



Full wwPDB EM Validation Report ⓘ

Jul 25, 2022 – 01:40 pm BST

PDB ID : 7Z10
EMDB ID : EMD-14436
Title : Monomeric respiratory complex IV isolated from *S. cerevisiae*
Authors : Marechal, A.; Hartley, A.; Ing, G.; Pinotsis, N.
Deposited on : 2022-02-24
Resolution : 3.87 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.dev8
Mogul : 1.8.4, 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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

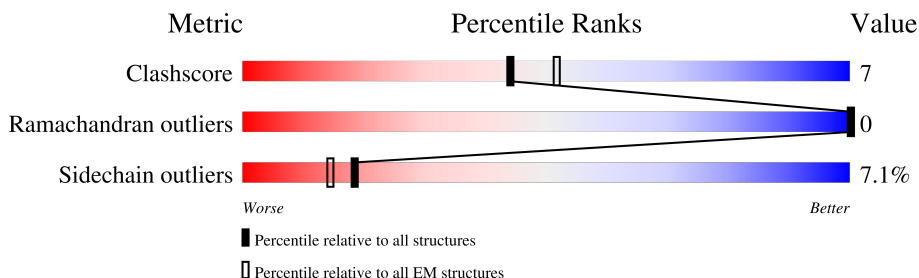
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.87 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.



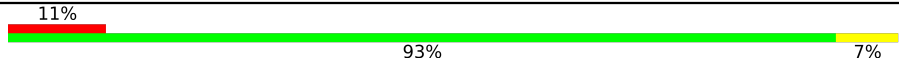
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	121	
5	e	133	
6	f	104	
7	g	59	
8	h	47	

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Mol	Chain	Length	Quality of chain
9	i	55	 11% 93% 7%

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
11	HEA	a	602	X	-	-	-
11	HEA	a	603	X	-	-	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 12574 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	534	4162	2778	649	713	22	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	236	1889	1242	286	351	10	0	0

- Molecule 3 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3.

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

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

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

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

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

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

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

- Molecule 7 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	47	383	261	62	59	1	0	0

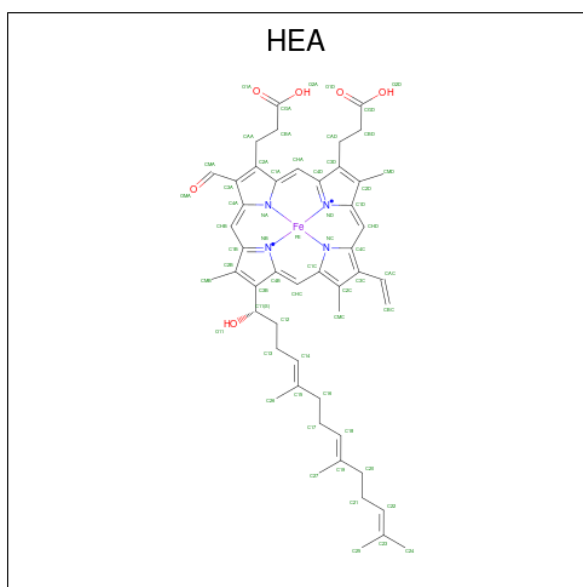
- Molecule 9 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9.

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

- Molecule 10 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 11 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).

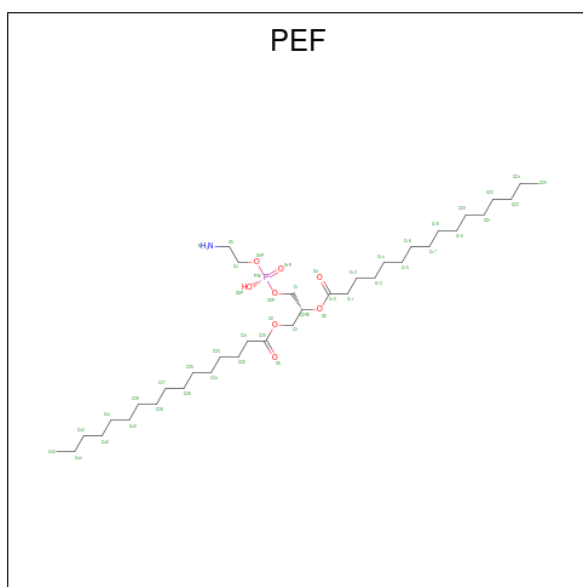


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
11	a	1	120	98	2	8	12	0
11	a	1	120	98	2	8	12	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

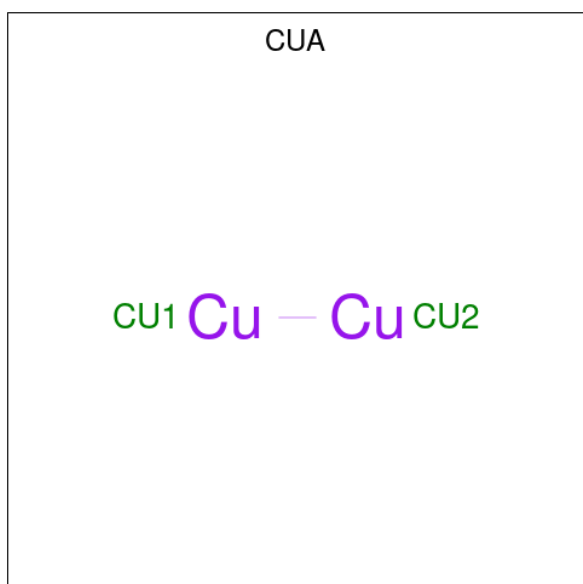
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
12	a	1	1	1	0

- Molecule 13 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: C₃₇H₇₄NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	a	1	80	60	2	16	2	0
13	a	1	80	60	2	16	2	0
13	c	1	36	26	1	8	1	0

- Molecule 14 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
14	b	1	Total	Cu	0
			2	2	

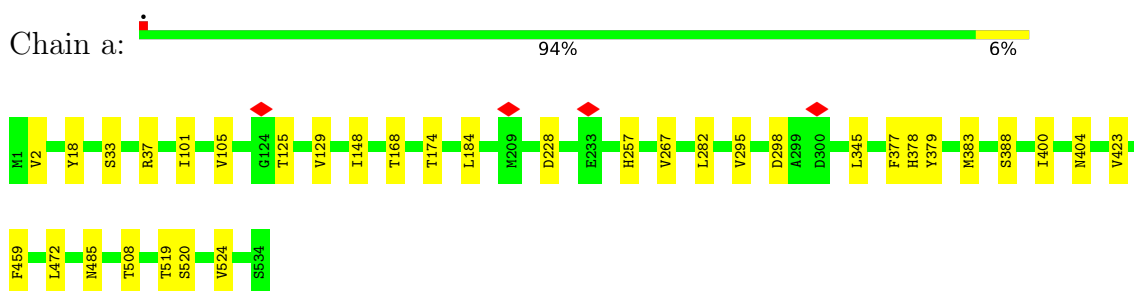
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

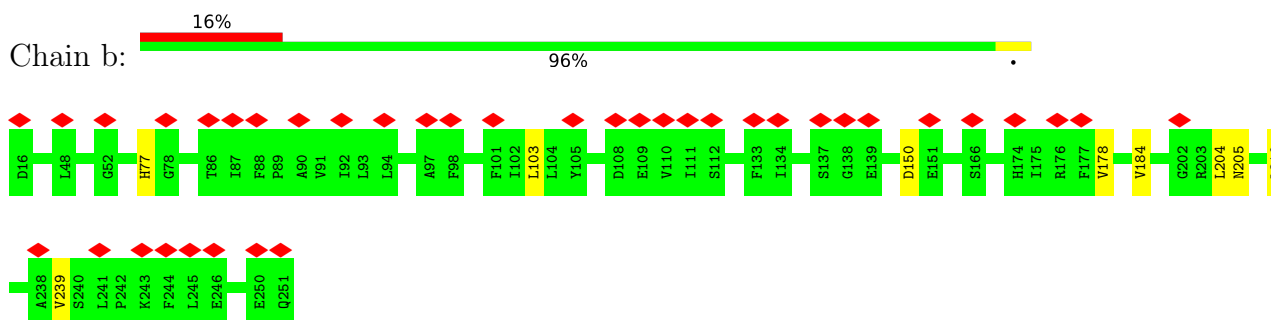
3 Residue-property plots

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.

