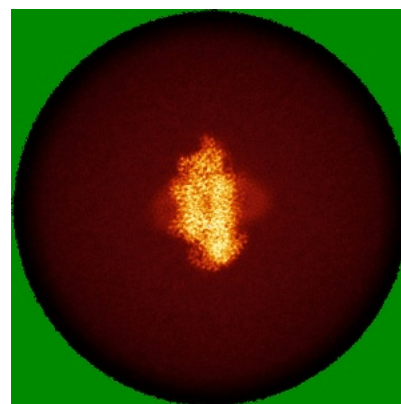
6.4.1 Primary map



X

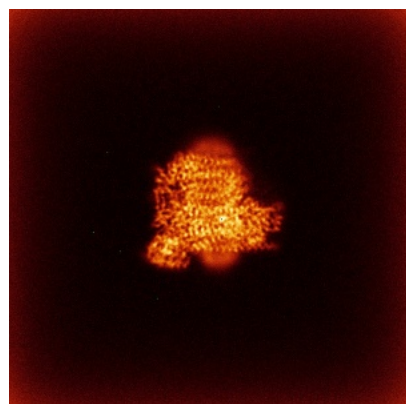


Y

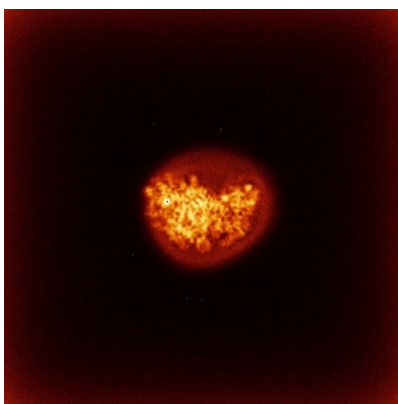


Z

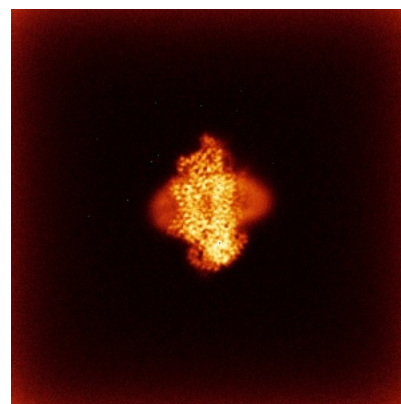
6.4.2 Raw map



X



Y

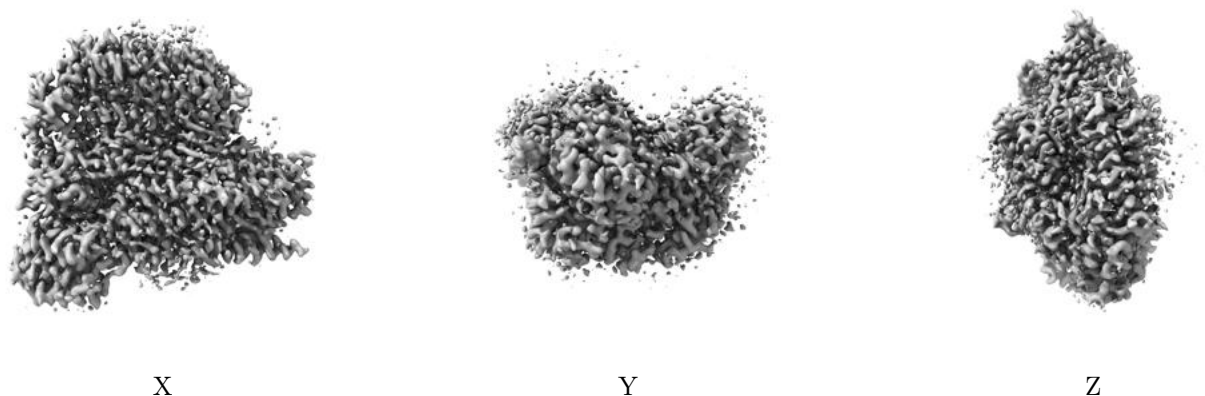


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

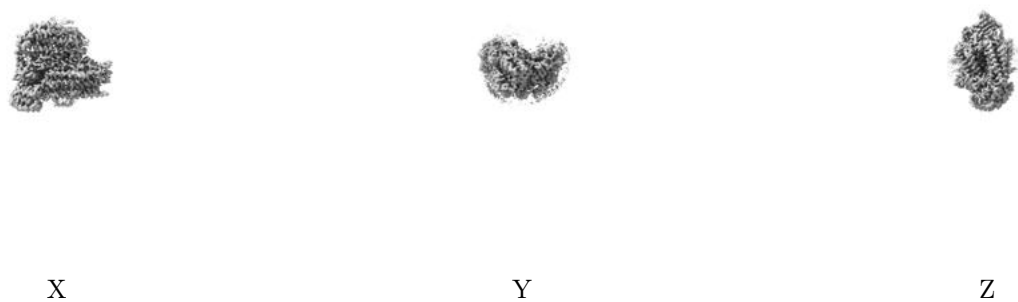
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.46. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

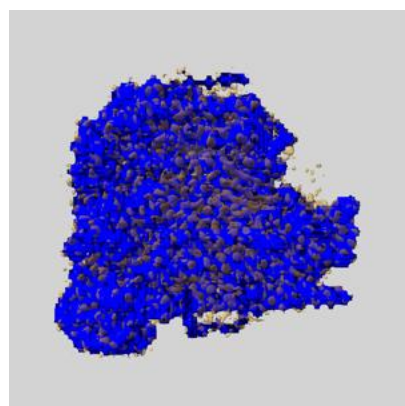
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

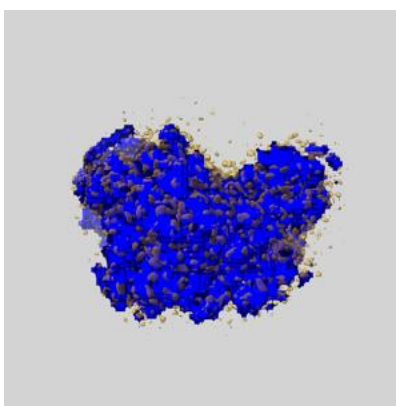
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

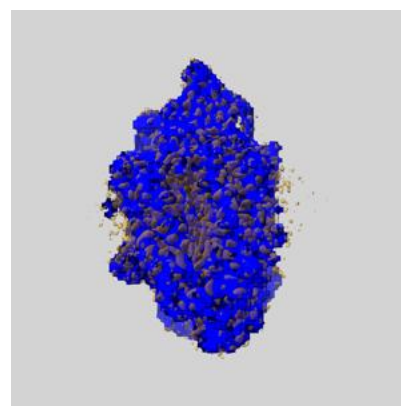
6.6.1 emd_27430_msk_1.map [i](#)



