Full wwPDB EM Validation Report (i)

Aug 4, 2026 – 09:32 AM EDT

PDB ID	:	8UCN / pdb_00008ucn
EMDB ID	:	EMD-42132
Title	:	Komagataella pastoris Cytochrome c oxidase in complex with human VMAT2 and Histamine
Authors	:	Ye, J.; Liu, B.; Li, W.
Deposited on	:	2023-09-26
Resolution	:	3.31 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

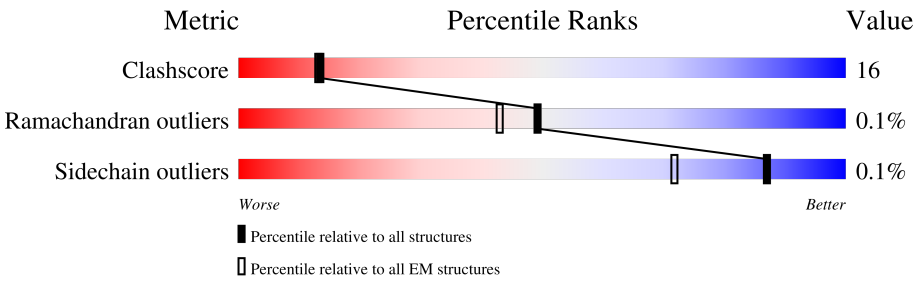
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

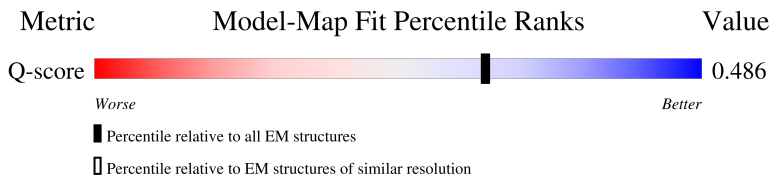
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.31 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	14550 (2.81 - 3.81)

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

Mol	Chain	Length	Quality of chain
1	A	514	5% 39% 32% 29%
2	a	535	67% 32%
3	b	236	• 72% 27%
4	c	268	5% 69% 30% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	d	117	68% 32%
6	e	124	78% 22%
7	f	100	72% 28%
8	g	58	78% 21%
9	h	48	79% 21%
10	i	56	80% 20%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 15312 atoms, of which 9 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 Synaptic vesicular amine transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	363	2713	1810	419	456	28	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	535	4169	2788	646	717	18	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	4	ILE	MET	conflict	UNP F2R0K8
a	16	ILE	MET	conflict	UNP F2R0K8
a	22	ILE	MET	conflict	UNP F2R0K8
a	33	ILE	MET	conflict	UNP F2R0K8
a	37	ILE	MET	conflict	UNP F2R0K8
a	49	ILE	MET	conflict	UNP F2R0K8
a	78	ILE	MET	conflict	UNP F2R0K8
a	85	LEU	THR	conflict	UNP F2R0K8
a	90	ILE	MET	conflict	UNP F2R0K8
a	121	ILE	MET	conflict	UNP F2R0K8
a	150	ILE	MET	conflict	UNP F2R0K8
a	158	ILE	MET	conflict	UNP F2R0K8
a	165	ILE	MET	conflict	UNP F2R0K8
a	168	ILE	MET	conflict	UNP F2R0K8
a	177	ILE	MET	conflict	UNP F2R0K8
a	232	ILE	MET	conflict	UNP F2R0K8
a	237	LEU	THR	conflict	UNP F2R0K8
a	250	ILE	MET	conflict	UNP F2R0K8
a	256	ILE	MET	conflict	UNP F2R0K8
a	260	ILE	MET	conflict	UNP F2R0K8
a	273	ILE	MET	conflict	UNP F2R0K8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
a	314	ILE	MET	conflict	UNP F2R0K8
a	320	ILE	MET	conflict	UNP F2R0K8
a	322	ILE	MET	conflict	UNP F2R0K8
a	334	ILE	MET	conflict	UNP F2R0K8
a	367	ILE	MET	conflict	UNP F2R0K8
a	401	LEU	THR	conflict	UNP F2R0K8
a	402	ILE	MET	conflict	UNP F2R0K8
a	421	ILE	MET	conflict	UNP F2R0K8
a	442	ILE	MET	conflict	UNP F2R0K8
a	455	ILE	MET	conflict	UNP F2R0K8
a	462	ILE	MET	conflict	UNP F2R0K8
a	464	ILE	MET	conflict	UNP F2R0K8
a	465	ILE	MET	conflict	UNP F2R0K8
a	510	ILE	MET	conflict	UNP F2R0K8
a	515	ILE	MET	conflict	UNP F2R0K8
a	524	LEU	THR	conflict	UNP F2R0K8

- Molecule 3 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	b	236	1896	1247	287	352	10	0	0

- Molecule 4 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	c	268	2163	1460	337	354	12	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	45	ILE	MET	conflict	UNP F2R0J6
c	55	ILE	MET	conflict	UNP F2R0J6
c	62	ILE	MET	conflict	UNP F2R0J6
c	81	ILE	MET	conflict	UNP F2R0J6
c	89	ILE	MET	conflict	UNP F2R0J6
c	101	ILE	MET	conflict	UNP F2R0J6
c	120	ILE	MET	conflict	UNP F2R0J6
c	129	ILE	MET	conflict	UNP F2R0J6
c	132	ILE	MET	conflict	UNP F2R0J6
c	143	ILE	MET	conflict	UNP F2R0J6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
c	247	ILE	MET	conflict	UNP F2R0J6
c	248	LEU	THR	conflict	UNP F2R0J6

- Molecule 5 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	d	117	910	576	147	183	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	e	124	1027	659	176	191	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	f	100	835	531	134	168	2	0	0

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	g	58	465	309	74	81	1	0	0

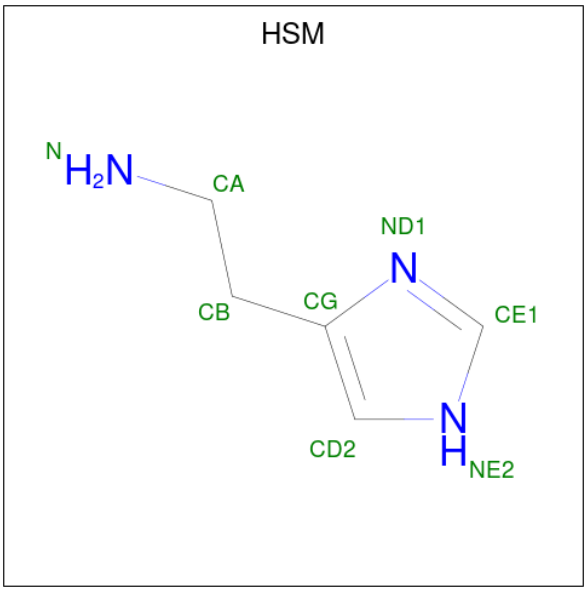
- Molecule 9 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	h	48	386	260	65	59	2	0	0

- Molecule 10 is a protein called Cytochrome c oxidase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	i	56	460	302	83	75	0	0

- Molecule 11 is HISTAMINE (CCD ID: HSM) (formula: $C_5H_9N_3$) (labeled as "Ligand of Interest" by depositor).

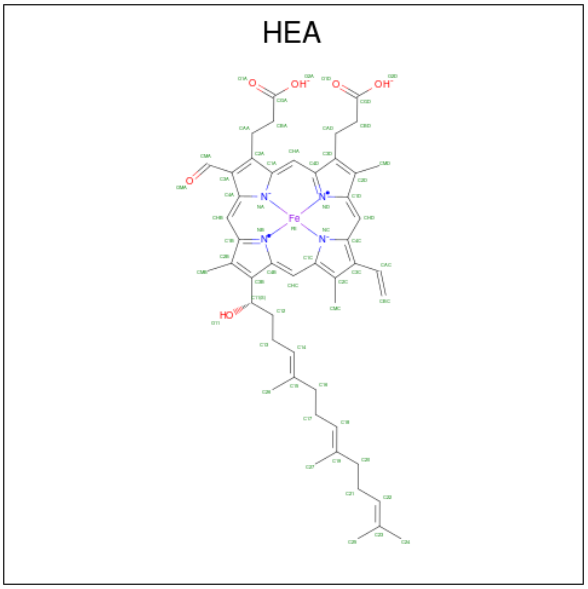


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
11	A	1	17	5	9	3	0

- Molecule 12 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

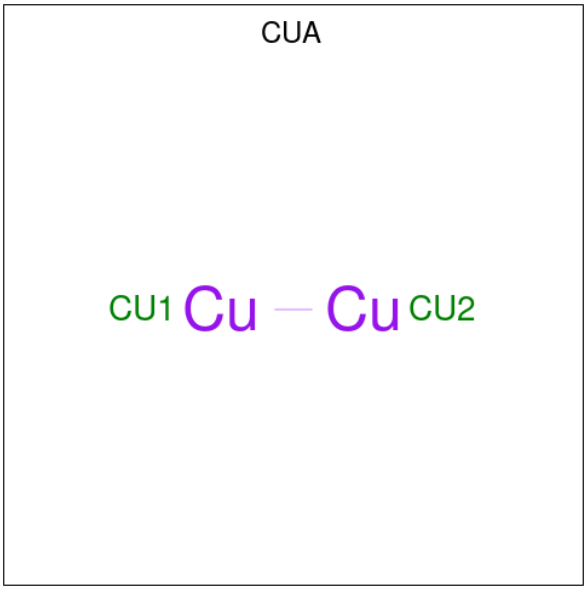
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
12	a	1	1	1	0

- Molecule 13 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



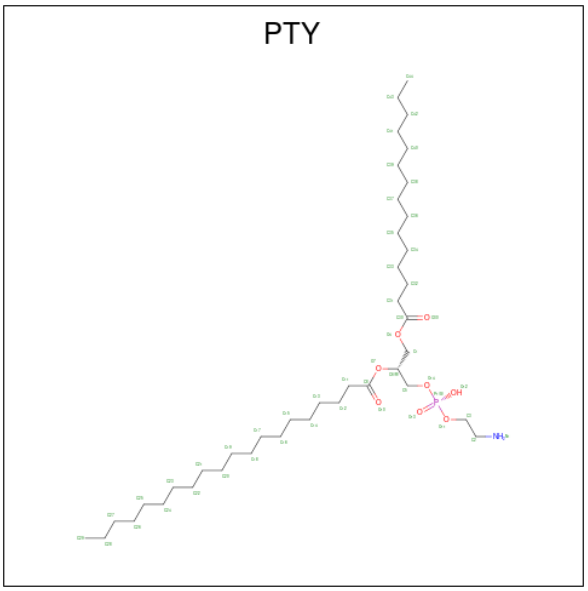
Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 60	C 49	Fe 1	N 4	O 6	0
13	a	1	Total 60	C 49	Fe 1	N 4	O 6	0

- Molecule 14 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	c	1	Total	C	N	O	P	0
			34	24	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
			33	23	1	8	1	
15	i	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

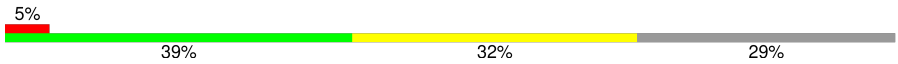
Mol	Chain	Residues	Atoms		AltConf
16	d	1	Total	Zn	0
			1	1	

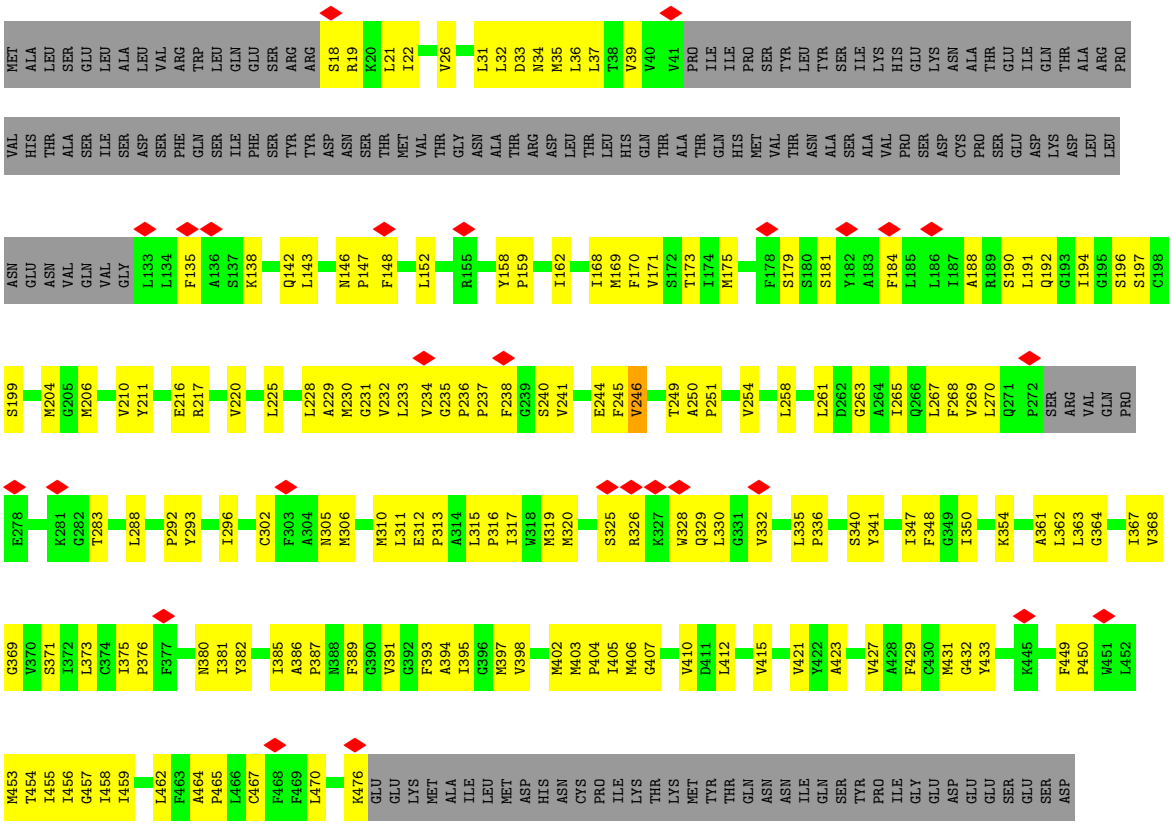
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Synaptic vesicular amine transporter

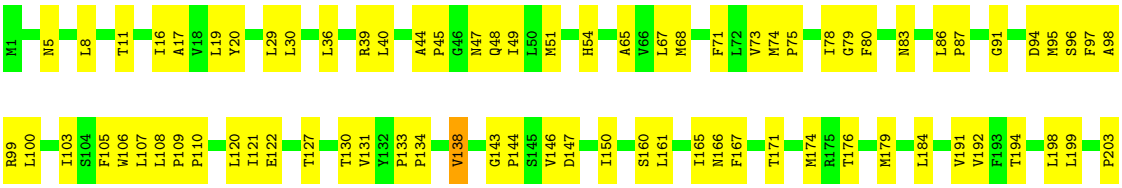
Chain A:

