



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 04:35 AM UTC

PDB ID : 6YMY / pdb_00006ymy
EMDB ID : EMD-10848
Title : Cytochrome c oxidase from *Saccharomyces cerevisiae*
Authors : Berndtsson, J.; Rathore, S.; Ott, M.
Deposited on : 2020-04-10
Resolution : 3.41 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:

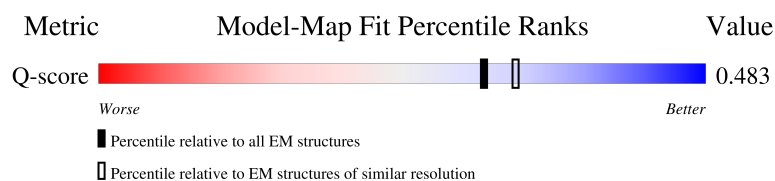
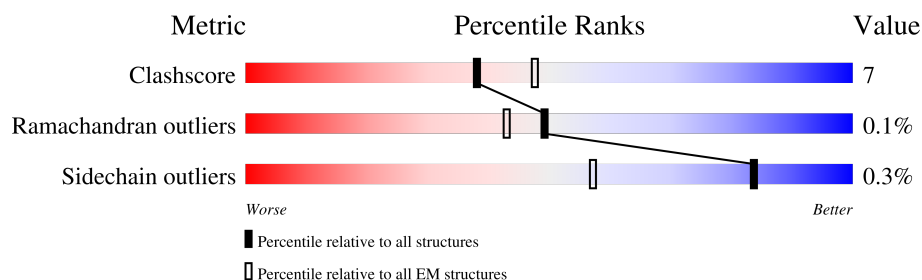
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.41 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	13997 (2.91 - 3.91)

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	530	
2	b	236	
3	c	268	
4	d	117	

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Mol	Chain	Length	Quality of chain
5	e	128	 87% 13%
6	f	99	 87% 13%
7	g	55	 91% 9%
8	h	51	 86% 14%
9	i	52	 83% 17%
10	j	78	 10% 87% 13%
11	k	114	 25% 87% 13%
12	m	38	 97%

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
15	PTY	e	201	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 14612 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	530	Total	C	N	O	S	0	0
			4126	2757	641	707	21		

- 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
			1888	1242	286	350	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	268	Total	C	N	O	S	0	0
			2138	1425	343	356	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	117	Total	C	N	O	S	0	0
			888	559	147	177	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	128	Total	C	N	O	S	0	0
			1008	639	175	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	99	Total	C	N	O	S	0	0
			828	533	134	160	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	g	55	Total	C	N	O	0	0
			456	310	77	69		

- 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	52	Total	C	N	O	S	0	0
			426	282	71	70	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	78	Total	C	N	O	S	0	0
			649	414	111	119	5		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			941	608	163	167	3		

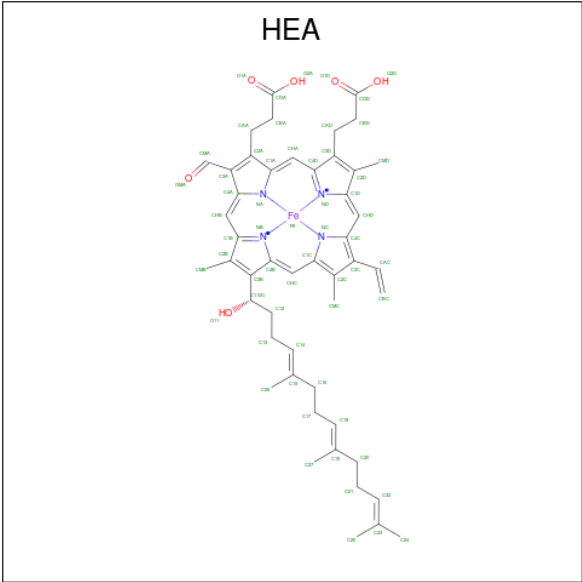
- Molecule 12 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	m	38	Total	C	N	O	S	0	0
			308	207	49	51	1		

- Molecule 13 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

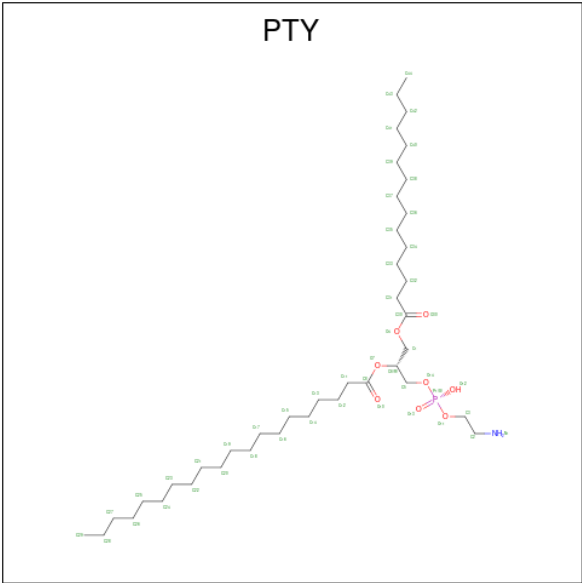
Mol	Chain	Residues	Atoms		AltConf
13	a	1	Total	Cu	0
			1	1	

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



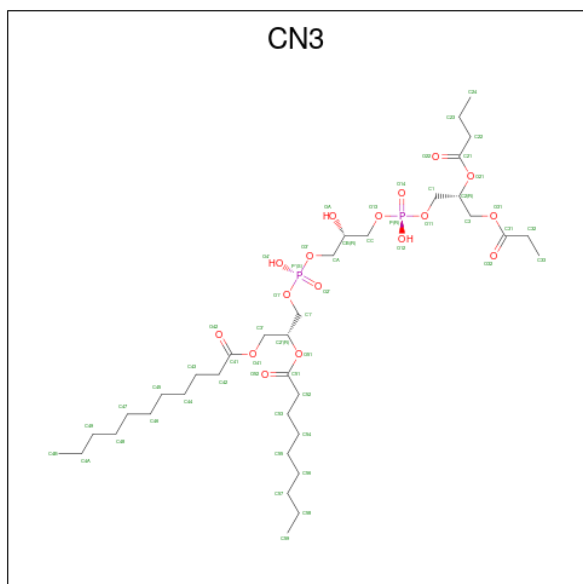
Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total	C	N	O	P	0
			35	25	1	8	1	
15	a	1	Total	C	N	O	P	0
			34	24	1	8	1	

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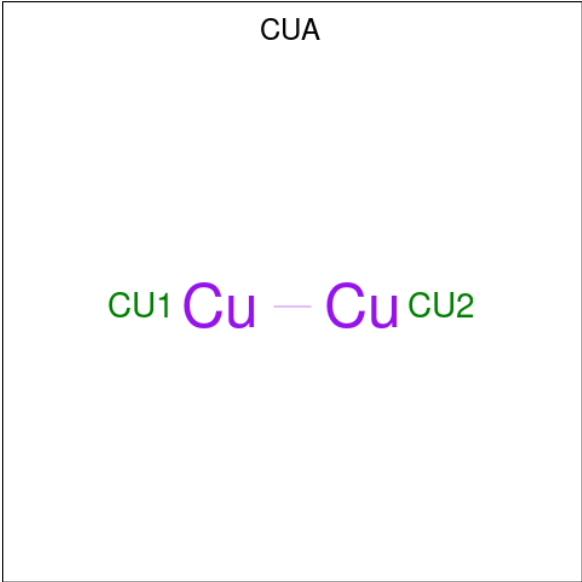
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	b	1	Total	C	N	O	P	0
			41	31	1	8	1	
15	c	1	Total	C	N	O	P	0
			40	30	1	8	1	
15	e	1	Total	C	N	O	P	0
			32	22	1	8	1	
15	i	1	Total	C	N	O	P	0
			30	20	1	8	1	

- Molecule 16 is (2R,5S,11R,14R)-5,8,11-trihydroxy-2-(nonanoyloxy)-5,11-dioxido-16-oxo-14-[(propanoyloxy)methyl]-4,6,10,12,15-pentaoxa-5,11-diphosphanadec-1-yl undecanoate (CCD ID: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



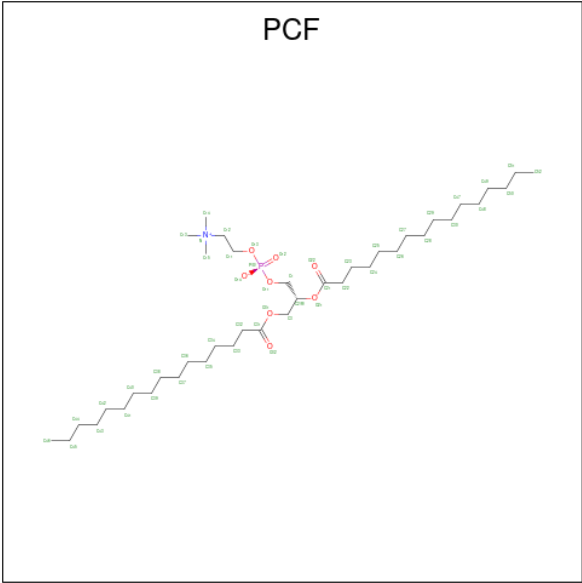
Mol	Chain	Residues	Atoms				AltConf
16	a	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 17 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



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

- Molecule 18 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C₄₀H₈₀NO₈P).



Mol	Chain	Residues	Atoms					AltConf
18	c	1	Total	C	N	O	P	0
			43	33	1	8	1	
18	e	1	Total	C	N	O	P	0
			36	26	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
18	m	1	Total	C	N	O	P	0
			38	28	1	8	1	

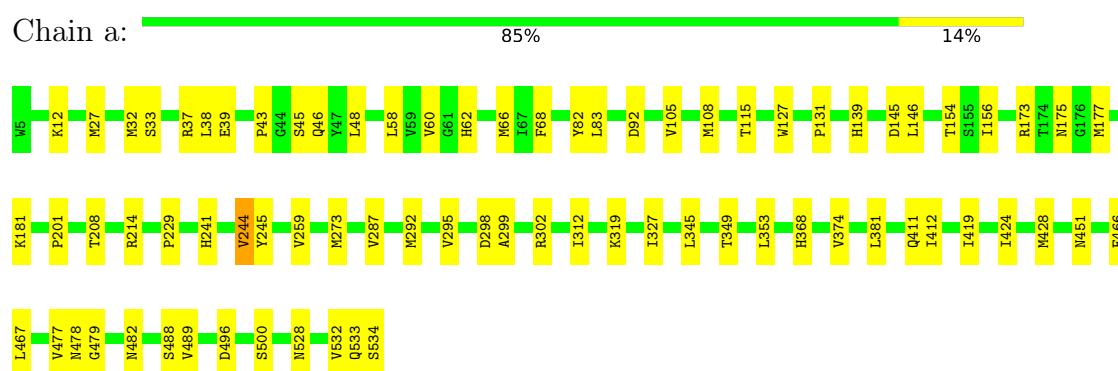
- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

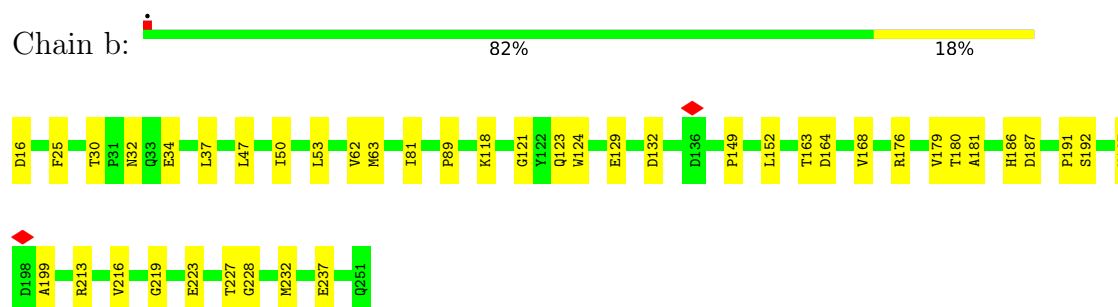
3 Residue-property plots

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.

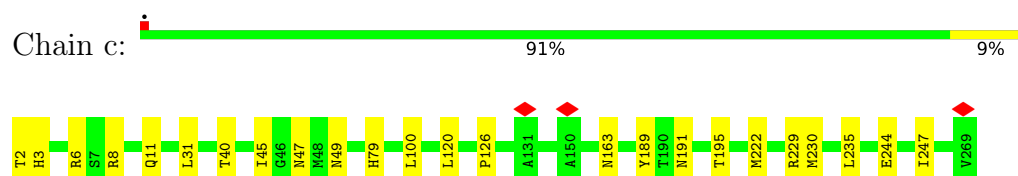
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3

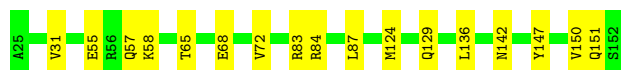


• Molecule 4: Cytochrome c oxidase subunit 4, mitochondrial

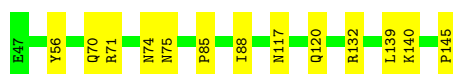
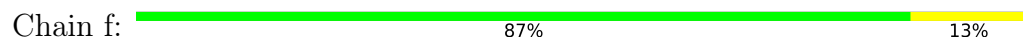




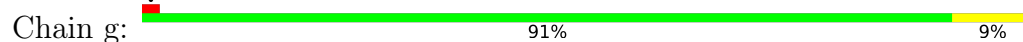
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



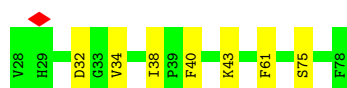
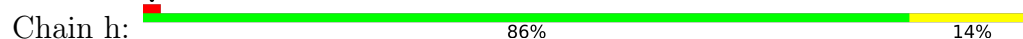
- Molecule 6: Cytochrome c oxidase subunit 6, mitochondrial



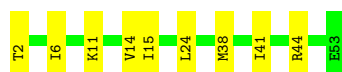
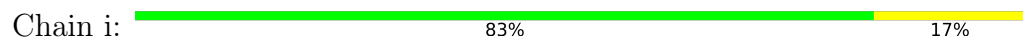
- Molecule 7: Cytochrome c oxidase subunit 7, mitochondrial



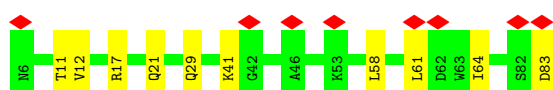
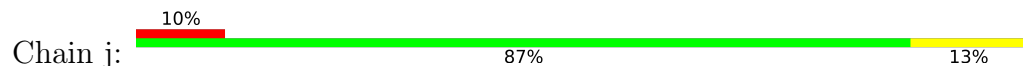
- Molecule 8: Cytochrome c oxidase subunit 8, mitochondrial



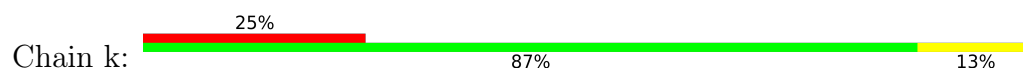
- Molecule 9: Cytochrome c oxidase subunit 9, mitochondrial

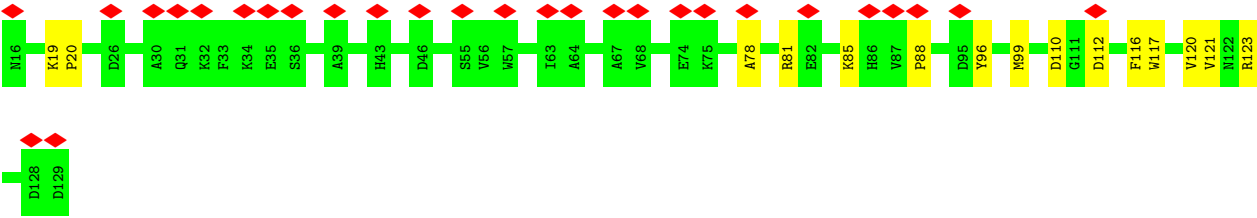


- Molecule 10: Cytochrome c oxidase subunit 12, mitochondrial



- Molecule 11: Cytochrome c oxidase subunit 13, mitochondrial





- Molecule 12: Cytochrome c oxidase subunit 26, mitochondrial

Chain m:

97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201223	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1.4	Depositor
Maximum defocus (nm)	-3.0	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.411	Depositor
Minimum map value	-1.211	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.41	Depositor
Map size (Å)	392.2, 392.2, 392.2	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0600001, 1.0600001, 1.0600001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CN3, HEA, CU, PCF, CUA, PTY

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	0.31	0/4254	0.55	0/5811
2	b	0.28	0/1940	0.51	0/2653
3	c	0.23	0/2210	0.45	0/3026
4	d	0.31	0/905	0.67	0/1231
5	e	0.30	0/1032	0.63	1/1396 (0.1%)
6	f	0.29	0/845	0.53	0/1143
7	g	0.25	0/472	0.53	0/645
8	h	0.23	0/423	0.46	0/569
9	i	0.25	0/438	0.48	0/590
10	j	0.21	0/671	0.51	0/910
11	k	0.22	0/974	0.56	0/1324
12	m	0.25	0/319	0.58	0/435
All	All	0.28	0/14483	0.54	1/19733 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	150	VAL	N-CA-C	5.75	115.63	106.88

There are no chirality outliers.