X



Y

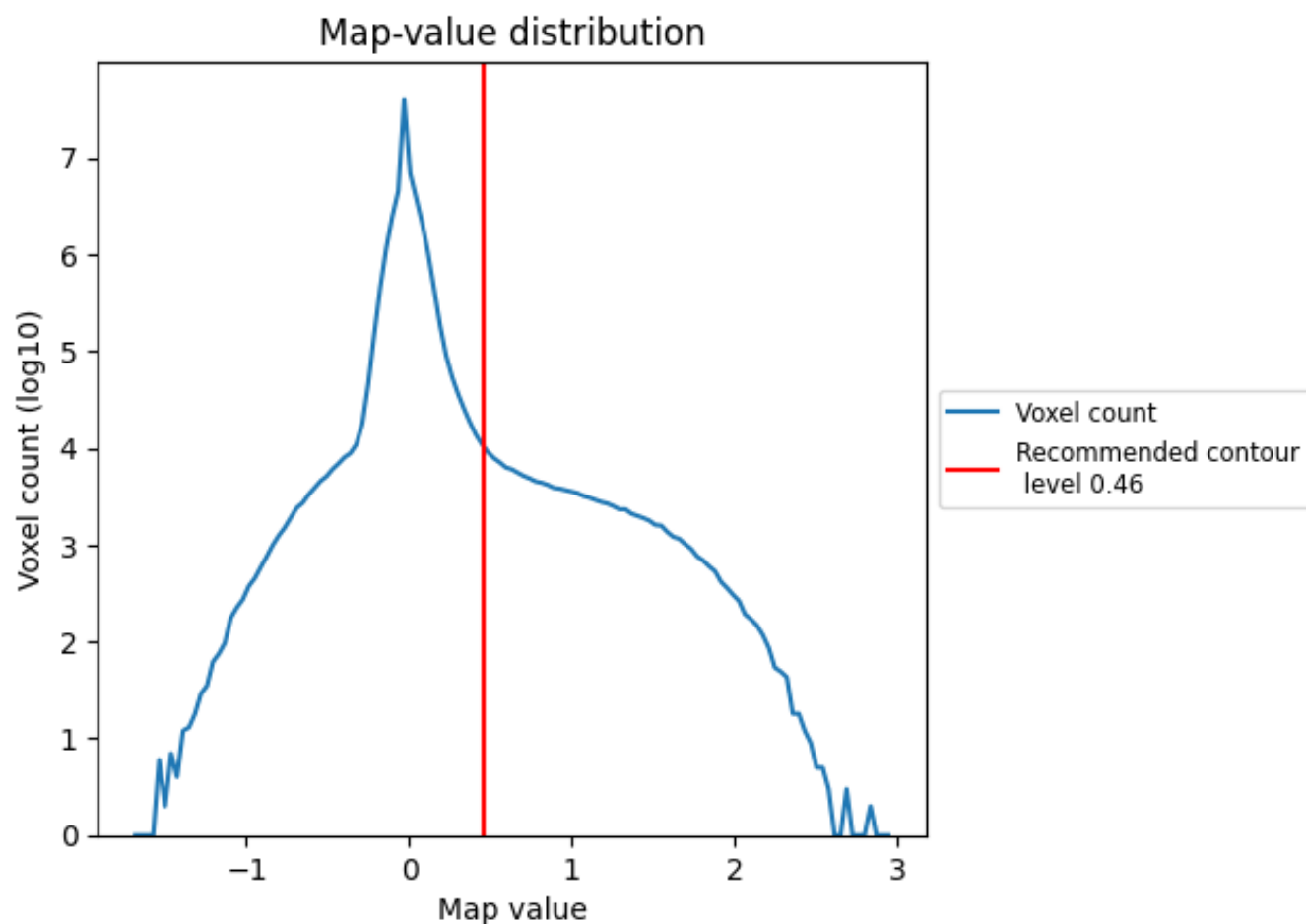


Z

7 Map analysis [i](#)