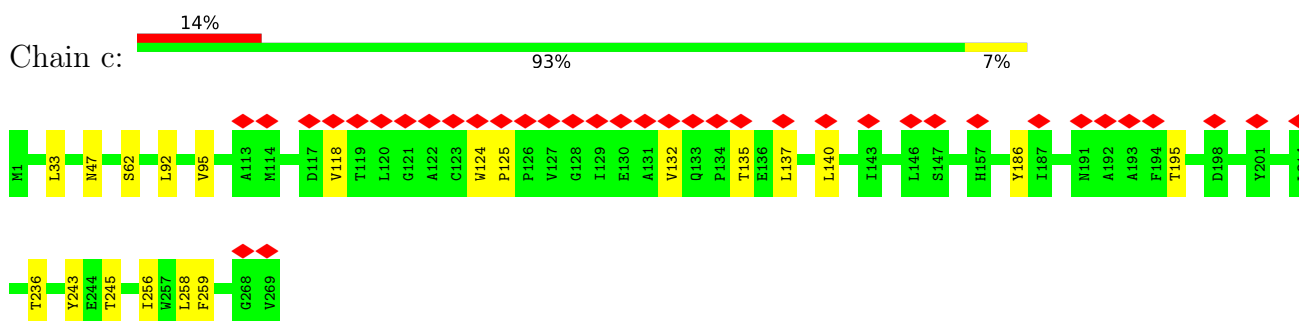
- Molecule 1: Cytochrome c oxidase subunit 1



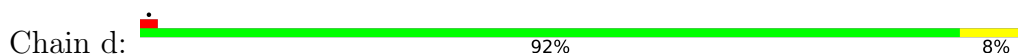
- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3

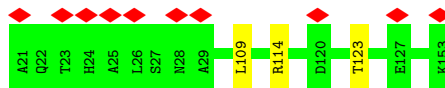


- Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial

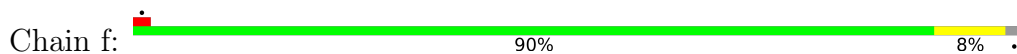




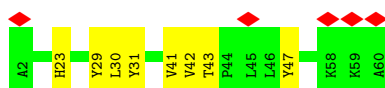
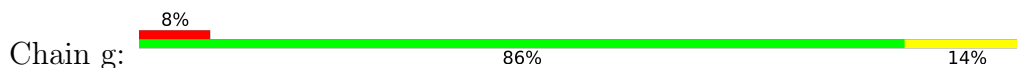
- Molecule 5: Cytochrome c oxidase polypeptide 5A, mitochondrial



- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial



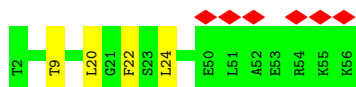
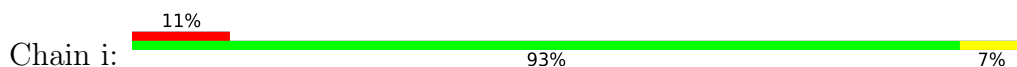
- Molecule 7: CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7



- Molecule 8: Cytochrome c oxidase polypeptide VIII, mitochondrial



- Molecule 9: CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.830	Depositor
Minimum map value	-14.394	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.6	Depositor
Map size (Å)	208.64, 208.64, 208.64	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.815, 0.815, 0.815	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: CU, MG, ZN, CUA, PEF, 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	0.43	0/4290	0.57	0/5857
2	b	0.33	0/1941	0.53	0/2653
3	c	0.34	0/2218	0.53	0/3036
4	d	0.36	0/932	0.55	1/1269 (0.1%)
5	e	0.32	0/1074	0.48	0/1451
6	f	0.37	0/868	0.48	0/1174
7	g	0.35	0/500	0.58	0/681
8	h	0.41	0/397	0.47	0/533
9	i	0.29	0/468	0.48	0/626
All	All	0.38	0/12688	0.54	1/17280 (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
3	c	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	143	LEU	C-N-CA	-5.72	107.41	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	520	SER	Peptide
3	c	124	TRP	Peptide
3	c	125	PRO	Peptide

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	4162	0	4192	0	0
2	b	1889	0	1866	0	0
3	c	2146	0	2137	0	0
4	d	913	0	910	0	0
5	e	1049	0	1030	0	0
6	f	851	0	822	0	0
7	g	484	0	517	0	0
8	h	383	0	386	0	0
9	i	456	0	469	0	0
10	a	1	0	0	0	0
11	a	120	0	108	0	0
12	a	1	0	0	0	0
13	a	80	0	112	0	0
13	c	36	0	45	0	0
14	b	2	0	0	0	0
15	d	1	0	0	0	0
All	All	12574	0	12594	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

There are no clashes within the asymmetric unit.

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	532/534 (100%)	499 (94%)	33 (6%)	0	100	100
2	b	234/236 (99%)	217 (93%)	17 (7%)	0	100	100
3	c	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
4	d	119/121 (98%)	95 (80%)	24 (20%)	0	100	100
5	e	131/133 (98%)	120 (92%)	11 (8%)	0	100	100
6	f	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
7	g	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
8	h	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
9	i	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
All	All	1538/1558 (99%)	1423 (92%)	115 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	447/447 (100%)	414 (93%)	33 (7%)	13	43
2	b	209/209 (100%)	200 (96%)	9 (4%)	29	56
3	c	228/228 (100%)	210 (92%)	18 (8%)	12	41
4	d	102/102 (100%)	93 (91%)	9 (9%)	10	37
5	e	110/110 (100%)	107 (97%)	3 (3%)	44	67
6	f	91/93 (98%)	83 (91%)	8 (9%)	10	37
7	g	50/50 (100%)	42 (84%)	8 (16%)	2	16
8	h	39/39 (100%)	37 (95%)	2 (5%)	24	53
9	i	46/46 (100%)	42 (91%)	4 (9%)	10	37
All	All	1322/1324 (100%)	1228 (93%)	94 (7%)	18	44

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	2	VAL
1	a	18	TYR
1	a	33	SER
1	a	37	ARG
1	a	101	ILE
1	a	105	VAL
1	a	125	THR
1	a	129	VAL
1	a	148	ILE
1	a	168	THR
1	a	174	THR
1	a	184	LEU
1	a	228	ASP
1	a	257	HIS
1	a	267	VAL
1	a	282	LEU
1	a	295	VAL
1	a	298	ASP
1	a	345	LEU
1	a	377	PHE
1	a	378	HIS
1	a	379	TYR
1	a	383	MET
1	a	388	SER
1	a	400	ILE
1	a	404	ASN
1	a	423	VAL
1	a	459	PHE
1	a	472	LEU
1	a	485	ASN
1	a	508	THR
1	a	519	THR
1	a	524	VAL
2	b	77	HIS
2	b	103	LEU
2	b	150	ASP
2	b	178	VAL
2	b	184	VAL
2	b	204	LEU
2	b	205	ASN
2	b	210	LEU
2	b	239	VAL

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Mol	Chain	Res	Type
3	c	33	LEU
3	c	47	ASN
3	c	62	SER
3	c	92	LEU
3	c	95	VAL
3	c	118	VAL
3	c	132	VAL
3	c	135	THR
3	c	137	LEU
3	c	140	LEU
3	c	186	TYR
3	c	195	THR
3	c	236	THR
3	c	243	TYR
3	c	245	THR
3	c	256	ILE
3	c	258	LEU
3	c	259	PHE
4	d	40	VAL
4	d	58	THR
4	d	75	LEU
4	d	80	VAL
4	d	99	ILE
4	d	100	ILE
4	d	104	ASP
4	d	114	SER
4	d	121	ILE
5	e	109	LEU
5	e	114	ARG
5	e	123	THR
6	f	60	PHE
6	f	81	LEU
6	f	98	VAL
6	f	115	VAL
6	f	124	TYR
6	f	126	ASP
6	f	135	LEU
6	f	137	VAL
7	g	23	HIS
7	g	29	TYR
7	g	30	LEU
7	g	31	TYR

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Mol	Chain	Res	Type
7	g	41	VAL
7	g	42	VAL
7	g	43	THR
7	g	47	TYR
8	h	34	VAL
8	h	47	THR
9	i	9	THR
9	i	20	LEU
9	i	22	PHE
9	i	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	81	ASN
1	a	99	ASN
1	a	164	ASN
1	a	234	HIS
1	a	399	GLN
1	a	475	GLN
1	a	478	ASN
1	a	482	ASN
1	a	485	ASN
2	b	40	HIS
2	b	157	GLN
3	c	239	HIS
5	e	129	GLN
6	f	70	GLN
8	h	53	HIS
9	i	42	ASN

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 9 ligands modelled in this entry, 3 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
14	CUA	b	301	2	0,1,1	-	-	-		
13	PEF	a	605	-	32,32,46	1.12	2 (6%)	35,37,51	1.26	4 (11%)
11	HEA	a	602	1	57,67,67	2.06	16 (28%)	61,103,103	2.54	25 (40%)
13	PEF	c	301	-	35,35,46	1.07	2 (5%)	38,40,51	1.14	3 (7%)
11	HEA	a	603	1	57,67,67	1.95	14 (24%)	61,103,103	2.48	24 (39%)
13	PEF	a	606	-	46,46,46	0.97	2 (4%)	49,51,51	1.09	3 (6%)