There are no planarity outliers.

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	4126	0	4150	73	0
2	b	1888	0	1868	33	0
3	c	2138	0	2125	18	0
4	d	888	0	885	27	0
5	e	1008	0	988	13	0
6	f	828	0	807	8	0
7	g	456	0	481	3	0
8	h	408	0	408	5	0
9	i	426	0	430	8	0
10	j	649	0	592	8	0
11	k	941	0	902	10	0
12	m	308	0	302	1	0
13	a	1	0	0	0	0
14	a	120	0	108	9	0
15	a	69	0	80	2	0
15	b	81	0	108	6	0
15	c	40	0	53	2	0
15	e	32	0	37	37	0
15	i	30	0	33	0	0
16	a	55	0	66	1	0
17	b	2	0	0	0	0
18	c	43	0	60	2	0
18	e	36	0	46	9	0
18	m	38	0	50	1	0
19	d	1	0	0	0	0
All	All	14612	0	14579	217	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.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:241:HIS:NE2	1:a:245:TYR:CE2	1.80	1.49
1:a:532:VAL:CG2	4:d:107:ARG:HH22	1.48	1.26
1:a:241:HIS:CD2	1:a:245:TYR:HE2	1.58	1.21
1:a:241:HIS:CD2	1:a:245:TYR:CE2	2.33	1.15
15:e:201:PTY:HC6	15:e:201:PTY:H131	1.21	1.14
1:a:241:HIS:NE2	1:a:245:TYR:HE2	1.18	1.14
1:a:532:VAL:HG23	4:d:107:ARG:NH2	1.69	1.08
15:e:201:PTY:O30	18:e:202:PCF:H242	1.55	1.06
15:e:201:PTY:H312	15:e:201:PTY:H122	1.10	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:532:VAL:CG2	4:d:107:ARG:NH2	2.19	1.04
1:a:532:VAL:HG21	4:d:107:ARG:HH22	1.18	1.03
15:e:201:PTY:H122	15:e:201:PTY:C31	1.91	1.00
15:e:201:PTY:H312	15:e:201:PTY:C12	1.97	0.95
2:b:16:ASP:N	2:b:192:SER:HG	1.63	0.94
15:e:201:PTY:H161	15:e:201:PTY:H121	1.46	0.93
15:e:201:PTY:O30	18:e:202:PCF:C24	2.23	0.87
15:e:201:PTY:C12	15:e:201:PTY:H182	2.04	0.87
15:e:201:PTY:H322	18:e:202:PCF:H262	1.60	0.82
15:e:201:PTY:H121	15:e:201:PTY:C16	2.09	0.81
15:e:201:PTY:H131	15:e:201:PTY:C6	2.08	0.78
1:a:181:LYS:HD2	1:a:533:GLN:NE2	2.00	0.76
15:e:201:PTY:H172	15:e:201:PTY:C21	2.14	0.76
15:e:201:PTY:H182	15:e:201:PTY:H111	1.67	0.76
15:e:201:PTY:O30	18:e:202:PCF:C23	2.34	0.75
15:e:201:PTY:H182	15:e:201:PTY:C11	2.17	0.74
1:a:532:VAL:HG21	4:d:107:ARG:NH2	1.96	0.67
1:a:534:SER:HB2	4:d:112:THR:HG22	1.77	0.67
1:a:241:HIS:NE2	1:a:245:TYR:CZ	2.46	0.66
15:e:201:PTY:H182	15:e:201:PTY:C13	2.26	0.65
2:b:121:GLY:HA3	2:b:186:HIS:CE1	2.31	0.65
15:e:201:PTY:H121	15:e:201:PTY:H182	1.81	0.63
15:e:201:PTY:C12	15:e:201:PTY:H161	2.22	0.63
2:b:186:HIS:CE1	2:b:232:MET:HE1	2.35	0.62
5:e:57:GLN:HE22	5:e:72:VAL:HG21	1.65	0.62
11:k:112:ASP:OD1	11:k:117:TRP:NE1	2.32	0.62
11:k:120:VAL:HG13	11:k:121:VAL:HG13	1.82	0.62
5:e:136:LEU:HD23	5:e:147:TYR:HB2	1.81	0.61
15:e:201:PTY:C18	15:e:201:PTY:H132	2.29	0.61
15:e:201:PTY:H182	15:e:201:PTY:H132	1.82	0.61
2:b:37:LEU:HD23	9:i:44:ARG:HH22	1.66	0.60
15:e:201:PTY:H112	18:e:202:PCF:H341	1.81	0.60
2:b:16:ASP:OD2	2:b:213:ARG:NH2	2.34	0.60
4:d:94:MET:SD	4:d:133:ARG:NH1	2.75	0.59
1:a:139:HIS:O	1:a:214:ARG:NH2	2.36	0.59
1:a:298:ASP:OD1	1:a:298:ASP:N	2.36	0.59
11:k:110:ASP:N	11:k:110:ASP:OD1	2.36	0.58
1:a:32:MET:HG2	1:a:58:LEU:HD22	1.86	0.58
15:e:201:PTY:O30	18:e:202:PCF:H232	2.02	0.58
1:a:68:PHE:HB3	1:a:154:THR:HG21	1.86	0.58
1:a:241:HIS:CD2	1:a:245:TYR:CD2	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:534:SER:N	4:d:110:GLY:O	2.36	0.57
1:a:108:MET:HB3	3:c:31:LEU:HB2	1.87	0.57
8:h:38:ILE:HG22	8:h:40:PHE:H	1.69	0.57
1:a:534:SER:CB	4:d:112:THR:HG22	2.34	0.56
2:b:168:VAL:HG12	2:b:237:GLU:HG3	1.87	0.56
9:i:38:MET:HA	9:i:41:ILE:HG22	1.86	0.56
1:a:478:ASN:O	1:a:482:ASN:ND2	2.38	0.56
4:d:102:SER:OG	4:d:103:TYR:N	2.38	0.56
15:e:201:PTY:HC31	15:e:201:PTY:C5	2.36	0.55
15:b:302:PTY:H131	9:i:14:VAL:HG11	1.88	0.55
15:e:201:PTY:C5	15:e:201:PTY:C3	2.85	0.55
15:e:201:PTY:H112	18:e:202:PCF:C34	2.37	0.55
2:b:124:TRP:HE1	2:b:228:GLY:H	1.55	0.55
5:e:124:MET:O	5:e:129:GLN:NE2	2.40	0.54
14:a:603:HEA:H22	2:b:50:ILE:HG21	1.89	0.54
2:b:34:GLU:OE2	9:i:44:ARG:NH1	2.40	0.54
15:e:201:PTY:C21	15:e:201:PTY:C17	2.85	0.54
15:e:201:PTY:C13	15:e:201:PTY:C18	2.85	0.54
1:a:479:GLY:HA2	1:a:482:ASN:HD22	1.73	0.54
2:b:176:ARG:NH2	10:j:12:VAL:O	2.41	0.54
5:e:142:ASN:HB2	5:e:147:TYR:HB3	1.90	0.54
15:e:201:PTY:H121	15:e:201:PTY:C17	2.37	0.54
2:b:186:HIS:HA	2:b:223:GLU:HB3	1.90	0.54
3:c:6:ARG:HH22	3:c:11:GLN:HA	1.72	0.53
10:j:61:LEU:HA	10:j:64:ILE:HD12	1.90	0.53
14:a:603:HEA:H242	2:b:89:PRO:HB3	1.89	0.53
4:d:60:LEU:O	4:d:68:ARG:NH1	2.41	0.53
2:b:25:PHE:HD2	2:b:37:LEU:HD13	1.74	0.53
3:c:6:ARG:O	3:c:6:ARG:NH1	2.39	0.52
15:e:201:PTY:H122	15:e:201:PTY:C30	2.37	0.52
1:a:259:VAL:HG13	1:a:327:ILE:HG23	1.91	0.52
2:b:179:VAL:HG12	2:b:199:ALA:HB2	1.91	0.52
11:k:88:PRO:O	11:k:123:ARG:NH1	2.40	0.52
2:b:121:GLY:HA3	2:b:186:HIS:HE1	1.71	0.52
1:a:528:ASN:ND2	4:d:106:TYR:OH	2.43	0.52
1:a:37:ARG:HH12	1:a:451:ASN:HD22	1.58	0.52
1:a:244:VAL:HG13	14:a:603:HEA:HBC1	1.91	0.52
2:b:30:THR:HG22	2:b:32:ASN:H	1.76	0.51
14:a:603:HEA:H253	2:b:50:ILE:HG13	1.91	0.51
15:e:201:PTY:C12	15:e:201:PTY:C18	2.85	0.51
1:a:181:LYS:HD2	1:a:533:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:63:GLU:HB2	4:d:68:ARG:HD3	1.93	0.51
1:a:488:SER:OG	1:a:489:VAL:N	2.44	0.51
2:b:180:THR:OG1	2:b:181:ALA:N	2.44	0.51
1:a:287:VAL:HG21	1:a:312:ILE:HD11	1.93	0.50
1:a:477:VAL:HG12	1:a:478:ASN:HD22	1.76	0.50
3:c:191:ASN:OD1	11:k:81:ARG:NH1	2.44	0.50
1:a:181:LYS:HD2	1:a:533:GLN:HE21	1.76	0.50
15:a:605:PTY:HN12	3:c:79:HIS:HE1	1.58	0.50
7:g:50:ASN:ND2	7:g:55:ILE:O	2.44	0.50
1:a:115:THR:HG23	1:a:146:LEU:HD13	1.94	0.50
1:a:299:ALA:HA	1:a:302:ARG:HD2	1.93	0.50
3:c:229:ARG:NH2	15:c:301:PTY:O12	2.40	0.50
1:a:534:SER:C	4:d:86:LEU:HG	2.36	0.50
2:b:187:ASP:HB2	2:b:223:GLU:HB2	1.93	0.50
1:a:466:PHE:HB3	16:a:606:CN3:H48	1.94	0.49
15:e:201:PTY:H121	15:e:201:PTY:C18	2.41	0.49
1:a:412:ILE:HG13	1:a:467:LEU:HD21	1.94	0.49
1:a:60:VAL:HG23	1:a:127:TRP:HA	1.95	0.49
8:h:32:ASP:OD2	8:h:32:ASP:N	2.44	0.49
1:a:43:PRO:O	1:a:46:GLN:NE2	2.46	0.49
1:a:201:PRO:HG2	3:c:100:LEU:HD23	1.95	0.49
4:d:115:PRO:HD2	4:d:118:SER:HB2	1.93	0.49
1:a:66:MET:HB3	14:a:602:HEA:HBC1	1.95	0.48
2:b:118:LYS:HE2	2:b:129:GLU:HG3	1.94	0.48
15:e:201:PTY:HC6	15:e:201:PTY:C13	2.15	0.48
4:d:134:CYS:HB3	4:d:138:GLY:H	1.78	0.48
1:a:488:SER:O	5:e:84:ARG:NH2	2.46	0.48
1:a:533:GLN:HG3	4:d:121:ILE:HD11	1.96	0.48
3:c:230:MET:HG3	3:c:235:LEU:HD12	1.95	0.47
1:a:82:TYR:HB3	1:a:83:LEU:HD12	1.96	0.47
1:a:273:MET:SD	1:a:319:LYS:NZ	2.81	0.47
1:a:177:MET:HA	1:a:533:GLN:OE1	2.15	0.47
3:c:163:ASN:N	3:c:163:ASN:OD1	2.46	0.47
15:e:201:PTY:H132	15:e:201:PTY:H181	1.96	0.47
15:b:302:PTY:H401	9:i:15:ILE:HD13	1.97	0.47
3:c:2:THR:OG1	3:c:3:HIS:N	2.46	0.47
3:c:189:TYR:HB3	11:k:116:PHE:HE2	1.79	0.47
1:a:43:PRO:HG2	5:e:124:MET:HE3	1.97	0.46
3:c:195:THR:HA	18:c:302:PCF:H133	1.96	0.46
1:a:45:SER:OG	1:a:48:LEU:O	2.33	0.46
5:e:129:GLN:OE1	5:e:151:GLN:N	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:46:LEU:HB3	4:d:65:GLY:HA2	1.97	0.46
3:c:120:LEU:HD13	3:c:126:PRO:HG3	1.97	0.46
5:e:55:GLU:HA	5:e:58:LYS:HZ3	1.80	0.46
2:b:81:ILE:HD13	15:b:302:PTY:H311	1.98	0.46
3:c:222:MET:HG3	15:c:301:PTY:H351	1.98	0.46
6:f:117:ASN:HB3	6:f:120:GLN:HG3	1.98	0.46
14:a:603:HEA:HHA	14:a:603:HEA:HAD1	1.68	0.45
2:b:62:VAL:HG12	2:b:63:MET:HE2	1.97	0.45
10:j:83:ASP:OD2	10:j:83:ASP:N	2.48	0.45
11:k:85:LYS:HB3	11:k:120:VAL:HG23	1.97	0.45
2:b:118:LYS:HZ2	10:j:58:LEU:H	1.63	0.45
4:d:52:LYS:HA	4:d:52:LYS:HD2	1.73	0.45
1:a:175:ASN:HD22	1:a:532:VAL:HG22	1.82	0.45
15:e:201:PTY:HC31	15:e:201:PTY:HC52	1.98	0.45
1:a:424:ILE:HG22	1:a:428:MET:HE3	1.97	0.45
2:b:163:THR:OG1	2:b:164:ASP:N	2.48	0.45
10:j:17:ARG:HH12	10:j:29:GLN:HG2	1.81	0.45
11:k:96:TYR:H	11:k:99:MET:HE2	1.81	0.45
1:a:105:VAL:HG21	1:a:156:ILE:HD11	1.97	0.45
2:b:123:GLN:O	2:b:123:GLN:NE2	2.48	0.45
1:a:496:ASP:O	5:e:83:ARG:NH2	2.50	0.45
6:f:85:PRO:HA	6:f:88:ILE:HG22	1.98	0.45
1:a:368:HIS:ND1	14:a:603:HEA:O1A	2.46	0.44
1:a:381:LEU:HD13	14:a:602:HEA:HAC	1.98	0.44
1:a:496:ASP:OD2	6:f:74:ASN:ND2	2.50	0.44
1:a:33:SER:HB2	1:a:62:HIS:CE1	2.52	0.44
1:a:39:GLU:OE2	1:a:46:GLN:N	2.42	0.44
1:a:292:MET:HE3	1:a:295:VAL:HG21	1.99	0.44
2:b:149:PRO:HD2	2:b:152:LEU:HB2	1.99	0.44
8:h:75:SER:O	8:h:75:SER:OG	2.29	0.44
15:b:302:PTY:H361	15:b:302:PTY:H331	1.86	0.43
11:k:19:LYS:HE2	11:k:19:LYS:HB3	1.88	0.43
1:a:131:PRO:HG2	1:a:229:PRO:HB3	2.00	0.43
1:a:532:VAL:HG12	4:d:86:LEU:HD23	2.00	0.43
15:a:605:PTY:H112	15:a:605:PTY:H141	1.82	0.43
4:d:40:VAL:O	4:d:45:THR:OG1	2.27	0.43
1:a:92:ASP:OD1	1:a:92:ASP:N	2.52	0.43
1:a:500:SER:OG	6:f:70:GLN:NE2	2.46	0.43
2:b:216:VAL:HA	2:b:237:GLU:HA	2.00	0.43
1:a:345:LEU:O	1:a:349:THR:OG1	2.34	0.43
2:b:191:PRO:HD3	2:b:219:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:53:LEU:HD21	15:b:302:PTY:H212	2.00	0.43
2:b:227:THR:OG1	2:b:228:GLY:N	2.51	0.43
3:c:244:GLU:HA	3:c:247:ILE:HD12	2.01	0.43
3:c:47:ASN:ND2	3:c:49:ASN:OD1	2.52	0.42
5:e:31:VAL:HG21	5:e:68:GLU:HG3	2.00	0.42
4:d:49:PRO:HD2	4:d:61:ASP:HA	2.01	0.42
4:d:58:THR:O	4:d:58:THR:OG1	2.36	0.42
1:a:302:ARG:NH2	10:j:21:GLN:OE1	2.52	0.42
1:a:374:VAL:HG11	14:a:602:HEA:HBA2	2.01	0.42
11:k:78:ALA:HA	11:k:81:ARG:HE	1.85	0.42
1:a:411:GLN:HE21	5:e:87:LEU:HD21	1.83	0.42
10:j:41:LYS:HD2	10:j:41:LYS:HA	1.82	0.42
7:g:12:PHE:O	7:g:22:ARG:NH1	2.53	0.42
4:d:55:THR:OG1	4:d:56:VAL:N	2.53	0.42
15:e:201:PTY:HC52	15:e:201:PTY:O10	2.20	0.42
9:i:24:LEU:HD23	9:i:24:LEU:HA	1.87	0.42
1:a:208:THR:HG21	18:c:302:PCF:H281	2.01	0.42
15:b:302:PTY:HC12	9:i:11:LYS:HG3	2.00	0.42
5:e:129:GLN:OE1	5:e:151:GLN:O	2.37	0.42
15:e:201:PTY:HC51	18:m:101:PCF:H153	2.02	0.42
18:e:202:PCF:H153	18:e:202:PCF:H112	1.84	0.42
1:a:145:ASP:OD2	1:a:214:ARG:NH1	2.53	0.41
5:e:65:THR:HB	5:e:68:GLU:HB2	2.01	0.41
1:a:12:LYS:HE2	1:a:12:LYS:HB3	1.85	0.41
1:a:38:LEU:HD12	1:a:38:LEU:HA	1.94	0.41
6:f:56:TYR:OH	6:f:75:ASN:O	2.36	0.41
1:a:27:MET:HG3	8:h:61:PHE:HD1	1.85	0.41
2:b:152:LEU:HD23	2:b:152:LEU:HA	1.93	0.41
3:c:40:THR:HB	3:c:45:ILE:HD12	2.02	0.41
4:d:137:CYS:O	6:f:71:ARG:NH2	2.54	0.41
9:i:2:THR:O	9:i:2:THR:OG1	2.37	0.41
1:a:173:ARG:H	1:a:173:ARG:HG2	1.63	0.41
7:g:8:LEU:HD23	7:g:8:LEU:HA	1.95	0.41
8:h:43:LYS:HE3	8:h:43:LYS:HB3	1.85	0.41
4:d:32:LYS:HD3	4:d:32:LYS:HA	1.76	0.40
10:j:11:THR:OG1	10:j:12:VAL:N	2.50	0.40
6:f:132:ARG:HH21	6:f:139:LEU:H	1.68	0.40
6:f:140:LYS:HE2	6:f:145:PRO:HG2	2.04	0.40
1:a:353:LEU:HD22	2:b:47:LEU:HD22	2.03	0.40
2:b:132:ASP:OD1	2:b:132:ASP:N	2.52	0.40
3:c:8:ARG:NH1	4:d:41:ASN:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:61:SER:O	12:m:61:SER:OG	2.35	0.40
1:a:419:ILE:HD12	1:a:419:ILE:HA	1.93	0.40
15:e:201:PTY:C11	18:e:202:PCF:H341	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	528/530 (100%)	489 (93%)	39 (7%)	0	100	100
2	b	234/236 (99%)	215 (92%)	19 (8%)	0	100	100
3	c	266/268 (99%)	252 (95%)	14 (5%)	0	100	100
4	d	115/117 (98%)	90 (78%)	25 (22%)	0	100	100
5	e	126/128 (98%)	115 (91%)	11 (9%)	0	100	100
6	f	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
7	g	53/55 (96%)	47 (89%)	6 (11%)	0	100	100
8	h	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
9	i	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
10	j	76/78 (97%)	66 (87%)	10 (13%)	0	100	100
11	k	112/114 (98%)	101 (90%)	10 (9%)	1 (1%)	14	41
12	m	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
All	All	1742/1766 (99%)	1586 (91%)	155 (9%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	k	20	PRO