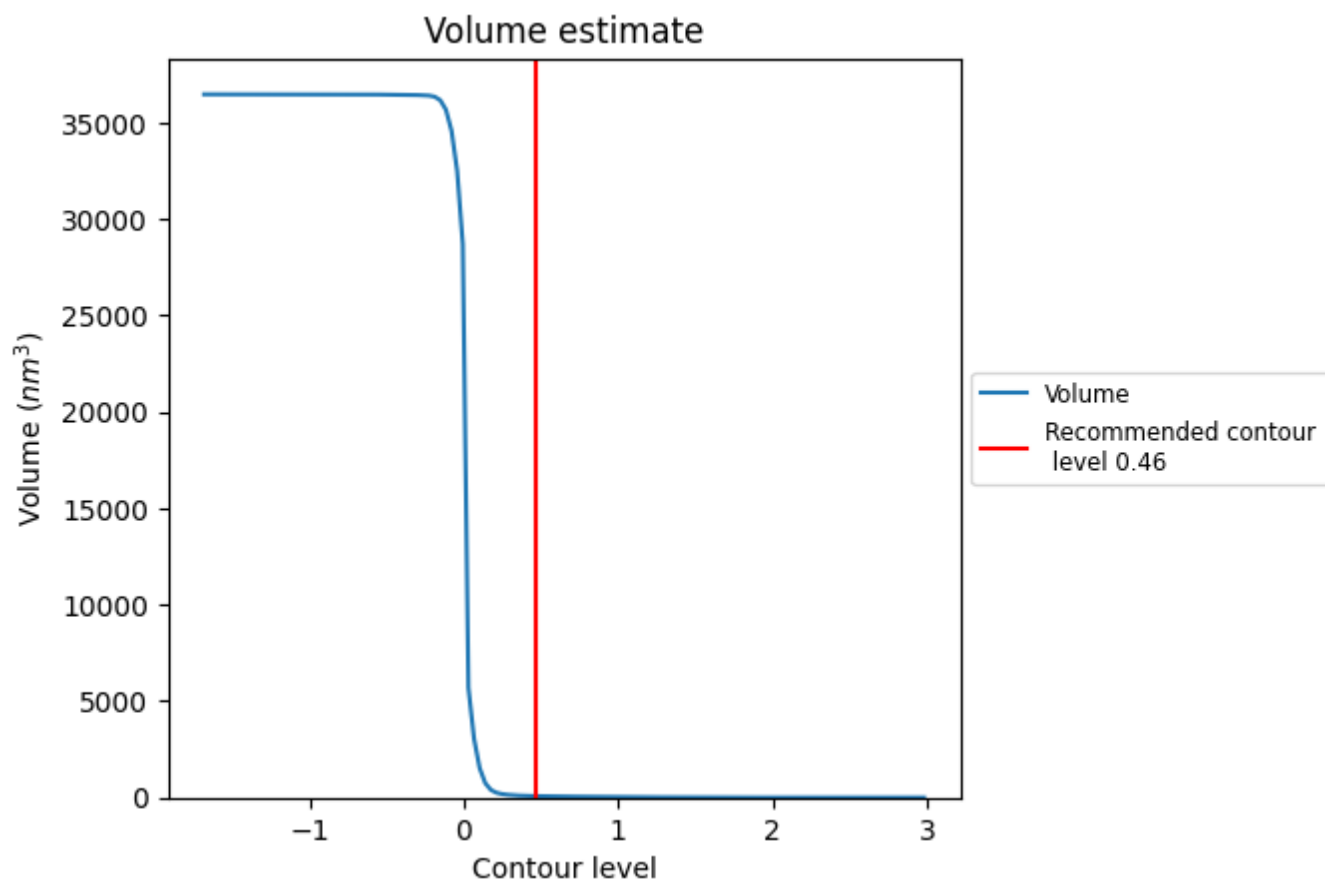
This section contains the results of statistical analysis of the map.