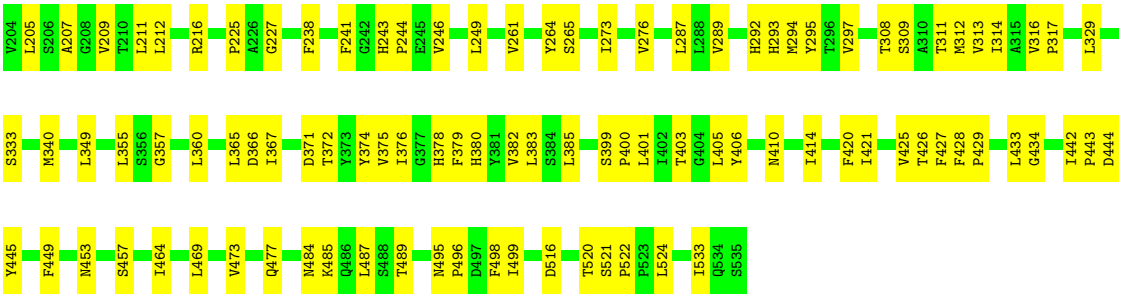




• Molecule 2: Cytochrome c oxidase subunit 1

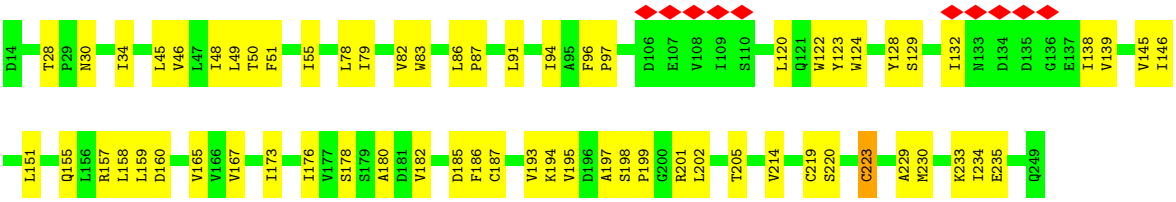
Chain a:





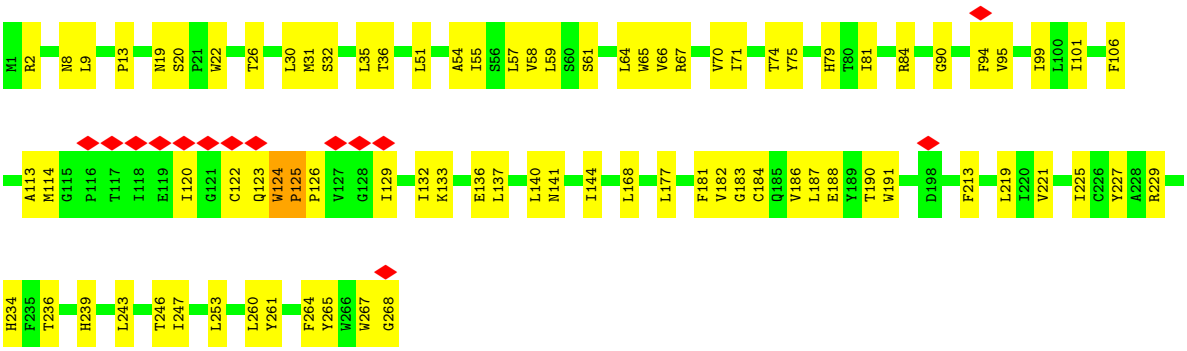
• Molecule 3: Cytochrome c oxidase subunit 2

Chain b:



• Molecule 4: Cytochrome c oxidase subunit 3

Chain c:

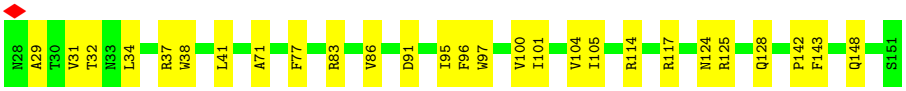


• Molecule 5: Cytochrome c oxidase subunit 4

Chain d:

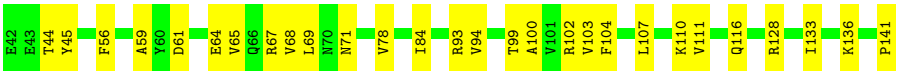
• Molecule 6: Cytochrome c oxidase subunit 5

Chain e:



• Molecule 7: Cytochrome c oxidase subunit 6

Chain f:

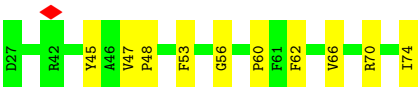


• Molecule 8: Cytochrome c oxidase subunit 7

Chain g:

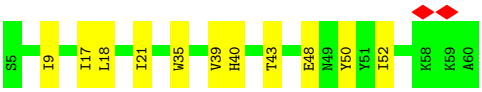
• Molecule 9: Cytochrome c oxidase subunit 8

Chain h:



• Molecule 10: Cytochrome c oxidase subunit 9

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84534	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.812	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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: CUA, HEA, PTY, HSM, ZN, CU

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	0.16	0/2776	0.40	1/3770 (0.0%)
2	a	0.23	0/4300	0.45	1/5878 (0.0%)
3	b	0.21	0/1947	0.47	0/2664
4	c	0.23	0/2234	0.47	0/3057
5	d	0.23	0/928	0.57	1/1260 (0.1%)
6	e	0.18	0/1055	0.41	0/1430
7	f	0.20	0/851	0.42	0/1148
8	g	0.19	0/478	0.45	1/647 (0.2%)
9	h	0.21	0/400	0.46	0/541
10	i	0.16	0/473	0.39	0/638
All	All	0.21	0/15442	0.45	4/21033 (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
4	c	0	1
6	e	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	VAL	N-CA-C	-7.66	105.09	111.91
2	a	138	VAL	N-CA-C	-6.01	106.90	112.43
5	d	52	ALA	N-CA-C	-5.38	107.97	114.75
8	g	9	ILE	N-CA-C	-5.28	107.32	112.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	c	124	TRP	Peptide
6	e	143	PHE	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	2713	0	2851	148	0
2	a	4169	0	4191	156	0
3	b	1896	0	1865	48	0
4	c	2163	0	2198	75	0
5	d	910	0	887	37	0
6	e	1027	0	1007	19	0
7	f	835	0	794	25	0
8	g	465	0	471	13	0
9	h	386	0	391	12	0
10	i	460	0	473	9	0
11	A	8	9	9	0	0
12	a	1	0	0	0	0
13	a	120	0	108	19	0
14	b	2	0	0	0	0
15	c	74	0	94	9	0
15	e	33	0	39	0	0
15	i	40	0	53	1	0
16	d	1	0	0	0	0
All	All	15303	9	15431	494	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 16.