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	443/443 (100%)	442 (100%)	1 (0%)	87	85
2	b	209/209 (100%)	208 (100%)	1 (0%)	81	80
3	c	227/227 (100%)	227 (100%)	0	100	100
4	d	99/99 (100%)	99 (100%)	0	100	100
5	e	106/106 (100%)	106 (100%)	0	100	100
6	f	88/88 (100%)	88 (100%)	0	100	100
7	g	48/48 (100%)	48 (100%)	0	100	100
8	h	41/41 (100%)	40 (98%)	1 (2%)	43	62
9	i	43/43 (100%)	42 (98%)	1 (2%)	44	62
10	j	70/70 (100%)	70 (100%)	0	100	100
11	k	100/100 (100%)	100 (100%)	0	100	100
12	m	32/32 (100%)	32 (100%)	0	100	100
All	All	1506/1506 (100%)	1502 (100%)	4 (0%)	84	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	244	VAL
2	b	197	VAL
8	h	34	VAL
9	i	6	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	175	ASN
1	a	234	HIS
1	a	257	HIS
1	a	328	HIS
1	a	376	HIS

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Mol	Chain	Res	Type
1	a	411	GLN
1	a	451	ASN
1	a	478	ASN
1	a	482	ASN
1	a	507	ASN
1	a	528	ASN
2	b	26	GLN
2	b	32	ASN
2	b	186	HIS
2	b	231	ASN
3	c	10	GLN
3	c	47	ASN
3	c	49	ASN
3	c	79	HIS
3	c	226	ASN
5	e	57	GLN
5	e	63	GLN
6	f	75	ASN
6	f	117	ASN
7	g	9	GLN
7	g	13	GLN
8	h	71	GLN
10	j	6	ASN
10	j	20	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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$
17	CUA	b	301	-	0,1,1	-	-	-		
15	PTY	b	302	-	39,39,49	0.99	4 (10%)	42,44,54	1.09	2 (4%)
18	PCF	c	302	-	42,42,49	0.64	0	48,50,57	0.58	0
15	PTY	e	201	-	31,31,49	1.10	2 (6%)	34,36,54	1.22	4 (11%)
14	HEA	a	602	1	67,67,67	1.18	7 (10%)	81,103,103	1.44	14 (17%)
14	HEA	a	603	1	67,67,67	1.26	8 (11%)	81,103,103	1.53	16 (19%)
16	CN3	a	606	-	54,54,54	0.51	0	60,66,66	1.19	4 (6%)
15	PTY	c	301	-	39,39,49	1.00	4 (10%)	42,44,54	1.15	3 (7%)
18	PCF	e	202	-	35,35,49	0.68	0	41,43,57	0.59	0
15	PTY	i	101	-	29,29,49	1.14	4 (13%)	32,34,54	1.23	2 (6%)
15	PTY	a	604	-	32,32,49	1.08	4 (12%)	35,37,54	1.13	2 (5%)
15	PTY	b	303	-	40,40,49	0.98	4 (10%)	43,45,54	1.13	2 (4%)
18	PCF	m	101	-	37,37,49	0.66	0	43,45,57	0.59	0
15	PTY	a	605	-	33,33,49	1.07	4 (12%)	36,38,54	1.17	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PTY	b	302	-	-	14/43/43/53	-
18	PCF	c	302	-	-	19/46/46/53	-
15	PTY	e	201	-	-	10/35/35/53	-
14	HEA	a	602	1	-	16/36/76/76	-
14	HEA	a	603	1	-	11/36/76/76	-
16	CN3	a	606	-	-	38/65/65/65	-
15	PTY	c	301	-	-	17/43/43/53	-
18	PCF	e	202	-	-	12/39/39/53	-
15	PTY	i	101	-	-	14/33/33/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PTY	a	604	-	-	12/36/36/53	-
15	PTY	b	303	-	-	21/44/44/53	-
18	PCF	m	101	-	-	15/41/41/53	-
15	PTY	a	605	-	-	16/37/37/53	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	603	HEA	CMA-C3A	-4.31	1.35	1.45
14	a	602	HEA	CMA-C3A	-4.01	1.36	1.45
15	e	201	PTY	O4-C30	4.00	1.45	1.33
15	e	201	PTY	O7-C8	3.58	1.44	1.34
15	c	301	PTY	O7-C6	-2.88	1.39	1.46
15	b	303	PTY	O7-C6	-2.80	1.40	1.46
15	a	605	PTY	O7-C6	-2.76	1.40	1.46
14	a	603	HEA	C4C-NC	-2.66	1.34	1.39
15	a	604	PTY	O7-C6	-2.64	1.40	1.46
15	b	302	PTY	O7-C6	-2.62	1.40	1.46
14	a	603	HEA	C1D-C2D	2.61	1.49	1.44
14	a	602	HEA	C4C-NC	-2.60	1.34	1.39
15	i	101	PTY	O7-C6	-2.60	1.40	1.46
15	i	101	PTY	O4-C30	2.47	1.40	1.33
15	c	301	PTY	O4-C30	2.44	1.40	1.33
15	b	303	PTY	O4-C30	2.42	1.40	1.33
15	b	302	PTY	O4-C30	2.41	1.40	1.33
14	a	603	HEA	CHC-C1C	-2.40	1.34	1.39
15	a	605	PTY	O4-C1	-2.38	1.39	1.45
15	a	605	PTY	O4-C30	2.36	1.40	1.33
14	a	603	HEA	CMD-C2D	2.33	1.55	1.50
15	a	604	PTY	O4-C1	-2.33	1.40	1.45
15	a	604	PTY	O4-C30	2.28	1.40	1.33
14	a	602	HEA	C4B-C3B	2.28	1.48	1.44
15	b	302	PTY	O4-C1	-2.27	1.40	1.45
15	i	101	PTY	O7-C8	2.22	1.40	1.34
14	a	603	HEA	C1D-ND	-2.21	1.36	1.40
15	a	605	PTY	O7-C8	2.20	1.40	1.34
15	c	301	PTY	O4-C1	-2.20	1.40	1.45
15	b	303	PTY	O4-C1	-2.18	1.40	1.45
15	b	302	PTY	O7-C8	2.17	1.40	1.34
14	a	602	HEA	CHC-C1C	-2.16	1.34	1.39
14	a	603	HEA	C3C-C2C	-2.15	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	i	101	PTY	O4-C1	-2.15	1.40	1.45
15	a	604	PTY	O7-C8	2.14	1.40	1.34
14	a	602	HEA	FE-NC	2.13	2.02	1.95
14	a	603	HEA	FE-NC	2.11	2.02	1.95
14	a	602	HEA	C1D-C2D	2.09	1.48	1.44
15	c	301	PTY	O7-C8	2.06	1.40	1.34
15	b	303	PTY	O7-C8	2.06	1.40	1.34
14	a	602	HEA	C3C-C2C	-2.03	1.34	1.41

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	101	PTY	O7-C8-C11	4.43	121.07	111.48
15	b	302	PTY	O7-C8-C11	4.22	120.60	111.48
16	a	606	CN3	O51-C51-C52	4.16	120.49	111.48
15	c	301	PTY	O7-C8-C11	4.03	120.19	111.48
15	b	303	PTY	O7-C8-C11	4.00	120.13	111.48
16	a	606	CN3	O21-C21-C22	3.99	120.11	111.48
15	a	604	PTY	O7-C8-C11	3.92	119.95	111.48
15	a	605	PTY	O7-C8-C11	3.91	119.95	111.48
15	e	201	PTY	C6-O7-C8	-3.86	108.55	117.80
14	a	603	HEA	CHB-C4A-NA	-3.66	120.47	124.45
14	a	602	HEA	CMD-C2D-C1D	3.49	130.49	125.03
14	a	602	HEA	CHB-C4A-NA	-3.38	120.77	124.45
14	a	603	HEA	CBD-CAD-C3D	3.35	121.79	112.53
14	a	603	HEA	C3D-C4D-ND	3.34	113.58	110.35
14	a	603	HEA	OMA-CMA-C3A	-3.24	118.31	125.62
14	a	603	HEA	CAD-C3D-C2D	3.13	133.72	127.87
14	a	603	HEA	CAD-C3D-C4D	-3.06	119.36	124.70
15	e	201	PTY	O7-C8-C11	3.04	118.06	111.48
14	a	602	HEA	C2A-C1A-NA	2.92	113.14	110.32
16	a	606	CN3	O31-C31-C32	2.89	119.92	111.15
16	a	606	CN3	O41-C41-C42	2.87	120.59	111.83
15	a	605	PTY	O4-C30-C31	2.87	120.58	111.83
14	a	603	HEA	CHA-C4D-C3D	-2.83	120.64	124.77
14	a	603	HEA	C1D-C2D-C3D	-2.82	104.01	106.98
15	i	101	PTY	O4-C30-C31	2.78	120.32	111.83
14	a	602	HEA	OMA-CMA-C3A	-2.75	119.40	125.62
14	a	602	HEA	C26-C15-C14	-2.70	116.68	123.63
14	a	602	HEA	C3C-C4C-NC	2.70	112.07	109.80
15	a	604	PTY	O4-C30-C31	2.68	120.01	111.83
15	b	303	PTY	O4-C30-C31	2.67	119.97	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	301	PTY	O4-C30-C31	2.59	119.75	111.83
14	a	603	HEA	C20-C19-C18	-2.59	115.36	121.17
14	a	603	HEA	CMD-C2D-C1D	2.57	129.05	125.03
14	a	603	HEA	C2A-C1A-NA	2.55	112.79	110.32
15	b	302	PTY	O4-C30-C31	2.46	119.32	111.83
14	a	602	HEA	C3D-C4D-ND	2.44	112.71	110.35
14	a	602	HEA	C2B-C1B-NB	2.38	112.66	109.90
14	a	602	HEA	C1D-C2D-C3D	-2.37	104.49	106.98
14	a	602	HEA	O1D-CGD-CBD	-2.35	115.63	123.09
14	a	602	HEA	C13-C14-C15	-2.34	122.27	127.62
14	a	603	HEA	CMB-C2B-C3B	-2.29	125.84	130.28
15	e	201	PTY	O4-C30-C31	2.28	118.78	111.83
14	a	602	HEA	O1A-CGA-CBA	-2.27	115.89	123.09
14	a	603	HEA	C3C-C4C-NC	2.25	111.69	109.80
14	a	603	HEA	CHD-C1D-ND	-2.22	121.62	124.37
15	c	301	PTY	C6-O7-C8	-2.21	112.52	117.80
14	a	603	HEA	O1D-CGD-CBD	-2.16	116.24	123.09
14	a	602	HEA	CHA-C4D-C3D	-2.15	121.64	124.77
14	a	602	HEA	CMB-C2B-C3B	-2.06	126.28	130.28
14	a	603	HEA	C2B-C1B-NB	2.04	112.26	109.90
15	e	201	PTY	C12-C11-C8	-2.03	106.25	113.69

There are no chirality outliers.