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.

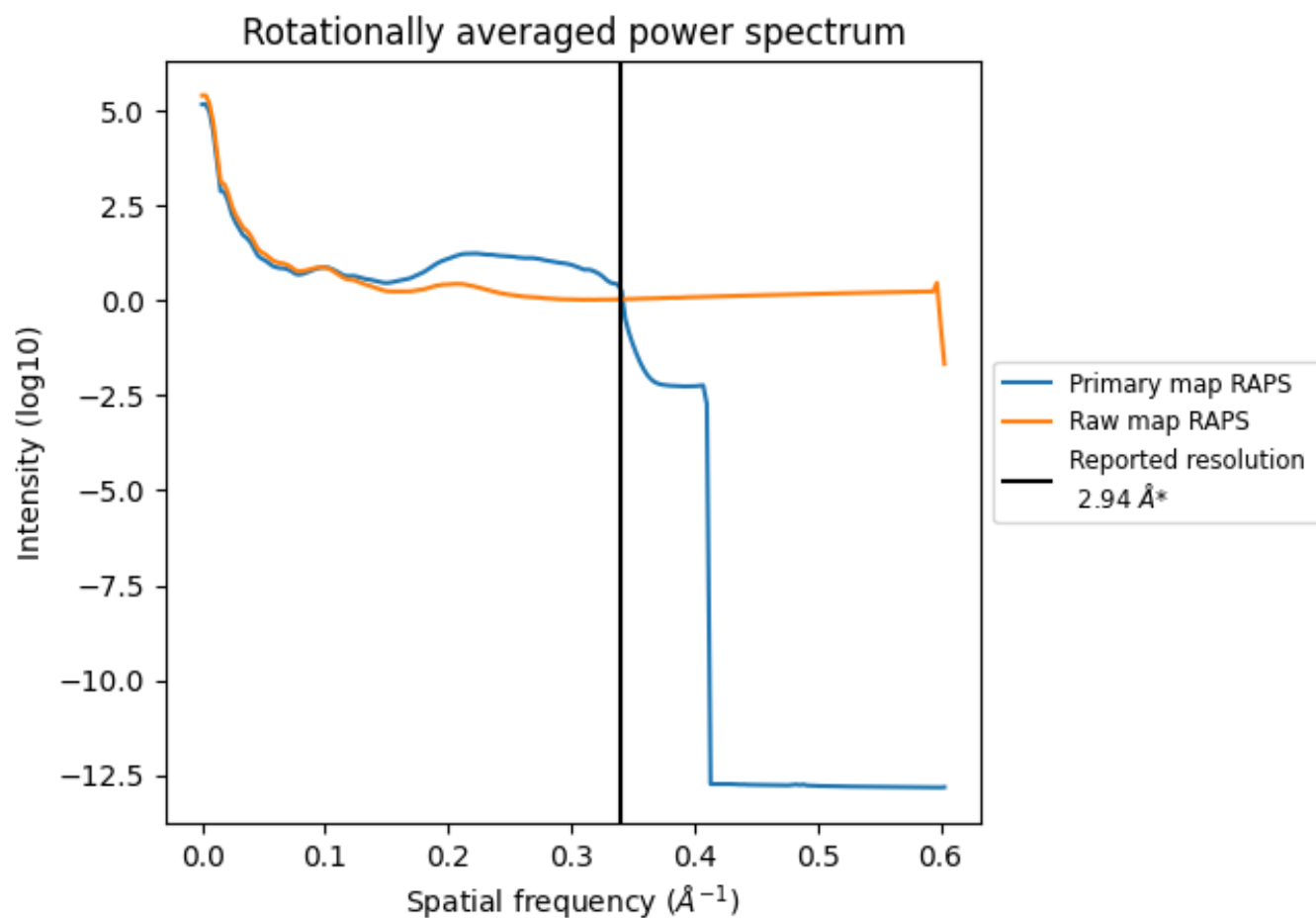
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 76 nm³; this corresponds to an approximate mass of 69 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 ⓘ