All (494) 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:363:LEU:HD22	1:A:397:MET:HE1	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:349:LEU:HD13	2:a:385:LEU:HD23	1.49	0.92
2:a:51:MET:HE3	9:h:74:ILE:HB	1.53	0.91
15:c:301:PTY:H151	15:c:301:PTY:H322	1.54	0.90
1:A:35:MET:HE2	1:A:238:PHE:HB2	1.61	0.82
1:A:142:GLN:HG3	1:A:197:SER:HB2	1.61	0.82
2:a:533:ILE:HG22	5:d:100:LEU:HD23	1.62	0.80
2:a:367:ILE:HD11	3:b:34:ILE:HD11	1.64	0.78
1:A:204:MET:HE2	1:A:403:MET:HE3	1.65	0.77
2:a:365:LEU:HD23	3:b:34:ILE:HG23	1.67	0.77
1:A:175:MET:HE1	1:A:184:PHE:HD2	1.55	0.72
1:A:181:SER:HB3	1:A:184:PHE:HD1	1.55	0.72
1:A:21:LEU:HD13	1:A:263:GLY:HA3	1.71	0.71
4:c:126:PRO:HG2	4:c:129:ILE:HD12	1.73	0.71
2:a:484:ASN:HA	2:a:487:LEU:HD13	1.73	0.71
2:a:449:PHE:O	2:a:453:ASN:ND2	2.25	0.69
2:a:264:TYR:HB2	2:a:340:MET:HE2	1.73	0.69
4:c:66:VAL:HG11	15:c:302:PTY:H322	1.74	0.69
1:A:329:GLN:HA	1:A:332:VAL:HG22	1.73	0.68
10:i:18:LEU:HD21	15:i:101:PTY:H331	1.76	0.68
13:a:603:HEA:H253	3:b:48:ILE:HD13	1.75	0.68
2:a:36:LEU:HD13	2:a:464:ILE:HD12	1.76	0.67
2:a:65:ALA:HB2	13:a:602:HEA:HAD1	1.77	0.67
4:c:35:LEU:HD13	8:g:51:THR:HG21	1.77	0.67
2:a:379:PHE:CG	13:a:603:HEA:HMD2	2.29	0.66
1:A:31:LEU:HD11	1:A:234:VAL:HG11	1.78	0.66
1:A:362:LEU:HD11	1:A:464:ALA:HB1	1.78	0.66
3:b:198:SER:OG	3:b:201:ARG:HG2	1.96	0.65
10:i:48:GLU:O	10:i:52:ILE:HG13	1.97	0.65
2:a:121:ILE:HD11	2:a:144:PRO:O	1.97	0.65
4:c:26:THR:HG22	4:c:61:SER:HB3	1.78	0.65
2:a:161:LEU:HD11	2:a:199:LEU:HD23	1.77	0.65
2:a:355:LEU:HD22	3:b:45:LEU:HD22	1.78	0.65
2:a:179:MET:CE	2:a:184:LEU:HD23	2.27	0.64
2:a:96:SER:OG	2:a:174:MET:SD	2.54	0.64
5:d:140:PRO:HB2	5:d:157:LEU:HD11	1.78	0.64
2:a:244:PRO:HG3	2:a:287:LEU:HD23	1.77	0.64
1:A:179:SER:HB2	1:A:184:PHE:HB3	1.79	0.64
2:a:264:TYR:HB2	2:a:340:MET:CE	2.28	0.64
2:a:533:ILE:HG21	5:d:100:LEU:HB3	1.80	0.64
2:a:44:ALA:HB3	2:a:48:GLN:HE22	1.63	0.63
1:A:143:LEU:HD11	1:A:431:MET:HE2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:182:VAL:HG13	4:c:213:PHE:CZ	2.34	0.63
2:a:316:VAL:HB	2:a:317:PRO:HD3	1.81	0.63
3:b:79:ILE:HG12	3:b:83:TRP:CZ3	2.34	0.63
9:h:47:VAL:HB	9:h:48:PRO:HD3	1.80	0.63
1:A:319:MET:HE3	1:A:330:LEU:HD23	1.81	0.63
6:e:77:PHE:HD1	6:e:83:ARG:HH12	1.47	0.63
5:d:113:LEU:HD23	5:d:156:LYS:HB3	1.80	0.62
3:b:96:PHE:HB3	3:b:97:PRO:HD3	1.80	0.62
7:f:136:LYS:HG3	7:f:141:PRO:HG3	1.81	0.62
1:A:158:TYR:HB2	1:A:159:PRO:HD3	1.82	0.62
2:a:376:ILE:HG23	2:a:380:HIS:NE2	2.14	0.62
4:c:229:ARG:HG2	4:c:234:HIS:HB2	1.81	0.62
2:a:357:GLY:HA3	13:a:603:HEA:HMB2	1.81	0.61
4:c:64:LEU:HD23	4:c:67:ARG:HD3	1.81	0.61
5:d:115:ASP:O	5:d:121:ARG:NH1	2.34	0.61
1:A:305:ASN:ND2	1:A:429:PHE:HA	2.15	0.61
1:A:37:LEU:HD12	1:A:138:LYS:HZ3	1.65	0.61
2:a:30:LEU:CD2	9:h:60:PRO:HD3	2.30	0.61
1:A:37:LEU:HD12	1:A:138:LYS:NZ	2.15	0.60
4:c:144:ILE:HG23	4:c:177:LEU:HD22	1.83	0.60
4:c:261:TYR:HA	4:c:265:TYR:HD2	1.65	0.60
1:A:250:ALA:HB3	1:A:251:PRO:HD3	1.82	0.60
4:c:221:VAL:O	4:c:225:ILE:HG13	2.01	0.60
1:A:158:TYR:O	1:A:162:ILE:HG13	2.02	0.60
4:c:113:ALA:HA	4:c:124:TRP:NE1	2.16	0.60
1:A:306:MET:CE	1:A:432:GLY:HA2	2.32	0.60
5:d:133:HIS:HE1	5:d:148:CYS:SG	2.25	0.60
4:c:122:CYS:O	4:c:123:GLN:HG3	2.02	0.59
7:f:111:VAL:CG1	7:f:116:GLN:HB2	2.32	0.59
1:A:170:PHE:O	1:A:173:THR:HG22	2.03	0.59
2:a:86:LEU:HB3	2:a:87:PRO:HD3	1.85	0.58
5:d:104:ARG:HD2	5:d:105:LYS:O	2.03	0.58
2:a:293:HIS:NE2	13:a:603:HEA:HHA	2.17	0.58
4:c:2:ARG:NH2	5:d:115:ASP:OD2	2.37	0.58
7:f:111:VAL:HG11	7:f:116:GLN:HB2	1.86	0.58
1:A:168:ILE:HA	1:A:171:VAL:HG12	1.85	0.58
5:d:140:PRO:HB2	5:d:157:LEU:CD1	2.33	0.58
7:f:100:ALA:HB1	7:f:133:ILE:HD13	1.85	0.58
2:a:40:LEU:HB3	2:a:49:ILE:CD1	2.34	0.58
3:b:120:LEU:HD23	3:b:180:ALA:HB3	1.86	0.58
8:g:43:SER:O	8:g:47:THR:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:399:SER:HB3	2:a:400:PRO:HD3	1.85	0.58
2:a:127:THR:OG1	2:a:131:VAL:HG12	2.04	0.58
2:a:74:MET:HB2	2:a:75:PRO:HD3	1.86	0.57
2:a:428:PHE:HB3	2:a:429:PRO:HD3	1.86	0.57
7:f:99:THR:O	7:f:103:VAL:HG23	2.04	0.57
1:A:138:LYS:HD2	1:A:192:GLN:HB3	1.87	0.57
3:b:165:VAL:CG2	3:b:234:ILE:HG12	2.34	0.57
1:A:380:ASN:HD22	1:A:382:TYR:HD2	1.53	0.57
2:a:349:LEU:HD13	2:a:385:LEU:CD2	2.29	0.57
3:b:86:LEU:HB2	3:b:87:PRO:HD3	1.86	0.57
4:c:113:ALA:HA	4:c:124:TRP:CE2	2.40	0.57
1:A:326:ARG:O	1:A:330:LEU:HG	2.04	0.57
4:c:133:LYS:HD2	4:c:136:GLU:OE2	2.05	0.57
1:A:302:CYS:O	1:A:306:MET:HG2	2.05	0.56
2:a:360:LEU:HD11	2:a:374:TYR:CD2	2.40	0.56
1:A:373:LEU:HD21	1:A:457:GLY:HA3	1.88	0.56
2:a:520:THR:HG21	2:a:524:LEU:CD2	2.35	0.56
5:d:60:LEU:O	5:d:78:THR:HA	2.05	0.56
2:a:372:THR:HG22	2:a:434:GLY:HA2	1.87	0.56
7:f:67:ARG:O	7:f:71:ASN:ND2	2.38	0.56
1:A:407:GLY:HA2	1:A:410:VAL:HG12	1.86	0.56
3:b:78:LEU:O	3:b:82:VAL:HG23	2.05	0.56
4:c:186:VAL:HG13	4:c:187:LEU:HD12	1.86	0.56
1:A:292:PRO:O	1:A:296:ILE:HG12	2.05	0.56
1:A:348:PHE:CE2	1:A:397:MET:HE2	2.41	0.56
2:a:73:VAL:CG1	2:a:249:LEU:HD22	2.35	0.56
2:a:121:ILE:CD1	2:a:144:PRO:HB2	2.35	0.56
6:e:96:PHE:O	6:e:100:VAL:HG23	2.06	0.56
4:c:70:VAL:O	4:c:74:THR:HG22	2.06	0.56
1:A:240:SER:HB3	1:A:245:PHE:CG	2.41	0.55
2:a:122:GLU:OE2	2:a:143:GLY:HA3	2.06	0.55
2:a:147:ASP:OD1	2:a:216:ARG:NH1	2.39	0.55
2:a:207:ALA:O	2:a:211:LEU:HD13	2.06	0.55
1:A:231:GLY:HA2	1:A:234:VAL:HG12	1.87	0.55
1:A:348:PHE:CE2	1:A:397:MET:HG2	2.42	0.55
4:c:67:ARG:O	4:c:71:ILE:HG13	2.06	0.55
2:a:357:GLY:HA3	13:a:603:HEA:CMB	2.36	0.55
10:i:35:TRP:CZ3	10:i:39:VAL:HG11	2.41	0.55
2:a:36:LEU:HB2	2:a:464:ILE:HD11	1.89	0.55
4:c:51:LEU:O	4:c:55:ILE:HG13	2.07	0.55
1:A:315:LEU:O	1:A:319:MET:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:O	1:A:476:LYS:HB2	2.07	0.55
2:a:121:ILE:HD11	2:a:144:PRO:HB2	1.89	0.55
2:a:294:MET:HE3	2:a:297:VAL:HG21	1.89	0.54
3:b:165:VAL:HG21	3:b:234:ILE:HG12	1.88	0.54
5:d:126:THR:C	5:d:133:HIS:HB3	2.31	0.54
1:A:175:MET:HE1	1:A:184:PHE:CD2	2.40	0.54
2:a:294:MET:CE	2:a:297:VAL:HG21	2.37	0.54
1:A:387:PRO:O	1:A:391:VAL:HG23	2.07	0.54
2:a:67:LEU:O	2:a:71:PHE:HB2	2.08	0.54
3:b:187:CYS:SG	3:b:194:LYS:HG3	2.47	0.54
8:g:40:LEU:O	8:g:44:VAL:HG23	2.07	0.54
1:A:240:SER:OG	1:A:241:VAL:N	2.40	0.54
1:A:347:ILE:HG22	1:A:348:PHE:CD1	2.41	0.54
2:a:533:ILE:CG2	5:d:100:LEU:HB3	2.37	0.54
4:c:74:THR:HG23	4:c:75:TYR:CD1	2.42	0.54
2:a:225:PRO:HG3	3:b:199:PRO:HB2	1.88	0.54
4:c:54:ALA:O	4:c:58:VAL:HG23	2.07	0.54
2:a:110:PRO:HB3	4:c:31:MET:HB2	1.88	0.54
2:a:499:ILE:HD13	7:f:102:ARG:HG3	1.90	0.54
4:c:94:PHE:CZ	15:c:301:PTY:H131	2.42	0.54
2:a:309:SER:O	2:a:313:VAL:HG23	2.07	0.54
1:A:315:LEU:HB3	1:A:316:PRO:HD3	1.89	0.54
2:a:19:LEU:HB3	2:a:105:PHE:CZ	2.42	0.54
3:b:146:ILE:HG22	3:b:160:ASP:O	2.08	0.54
1:A:368:VAL:HB	1:A:394:ALA:CB	2.37	0.54
1:A:373:LEU:CD2	1:A:457:GLY:HA3	2.38	0.54
1:A:236:PRO:HB2	1:A:237:PRO:CD	2.38	0.53
3:b:165:VAL:HG22	3:b:233:LYS:O	2.08	0.53
2:a:150:ILE:CG2	2:a:209:VAL:HB	2.37	0.53
2:a:165:ILE:HG21	4:c:94:PHE:CE2	2.43	0.53
2:a:91:GLY:HA3	2:a:176:THR:CG2	2.38	0.53
1:A:293:TYR:HD1	1:A:470:LEU:HD23	1.74	0.53
1:A:449:PHE:HB3	1:A:450:PRO:HD3	1.91	0.53
3:b:176:ILE:CG2	3:b:202:LEU:HD12	2.39	0.53
5:d:51:ILE:HD11	5:d:92:ILE:CD1	2.38	0.53
1:A:402:MET:O	1:A:405:ILE:HG22	2.08	0.53
1:A:283:THR:HB	1:A:288:LEU:HD11	1.90	0.53
1:A:254:VAL:O	1:A:258:LEU:HD23	2.09	0.53
1:A:283:THR:HG23	1:A:415:VAL:HG13	1.91	0.53
2:a:54:HIS:ND1	2:a:443:PRO:HG2	2.24	0.53
13:a:602:HEA:H122	13:a:602:HEA:HHC	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:64:GLU:O	7:f:68:VAL:HG23	2.09	0.53
1:A:306:MET:HE2	1:A:432:GLY:HA2	1.91	0.53
2:a:65:ALA:HB2	13:a:602:HEA:CAD	2.37	0.53
2:a:383:LEU:HD13	13:a:602:HEA:HAC	1.90	0.53
3:b:129:SER:O	3:b:132:ILE:HD11	2.09	0.52
4:c:32:SER:HB2	8:g:47:THR:HG21	1.91	0.52
4:c:84:ARG:HD3	4:c:239:HIS:CD2	2.45	0.52
5:d:54:VAL:HG11	5:d:83:TYR:HE1	1.74	0.52
1:A:216:GLU:O	1:A:220:VAL:HG22	2.09	0.52
2:a:44:ALA:HB3	2:a:48:GLN:NE2	2.23	0.52
13:a:603:HEA:H253	3:b:48:ILE:CD1	2.39	0.52
4:c:79:HIS:N	5:d:81:GLU:OE2	2.42	0.52
4:c:94:PHE:CE2	15:c:301:PTY:H131	2.43	0.52
1:A:169:MET:HE1	1:A:199:SER:OG	2.08	0.52
1:A:362:LEU:CD1	1:A:464:ALA:HB1	2.39	0.52
2:a:165:ILE:HD13	4:c:94:PHE:CE2	2.45	0.52
4:c:168:LEU:HB3	4:c:227:TYR:HE1	1.74	0.52
1:A:393:PHE:CE2	1:A:397:MET:HE3	2.44	0.52
2:a:433:LEU:CD2	2:a:449:PHE:HB3	2.40	0.52
7:f:78:VAL:HG21	10:i:9:ILE:HD13	1.92	0.52
1:A:386:ALA:HB3	1:A:387:PRO:HD3	1.91	0.52
1:A:328:TRP:O	1:A:332:VAL:HG13	2.10	0.52
1:A:335:LEU:HB3	1:A:336:PRO:HD3	1.92	0.52
2:a:160:SER:HB3	2:a:198:LEU:HD22	1.91	0.52
2:a:469:LEU:O	2:a:473:VAL:HG23	2.09	0.51
2:a:261:VAL:HG13	2:a:329:LEU:HD12	1.90	0.51
10:i:40:HIS:O	10:i:43:THR:OG1	2.26	0.51
4:c:229:ARG:O	4:c:234:HIS:HB2	2.10	0.51
2:a:120:LEU:O	9:h:70:ARG:NH1	2.41	0.51
2:a:171:THR:HG21	2:a:192:VAL:HG22	1.92	0.51
6:e:31:VAL:HG13	6:e:71:ALA:HB2	1.93	0.51
1:A:22:ILE:HD11	1:A:206:MET:HE2	1.93	0.51
1:A:34:ASN:ND2	1:A:228:LEU:HD12	2.25	0.51
4:c:95:VAL:O	4:c:99:ILE:HG13	2.11	0.51
8:g:34:ILE:HB	8:g:35:PRO:HD3	1.93	0.51
1:A:148:PHE:CE2	1:A:152:LEU:HD11	2.46	0.51
1:A:225:LEU:HD11	1:A:403:MET:HG3	1.93	0.51
2:a:133:PRO:HG2	2:a:134:PRO:HD3	1.93	0.51
1:A:143:LEU:HA	1:A:146:ASN:ND2	2.26	0.51
2:a:95:MET:HE1	2:a:167:PHE:CE1	2.46	0.51
2:a:30:LEU:HD23	9:h:60:PRO:HD3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:520:THR:HG23	2:a:522:PRO:O	2.11	0.51
1:A:455:ILE:O	1:A:459:ILE:HG13	2.11	0.51
13:a:602:HEA:H122	13:a:602:HEA:CHC	2.41	0.51
1:A:340:SER:OG	1:A:393:PHE:N	2.43	0.50
2:a:244:PRO:HG3	2:a:287:LEU:CD2	2.41	0.50
4:c:190:THR:HG23	4:c:191:TRP:CD1	2.46	0.50
1:A:423:ALA:O	1:A:427:VAL:HG23	2.10	0.50
5:d:140:PRO:C	5:d:157:LEU:HD11	2.36	0.50
3:b:132:ILE:HG12	3:b:138:ILE:HG12	1.92	0.50
6:e:97:TRP:O	6:e:101:ILE:HG13	2.12	0.50
6:e:100:VAL:O	6:e:104:VAL:HG23	2.12	0.50
2:a:51:MET:CE	9:h:74:ILE:HB	2.35	0.50
2:a:171:THR:HG21	2:a:192:VAL:CG2	2.41	0.50
3:b:122:TRP:HA	3:b:230:MET:CE	2.42	0.50
6:e:34:LEU:HD22	6:e:38:TRP:HE3	1.77	0.50
5:d:133:HIS:NE2	5:d:150:GLU:HB3	2.25	0.50
5:d:137:TRP:O	5:d:138:LEU:HD23	2.11	0.50
1:A:36:LEU:O	1:A:39:VAL:HG23	2.11	0.50
2:a:383:LEU:HG	13:a:603:HEA:HBC2	1.93	0.50
4:c:26:THR:HG22	4:c:61:SER:CB	2.41	0.50
7:f:78:VAL:HG21	10:i:9:ILE:CD1	2.41	0.50
4:c:187:LEU:HA	4:c:190:THR:HG22	1.94	0.50
1:A:236:PRO:HB2	1:A:237:PRO:HD3	1.92	0.49
1:A:267:LEU:HD23	1:A:268:PHE:CZ	2.47	0.49
4:c:183:GLY:O	4:c:186:VAL:HG12	2.12	0.49
4:c:229:ARG:HG2	4:c:234:HIS:CB	2.41	0.49
15:c:301:PTY:H322	15:c:301:PTY:C15	2.33	0.49
6:e:29:ALA:HA	6:e:32:THR:HG22	1.94	0.49
2:a:5:ASN:O	4:c:19:ASN:ND2	2.46	0.49
4:c:36:THR:CG2	8:g:47:THR:HG22	2.43	0.49
4:c:141:ASN:HB3	4:c:181:PHE:CE2	2.47	0.49
2:a:383:LEU:HG	13:a:603:HEA:CBC	2.43	0.49
1:A:403:MET:HB2	1:A:404:PRO:HD3	1.95	0.49
3:b:128:TYR:HB2	3:b:139:VAL:HG13	1.94	0.49
4:c:137:LEU:HD11	4:c:184:CYS:SG	2.53	0.49
1:A:306:MET:HE1	1:A:432:GLY:HA2	1.95	0.49
4:c:124:TRP:HB3	4:c:125:PRO:HD3	1.94	0.49
4:c:243:LEU:O	4:c:247:ILE:HG13	2.13	0.49
1:A:265:ILE:O	1:A:269:VAL:HB	2.12	0.49
2:a:314:ILE:O	2:a:317:PRO:HD2	2.13	0.49
2:a:349:LEU:HD11	2:a:420:PHE:CE1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:HA	1:A:332:VAL:CG2	2.42	0.49
4:c:260:LEU:O	4:c:264:PHE:HB2	2.11	0.49
1:A:354:LYS:HE3	4:c:268:GLY:C	2.38	0.48
3:b:165:VAL:HG23	3:b:234:ILE:HA	1.94	0.48
5:d:102:ALA:HB1	5:d:130:ALA:HB2	1.95	0.48
1:A:302:CYS:SG	1:A:306:MET:HE3	2.52	0.48
1:A:354:LYS:HD3	4:c:267:TRP:CD1	2.48	0.48
3:b:185:ASP:OD2	3:b:220:SER:HB2	2.13	0.48
4:c:66:VAL:CG1	15:c:302:PTY:H322	2.42	0.48
1:A:350:ILE:HD12	4:c:114:MET:HE1	1.95	0.48
2:a:11:THR:HG23	2:a:98:ALA:CB	2.43	0.48
1:A:373:LEU:O	1:A:376:PRO:HD2	2.13	0.48
3:b:186:PHE:O	3:b:194:LYS:HA	2.12	0.48
4:c:81:ILE:HG13	5:d:84:GLU:OE1	2.13	0.48
7:f:78:VAL:HG12	7:f:110:LYS:HG2	1.94	0.48
1:A:244:GLU:HG3	2:a:273:ILE:CG2	2.43	0.48
3:b:145:VAL:HG11	3:b:229:ALA:HB1	1.94	0.48
6:e:91:ASP:O	6:e:95:ILE:HG13	2.12	0.48
1:A:348:PHE:HE2	1:A:397:MET:HE2	1.78	0.48
2:a:133:PRO:CG	2:a:134:PRO:HD3	2.43	0.48
1:A:363:LEU:O	1:A:367:ILE:HG12	2.13	0.48
6:e:34:LEU:HD22	6:e:38:TRP:CE3	2.48	0.48
7:f:65:VAL:HG21	7:f:94:VAL:HG21	1.96	0.48
2:a:205:LEU:HD22	2:a:241:PHE:CE2	2.49	0.48
3:b:165:VAL:CG2	3:b:234:ILE:HA	2.44	0.48
3:b:187:CYS:HA	3:b:193:VAL:O	2.14	0.48
1:A:18:SER:N	1:A:267:LEU:HD13	2.29	0.48
2:a:410:ASN:O	2:a:414:ILE:HG13	2.13	0.48
1:A:454:THR:O	1:A:458:ILE:HD12	2.14	0.48
2:a:68:MET:SD	13:a:602:HEA:HMC3	2.54	0.48
1:A:190:SER:O	1:A:191:LEU:HB2	2.13	0.47
2:a:498:PHE:CE2	7:f:102:ARG:HD2	2.49	0.47
1:A:317:ILE:HD12	1:A:317:ILE:H	1.79	0.47
2:a:146:VAL:O	2:a:150:ILE:HG13	2.14	0.47
1:A:375:ILE:HB	1:A:376:PRO:HD3	1.96	0.47
7:f:84:ILE:HD13	7:f:107:LEU:HD11	1.96	0.47
2:a:360:LEU:HD11	2:a:374:TYR:HD2	1.78	0.47
1:A:246:VAL:HG12	1:A:246:VAL:O	2.15	0.47
2:a:203:PRO:HB3	4:c:101:ILE:HG12	1.96	0.47
2:a:265:SER:HA	2:a:333:SER:O	2.15	0.47
1:A:33:ASP:OD1	1:A:196:SER:OG	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:HB2	1:A:147:PRO:HD3	1.96	0.47
1:A:310:MET:O	1:A:313:PRO:HD2	2.14	0.47
1:A:373:LEU:CD2	1:A:454:THR:HA	2.45	0.47
1:A:406:MET:HG3	1:A:421:VAL:CG1	2.45	0.47
1:A:453:MET:HA	1:A:456:ILE:HG22	1.97	0.47
2:a:121:ILE:O	2:a:122:GLU:HG3	2.15	0.47
4:c:32:SER:CB	8:g:47:THR:HG21	2.45	0.47
1:A:283:THR:HG23	1:A:415:VAL:CG1	2.44	0.47
1:A:368:VAL:HB	1:A:394:ALA:HB3	1.97	0.47
2:a:78:ILE:HG23	2:a:167:PHE:HE2	1.80	0.47
1:A:381:ILE:O	1:A:385:ILE:HG13	2.15	0.47
2:a:308:THR:O	2:a:312:MET:HG3	2.15	0.47
2:a:499:ILE:CD1	7:f:102:ARG:HG3	2.44	0.47
4:c:8:ASN:C	4:c:9:LEU:HD12	2.40	0.47
1:A:230:MET:O	1:A:234:VAL:HG12	2.15	0.46
4:c:132:ILE:HD13	4:c:188:GLU:OE2	2.15	0.46
1:A:348:PHE:HE2	1:A:397:MET:HG2	1.80	0.46
2:a:36:LEU:HD13	2:a:464:ILE:CD1	2.44	0.46
3:b:120:LEU:HD12	3:b:123:TYR:CE2	2.49	0.46
7:f:61:ASP:O	7:f:65:VAL:HG23	2.15	0.46
5:d:51:ILE:HD11	5:d:92:ILE:HD12	1.98	0.46
2:a:130:THR:HG22	2:a:238:PHE:CE2	2.50	0.46
8:g:55:CYS:O	9:h:70:ARG:NH2	2.48	0.46
1:A:364:GLY:O	1:A:394:ALA:HB1	2.15	0.46
2:a:179:MET:HE2	2:a:184:LEU:HD23	1.97	0.46
2:a:273:ILE:HA	2:a:276:VAL:HG12	1.97	0.46
2:a:295:TYR:HB2	2:a:366:ASP:OD2	2.15	0.46
2:a:521:SER:HB2	2:a:522:PRO:CD	2.45	0.46
5:d:113:LEU:HD21	5:d:156:LYS:HD3	1.98	0.46
2:a:165:ILE:HD13	4:c:94:PHE:CD2	2.51	0.46
3:b:124:TRP:HE1	3:b:230:MET:HG2	1.80	0.46
1:A:394:ALA:O	1:A:397:MET:HB2	2.15	0.46
2:a:39:ARG:CG	2:a:457:SER:HA	2.45	0.46
2:a:227:GLY:O	4:c:120:ILE:HD11	2.15	0.46
1:A:175:MET:O	1:A:179:SER:OG	2.32	0.46
2:a:146:VAL:HG12	2:a:150:ILE:HD11	1.96	0.46
1:A:135:PHE:HZ	1:A:433:TYR:HD1	1.64	0.46
1:A:320:MET:SD	1:A:330:LEU:HD21	2.56	0.46
3:b:79:ILE:HG12	3:b:83:TRP:HZ3	1.78	0.46
4:c:140:LEU:O	4:c:144:ILE:HG13	2.15	0.46
9:h:62:PHE:O	9:h:66:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:312:MET:HB3	3:b:91:LEU:HD22	1.97	0.45
2:a:421:ILE:O	2:a:425:VAL:HG23	2.15	0.45
13:a:603:HEA:H261	13:a:603:HEA:H172	1.72	0.45
3:b:46:VAL:O	3:b:50:THR:HG23	2.16	0.45
3:b:51:PHE:CZ	3:b:55:ILE:HD11	2.52	0.45
2:a:30:LEU:HD23	9:h:56:GLY:O	2.16	0.45
2:a:289:VAL:O	2:a:289:VAL:HG13	2.16	0.45
2:a:533:ILE:CG2	5:d:100:LEU:HD23	2.41	0.45
1:A:234:VAL:HG13	1:A:235:GLY:H	1.81	0.45
1:A:341:TYR:HE1	1:A:395:ILE:HG22	1.81	0.45
2:a:45:PRO:HB3	3:b:157:ARG:NH2	2.31	0.45
15:c:301:PTY:H162	15:c:302:PTY:H202	1.99	0.45
5:d:51:ILE:O	5:d:51:ILE:HG13	2.16	0.45
8:g:20:LYS:HB3	8:g:21:PRO:HD2	1.98	0.45
2:a:179:MET:HE1	2:a:184:LEU:HD23	1.98	0.45
13:a:602:HEA:H261	13:a:602:HEA:H172	1.69	0.45
3:b:151:LEU:HD22	3:b:155:GLN:HB2	1.98	0.45
1:A:319:MET:HB3	1:A:325:SER:OG	2.16	0.45
2:a:79:GLY:O	2:a:83:ASN:HB2	2.16	0.45
1:A:341:TYR:CE1	1:A:395:ILE:HG22	2.52	0.45
2:a:16:ILE:HG22	2:a:20:TYR:CE2	2.52	0.45
2:a:17:ALA:HA	2:a:20:TYR:HD2	1.80	0.45
2:a:243:HIS:O	2:a:246:VAL:HG22	2.17	0.45
1:A:142:GLN:CG	1:A:197:SER:HB2	2.41	0.45
1:A:305:ASN:HD22	1:A:429:PHE:HA	1.82	0.45
2:a:11:THR:HG23	2:a:98:ALA:HB3	1.99	0.45
4:c:26:THR:CG2	4:c:61:SER:HB3	2.45	0.45
6:e:101:ILE:O	6:e:105:ILE:HG13	2.17	0.45
7:f:78:VAL:CG2	10:i:9:ILE:HB	2.46	0.45
4:c:22:TRP:HB3	4:c:65:TRP:CD1	2.52	0.44
2:a:375:VAL:O	2:a:378:HIS:HB3	2.16	0.44
1:A:191:LEU:HA	1:A:194:ILE:HG22	1.99	0.44
6:e:77:PHE:HB3	7:f:102:ARG:NH1	2.33	0.44
1:A:206:MET:O	1:A:210:VAL:HG23	2.17	0.44
2:a:121:ILE:HG22	8:g:55:CYS:SG	2.58	0.44
2:a:261:VAL:CG1	2:a:329:LEU:HD12	2.46	0.44
2:a:360:LEU:HB3	13:a:603:HEA:CMA	2.47	0.44
2:a:403:THR:CG2	2:a:405:LEU:HD12	2.47	0.44
9:h:45:TYR:C	9:h:48:PRO:HD2	2.42	0.44
1:A:175:MET:HG3	1:A:188:ALA:HB2	1.99	0.44
1:A:394:ALA:O	1:A:398:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:17:ALA:HB1	2:a:80:PHE:HA	1.98	0.44
2:a:401:LEU:HD21	2:a:516:ASP:O	2.17	0.44
2:a:496:PRO:HB2	6:e:83:ARG:HH21	1.82	0.44
2:a:150:ILE:HG23	2:a:209:VAL:HB	1.98	0.44
3:b:94:ILE:O	3:b:97:PRO:HD2	2.17	0.44
1:A:237:PRO:HB3	1:A:240:SER:HB2	1.98	0.44
1:A:431:MET:HE3	1:A:431:MET:HB2	1.91	0.44
2:a:99:ARG:HD3	4:c:20:SER:OG	2.18	0.44
1:A:32:LEU:CD2	1:A:36:LEU:HD12	2.47	0.44
4:c:106:PHE:HZ	4:c:260:LEU:HD12	1.82	0.44
1:A:179:SER:HB2	1:A:184:PHE:CB	2.46	0.44
2:a:40:LEU:HB3	2:a:49:ILE:HD11	2.00	0.44
4:c:90:GLY:O	4:c:94:PHE:HD2	2.01	0.44
2:a:45:PRO:HB3	3:b:157:ARG:HH21	1.83	0.43
2:a:97:PHE:O	2:a:166:ASN:ND2	2.50	0.43
3:b:195:VAL:HG11	3:b:205:THR:HG23	2.00	0.43
5:d:50:SER:HB2	5:d:90:GLU:OE2	2.18	0.43
7:f:104:PHE:CZ	7:f:128:ARG:HD2	2.53	0.43
1:A:462:LEU:O	1:A:465:PRO:HD2	2.19	0.43
2:a:212:LEU:O	2:a:216:ARG:HG3	2.18	0.43
2:a:495:ASN:OD1	2:a:496:PRO:HD2	2.18	0.43
3:b:219:CYS:SG	3:b:220:SER:N	2.91	0.43
5:d:138:LEU:HD13	5:d:146:ALA:HB1	2.00	0.43
1:A:143:LEU:HA	1:A:146:ASN:HD22	1.83	0.43
1:A:311:LEU:HA	1:A:453:MET:HE1	2.00	0.43
1:A:464:ALA:HB3	1:A:465:PRO:HD3	1.99	0.43
2:a:289:VAL:HG22	2:a:292:HIS:HD1	1.84	0.43
1:A:19:ARG:HB3	1:A:211:TYR:OH	2.18	0.43
4:c:67:ARG:O	4:c:70:VAL:HG12	2.18	0.43
6:e:124:ASN:OD1	6:e:125:ARG:N	2.50	0.43
2:a:191:VAL:O	2:a:194:THR:HG22	2.19	0.43
2:a:289:VAL:HG21	2:a:311:THR:OG1	2.19	0.43
2:a:376:ILE:HA	2:a:379:PHE:CE2	2.54	0.43
2:a:379:PHE:CD2	13:a:603:HEA:HMD2	2.54	0.43
1:A:181:SER:HB3	1:A:184:PHE:CD1	2.43	0.43
2:a:360:LEU:CB	13:a:603:HEA:HMA	2.49	0.43
6:e:37:ARG:O	6:e:41:LEU:HG	2.19	0.43
6:e:142:PRO:HB3	10:i:50:TYR:CZ	2.54	0.43
1:A:350:ILE:HD12	4:c:114:MET:CE	2.48	0.42
2:a:29:LEU:HD11	9:h:53:PHE:CD1	2.54	0.42
5:d:121:ARG:O	5:d:140:PRO:HD2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:31:VAL:O	6:e:34:LEU:HG	2.19	0.42
1:A:453:MET:O	1:A:456:ILE:HG22	2.19	0.42
2:a:100:LEU:O	2:a:103:ILE:HG22	2.18	0.42
2:a:294:MET:HG3	2:a:294:MET:O	2.19	0.42
2:a:371:ASP:CB	3:b:220:SER:HB3	2.49	0.42
3:b:28:THR:HG22	3:b:30:ASN:H	1.84	0.42
5:d:83:TYR:CD2	5:d:94:VAL:HG11	2.55	0.42
7:f:44:THR:HG22	7:f:45:TYR:H	1.84	0.42
1:A:340:SER:HB2	1:A:389:PHE:CD2	2.54	0.42
1:A:368:VAL:HB	1:A:394:ALA:HB1	2.01	0.42
4:c:22:TRP:CH2	4:c:64:LEU:HD13	2.54	0.42
4:c:236:THR:OG1	4:c:239:HIS:HB3	2.19	0.42
5:d:44:GLN:N	5:d:61:VAL:HG11	2.34	0.42
6:e:128:GLN:HB3	6:e:148:GLN:O	2.18	0.42
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.89	0.42
1:A:312:GLU:HG2	1:A:313:PRO:HD3	2.01	0.42
2:a:138:VAL:HG12	2:a:138:VAL:O	2.20	0.42
3:b:182:VAL:HG21	3:b:223:CYS:HB3	2.01	0.42
3:b:178:SER:O	3:b:197:ALA:HB1	2.20	0.42
1:A:179:SER:CB	1:A:184:PHE:HB3	2.49	0.42
1:A:312:GLU:CG	1:A:313:PRO:HD3	2.50	0.42
2:a:8:LEU:HD23	2:a:106:TRP:CZ2	2.55	0.42
2:a:94:ASP:O	2:a:174:MET:HE1	2.20	0.42
5:d:54:VAL:HG11	5:d:83:TYR:CE1	2.53	0.42
1:A:22:ILE:HD11	1:A:206:MET:CE	2.49	0.42
1:A:35:MET:CE	1:A:238:PHE:HB2	2.41	0.42
3:b:167:VAL:HB	3:b:173:ILE:HD11	2.01	0.42
4:c:94:PHE:CE1	15:c:301:PTY:H131	2.55	0.42
4:c:168:LEU:HD22	4:c:227:TYR:CE1	2.55	0.42
5:d:102:ALA:CB	5:d:130:ALA:HB2	2.50	0.42
1:A:34:ASN:ND2	1:A:229:ALA:H	2.18	0.42
4:c:64:LEU:CD2	4:c:67:ARG:HD3	2.49	0.42
2:a:47:ASN:HB3	2:a:51:MET:O	2.20	0.42
2:a:399:SER:OG	2:a:477:GLN:NE2	2.48	0.42
2:a:489:THR:HG23	6:e:86:VAL:HG22	2.02	0.41
3:b:158:LEU:O	3:b:159:LEU:HD23	2.19	0.41
6:e:114:ARG:O	6:e:117:ARG:NE	2.47	0.41
7:f:56:PHE:HZ	7:f:69:LEU:HD23	1.83	0.41
8:g:9:ILE:HG22	8:g:9:ILE:O	2.19	0.41
2:a:442:ILE:O	2:a:442:ILE:HG13	2.20	0.41
10:i:17:ILE:O	10:i:21:ILE:HG13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD22	1:A:397:MET:CE	2.35	0.41
1:A:32:LEU:HD23	1:A:36:LEU:HD12	2.02	0.41
3:b:49:LEU:HD12	3:b:49:LEU:HA	1.94	0.41
4:c:55:ILE:O	4:c:59:LEU:HD12	2.20	0.41
4:c:243:LEU:HA	4:c:246:THR:HG22	2.03	0.41
5:d:150:GLU:O	7:f:67:ARG:NH2	2.54	0.41
1:A:204:MET:CE	1:A:403:MET:HE3	2.43	0.41
5:d:61:VAL:HG23	5:d:62:GLY:H	1.85	0.41
2:a:289:VAL:HG22	2:a:292:HIS:ND1	2.35	0.41
8:g:18:THR:O	8:g:19:ASN:HB2	2.21	0.41
9:h:70:ARG:O	9:h:70:ARG:HG2	2.21	0.41
2:a:36:LEU:HD22	2:a:464:ILE:CD1	2.51	0.41
4:c:57:LEU:HD13	8:g:40:LEU:HD12	2.03	0.41
7:f:78:VAL:HG12	7:f:110:LYS:CG	2.51	0.41
1:A:31:LEU:HD11	1:A:234:VAL:CG1	2.48	0.41
1:A:233:LEU:HD11	1:A:335:LEU:HD11	2.03	0.41
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.91	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.84	0.41
1:A:369:GLY:O	1:A:373:LEU:HG	2.21	0.41
2:a:444:ASP:OD2	2:a:445:TYR:N	2.54	0.41
7:f:59:ALA:O	7:f:93:ARG:NH1	2.54	0.41
1:A:217:ARG:HA	1:A:220:VAL:HG22	2.04	0.40
1:A:371:SER:OG	1:A:387:PRO:O	2.38	0.40
2:a:406:TYR:CD2	2:a:485:LYS:HB3	2.56	0.40
5:d:65:ALA:CB	5:d:71:PRO:HB3	2.51	0.40
1:A:245:PHE:O	1:A:249:THR:HG22	2.22	0.40
2:a:40:LEU:HB3	2:a:49:ILE:HD12	2.01	0.40
2:a:108:LEU:HB2	2:a:109:PRO:HD3	2.03	0.40
2:a:426:THR:HG23	2:a:427:PHE:CD2	2.56	0.40
3:b:214:VAL:HG12	3:b:235:GLU:HG2	2.02	0.40
4:c:94:PHE:CD2	15:c:301:PTY:H131	2.57	0.40
1:A:22:ILE:O	1:A:26:VAL:HG23	2.21	0.40
4:c:13:PRO:HB3	5:d:95:PHE:CE2	2.56	0.40
1:A:361:ALA:HB3	1:A:467:CYS:SG	2.61	0.40
2:a:379:PHE:HA	2:a:382:VAL:HG22	2.03	0.40
5:d:138:LEU:HB3	5:d:146:ALA:HB1	2.03	0.40
5:d:141:THR:HG22	5:d:142:THR:N	2.37	0.40
1:A:34:ASN:ND2	1:A:232:VAL:HG23	2.36	0.40
1:A:329:GLN:CA	1:A:332:VAL:HG22	2.47	0.40
2:a:107:LEU:HD21	4:c:30:LEU:HD12	2.02	0.40
4:c:219:LEU:HD11	4:c:253:LEU:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:f:56:PHE:CZ	7:f:69:LEU:HD23	2.57	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	357/514 (70%)	341 (96%)	16 (4%)	0	100	100
2	a	533/535 (100%)	507 (95%)	26 (5%)	0	100	100
3	b	234/236 (99%)	218 (93%)	16 (7%)	0	100	100
4	c	266/268 (99%)	250 (94%)	15 (6%)	1 (0%)	30	60
5	d	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
6	e	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
7	f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
8	g	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
9	h	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
10	i	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
All	All	1881/2056 (92%)	1776 (94%)	104 (6%)	1 (0%)	49	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	c	125	PRO