All (215) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	a	602	HEA	C2A-C3A-CMA-OMA
14	a	602	HEA	C4A-C3A-CMA-OMA
14	a	602	HEA	C13-C14-C15-C26
14	a	602	HEA	C17-C18-C19-C27
14	a	603	HEA	C2A-C3A-CMA-OMA
14	a	603	HEA	C4A-C3A-CMA-OMA
15	a	604	PTY	C3-O11-P1-O13
15	a	604	PTY	C3-O11-P1-O14
15	a	605	PTY	C3-O11-P1-O12
15	a	605	PTY	C3-O11-P1-O14
15	a	605	PTY	C5-O14-P1-O13
15	b	303	PTY	O10-C8-O7-C6
15	b	303	PTY	C11-C8-O7-C6
15	b	303	PTY	C5-O14-P1-O11
15	b	303	PTY	C5-O14-P1-O12
15	b	303	PTY	C5-O14-P1-O13

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Mol	Chain	Res	Type	Atoms
15	c	301	PTY	N1-C2-C3-O11
15	c	301	PTY	O14-C5-C6-O7
15	e	201	PTY	C11-C8-O7-C6
15	e	201	PTY	C3-O11-P1-O12
15	e	201	PTY	C3-O11-P1-O13
15	e	201	PTY	C3-O11-P1-O14
15	i	101	PTY	O4-C1-C6-O7
15	i	101	PTY	O10-C8-O7-C6
15	i	101	PTY	C11-C8-O7-C6
15	i	101	PTY	C5-O14-P1-O13
16	a	606	CN3	C1-O11-P-O12
16	a	606	CN3	C1-O11-P-O13
16	a	606	CN3	C1-O11-P-O14
16	a	606	CN3	CC-O13-P-O11
16	a	606	CN3	CC-O13-P-O12
16	a	606	CN3	C1'-O1'-P'-O2'
16	a	606	CN3	C1'-O1'-P'-O3'
16	a	606	CN3	CA-O3'-P'-O1'
16	a	606	CN3	CA-O3'-P'-O4'
16	a	606	CN3	O1'-C1'-C2'-O51
16	a	606	CN3	C52-C51-O51-C2'
18	c	302	PCF	C1-O11-P-O12
18	c	302	PCF	C1-O11-P-O13
18	c	302	PCF	O13-C11-C12-N
18	c	302	PCF	C22-C21-O21-C2
18	m	101	PCF	C1-O11-P-O14
18	m	101	PCF	C11-O13-P-O11
18	m	101	PCF	C11-O13-P-O12
18	m	101	PCF	C11-O13-P-O14
18	m	101	PCF	O13-C11-C12-N
15	a	605	PTY	O30-C30-O4-C1
14	a	602	HEA	C21-C22-C23-C25
15	a	604	PTY	O30-C30-O4-C1
15	e	201	PTY	O10-C8-O7-C6
16	a	606	CN3	O52-C51-O51-C2'
18	c	302	PCF	O22-C21-O21-C2
15	a	604	PTY	C31-C30-O4-C1
15	a	605	PTY	C31-C30-O4-C1
16	a	606	CN3	OA-CB-CC-O13
14	a	602	HEA	C17-C18-C19-C20
16	a	606	CN3	O3'-CA-CB-CC
18	c	302	PCF	C11-C12-N-C13

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Mol	Chain	Res	Type	Atoms
18	c	302	PCF	C11-C12-N-C15
16	a	606	CN3	O3'-CA-CB-OA
16	a	606	CN3	O21-C2-C3-O31
14	a	602	HEA	C21-C22-C23-C24
15	a	604	PTY	C8-C11-C12-C13
15	b	302	PTY	C8-C11-C12-C13
15	b	303	PTY	C30-C31-C32-C33
15	a	605	PTY	C30-C31-C32-C33
14	a	603	HEA	C4D-C3D-CAD-CBD
15	a	605	PTY	C11-C8-O7-C6
15	a	605	PTY	O10-C8-O7-C6
18	e	202	PCF	C21-C22-C23-C24
15	b	303	PTY	C33-C34-C35-C36
15	e	201	PTY	C14-C15-C16-C17
14	a	602	HEA	C4C-C3C-CAC-CBC
15	i	101	PTY	C8-C11-C12-C13
16	a	606	CN3	C51-C52-C53-C54
15	c	301	PTY	C33-C34-C35-C36
15	a	605	PTY	C12-C13-C14-C15
18	c	302	PCF	C11-C12-N-C14
15	b	303	PTY	C34-C35-C36-C37
15	b	302	PTY	C30-C31-C32-C33
16	a	606	CN3	C42-C41-O41-C3'
18	c	302	PCF	C32-C31-O31-C3
15	e	201	PTY	C15-C16-C17-C18
15	b	303	PTY	C32-C33-C34-C35
18	c	302	PCF	C36-C37-C38-C39
15	a	605	PTY	C31-C32-C33-C34
16	a	606	CN3	C52-C53-C54-C55
15	c	301	PTY	C11-C8-O7-C6
18	m	101	PCF	C22-C21-O21-C2
15	c	301	PTY	O10-C8-O7-C6
15	e	201	PTY	C8-C11-C12-C13
15	c	301	PTY	C17-C18-C19-C20
15	a	605	PTY	C13-C14-C15-C16
18	c	302	PCF	C31-C32-C33-C34
15	a	604	PTY	C13-C14-C15-C16
15	b	303	PTY	C18-C19-C20-C21
15	c	301	PTY	C34-C35-C36-C37
15	a	605	PTY	C32-C33-C34-C35
15	i	101	PTY	C13-C14-C15-C16
16	a	606	CN3	O42-C41-O41-C3'

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Mol	Chain	Res	Type	Atoms
15	b	302	PTY	O14-C5-C6-C1
16	a	606	CN3	O11-C1-C2-C3
16	a	606	CN3	O1'-C1'-C2'-C3'
18	m	101	PCF	O22-C21-O21-C2
18	c	302	PCF	O32-C31-O31-C3
15	b	302	PTY	O4-C1-C6-C5
16	a	606	CN3	C1-C2-C3-O31
18	e	202	PCF	C1-C2-C3-O31
14	a	603	HEA	C27-C19-C20-C21
15	e	201	PTY	C31-C30-O4-C1
15	b	303	PTY	C12-C13-C14-C15
18	e	202	PCF	C23-C24-C25-C26
15	b	302	PTY	O4-C1-C6-O7
14	a	603	HEA	C2D-C3D-CAD-CBD
15	b	303	PTY	O4-C30-C31-C32
18	e	202	PCF	C32-C31-O31-C3
15	a	604	PTY	O14-C5-C6-C1
15	c	301	PTY	C12-C13-C14-C15
18	e	202	PCF	C25-C26-C27-C28
15	b	303	PTY	O4-C1-C6-C5
16	a	606	CN3	O11-C1-C2-O21
18	m	101	PCF	O11-C1-C2-O21
15	b	303	PTY	O4-C1-C6-O7
18	e	202	PCF	O21-C2-C3-O31
16	a	606	CN3	C43-C44-C45-C46
16	a	606	CN3	CA-CB-CC-O13
15	i	101	PTY	O14-C5-C6-C1
18	m	101	PCF	O11-C1-C2-C3
15	a	605	PTY	C14-C15-C16-C17
15	c	301	PTY	C31-C32-C33-C34
18	c	302	PCF	C22-C23-C24-C25
15	e	201	PTY	O30-C30-O4-C1
18	e	202	PCF	O32-C31-O31-C3
18	e	202	PCF	C28-C29-C30-C47
18	c	302	PCF	C1-C2-C3-O31
15	c	301	PTY	C11-C12-C13-C14
15	b	302	PTY	C32-C33-C34-C35
18	e	202	PCF	O13-C11-C12-N
14	a	603	HEA	C4C-C3C-CAC-CBC
15	b	302	PTY	C31-C32-C33-C34
15	b	303	PTY	O14-C5-C6-C1
15	c	301	PTY	O14-C5-C6-C1

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Mol	Chain	Res	Type	Atoms
15	b	303	PTY	C16-C17-C18-C19
16	a	606	CN3	C45-C46-C47-C48
15	a	604	PTY	O14-C5-C6-O7
15	a	605	PTY	O14-C5-C6-O7
15	b	302	PTY	O14-C5-C6-O7
15	b	303	PTY	O14-C5-C6-O7
15	i	101	PTY	O14-C5-C6-O7
15	i	101	PTY	C30-C31-C32-C33
15	b	302	PTY	C11-C12-C13-C14
15	i	101	PTY	O4-C1-C6-C5
14	a	602	HEA	C11-C12-C13-C14
15	a	605	PTY	N1-C2-C3-O11
15	b	302	PTY	N1-C2-C3-O11
15	b	303	PTY	C3-O11-P1-O13
15	i	101	PTY	C5-O14-P1-O11
16	a	606	CN3	CA-O3'-P'-O2'
18	e	202	PCF	C11-O13-P-O12
18	m	101	PCF	C1-O11-P-O12
18	m	101	PCF	C1-O11-P-O13
18	c	302	PCF	C35-C36-C37-C38
14	a	602	HEA	C2C-C3C-CAC-CBC
14	a	603	HEA	C2C-C3C-CAC-CBC
16	a	606	CN3	CB-CC-O13-P
18	m	101	PCF	C28-C29-C30-C47
15	a	605	PTY	O14-C5-C6-C1
18	m	101	PCF	C36-C37-C38-C39
16	a	606	CN3	C32-C31-O31-C3
15	b	303	PTY	C11-C12-C13-C14
15	c	301	PTY	C31-C30-O4-C1
16	a	606	CN3	O32-C31-O31-C3
14	a	603	HEA	C18-C19-C20-C21
15	b	303	PTY	O30-C30-C31-C32
15	c	301	PTY	O30-C30-O4-C1
15	a	604	PTY	C16-C17-C18-C19
15	c	301	PTY	C14-C15-C16-C17
18	m	101	PCF	C22-C23-C24-C25
14	a	602	HEA	CAA-CBA-CGA-O2A
18	c	302	PCF	C2-C1-O11-P
15	a	604	PTY	C31-C32-C33-C34
18	c	302	PCF	O21-C2-C3-O31
14	a	602	HEA	CAD-CBD-CGD-O1D
14	a	602	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	a	603	HEA	CAA-CBA-CGA-O1A
14	a	603	HEA	CAA-CBA-CGA-O2A
15	i	101	PTY	C6-C5-O14-P1
15	a	604	PTY	C11-C12-C13-C14
15	a	604	PTY	C12-C11-C8-O7
15	b	303	PTY	C31-C32-C33-C34
18	e	202	PCF	C22-C23-C24-C25
15	b	302	PTY	C38-C39-C40-C41
18	m	101	PCF	C21-C22-C23-C24
15	b	302	PTY	C12-C11-C8-O7
14	a	602	HEA	CAA-CBA-CGA-O1A
14	a	603	HEA	CAD-CBD-CGD-O2D
15	c	301	PTY	C35-C36-C37-C38
15	c	301	PTY	C37-C38-C39-C40
16	a	606	CN3	O32-C31-C32-C33
18	c	302	PCF	O11-C1-C2-O21
18	e	202	PCF	C33-C34-C35-C36
18	c	302	PCF	C25-C26-C27-C28
16	a	606	CN3	O31-C31-C32-C33
15	i	101	PTY	O30-C30-O4-C1
16	a	606	CN3	O51-C51-C52-C53
15	b	302	PTY	C36-C37-C38-C39
16	a	606	CN3	C54-C55-C56-C57
14	a	602	HEA	C3A-C2A-CAA-CBA
16	a	606	CN3	O22-C21-O21-C2
15	i	101	PTY	C31-C30-O4-C1
15	b	302	PTY	C37-C38-C39-C40
15	c	301	PTY	C12-C11-C8-O7
14	a	602	HEA	CAD-CBD-CGD-O2D
16	a	606	CN3	C22-C21-O21-C2
16	a	606	CN3	O52-C51-C52-C53

There are no ring outliers.

10 monomers are involved in 60 short contacts:

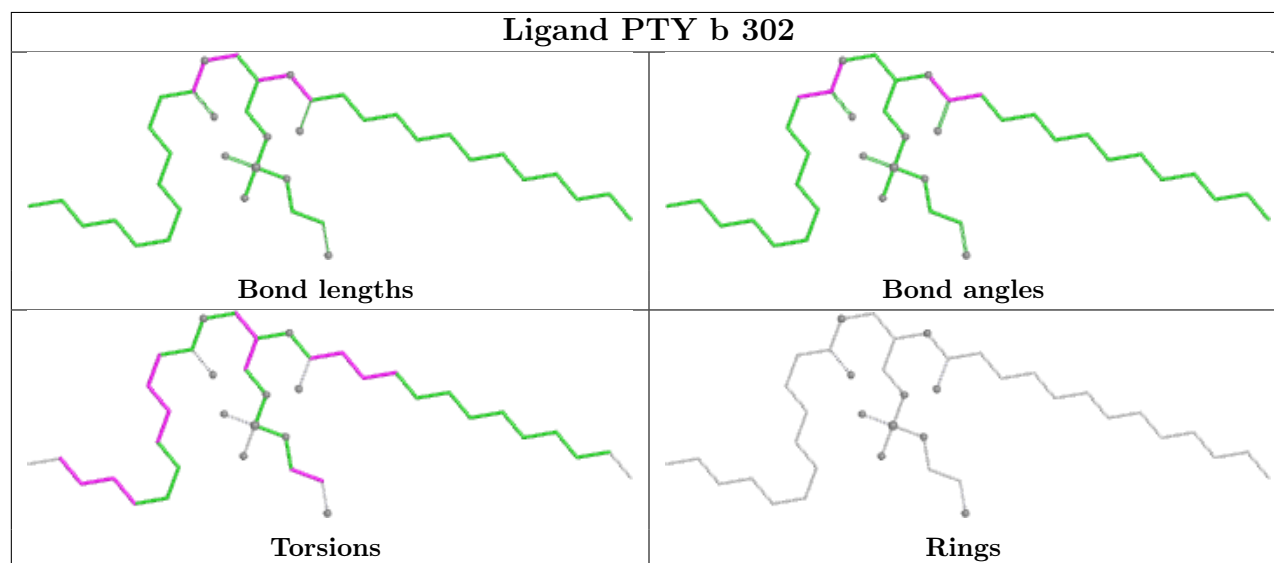
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	302	PTY	6	0
18	c	302	PCF	2	0
15	e	201	PTY	37	0
14	a	602	HEA	3	0
14	a	603	HEA	6	0
16	a	606	CN3	1	0