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	PEF	a	605	-	-	13/36/36/50	-
11	HEA	a	602	1	2/2/7/16	12/32/76/76	-
13	PEF	c	301	-	-	10/39/39/50	-
11	HEA	a	603	1	2/2/7/16	7/32/76/76	-
13	PEF	a	606	-	-	20/50/50/50	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	602	HEA	C3A-C2A	5.29	1.47	1.40
11	a	602	HEA	C3B-C2B	5.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	603	HEA	C3B-C2B	5.02	1.46	1.34
11	a	602	HEA	C3D-C2D	4.94	1.47	1.36
11	a	603	HEA	C3A-C2A	4.91	1.47	1.40
11	a	602	HEA	C3C-C2C	4.88	1.47	1.40
11	a	603	HEA	C3D-C2D	4.79	1.46	1.36
11	a	602	HEA	CHD-C1D	4.75	1.47	1.35
11	a	603	HEA	CHD-C1D	4.61	1.46	1.35
11	a	603	HEA	CHC-C4B	4.41	1.46	1.35
11	a	602	HEA	CHC-C4B	4.35	1.46	1.35
13	a	606	PEF	O3-C30	4.17	1.45	1.33
13	a	606	PEF	O2-C10	4.14	1.46	1.34
13	a	605	PEF	O3-C30	4.10	1.45	1.33
13	c	301	PEF	O3-C30	4.05	1.45	1.33
13	c	301	PEF	O2-C10	4.03	1.45	1.34
13	a	605	PEF	O2-C10	4.00	1.45	1.34
11	a	603	HEA	C3C-C2C	3.73	1.45	1.40
11	a	603	HEA	C1D-ND	-3.38	1.34	1.40
11	a	602	HEA	C1D-ND	-3.37	1.34	1.40
11	a	602	HEA	C4B-NB	-3.26	1.34	1.40
11	a	603	HEA	C4B-NB	-2.96	1.35	1.40
11	a	602	HEA	C2A-C1A	2.95	1.49	1.42
11	a	603	HEA	FE-NB	2.81	2.10	1.96
11	a	603	HEA	FE-ND	2.77	2.10	1.96
11	a	602	HEA	FE-NB	2.76	2.10	1.96
11	a	602	HEA	FE-ND	2.60	2.09	1.96
11	a	602	HEA	C4B-C3B	2.50	1.48	1.44
11	a	602	HEA	C1B-NB	-2.45	1.33	1.38
11	a	603	HEA	C2A-C1A	2.43	1.48	1.42
11	a	602	HEA	C4D-C3D	2.42	1.49	1.45
11	a	603	HEA	C4B-C3B	2.32	1.48	1.44
11	a	603	HEA	C1B-NB	-2.23	1.34	1.38
11	a	603	HEA	C4D-ND	-2.20	1.34	1.38
11	a	602	HEA	CHA-C4D	2.19	1.47	1.41
11	a	602	HEA	C4C-CHD	2.08	1.46	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	603	HEA	C3D-C4D-ND	7.21	117.34	110.36
11	a	602	HEA	C2B-C1B-NB	5.98	117.04	109.88
11	a	603	HEA	C2D-C1D-ND	5.52	116.38	109.84
11	a	603	HEA	C3B-C4B-NB	5.42	116.26	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	603	HEA	C2B-C1B-NB	5.41	116.36	109.88
11	a	602	HEA	C3B-C4B-NB	5.40	116.24	109.84
11	a	602	HEA	C3D-C4D-ND	5.16	115.35	110.36
11	a	602	HEA	C2D-C1D-ND	4.86	115.59	109.84
11	a	602	HEA	CMC-C2C-C3C	4.73	133.52	124.68
11	a	602	HEA	CHB-C1B-NB	-4.49	119.55	124.43
13	a	605	PEF	O2-C10-C11	4.41	121.00	111.50
11	a	602	HEA	C3C-C4C-NC	4.36	114.85	109.21
13	a	606	PEF	O2-C10-C11	4.24	120.64	111.50
11	a	603	HEA	C1D-C2D-C3D	-4.12	102.62	106.96
13	c	301	PEF	O2-C10-C11	4.03	120.19	111.50
11	a	602	HEA	C26-C15-C16	4.01	122.02	115.27
11	a	603	HEA	C13-C12-C11	-3.94	108.43	114.35
11	a	602	HEA	C1B-C2B-C3B	-3.85	102.20	106.80
11	a	603	HEA	C3C-C4C-NC	3.74	114.04	109.21
11	a	602	HEA	CHA-C4D-ND	-3.73	120.38	124.43
11	a	603	HEA	C4D-C3D-C2D	-3.66	101.56	106.90
11	a	602	HEA	CAD-C3D-C4D	3.64	131.01	124.66
11	a	602	HEA	C1D-C2D-C3D	-3.64	103.13	106.96
11	a	602	HEA	CAD-CBD-CGD	-3.40	106.29	113.60
11	a	602	HEA	C13-C12-C11	-3.40	109.25	114.35
11	a	603	HEA	CBA-CAA-C2A	-3.38	106.91	112.60
11	a	602	HEA	C4D-C3D-C2D	-3.33	102.05	106.90
11	a	603	HEA	C1B-C2B-C3B	-3.28	102.88	106.80
11	a	603	HEA	CHA-C4D-ND	-3.23	120.92	124.43
11	a	603	HEA	CMC-C2C-C3C	3.17	130.60	124.68
11	a	603	HEA	C4B-C3B-C2B	-3.14	102.05	107.41
11	a	603	HEA	CAD-CBD-CGD	-3.10	106.93	113.60
11	a	602	HEA	C4B-C3B-C2B	-3.04	102.21	107.41
13	a	606	PEF	C2-O2-C10	-2.96	110.51	117.79
11	a	603	HEA	C1D-ND-C4D	-2.89	102.09	105.07
11	a	603	HEA	CMB-C2B-C1B	2.85	129.38	125.04
13	a	605	PEF	C2-O2-C10	-2.74	111.04	117.79
11	a	603	HEA	CHB-C1B-NB	-2.72	121.47	124.43
11	a	602	HEA	C4B-NB-C1B	-2.67	102.31	105.07
13	a	606	PEF	O3-C30-C31	2.59	120.03	111.91
11	a	603	HEA	C13-C14-C15	-2.57	121.48	127.66
11	a	603	HEA	C4B-NB-C1B	-2.55	102.44	105.07
11	a	602	HEA	C27-C19-C20	2.52	119.51	115.27
11	a	602	HEA	CHC-C4B-NB	-2.46	121.34	124.38
11	a	603	HEA	C25-C23-C24	2.39	119.88	114.60
11	a	602	HEA	C4A-CHB-C1B	-2.36	119.45	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	602	HEA	CMB-C2B-C1B	2.34	128.61	125.04
11	a	603	HEA	CHD-C1D-C2D	-2.34	120.25	126.72
11	a	602	HEA	OMA-CMA-C3A	-2.32	119.85	124.91
13	c	301	PEF	C2-O2-C10	-2.32	112.09	117.79
11	a	602	HEA	C13-C14-C15	-2.31	122.09	127.66
11	a	603	HEA	C26-C15-C16	2.20	118.97	115.27
11	a	603	HEA	C17-C18-C19	-2.18	122.40	127.66
13	a	605	PEF	O2-C10-O4	-2.14	118.53	123.70
11	a	602	HEA	C17-C18-C19	-2.14	122.50	127.66
11	a	603	HEA	CHA-C4D-C3D	-2.11	121.74	124.84
13	a	605	PEF	C32-C31-C30	-2.09	106.01	113.62
13	c	301	PEF	O3-C30-C31	2.05	118.35	111.91
11	a	602	HEA	C21-C22-C23	-2.04	120.79	127.75

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	a	602	HEA	ND
11	a	602	HEA	NB
11	a	603	HEA	ND
11	a	603	HEA	NB