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	289/427 (68%)	289 (100%)	0	100	100
2	a	452/452 (100%)	452 (100%)	0	100	100
3	b	212/212 (100%)	211 (100%)	1 (0%)	81	82
4	c	234/234 (100%)	234 (100%)	0	100	100
5	d	99/99 (100%)	99 (100%)	0	100	100
6	e	110/110 (100%)	110 (100%)	0	100	100
7	f	90/90 (100%)	90 (100%)	0	100	100
8	g	48/48 (100%)	48 (100%)	0	100	100
9	h	41/41 (100%)	41 (100%)	0	100	100
10	i	47/47 (100%)	47 (100%)	0	100	100
All	All	1622/1760 (92%)	1621 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	223	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
4	c	238	ASN
5	d	145	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	603	-	67,67,67	1.02	5 (7%)	81,103,103	2.22	29 (35%)
14	CUA	b	301	3	0,1,1	-	-	-		
13	HEA	a	602	-	67,67,67	1.05	4 (5%)	81,103,103	2.14	28 (34%)
11	HSM	A	601	-	8,8,8	1.29	1 (12%)	9,9,9	1.01	0
15	PTY	c	302	-	39,39,49	0.45	0	42,44,54	1.26	4 (9%)
15	PTY	e	201	-	32,32,49	0.49	0	35,37,54	1.36	4 (11%)
15	PTY	i	101	-	39,39,49	0.44	0	42,44,54	1.29	4 (9%)
15	PTY	c	301	-	33,33,49	0.46	0	36,38,54	1.37	4 (11%)