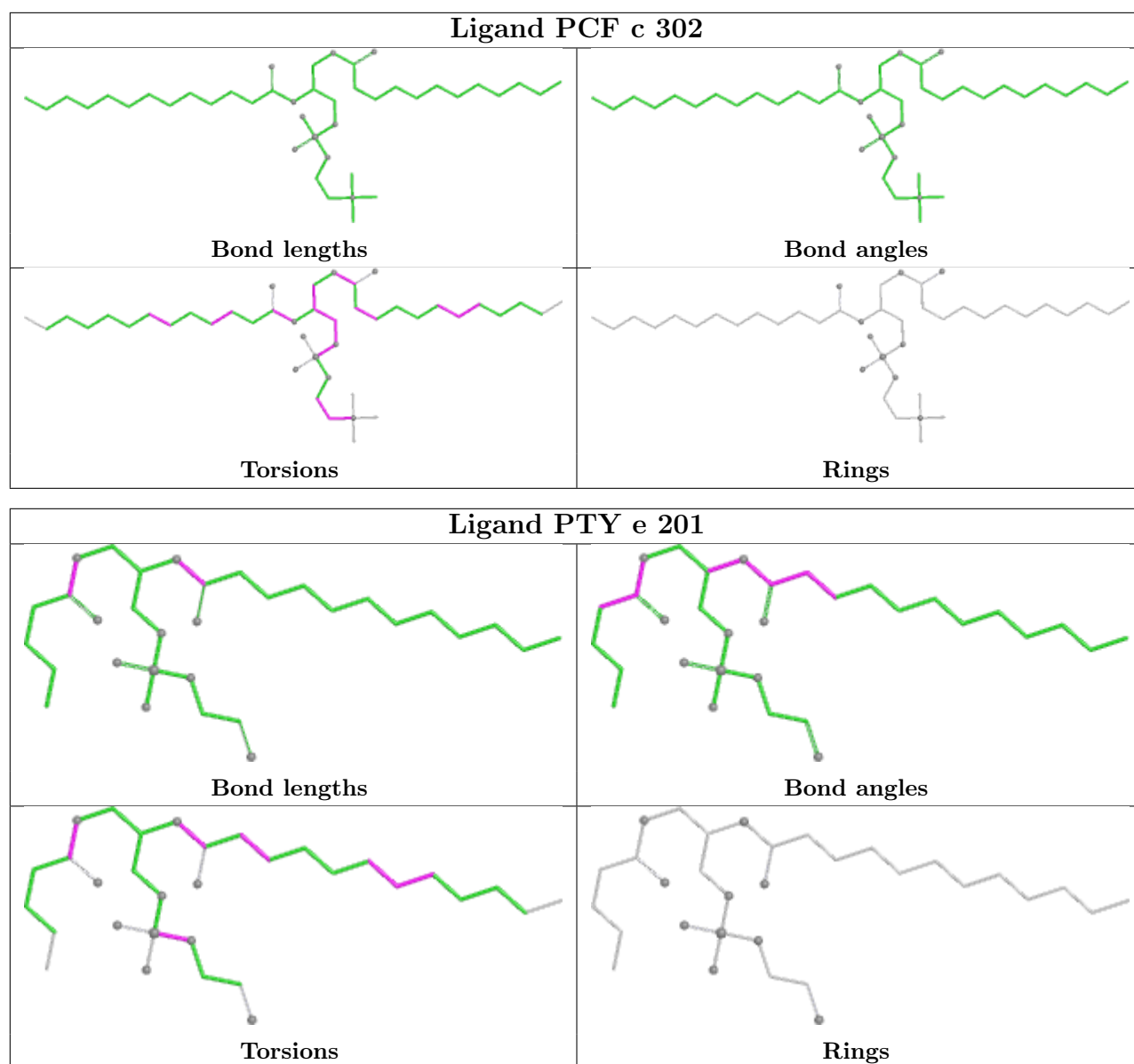
Continued on next page...

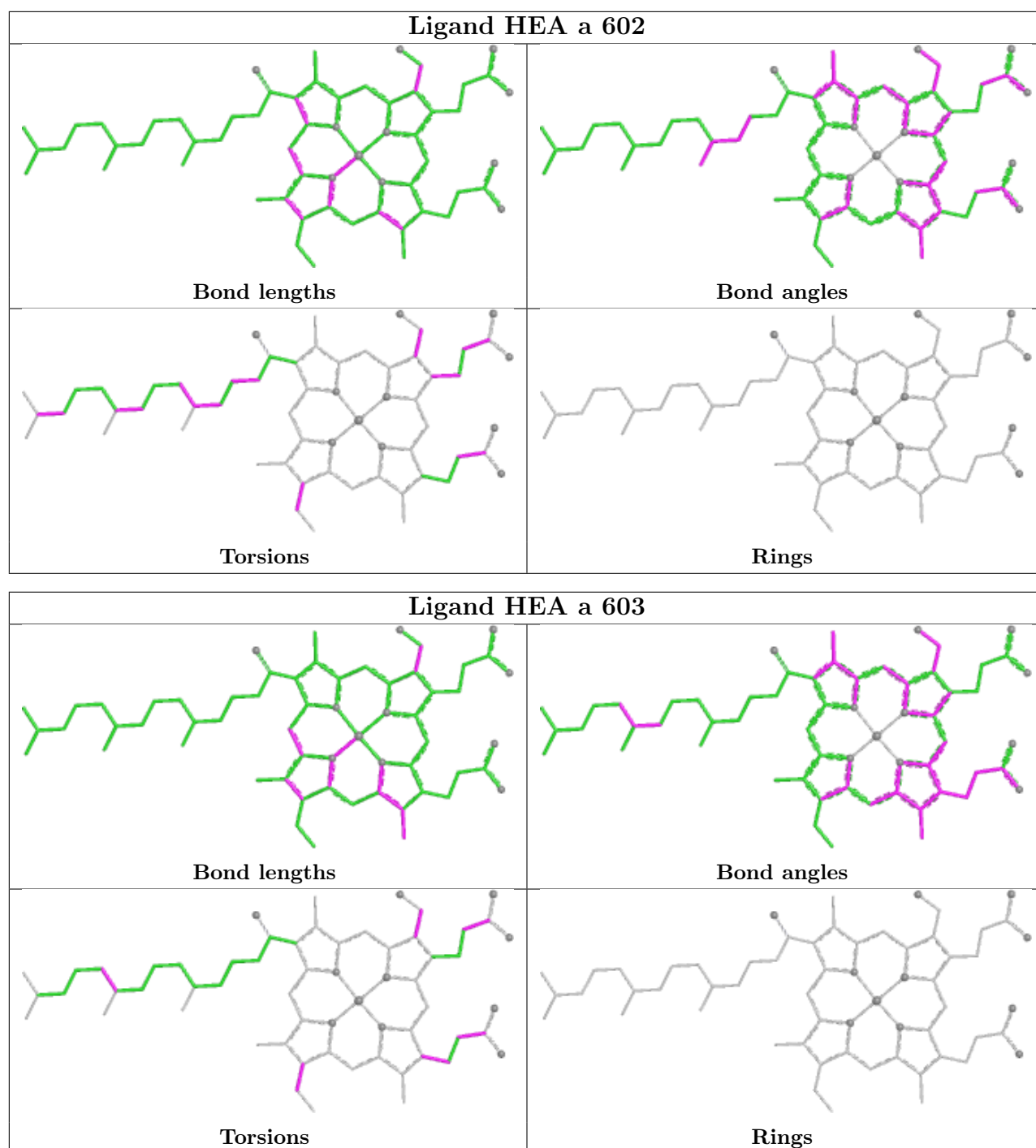
Continued from previous page...

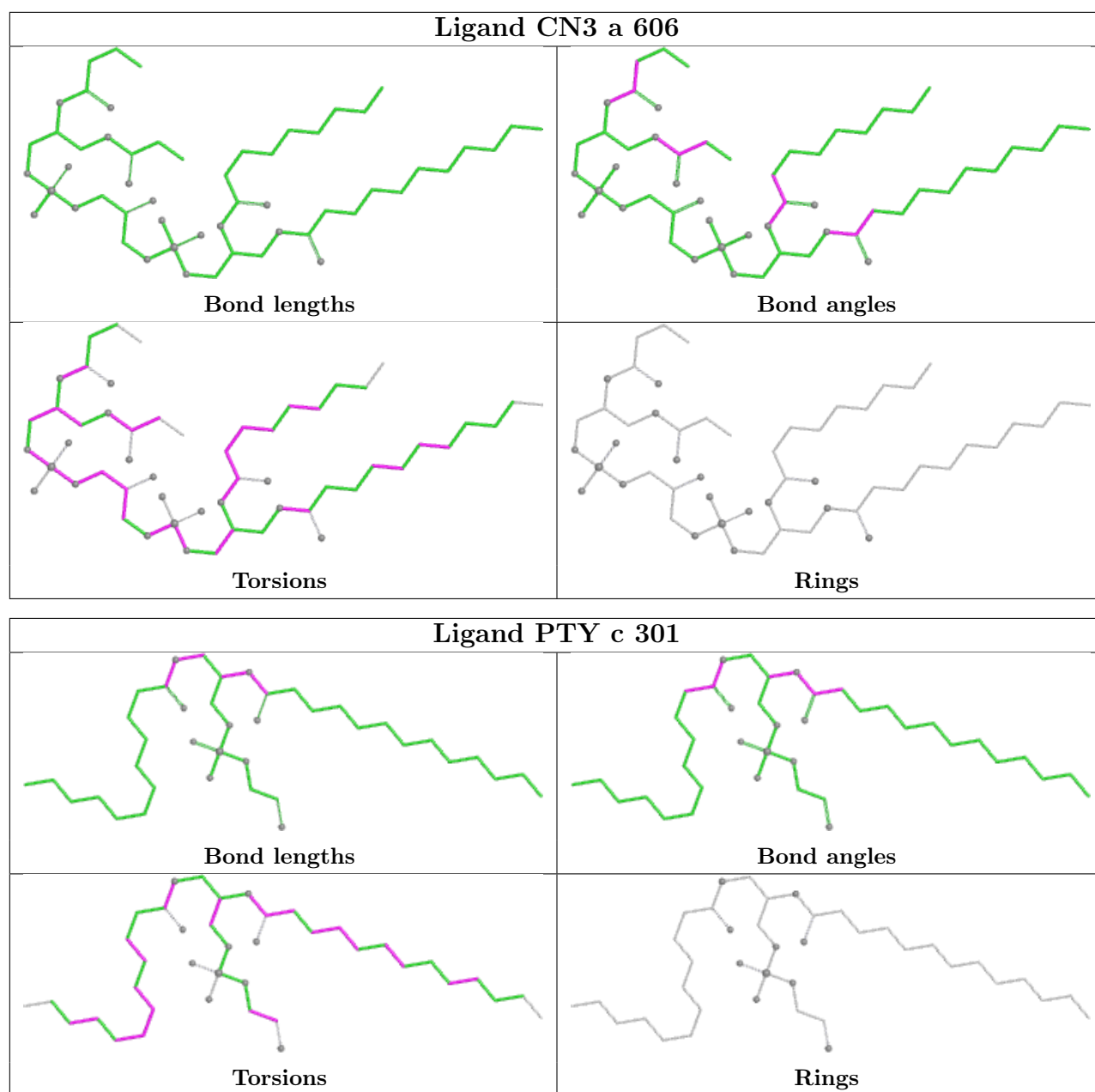
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c	301	PTY	2	0
18	e	202	PCF	9	0
18	m	101	PCF	1	0
15	a	605	PTY	2	0

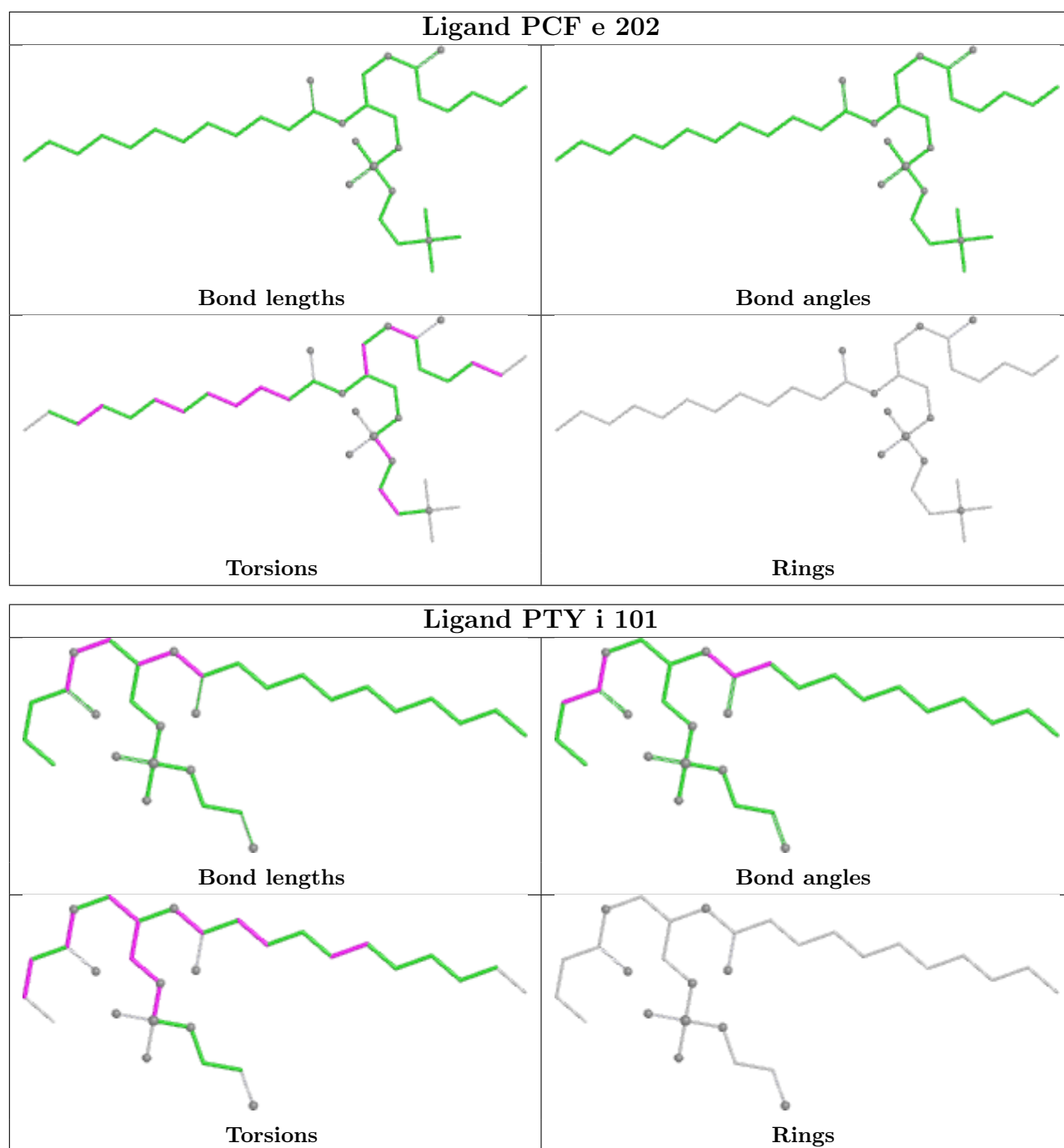
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