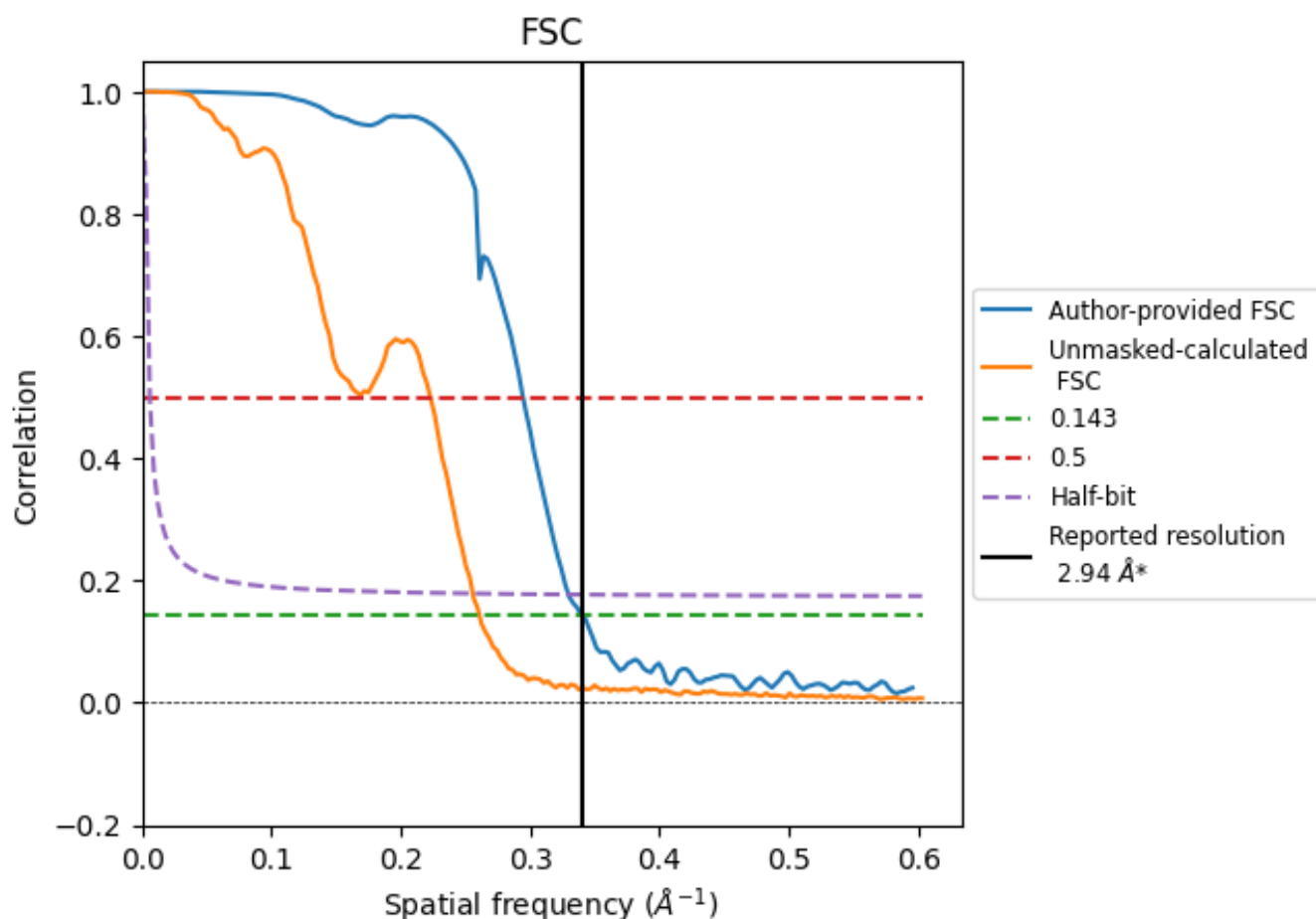


*Reported resolution corresponds to spatial frequency of 0.340 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.340 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

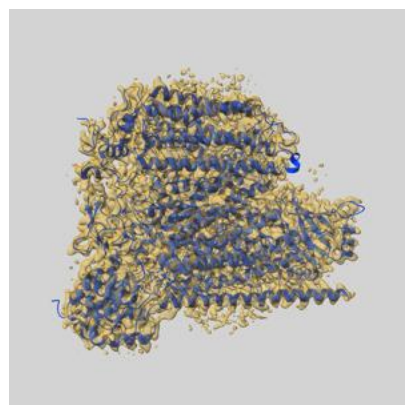
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.94	-	-
Author-provided FSC curve	2.94	3.40	3.03
Unmasked-calculated*	3.84	4.49	3.