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	a	602	HEA	C2A-CAA-CBA-CGA
11	a	602	HEA	C11-C12-C13-C14
11	a	602	HEA	C14-C15-C16-C17
11	a	602	HEA	C26-C15-C16-C17
13	a	605	PEF	C1-O3P-P-O1P
13	a	605	PEF	C1-O3P-P-O2P
13	a	605	PEF	C1-O3P-P-O4P
13	a	606	PEF	C11-C10-O2-C2
13	a	606	PEF	C1-O3P-P-O1P
13	a	606	PEF	C1-O3P-P-O2P
13	a	606	PEF	C1-O3P-P-O4P
13	c	301	PEF	C1-O3P-P-O2P
13	a	606	PEF	O4-C10-O2-C2
13	c	301	PEF	C1-O3P-P-O4P
13	a	606	PEF	C38-C39-C40-C41
13	a	606	PEF	C20-C21-C22-C23
13	c	301	PEF	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
13	a	606	PEF	C39-C40-C41-C42
13	c	301	PEF	C30-C31-C32-C33
13	a	606	PEF	C10-C11-C12-C13
13	a	606	PEF	C37-C38-C39-C40
11	a	603	HEA	C2A-CAA-CBA-CGA
13	a	606	PEF	C33-C34-C35-C36
13	a	605	PEF	C11-C10-O2-C2
13	a	605	PEF	O4-C10-O2-C2
13	a	606	PEF	C15-C16-C17-C18
11	a	602	HEA	C3D-CAD-CBD-CGD
13	c	301	PEF	C1-C2-C3-O3
13	a	606	PEF	O4P-C4-C5-N
13	a	605	PEF	C1-C2-C3-O3
13	a	606	PEF	C4-O4P-P-O3P
13	a	605	PEF	O2-C2-C3-O3
13	c	301	PEF	C11-C12-C13-C14
13	c	301	PEF	C4-O4P-P-O3P
13	a	605	PEF	O3P-C1-C2-C3
13	c	301	PEF	O3P-C1-C2-C3
13	a	606	PEF	C21-C22-C23-C24
13	a	605	PEF	O3P-C1-C2-O2
13	c	301	PEF	O3P-C1-C2-O2
13	c	301	PEF	O2-C2-C3-O3
11	a	602	HEA	C15-C16-C17-C18
13	a	605	PEF	C4-O4P-P-O3P
13	a	606	PEF	C31-C32-C33-C34
11	a	602	HEA	C2D-C3D-CAD-CBD
11	a	602	HEA	CAA-CBA-CGA-O2A
11	a	602	HEA	CAA-CBA-CGA-O1A
11	a	603	HEA	CAD-CBD-CGD-O1D
13	a	606	PEF	C40-C41-C42-C43
11	a	603	HEA	C26-C15-C16-C17
11	a	603	HEA	CAD-CBD-CGD-O2D
11	a	603	HEA	C2D-C3D-CAD-CBD
11	a	603	HEA	C14-C15-C16-C17
11	a	603	HEA	C4D-C3D-CAD-CBD
13	a	605	PEF	O2-C10-C11-C12
11	a	602	HEA	C4D-C3D-CAD-CBD
13	a	606	PEF	O3-C30-C31-C32
11	a	602	HEA	C19-C20-C21-C22
13	a	606	PEF	C4-O4P-P-O1P
13	a	605	PEF	O4-C10-C11-C12

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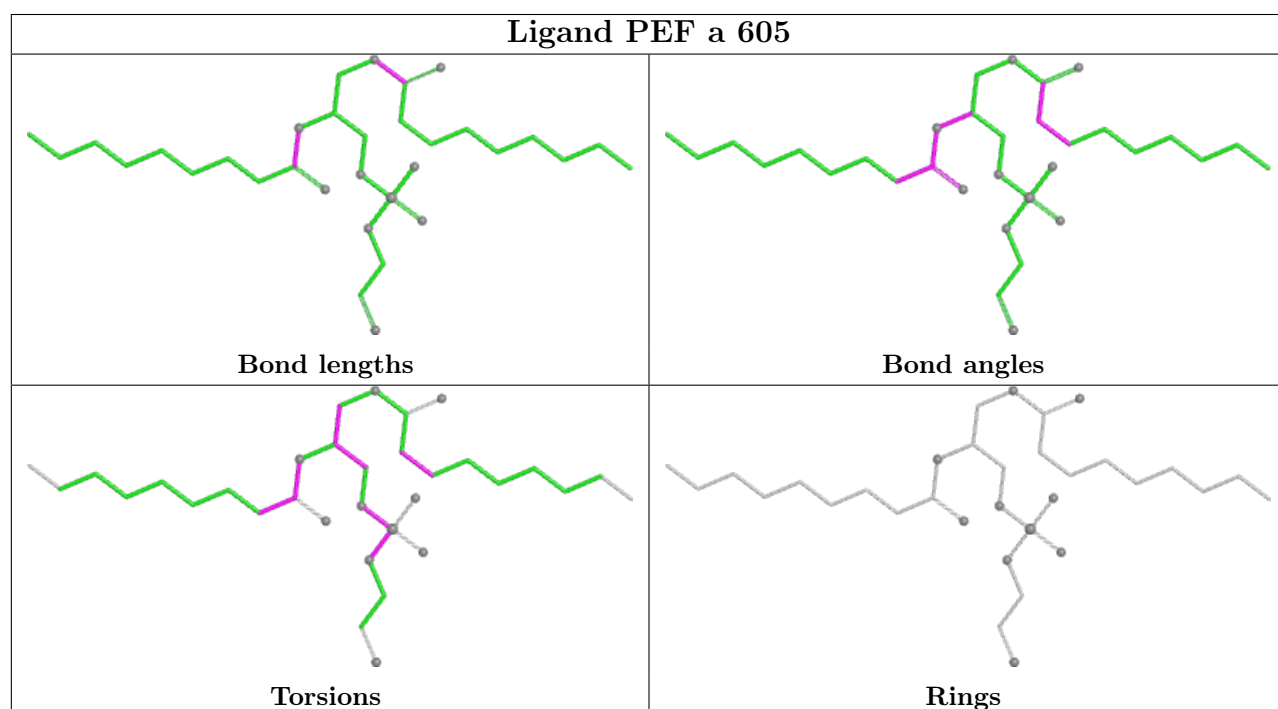
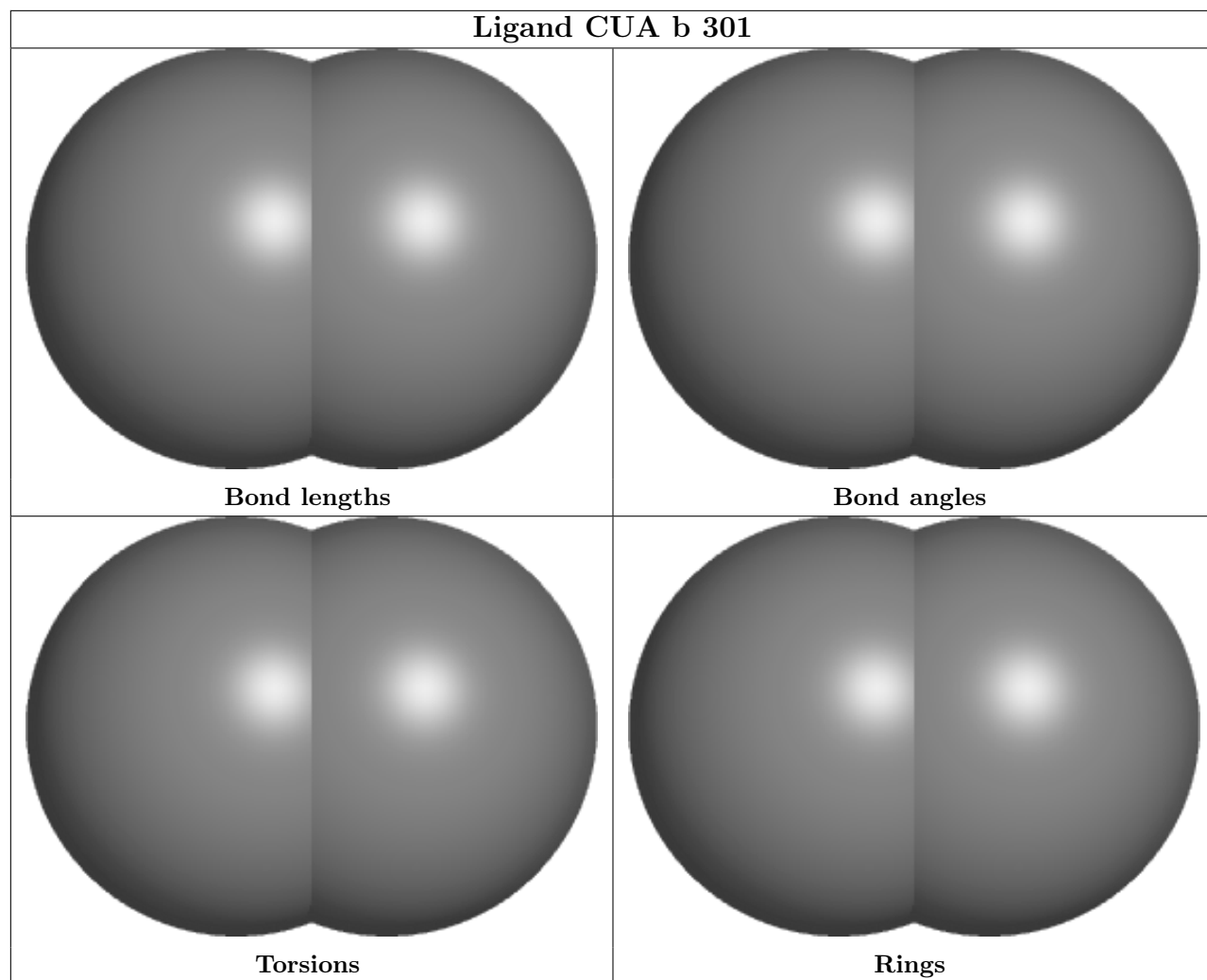
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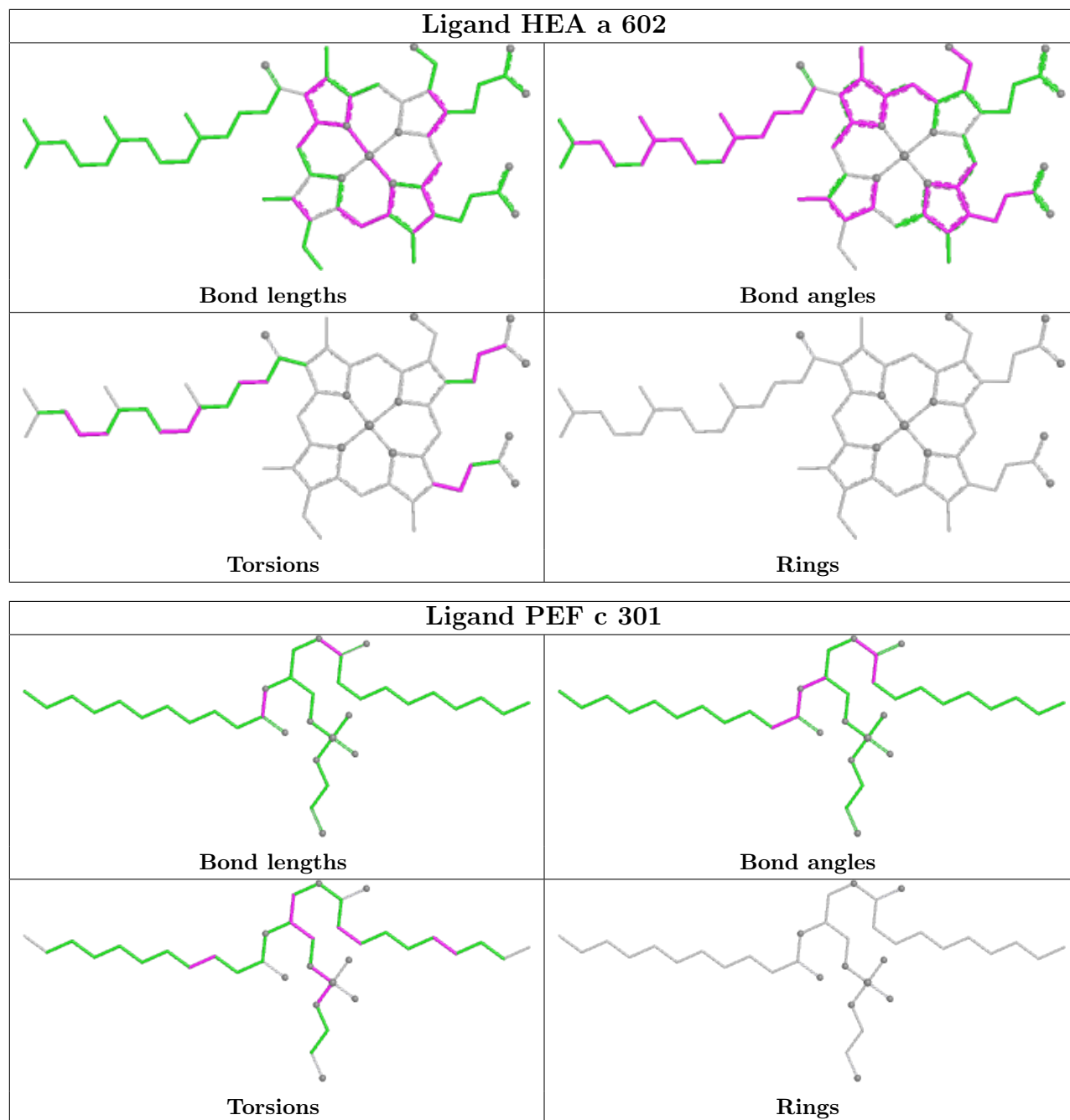
Mol	Chain	Res	Type	Atoms
13	a	606	PEF	O5-C30-C31-C32
13	a	605	PEF	C30-C31-C32-C33
11	a	602	HEA	C20-C21-C22-C23