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	603	-	-	16/36/76/76	-
13	HEA	a	602	-	-	14/36/76/76	-
15	PTY	c	302	-	-	6/43/43/53	-
11	HSM	A	601	-	-	3/3/3/3	0/1/1/1
15	PTY	e	201	-	-	9/36/36/53	-
15	PTY	i	101	-	-	14/43/43/53	-
15	PTY	c	301	-	-	13/37/37/53	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	603	HEA	C1A-C2A	-4.03	1.38	1.45
13	a	602	HEA	C1A-C2A	-3.72	1.38	1.45
13	a	602	HEA	C3A-C4A	-3.48	1.40	1.46
13	a	603	HEA	C3A-C4A	-3.18	1.40	1.46
11	A	601	HSM	CG-ND1	-2.61	1.31	1.38
13	a	603	HEA	C1D-ND	-2.56	1.35	1.40
13	a	602	HEA	C1D-ND	-2.52	1.35	1.40
13	a	603	HEA	C4B-NB	-2.29	1.36	1.40
13	a	602	HEA	C4B-NB	-2.27	1.36	1.40
13	a	603	HEA	C1C-C2C	-2.18	1.38	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	603	HEA	CHA-C1A-NA	-6.38	117.51	124.45
13	a	602	HEA	CHB-C4A-NA	-6.17	117.73	124.45
13	a	603	HEA	CHA-C1A-C2A	5.27	133.19	124.86
13	a	603	HEA	C1A-CHA-C4D	-5.26	114.84	126.02
13	a	602	HEA	C4A-CHB-C1B	-5.11	115.16	126.02
13	a	603	HEA	CHA-C4D-ND	-4.82	119.23	124.42
13	a	602	HEA	CHB-C4A-C3A	4.60	132.96	125.21
13	a	603	HEA	C1C-CHC-C4B	-4.54	115.57	126.25
13	a	602	HEA	C4C-CHD-C1D	-4.51	115.64	126.25
13	a	603	HEA	CHC-C4B-NB	-4.43	118.89	124.37
15	c	301	PTY	O7-C8-C11	4.36	120.90	111.48
15	e	201	PTY	O7-C8-C11	4.20	120.58	111.48
15	i	101	PTY	O7-C8-C11	4.16	120.48	111.48
13	a	602	HEA	CHB-C1B-NB	-3.93	120.19	124.42
13	a	602	HEA	CHA-C1A-C2A	3.86	130.96	124.86
13	a	603	HEA	C3C-C4C-NC	-3.83	106.57	109.80
13	a	603	HEA	CHA-C4D-C3D	3.75	130.24	124.77
15	c	302	PTY	O7-C8-C11	3.73	119.55	111.48
13	a	603	HEA	C17-C18-C19	-3.73	119.09	127.62
13	a	602	HEA	CHD-C4C-NC	-3.58	117.37	123.86
13	a	602	HEA	CHC-C4B-NB	-3.55	119.97	124.37
13	a	603	HEA	CHC-C1C-NC	-3.44	117.62	123.86
15	c	302	PTY	P1-O11-C3	-3.39	105.12	121.26
13	a	602	HEA	CHD-C1D-ND	-3.33	120.25	124.37
13	a	603	HEA	C13-C14-C15	-3.29	120.10	127.62
13	a	602	HEA	CHB-C1B-C2B	3.27	130.19	125.03
13	a	602	HEA	C13-C14-C15	-3.25	120.19	127.62
13	a	603	HEA	C13-C12-C11	-3.25	109.21	114.39
13	a	603	HEA	CHB-C4A-C3A	3.23	130.66	125.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	i	101	PTY	P1-O11-C3	-3.22	105.94	121.26
13	a	602	HEA	CHA-C1A-NA	-3.15	121.02	124.45
15	c	301	PTY	P1-O11-C3	-3.15	106.27	121.26
15	e	201	PTY	P1-O11-C3	-3.13	106.35	121.26
13	a	602	HEA	C13-C12-C11	-3.03	109.55	114.39
13	a	603	HEA	OMA-CMA-C3A	-2.97	118.92	125.62
13	a	602	HEA	C17-C18-C19	-2.89	121.00	127.62
13	a	602	HEA	CHA-C4D-C3D	2.87	128.96	124.77
15	c	301	PTY	O4-C30-C31	2.76	120.25	111.83
13	a	602	HEA	C27-C19-C20	2.68	119.87	115.23
15	e	201	PTY	P1-O14-C5	-2.64	106.22	121.35
15	e	201	PTY	O4-C30-C31	2.64	119.88	111.83
15	i	101	PTY	P1-O14-C5	-2.61	106.39	121.35
15	c	302	PTY	P1-O14-C5	-2.61	106.39	121.35
13	a	603	HEA	CMB-C2B-C3B	-2.59	125.27	130.28
13	a	602	HEA	CHA-C4D-ND	-2.56	121.67	124.42
15	i	101	PTY	O4-C30-C31	2.54	119.58	111.83
13	a	602	HEA	C4B-NB-C1B	2.45	108.11	105.21
13	a	603	HEA	C27-C19-C20	2.45	119.47	115.23
13	a	602	HEA	C26-C15-C16	2.44	119.47	115.23
15	c	302	PTY	O4-C30-C31	2.41	119.18	111.83
13	a	602	HEA	C2A-C1A-NA	-2.40	108.01	110.32
13	a	603	HEA	CHB-C1B-C2B	2.39	128.81	125.03
13	a	603	HEA	C21-C22-C23	-2.39	119.67	127.64
13	a	603	HEA	CHC-C1C-C2C	2.35	134.25	127.43
15	c	301	PTY	P1-O14-C5	-2.32	108.08	121.35
13	a	603	HEA	CHB-C1B-NB	-2.31	121.94	124.42
13	a	602	HEA	C12-C11-C3B	2.31	115.73	112.12
13	a	603	HEA	CHB-C4A-NA	-2.31	121.94	124.45
13	a	602	HEA	C25-C23-C24	2.28	119.83	114.59
13	a	603	HEA	C26-C15-C16	2.27	119.16	115.23
13	a	602	HEA	C21-C22-C23	-2.26	120.09	127.64
13	a	603	HEA	CHD-C1D-ND	-2.19	121.66	124.37
13	a	603	HEA	C25-C23-C24	2.14	119.51	114.59
13	a	603	HEA	C4A-C3A-C2A	2.13	108.66	106.81
13	a	603	HEA	C1D-ND-C4D	2.13	107.73	105.21
13	a	602	HEA	C3C-C2C-C1C	2.12	109.67	107.17
13	a	603	HEA	CHC-C4B-C3B	2.11	131.13	125.80
13	a	602	HEA	C1D-ND-C4D	2.10	107.69	105.21
13	a	603	HEA	O2D-CGD-CBD	2.09	120.59	114.00
13	a	602	HEA	C2C-C1C-NC	-2.06	106.84	110.14
13	a	602	HEA	CBA-CAA-C2A	-2.05	106.86	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	603	HEA	C4A-CHB-C1B	-2.00	121.76	126.02
13	a	602	HEA	OMA-CMA-C3A	-2.00	121.11	125.62

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	601	HSM	N-CA-CB-CG
13	a	602	HEA	C12-C11-C3B-C2B
13	a	602	HEA	C12-C11-C3B-C4B
13	a	602	HEA	C3B-C11-C12-C13
13	a	603	HEA	C4A-C3A-CMA-OMA
13	a	603	HEA	C2C-C3C-CAC-CBC
13	a	603	HEA	C4C-C3C-CAC-CBC
13	a	603	HEA	C26-C15-C16-C17
15	c	301	PTY	N1-C2-C3-O11
15	c	301	PTY	O10-C8-O7-C6
15	c	301	PTY	C5-O14-P1-O11
15	c	301	PTY	C5-O14-P1-O12
15	c	301	PTY	C5-O14-P1-O13
15	c	302	PTY	N1-C2-C3-O11
15	e	201	PTY	N1-C2-C3-O11
15	e	201	PTY	O14-C5-C6-O7
15	i	101	PTY	N1-C2-C3-O11
15	e	201	PTY	O30-C30-O4-C1
15	e	201	PTY	C31-C30-O4-C1
15	c	301	PTY	C11-C8-O7-C6
13	a	602	HEA	C26-C15-C16-C17
13	a	602	HEA	C15-C16-C17-C18
13	a	603	HEA	C4D-C3D-CAD-CBD
15	c	302	PTY	O4-C1-C6-O7
13	a	603	HEA	C2D-C3D-CAD-CBD
15	e	201	PTY	C8-C11-C12-C13
13	a	602	HEA	O11-C11-C12-C13
15	c	301	PTY	C30-C31-C32-C33
15	e	201	PTY	O14-C5-C6-C1
15	c	301	PTY	O4-C1-C6-C5
15	c	302	PTY	O4-C1-C6-C5
15	i	101	PTY	O4-C1-C6-C5
15	i	101	PTY	C12-C13-C14-C15
13	a	603	HEA	C2A-C3A-CMA-OMA
13	a	603	HEA	C3B-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	603	HEA	C17-C18-C19-C27
13	a	603	HEA	C1A-C2A-CAA-CBA
15	c	301	PTY	C34-C35-C36-C37
13	a	602	HEA	C4C-C3C-CAC-CBC
15	i	101	PTY	C19-C20-C21-C22
15	i	101	PTY	O4-C1-C6-O7
13	a	602	HEA	C19-C20-C21-C22
13	a	603	HEA	O11-C11-C12-C13
15	i	101	PTY	C15-C16-C17-C18
15	c	301	PTY	O4-C1-C6-O7
13	a	603	HEA	O11-C11-C3B-C4B
13	a	603	HEA	C3A-C2A-CAA-CBA
13	a	603	HEA	O11-C11-C3B-C2B
15	i	101	PTY	C5-O14-P1-O11
15	i	101	PTY	C5-O14-P1-O12
15	i	101	PTY	C5-O14-P1-O13
15	i	101	PTY	C31-C32-C33-C34
11	A	601	HSM	CA-CB-CG-CD2
15	i	101	PTY	C13-C14-C15-C16
15	c	302	PTY	C37-C38-C39-C40
15	e	201	PTY	C34-C35-C36-C37
15	c	302	PTY	C17-C18-C19-C20
15	c	301	PTY	C12-C13-C14-C15
13	a	602	HEA	CAA-CBA-CGA-O2A
11	A	601	HSM	CA-CB-CG-ND1
13	a	602	HEA	CAA-CBA-CGA-O1A
13	a	603	HEA	CAA-CBA-CGA-O1A
13	a	603	HEA	CAA-CBA-CGA-O2A
13	a	602	HEA	CAD-CBD-CGD-O2D
15	i	101	PTY	C30-C31-C32-C33
15	c	302	PTY	C36-C37-C38-C39
15	e	201	PTY	C11-C12-C13-C14
15	c	301	PTY	C12-C11-C8-O7
13	a	602	HEA	C2C-C3C-CAC-CBC
13	a	602	HEA	C14-C15-C16-C17
13	a	602	HEA	CAD-CBD-CGD-O1D
15	e	201	PTY	C12-C13-C14-C15
15	i	101	PTY	C34-C35-C36-C37
15	c	301	PTY	C12-C11-C8-O10
15	i	101	PTY	C12-C11-C8-O7

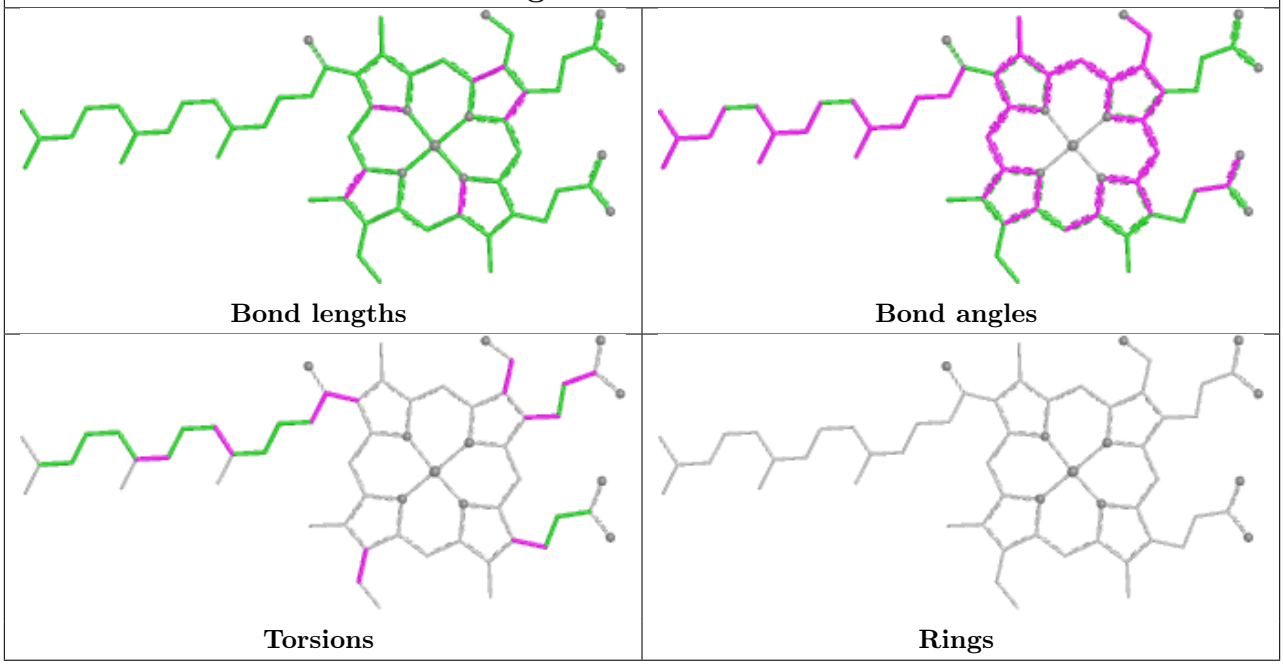
There are no ring outliers.