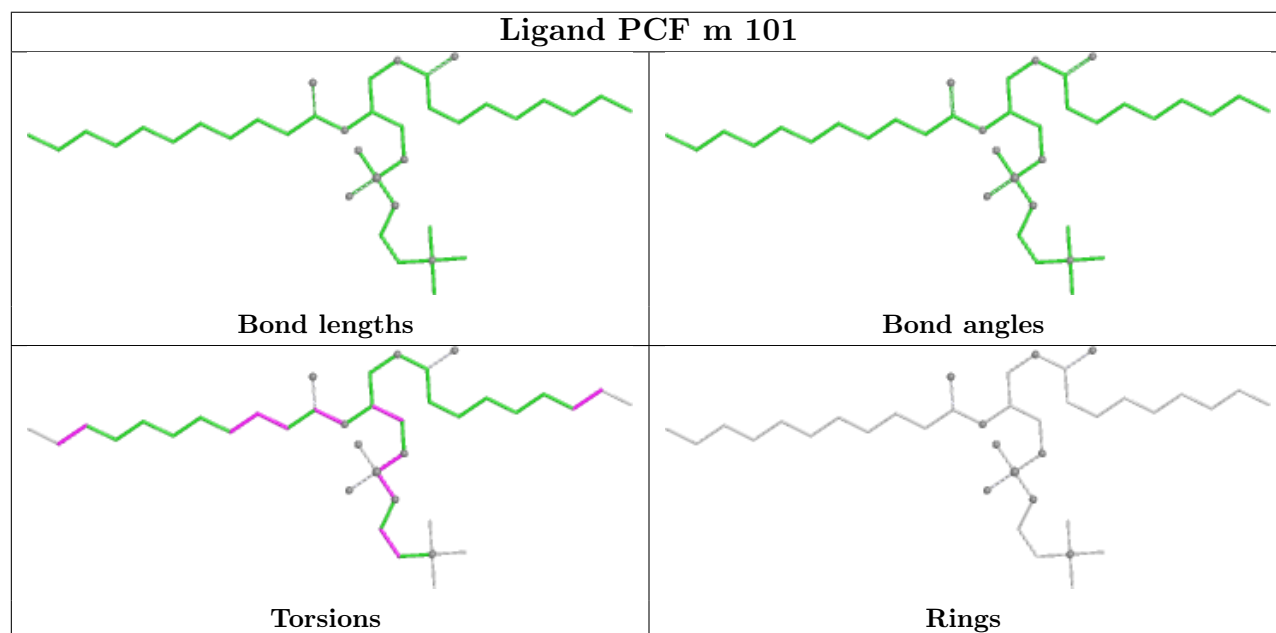
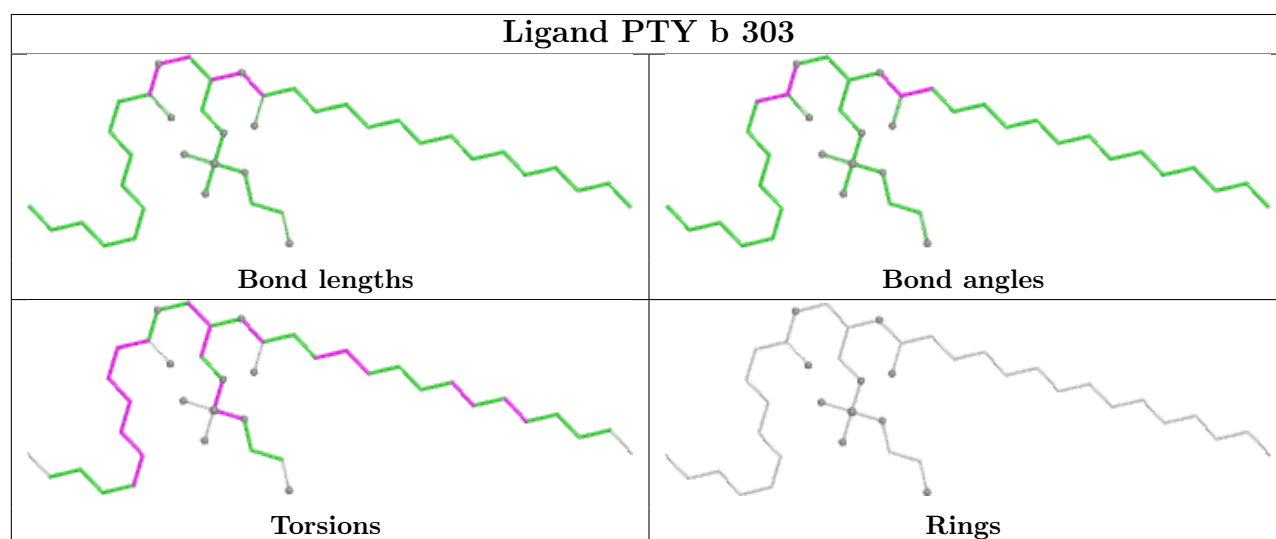
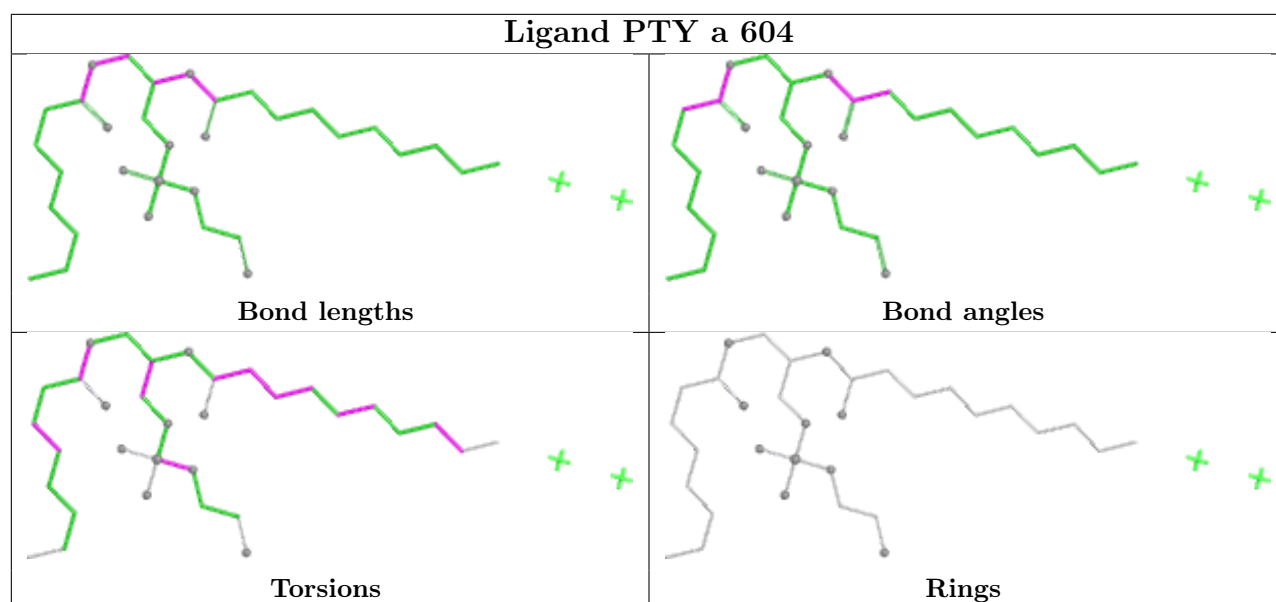


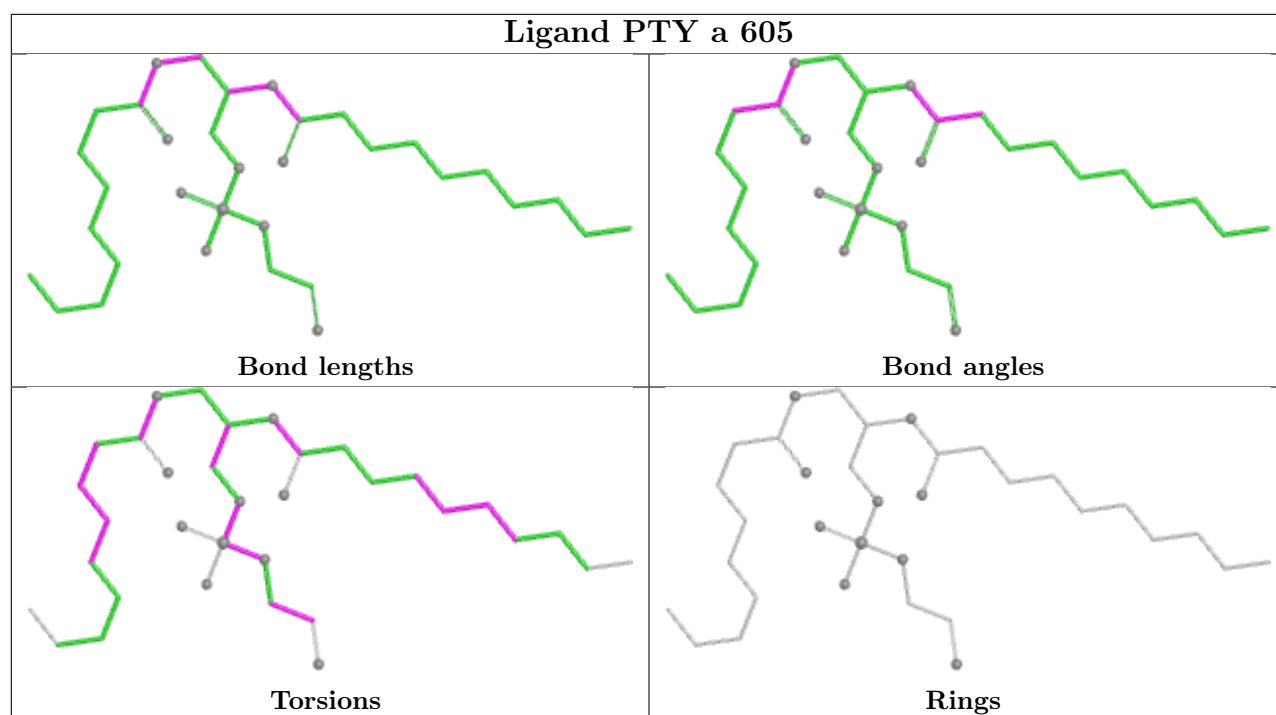












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

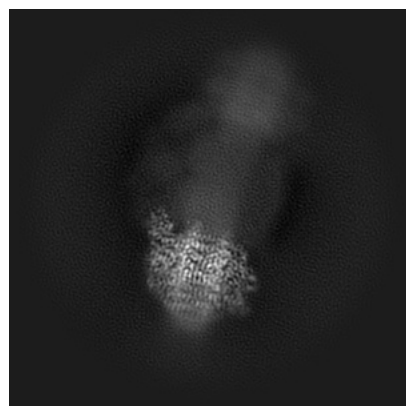
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10848. These allow visual inspection of the internal detail of the map and identification of artifacts.

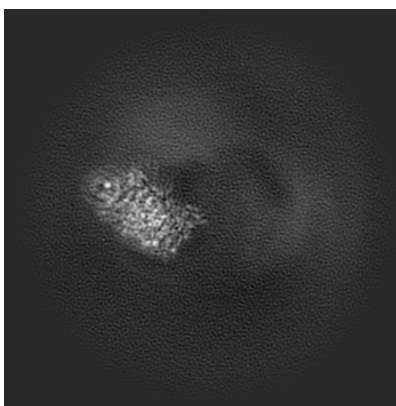
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

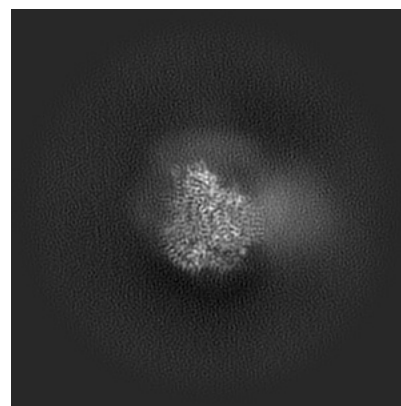
6.1.1 Primary map



X

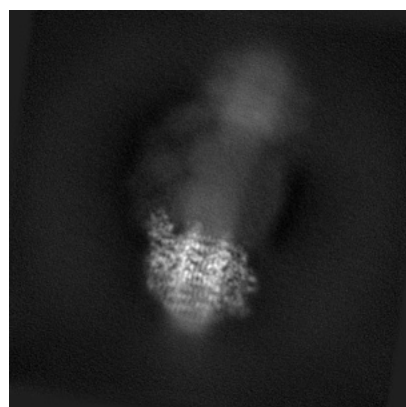


Y

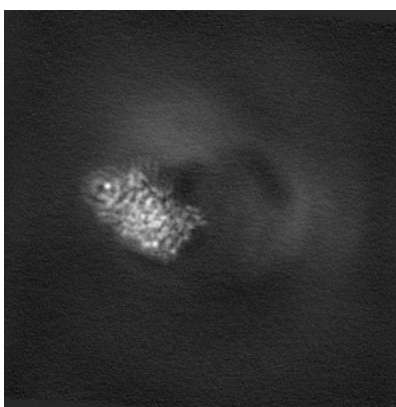


Z

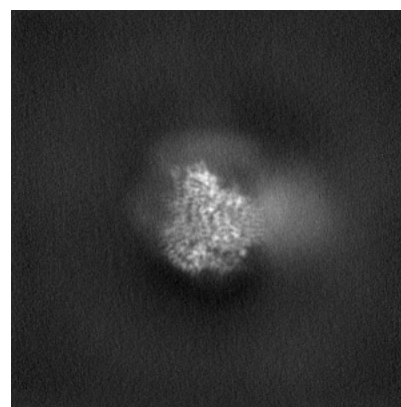
6.1.2 Raw map



X



Y

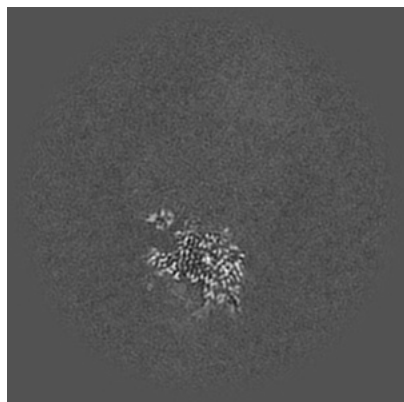


Z

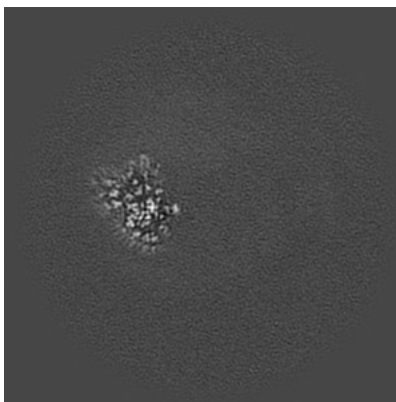
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

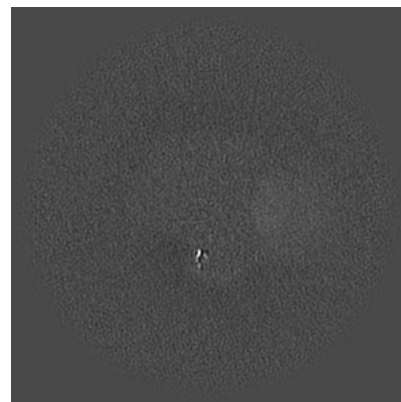
6.2.1 Primary map



X Index: 185

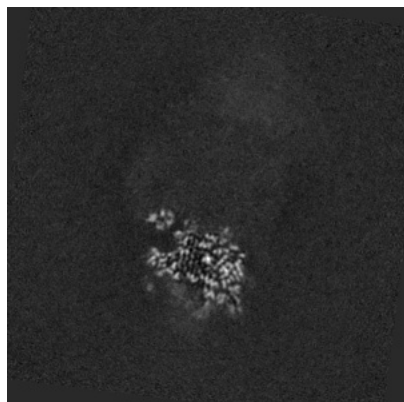


Y Index: 185

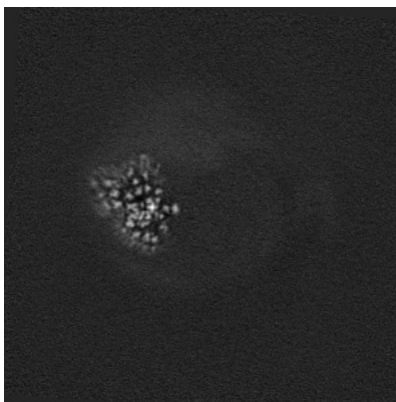


Z Index: 185

6.2.2 Raw map



X Index: 185



Y Index: 185

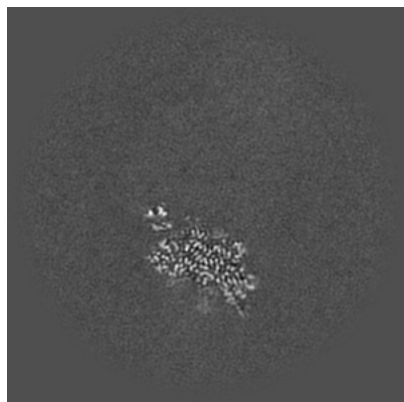


Z Index: 185

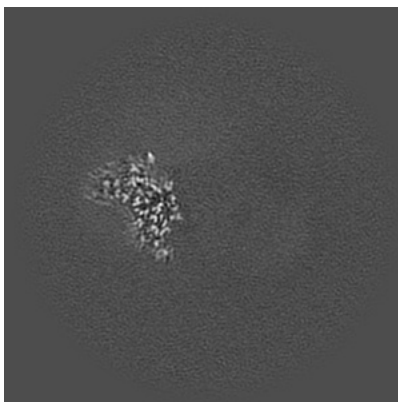
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