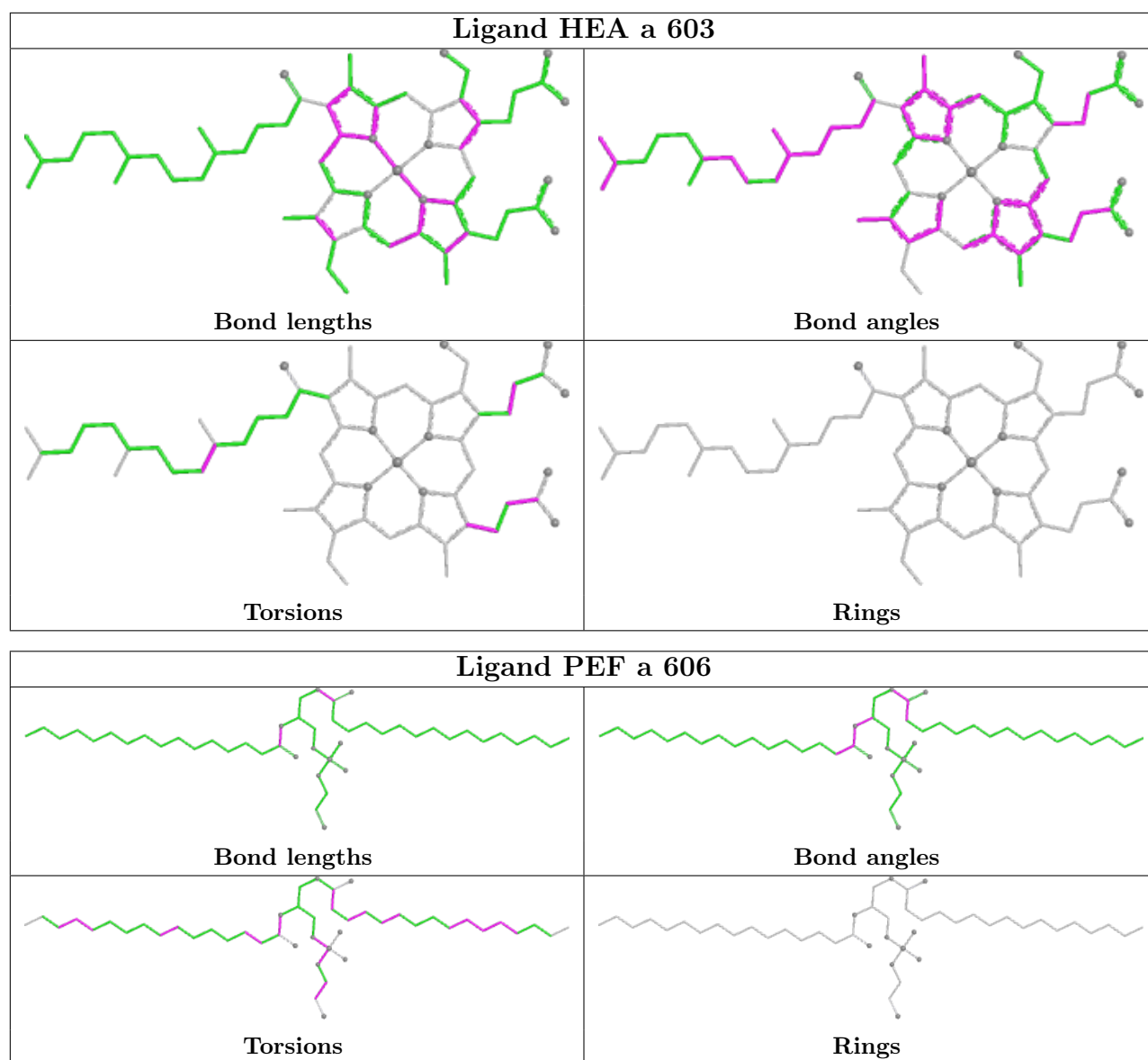
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

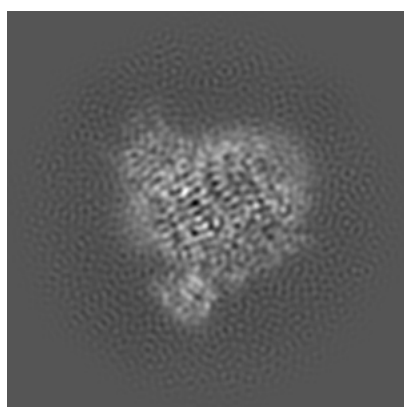
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14436. These allow visual inspection of the internal detail of the map and identification of artifacts.