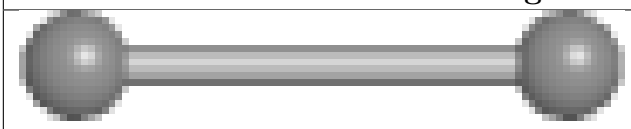
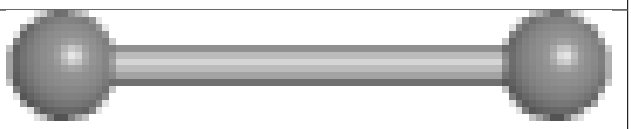
5 monomers are involved in 29 short contacts:

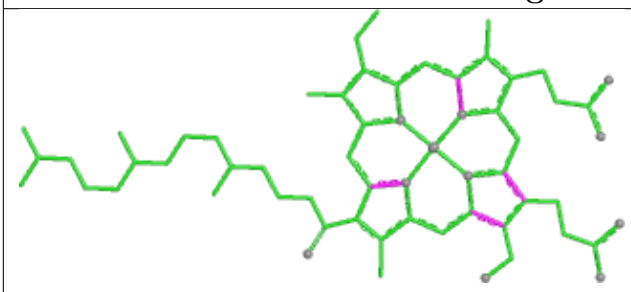
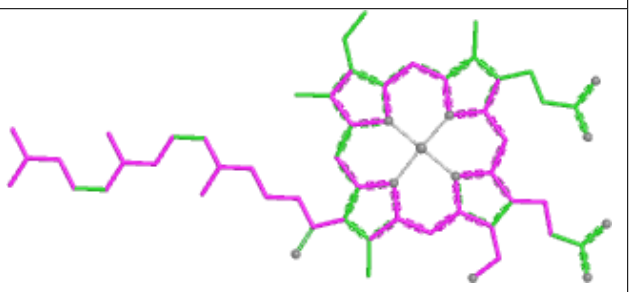
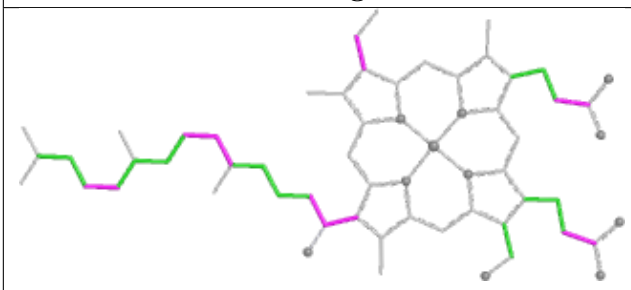
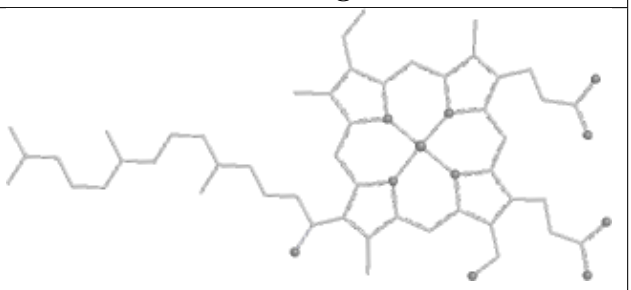
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	603	HEA	12	0
13	a	602	HEA	7	0
15	c	302	PTY	3	0
15	i	101	PTY	1	0
15	c	301	PTY	7	0

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

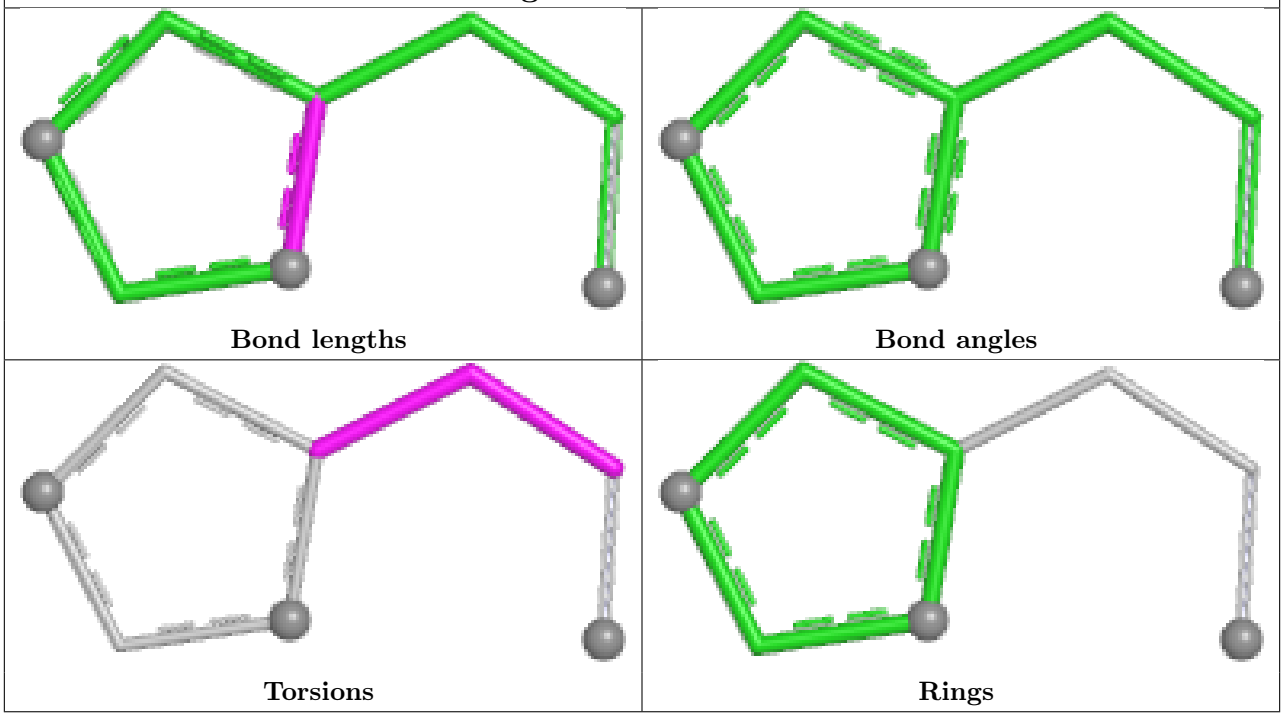
Ligand HEA a 603



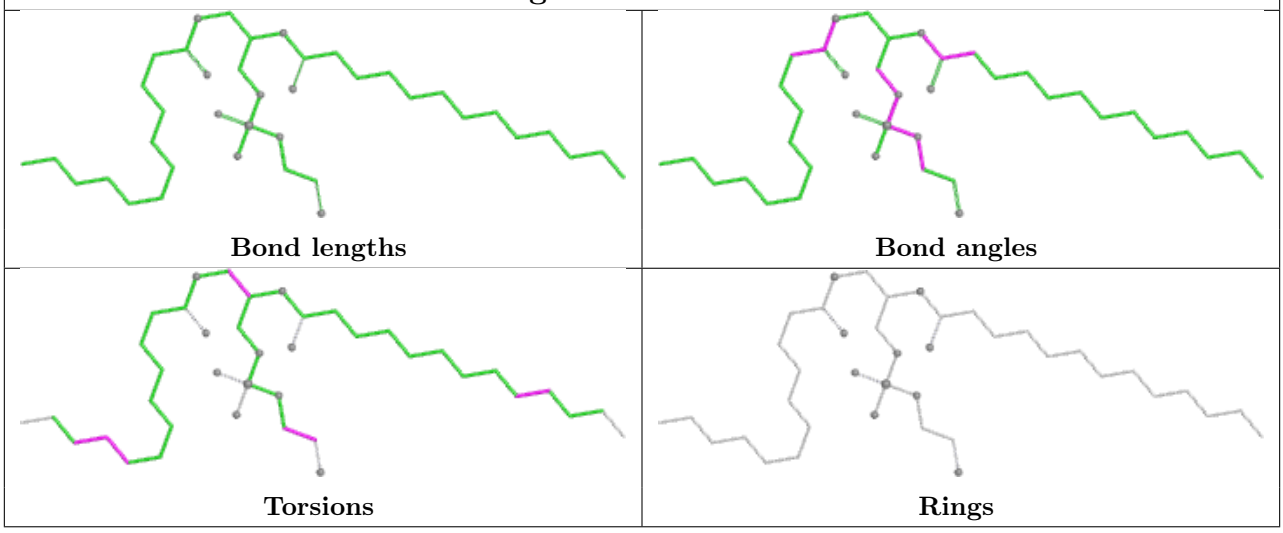
Ligand CUA b 301	
 Bond lengths	 Bond angles
Torsions	Rings

Ligand HEA a 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

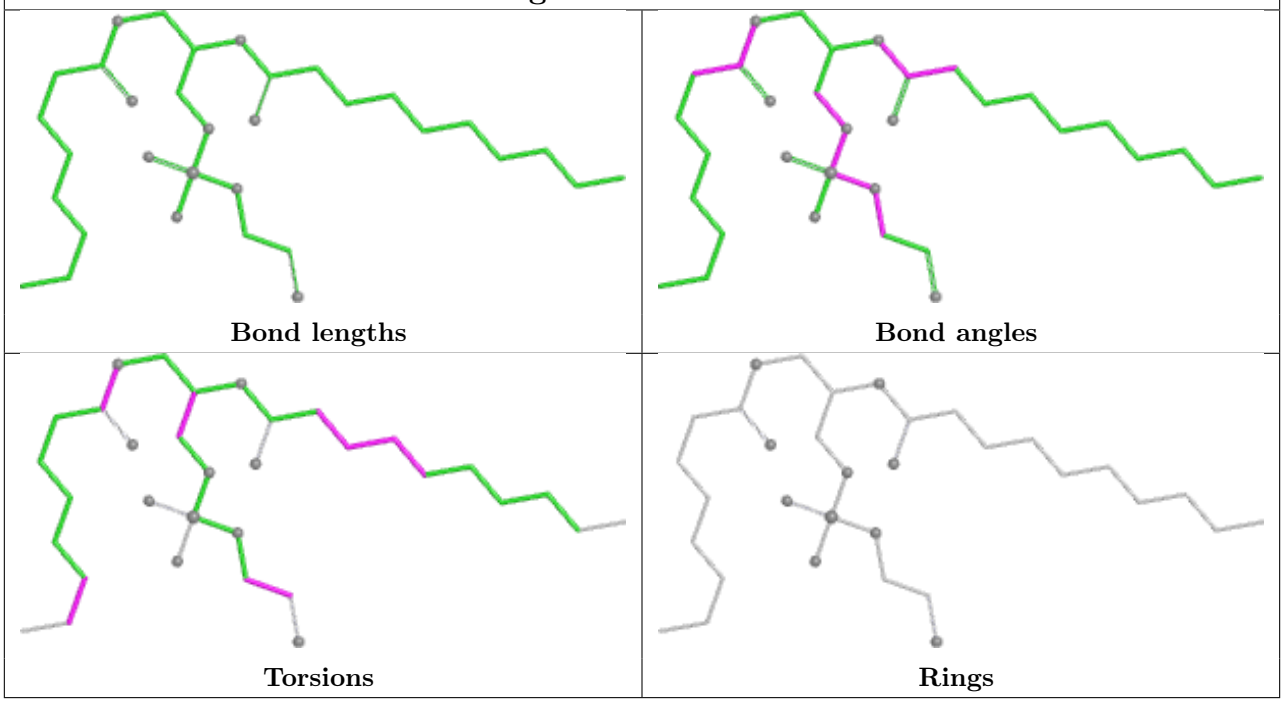
Ligand HSM A 601



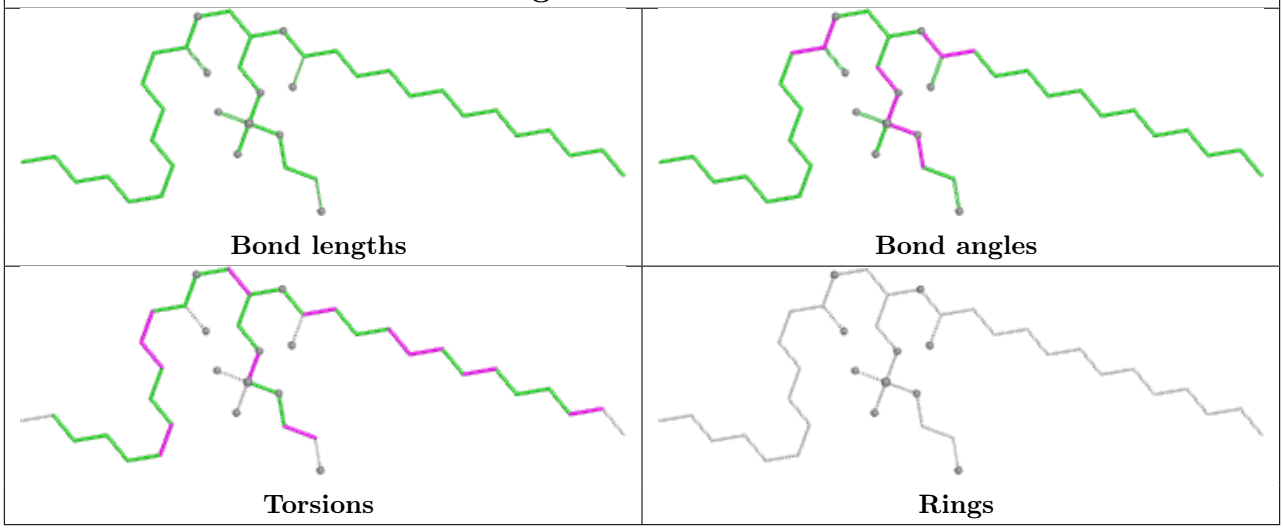
Ligand PTY c 302

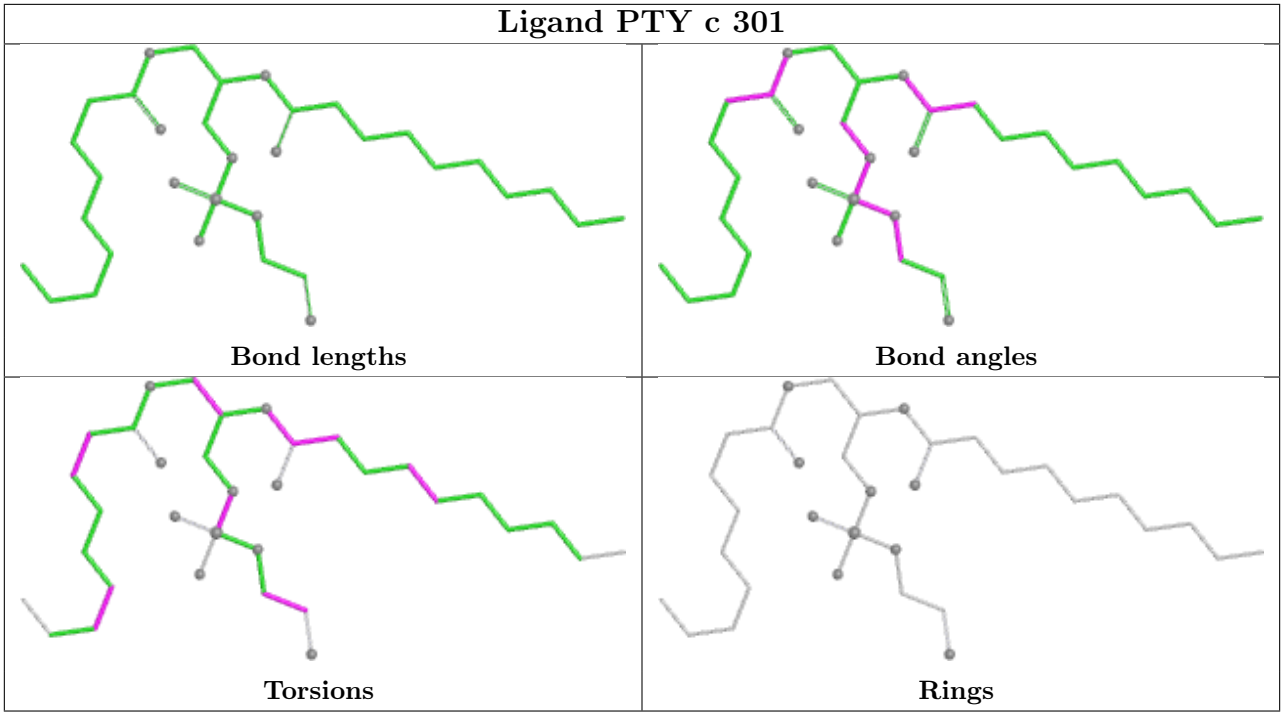


Ligand PTY e 201



Ligand PTY i 101





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.

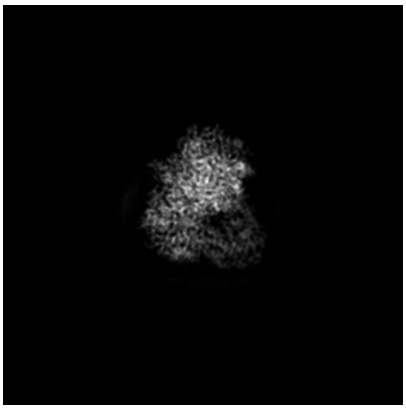
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-42132. These allow visual inspection of the internal detail of the map and identification of artifacts.