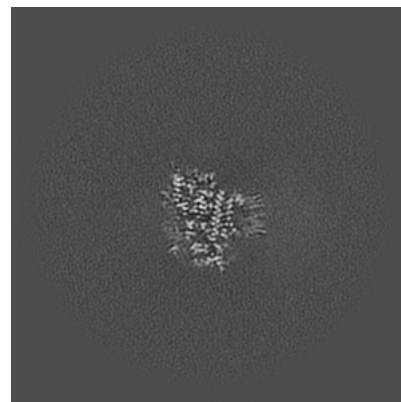
6.3.1 Primary map



X Index: 178

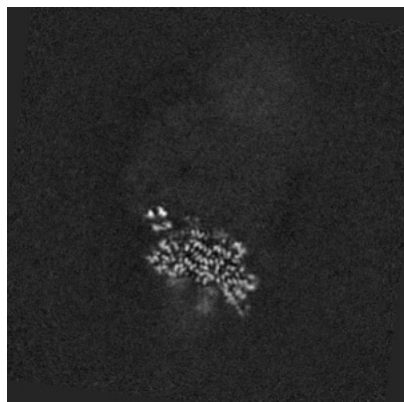


Y Index: 162

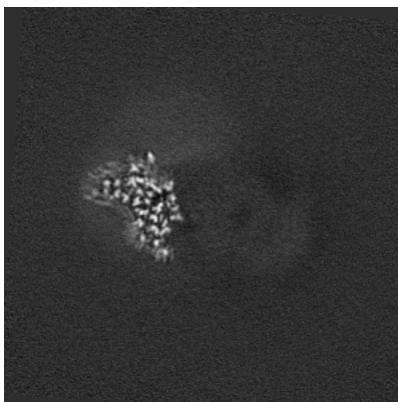


Z Index: 133

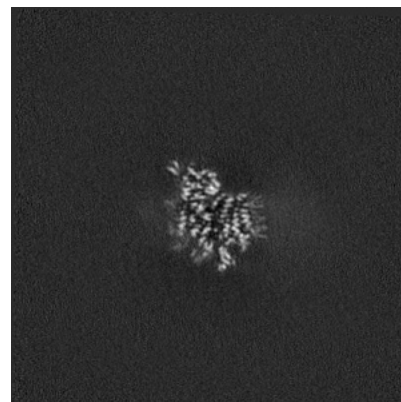
6.3.2 Raw map



X Index: 178



Y Index: 162

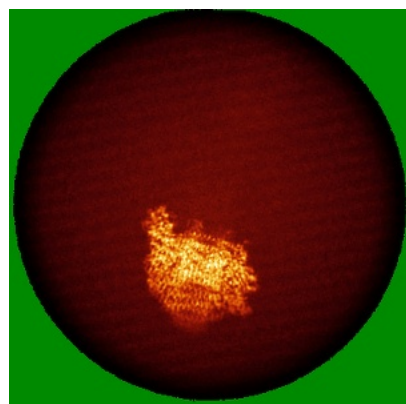


Z Index: 126

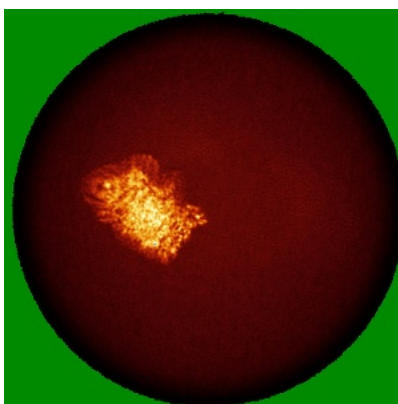
The images above show the largest variance slices of the map in three orthogonal directions.

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

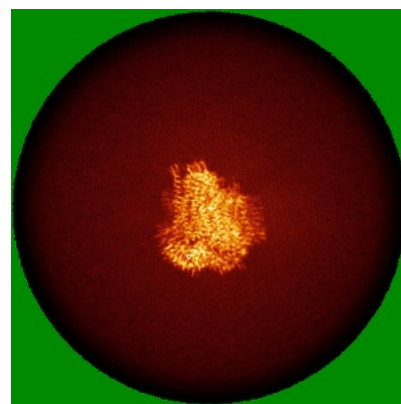
6.4.1 Primary map



X

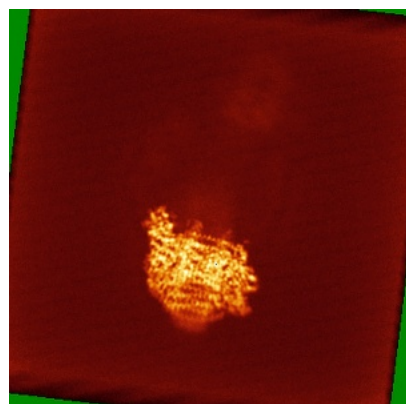


Y

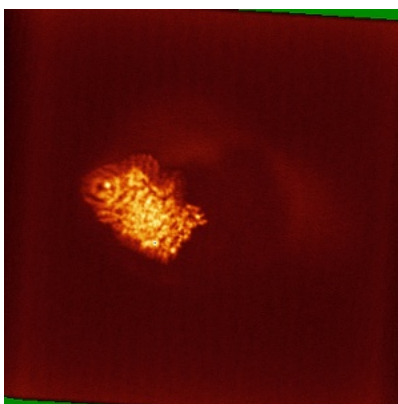


Z

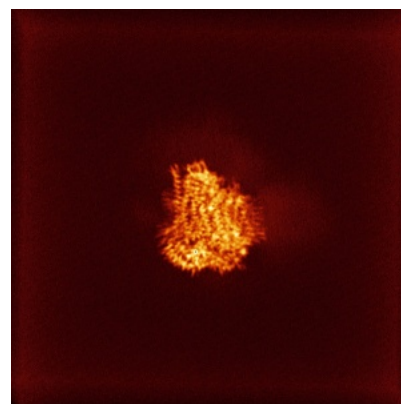
6.4.2 Raw map



X



Y

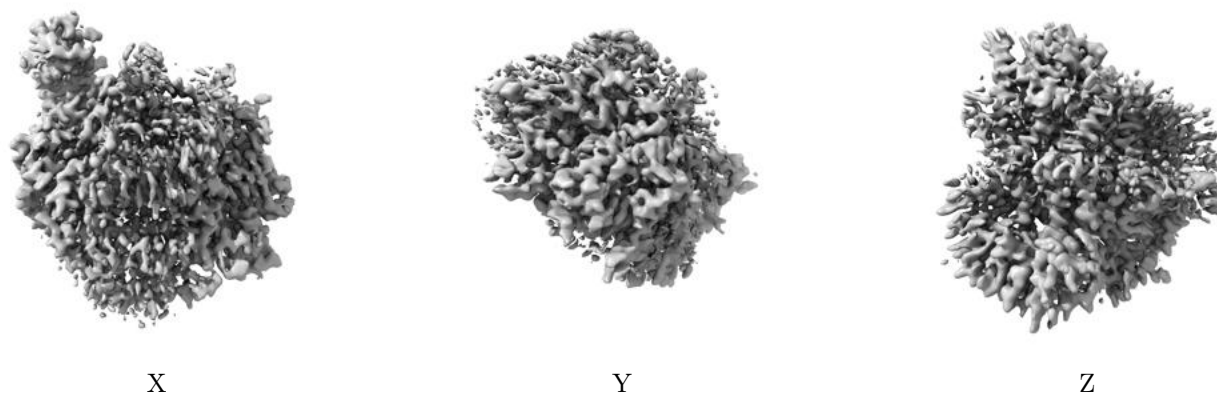


Z

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 0.41. 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.

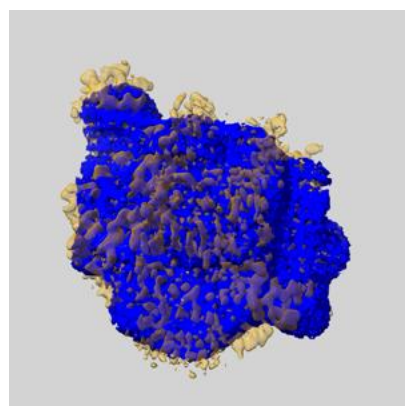
6.6 Mask visualisation [i](#)

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

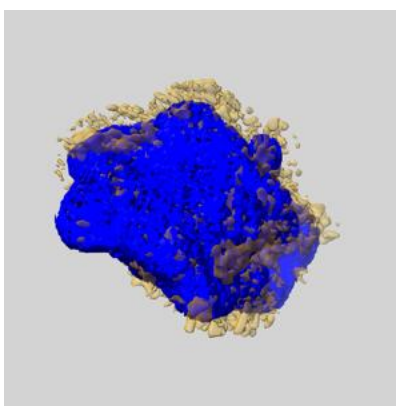
A mask typically either:

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

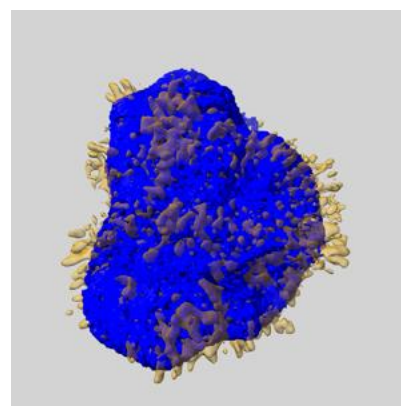
6.6.1 emd_10848_msk_1.map [i](#)



X



Y

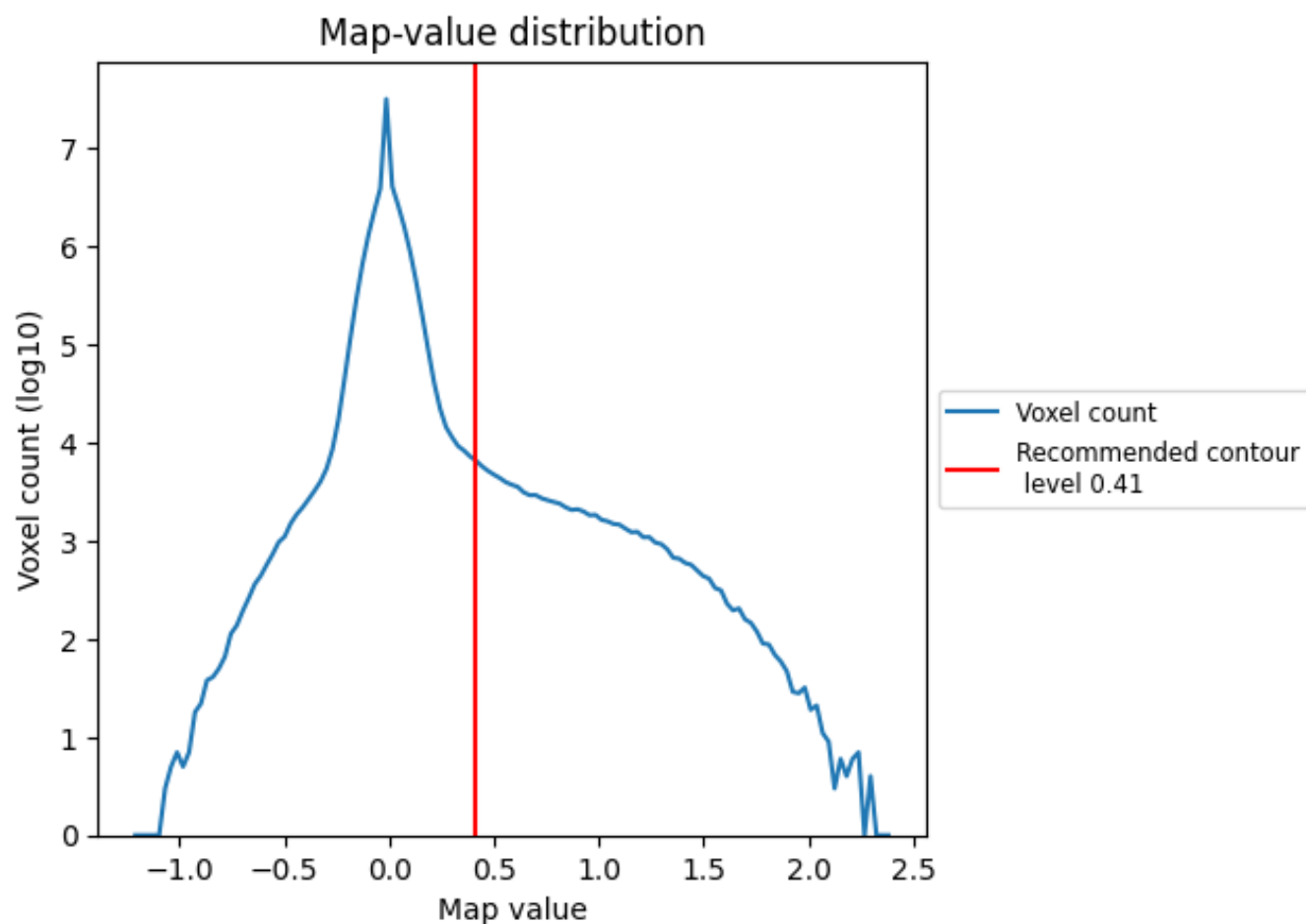


Z

7 Map analysis [i](#)

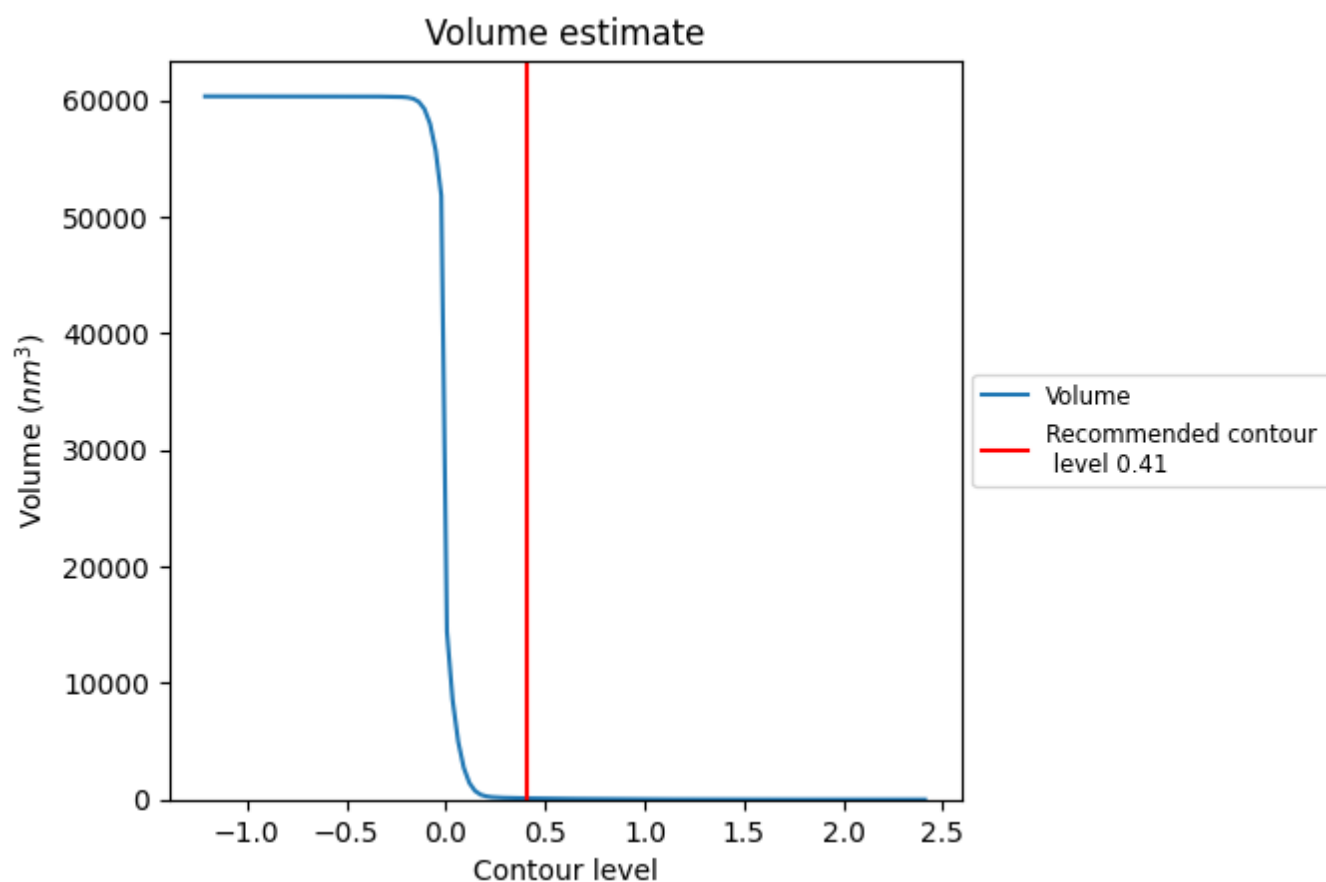
This section contains the results of statistical analysis of the map.