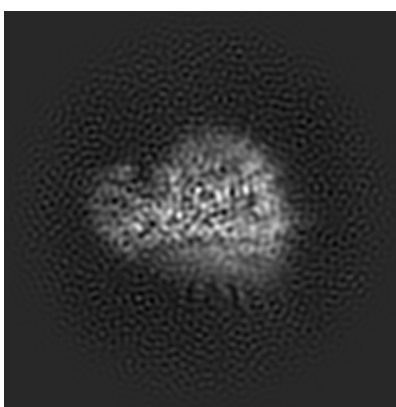
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

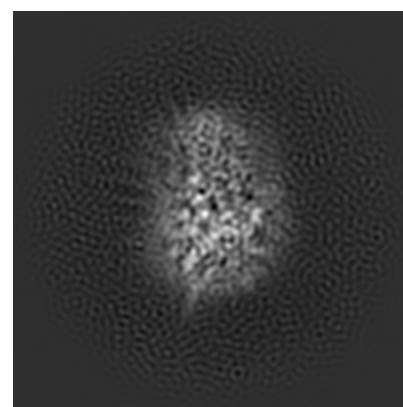
6.1.1 Primary map



X



Y

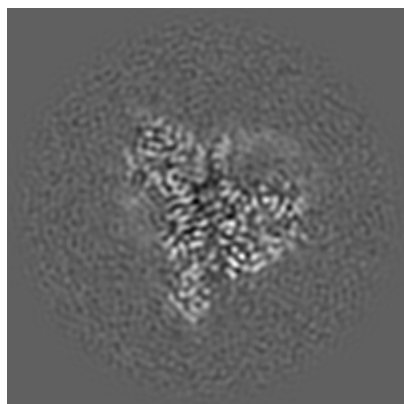


Z

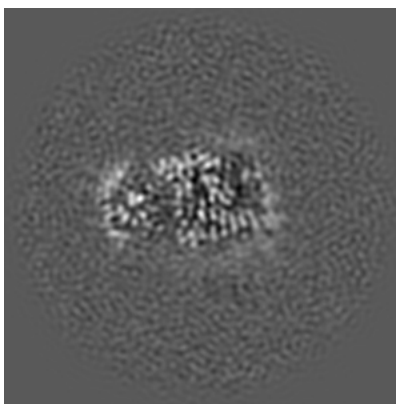
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

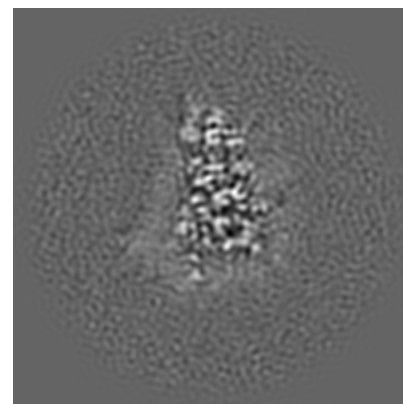
6.2.1 Primary map



X Index: 128



Y Index: 128

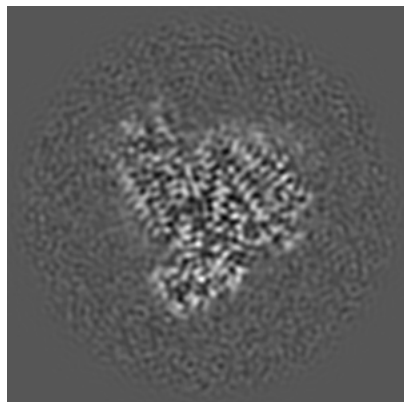


Z Index: 128

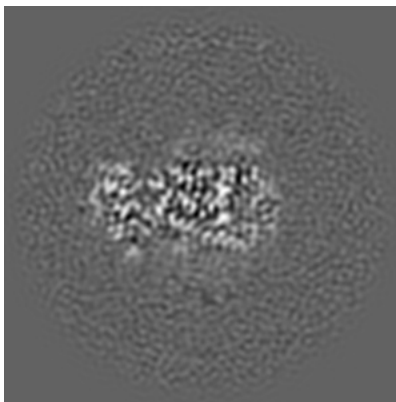
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

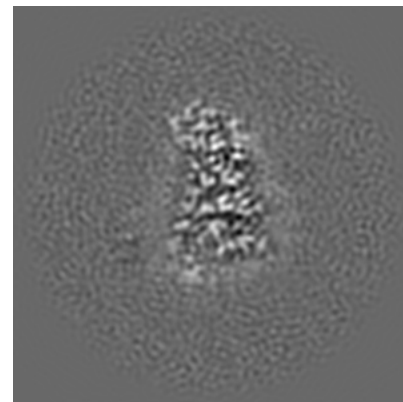
6.3.1 Primary map



X Index: 117



Y Index: 113



Z Index: 133

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 3.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