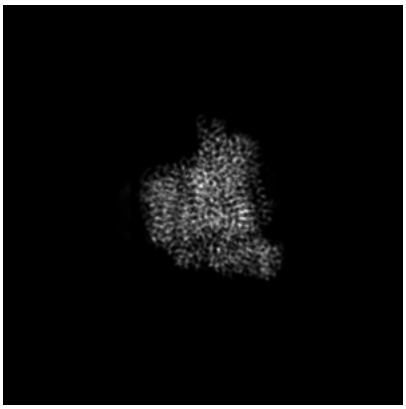
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

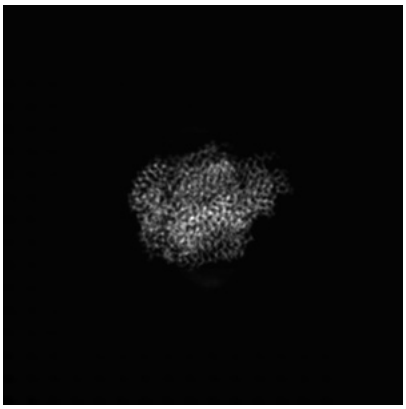
6.1.1 Primary map



X

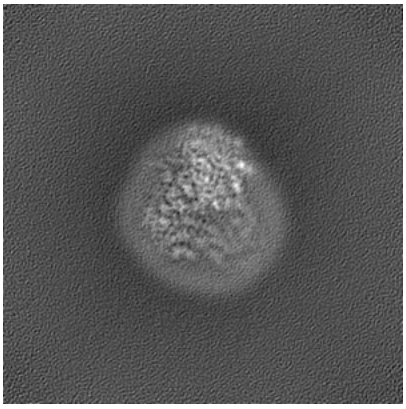


Y

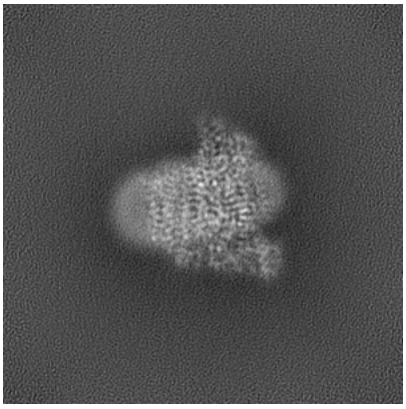


Z

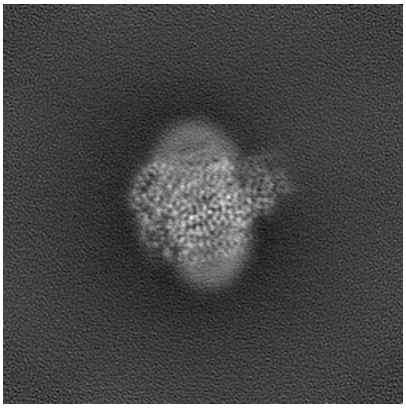
6.1.2 Raw map



X



Y



Z

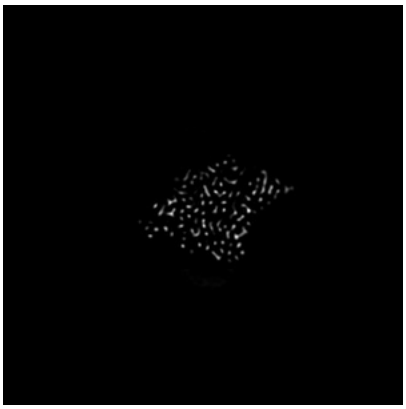
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

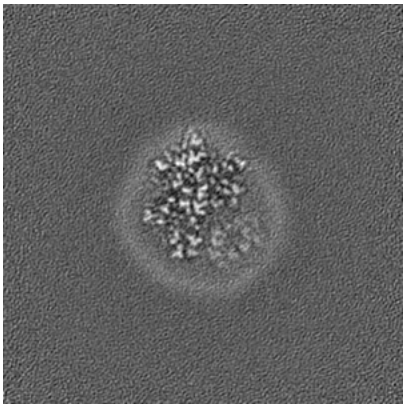
6.2.1 Primary map

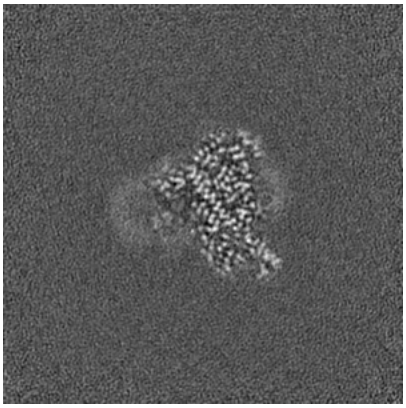
X Index: 128

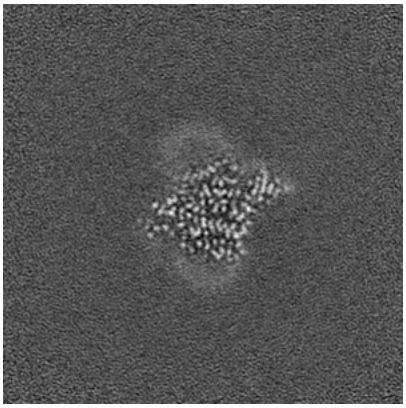
Y Index: 128


Z Index: 128

6.2.2 Raw 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)

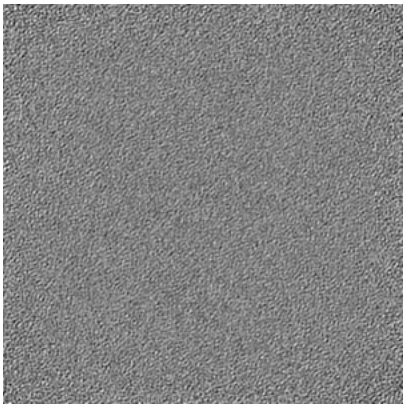
6.3.1 Primary map

X Index: 119

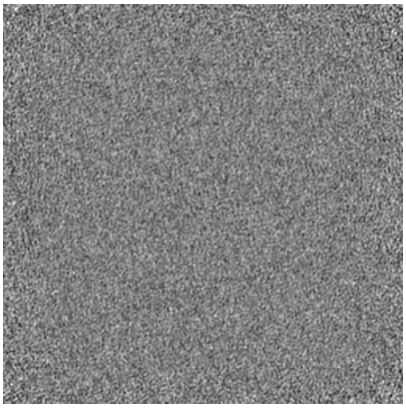
Y Index: 126

Z Index: 137

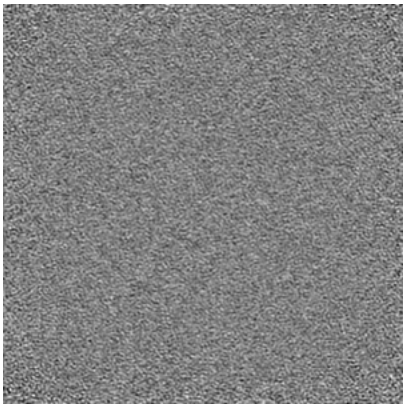
6.3.2 Raw map



X Index: 0



Y Index: 0

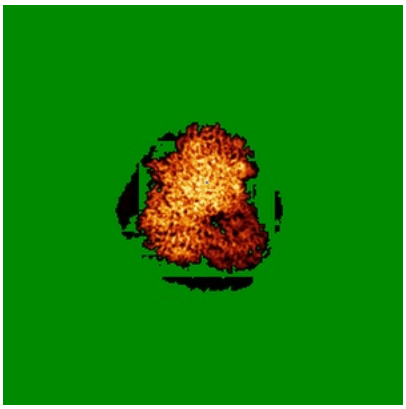


Z Index: 255

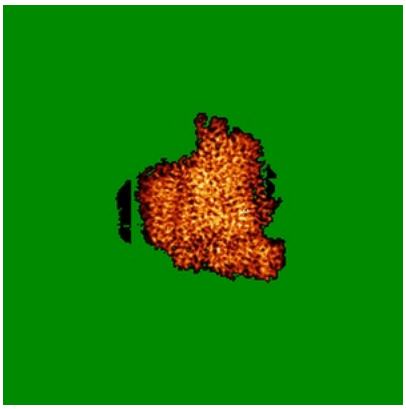
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

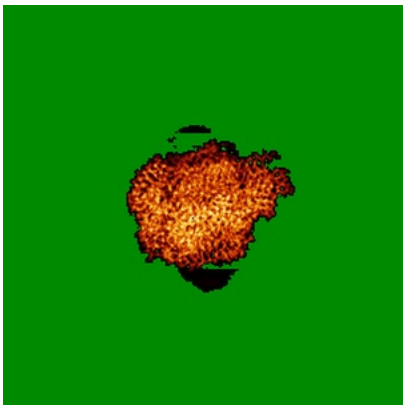
6.4.1 Primary map



X

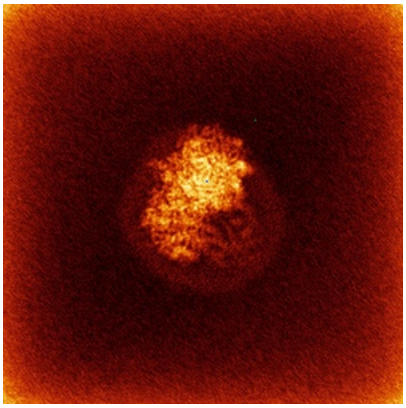


Y

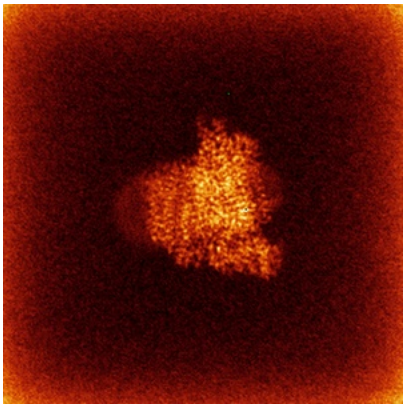


Z

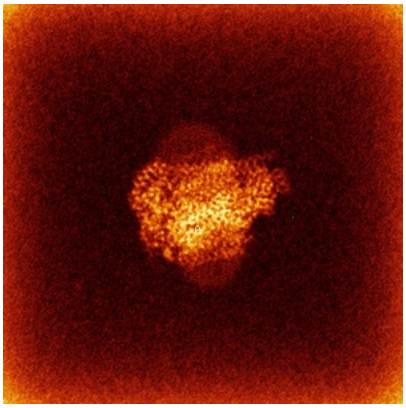
6.4.2 Raw map



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.

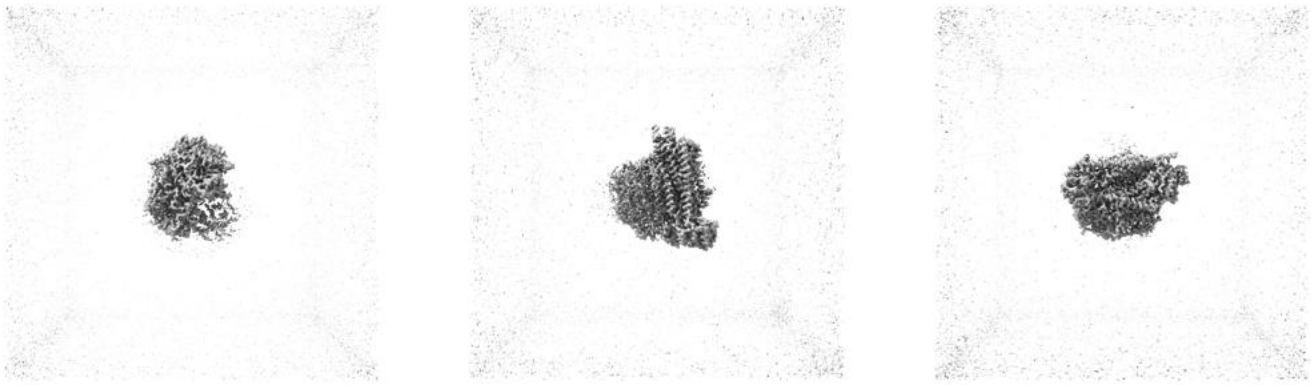
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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



X Y Z

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.

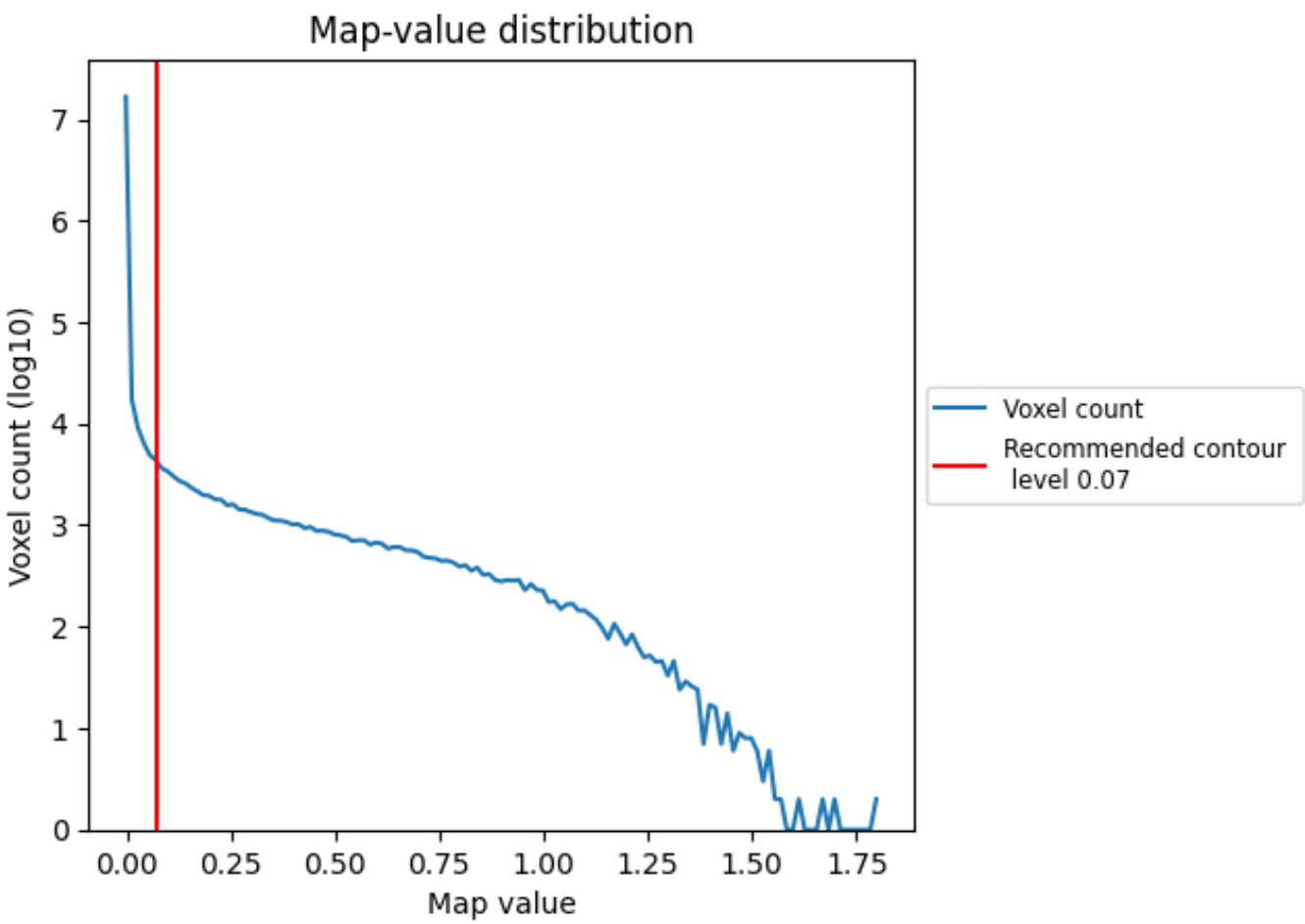
6.6 Mask visualisation (i)