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.

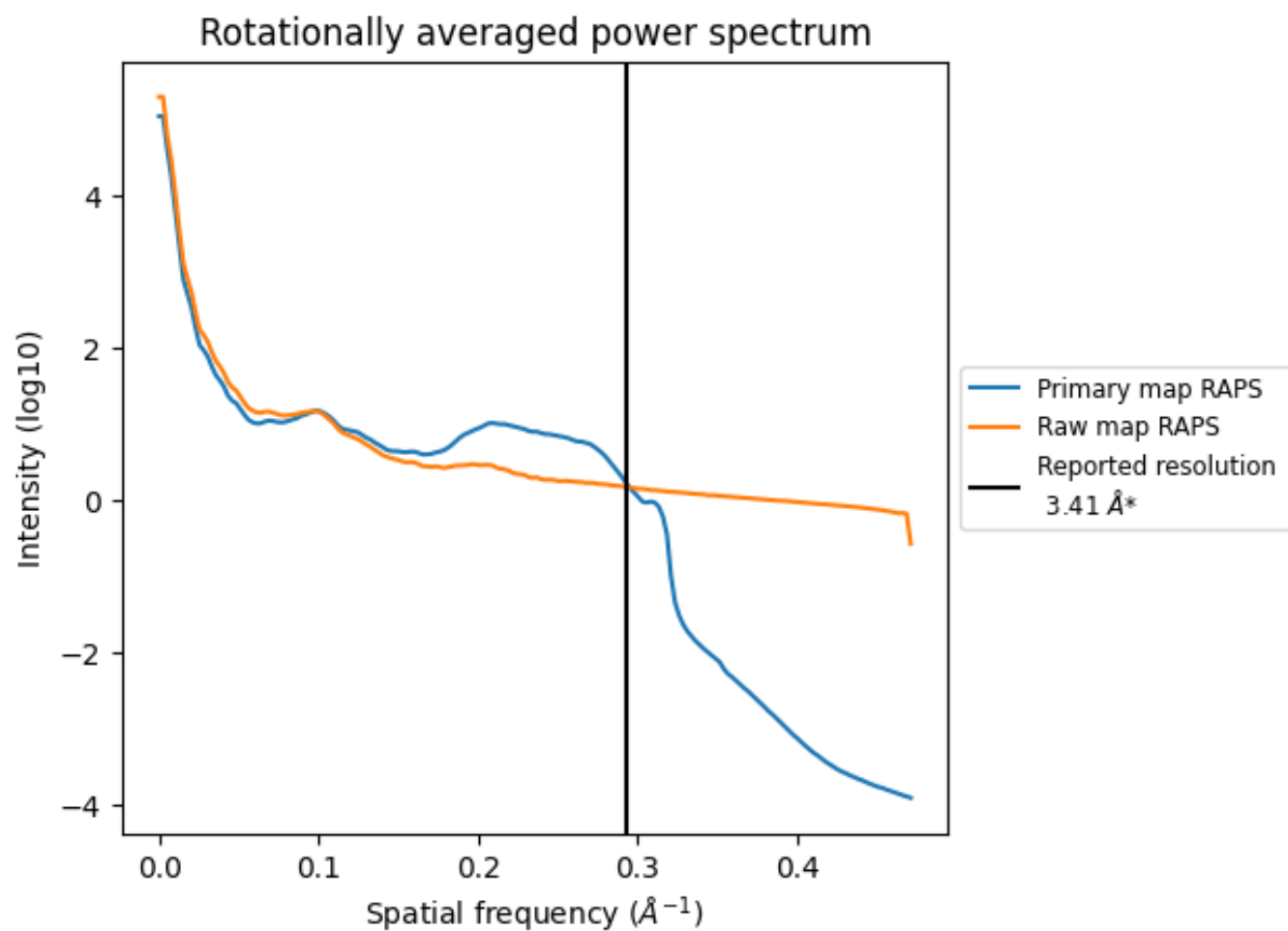
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 $0.293 \text{ \AA}^{-1}$

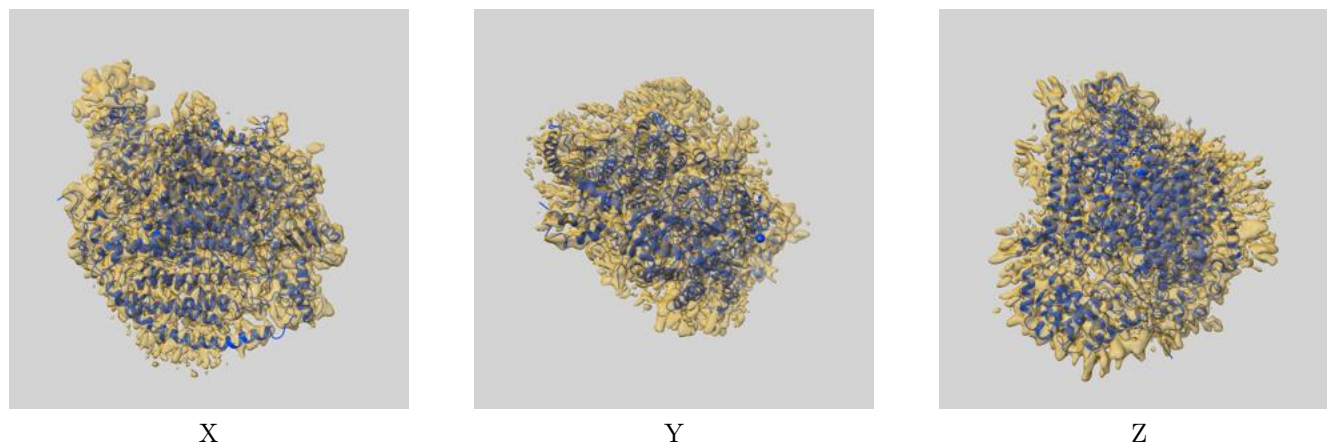
8 Fourier-Shell correlation

This section was not generated.

9 Map-model fit [i](#)

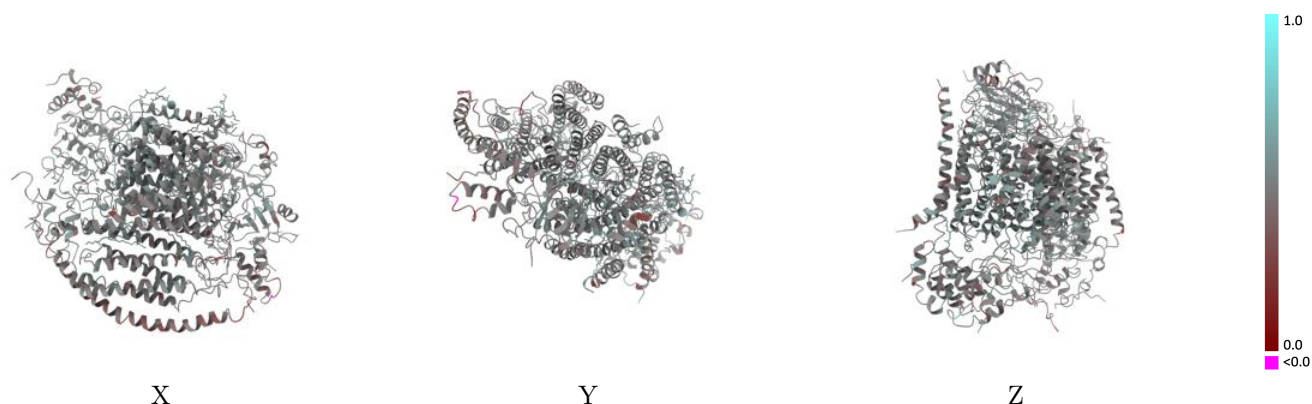
This section contains information regarding the fit between EMDB map EMD-10848 and PDB model 6YMY. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



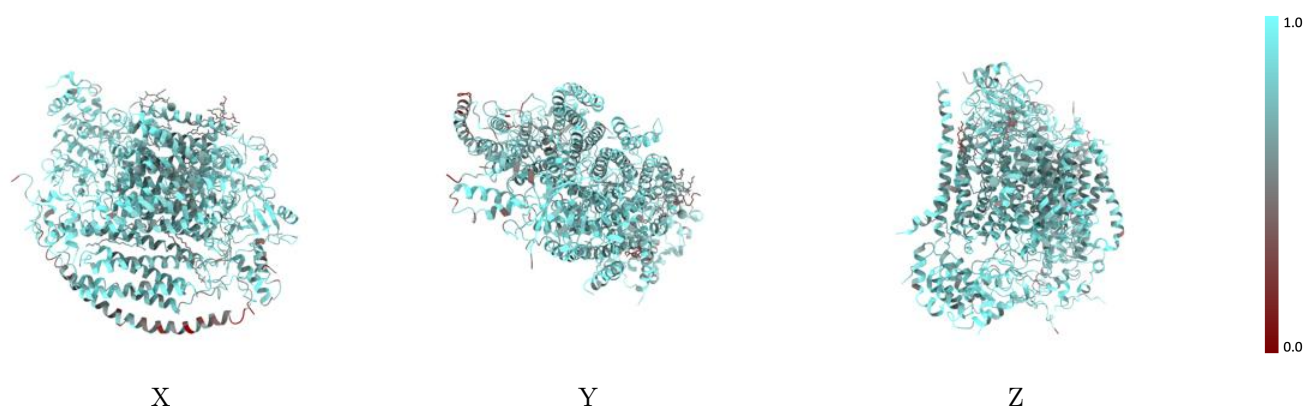
The images above show the 3D surface view of the map at the recommended contour level 0.41 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



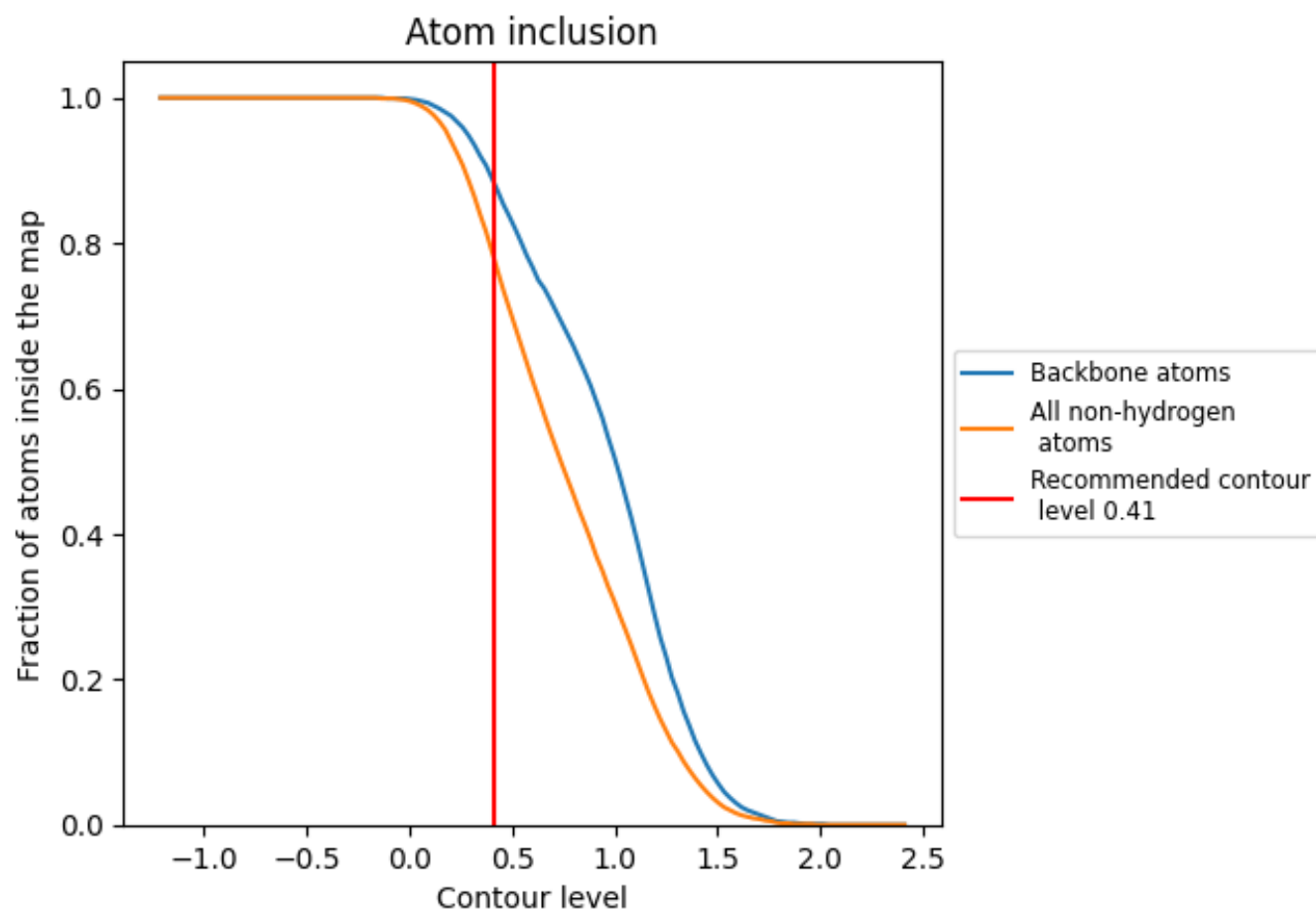
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.41).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.41) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.4830
a	0.7970	0.5060
b	0.8020	0.4950
c	0.7870	0.4830
d	0.8210	0.4760
e	0.7810	0.4710
f	0.8270	0.4750
g	0.8420	0.4810
h	0.8060	0.4900
i	0.7710	0.4730
j	0.7430	0.4430
k	0.5830	0.4130
m	0.7460	0.4720

1.0

0.0

<0.0