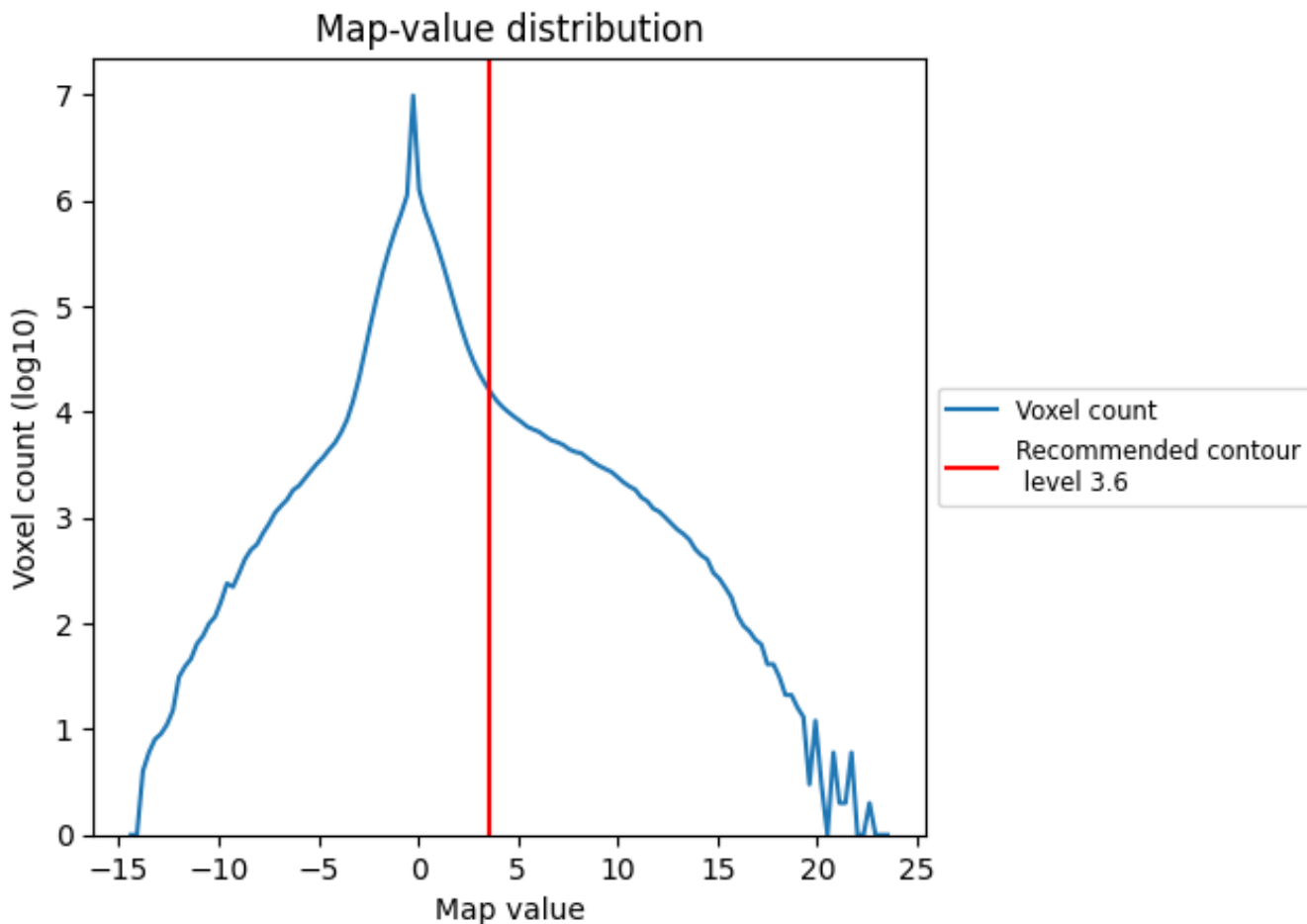
6.5 Mask visualisation

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

7 Map analysis [i](#)

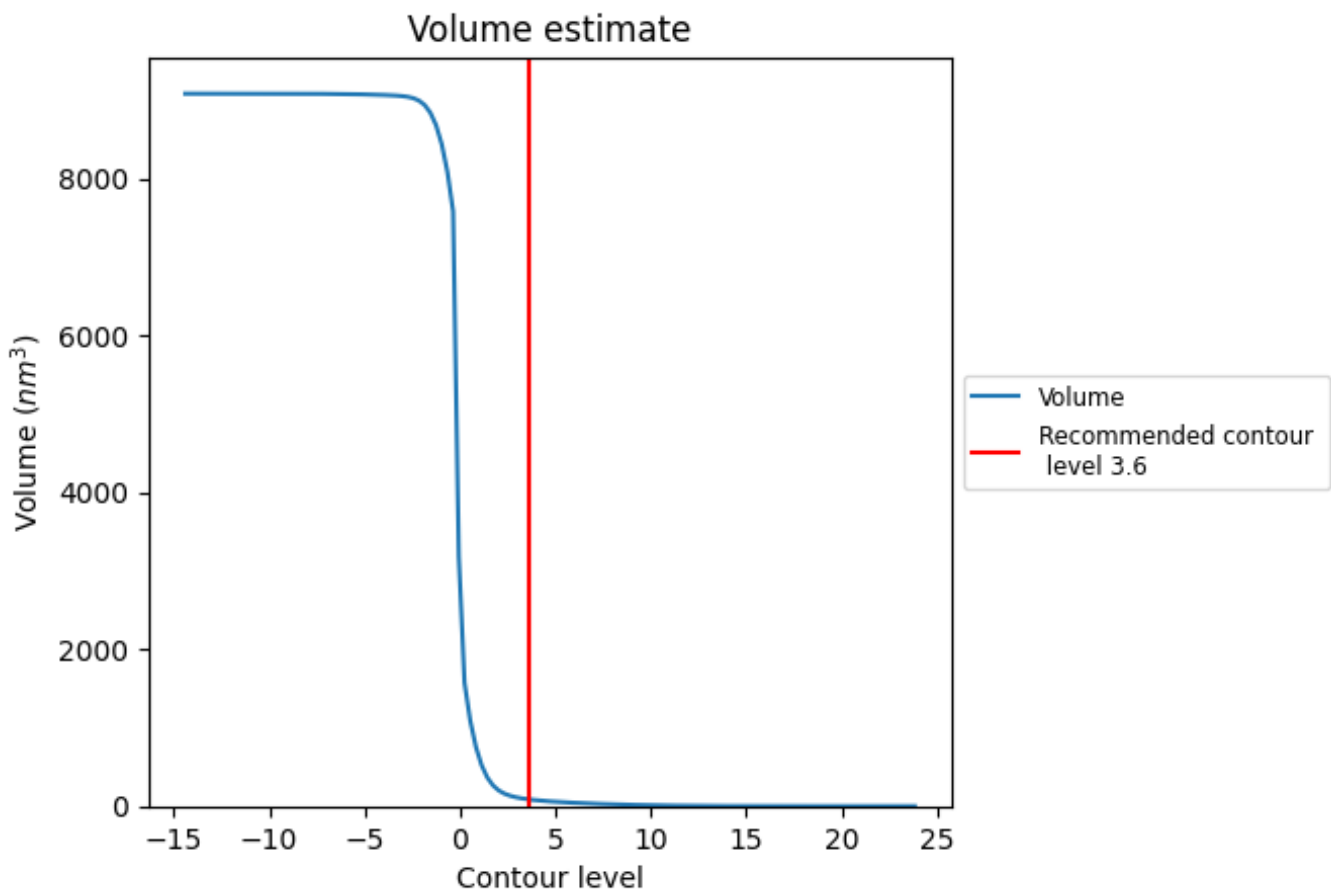
This section contains the results of statistical analysis of the map.

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.

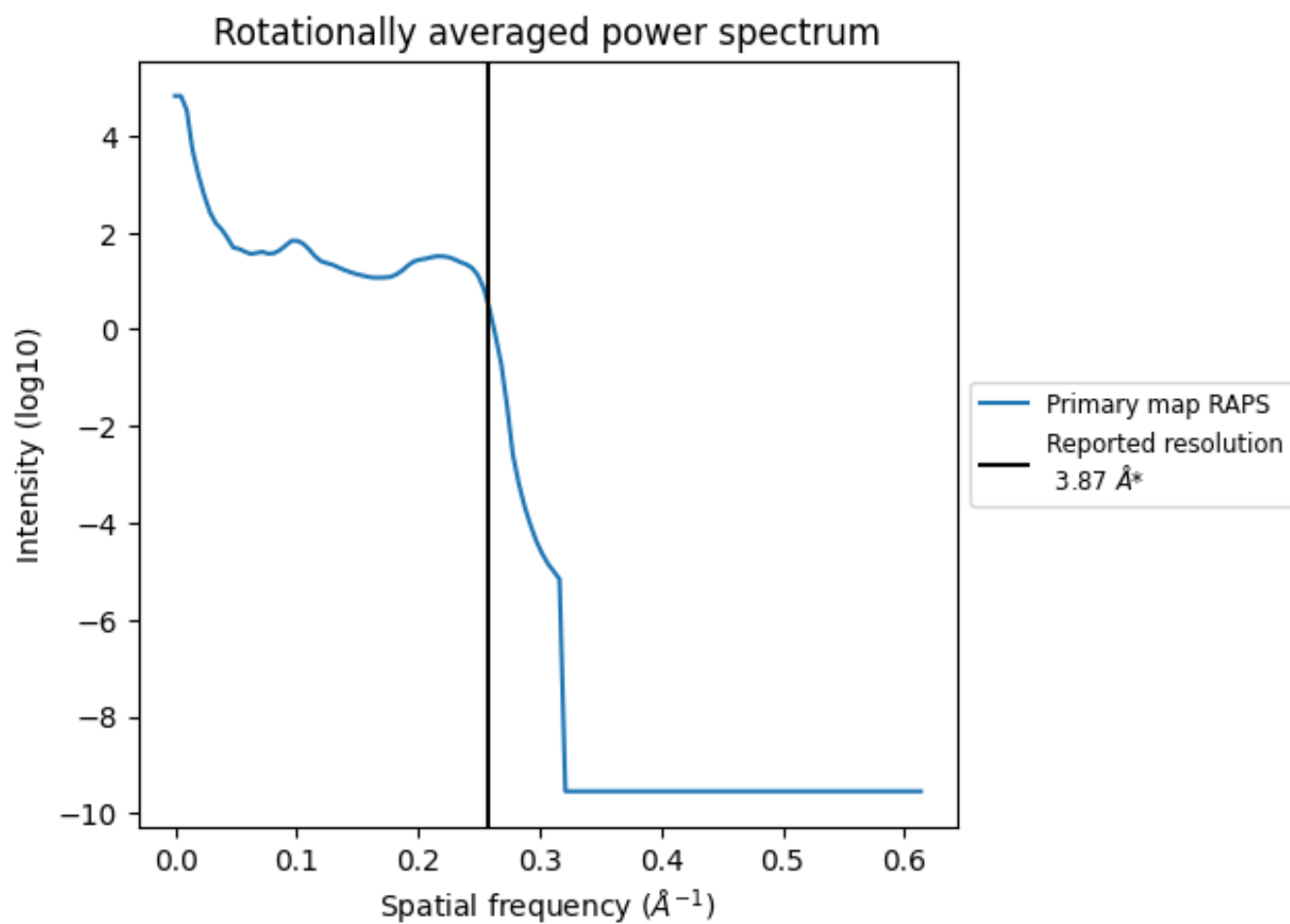
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 86 nm^3 ; this corresponds to an approximate mass of 78 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 [\(i\)](#)