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.84 differs from the reported value 2.94 by more than 10 %

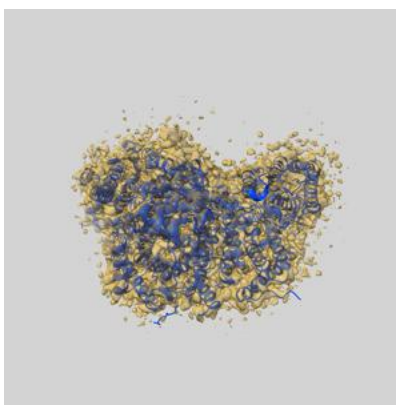
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27430 and PDB model 8DH6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

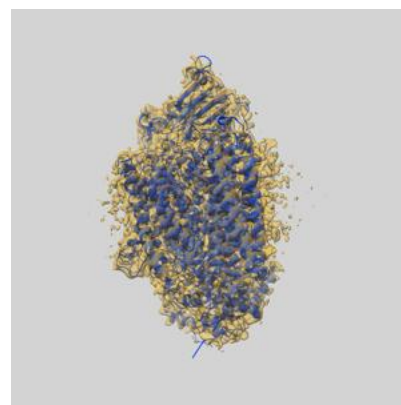
9.1 Map-model overlay [i](#)



X



Y



Z

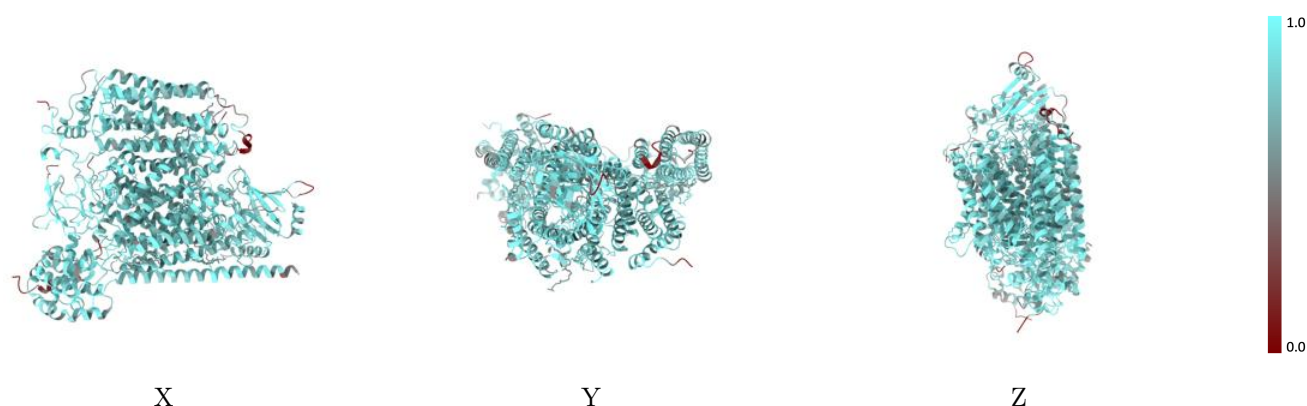
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