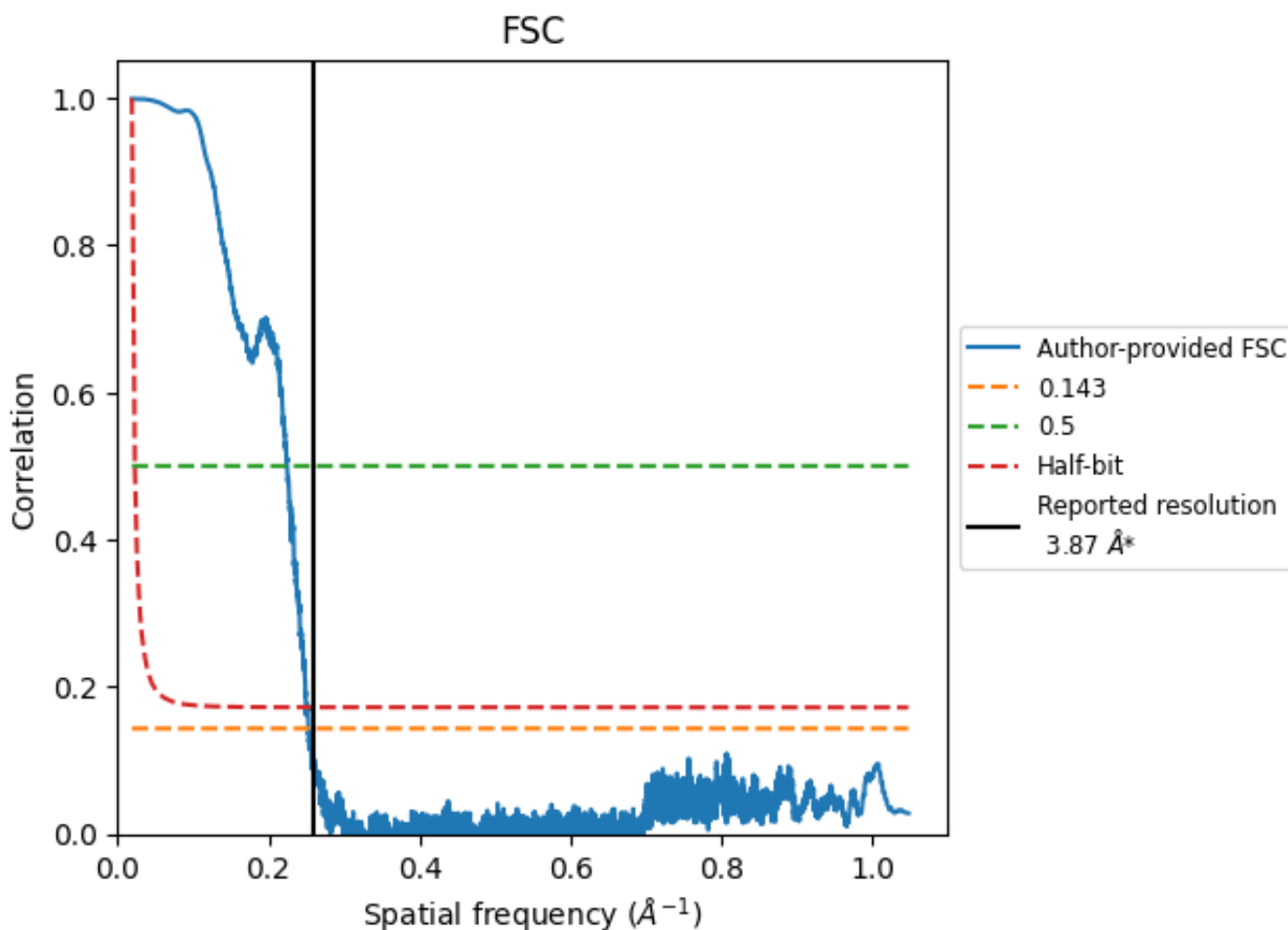


*Reported resolution corresponds to spatial frequency of 0.258 Å⁻¹

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 0.258 Å⁻¹

8.2 Resolution estimates [i](#)

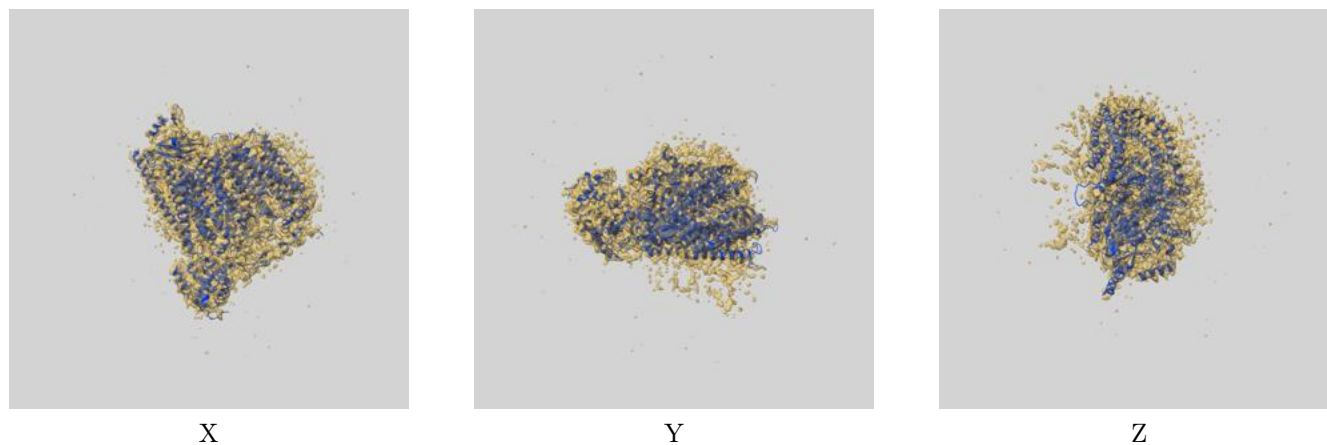
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.87	-	-
Author-provided FSC curve	3.95	4.45	4.00
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

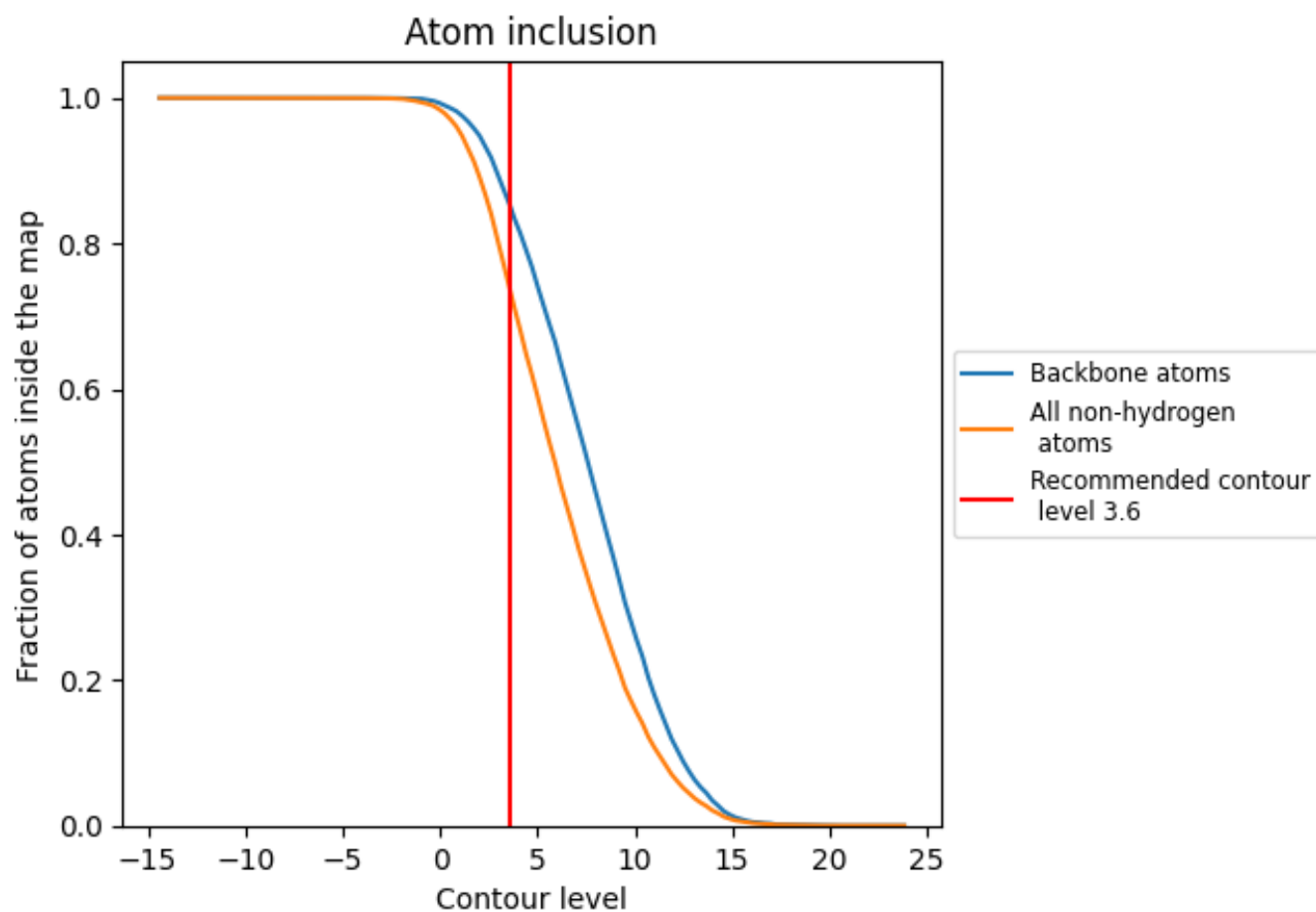
This section contains information regarding the fit between EMDB map EMD-14436 and PDB model 7Z10. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.6 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 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.