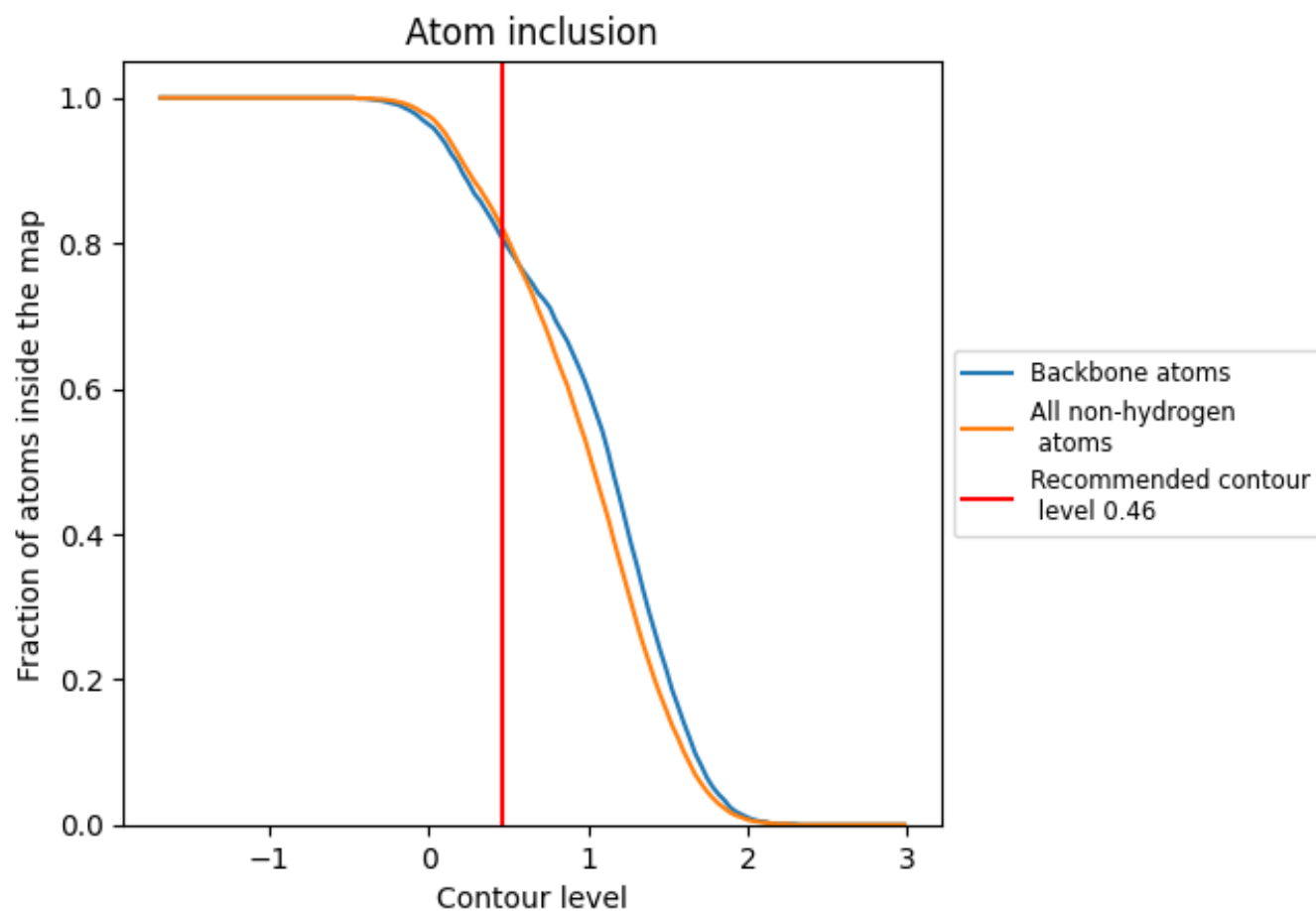
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.46).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.5340
a	0.8700	0.5600
b	0.8120	0.5300
c	0.8050	0.5310
d	0.7900	0.5100
e	0.7290	0.4820
f	0.7950	0.5210
g	0.8440	0.5390
h	0.8360	0.5380
i	0.7670	0.5100

1.0

0.0

<0.0