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

7 Map analysis (i)

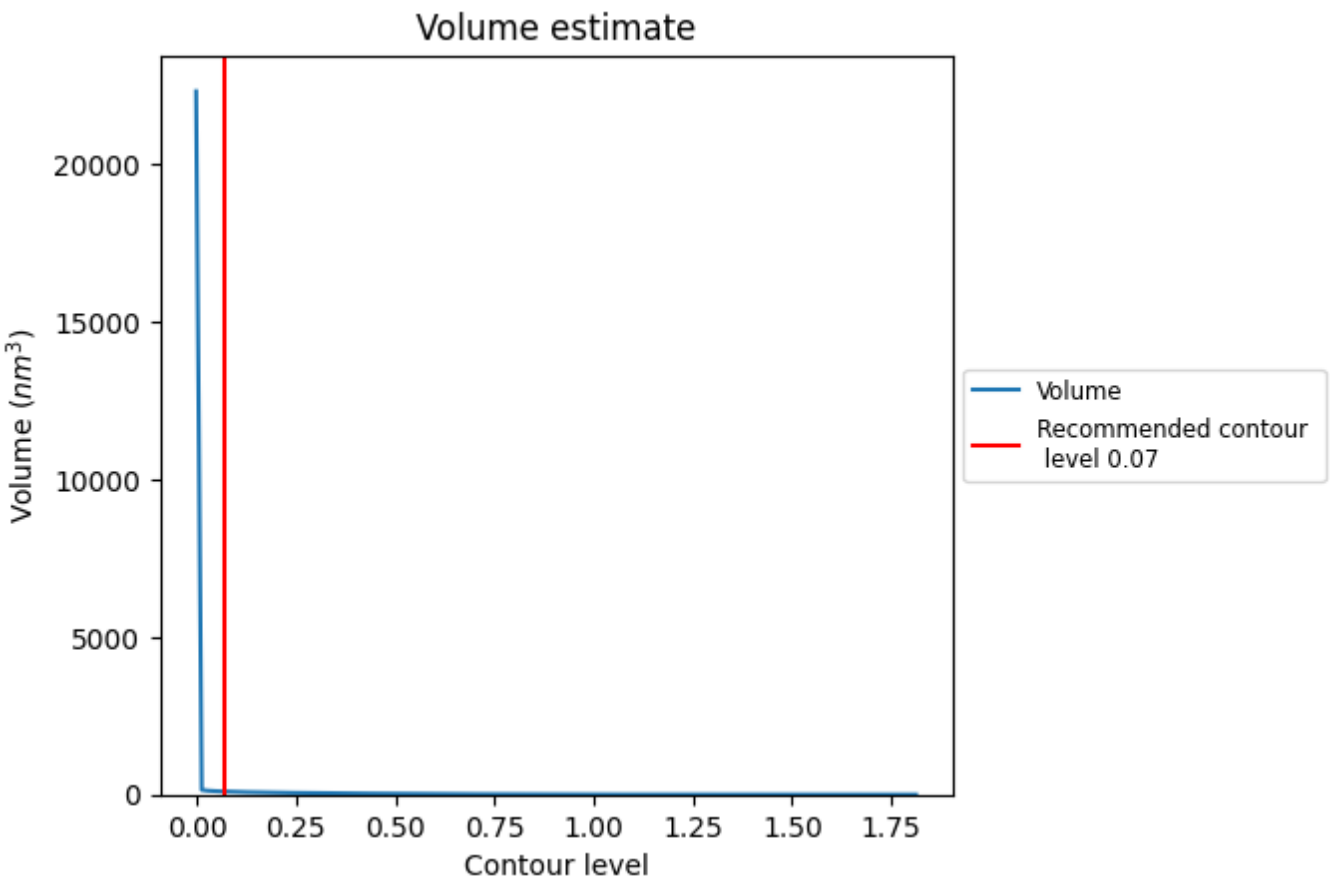
This section contains the results of statistical analysis of the map.

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.

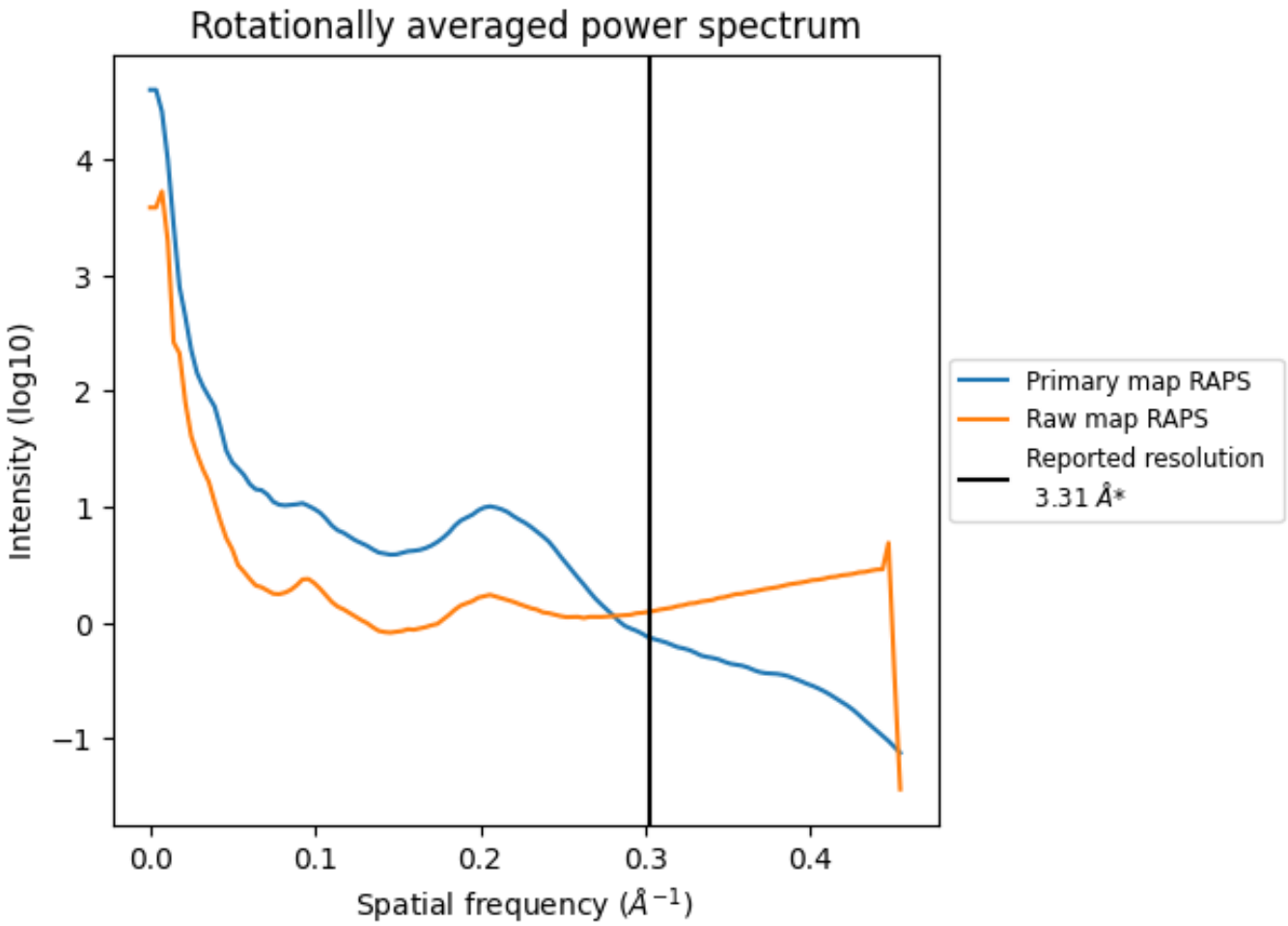
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 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)

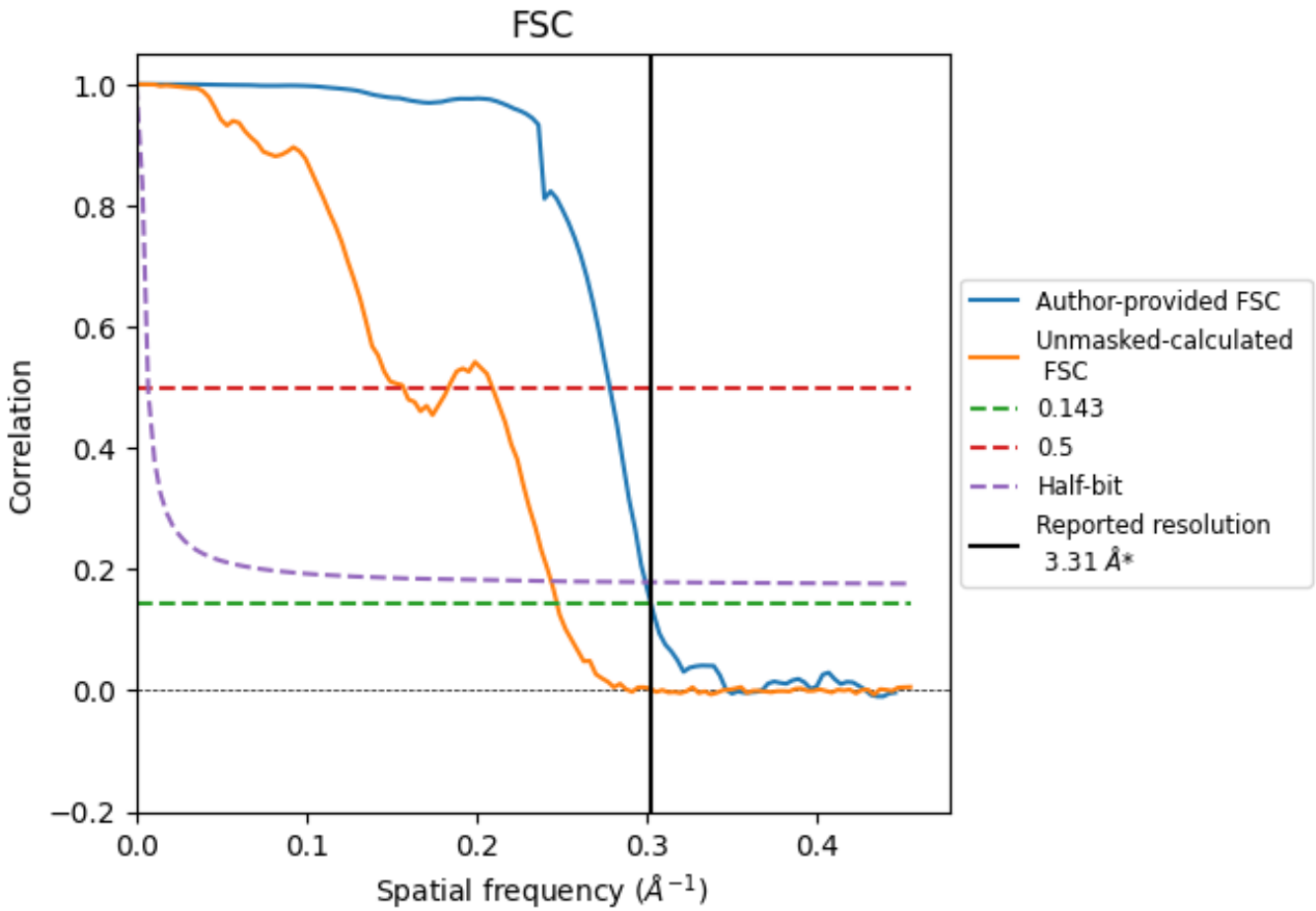


*Reported resolution corresponds to spatial frequency of 0.302 Å^{-1}

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 0.302 Å^{-1}

8.2 Resolution estimates (i)

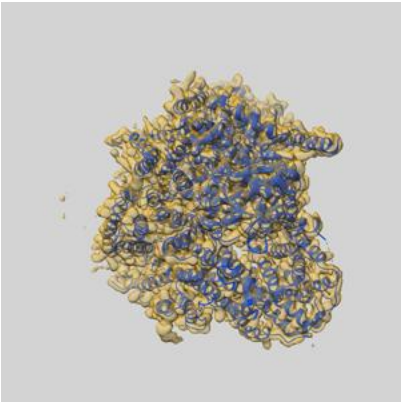
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.31	3.60	3.34
Unmasked-calculated*	4.05	6.38	4.11

*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 4.05 differs from the reported value 3.31 by more than 10 %

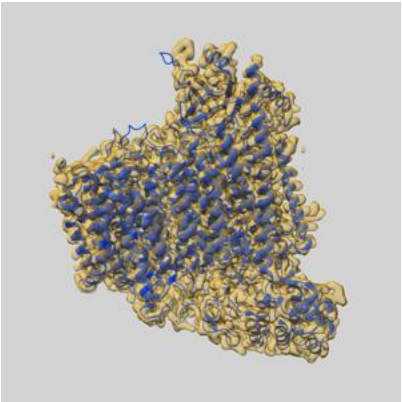
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42132 and PDB model 8UCN. Per-residue inclusion information can be found in section 3 on page 10.

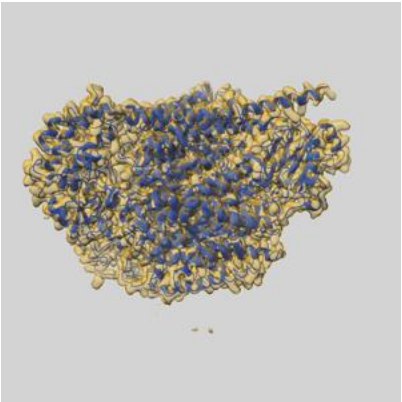
9.1 Map-model overlay (i)



X



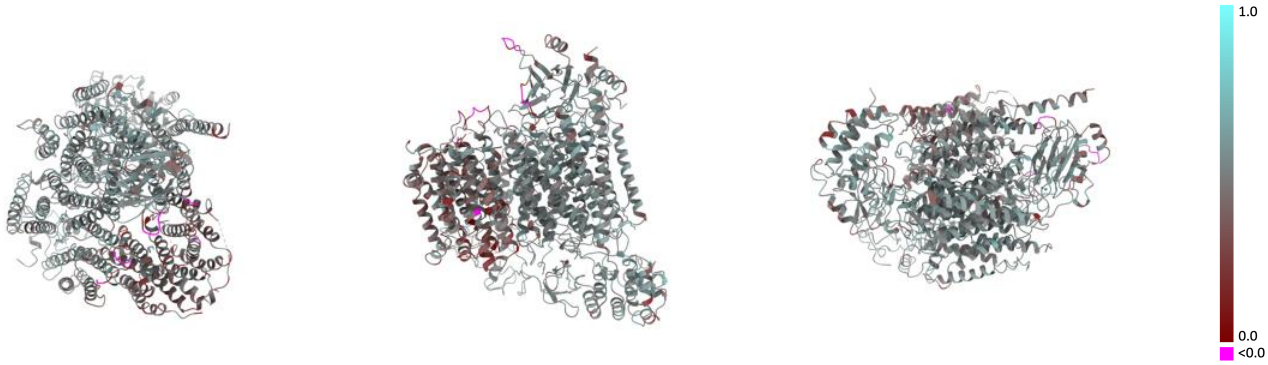
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

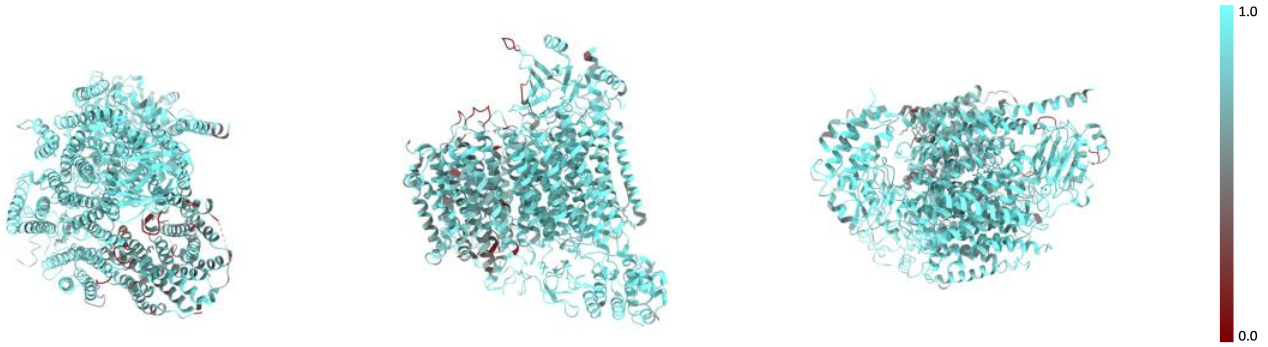
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

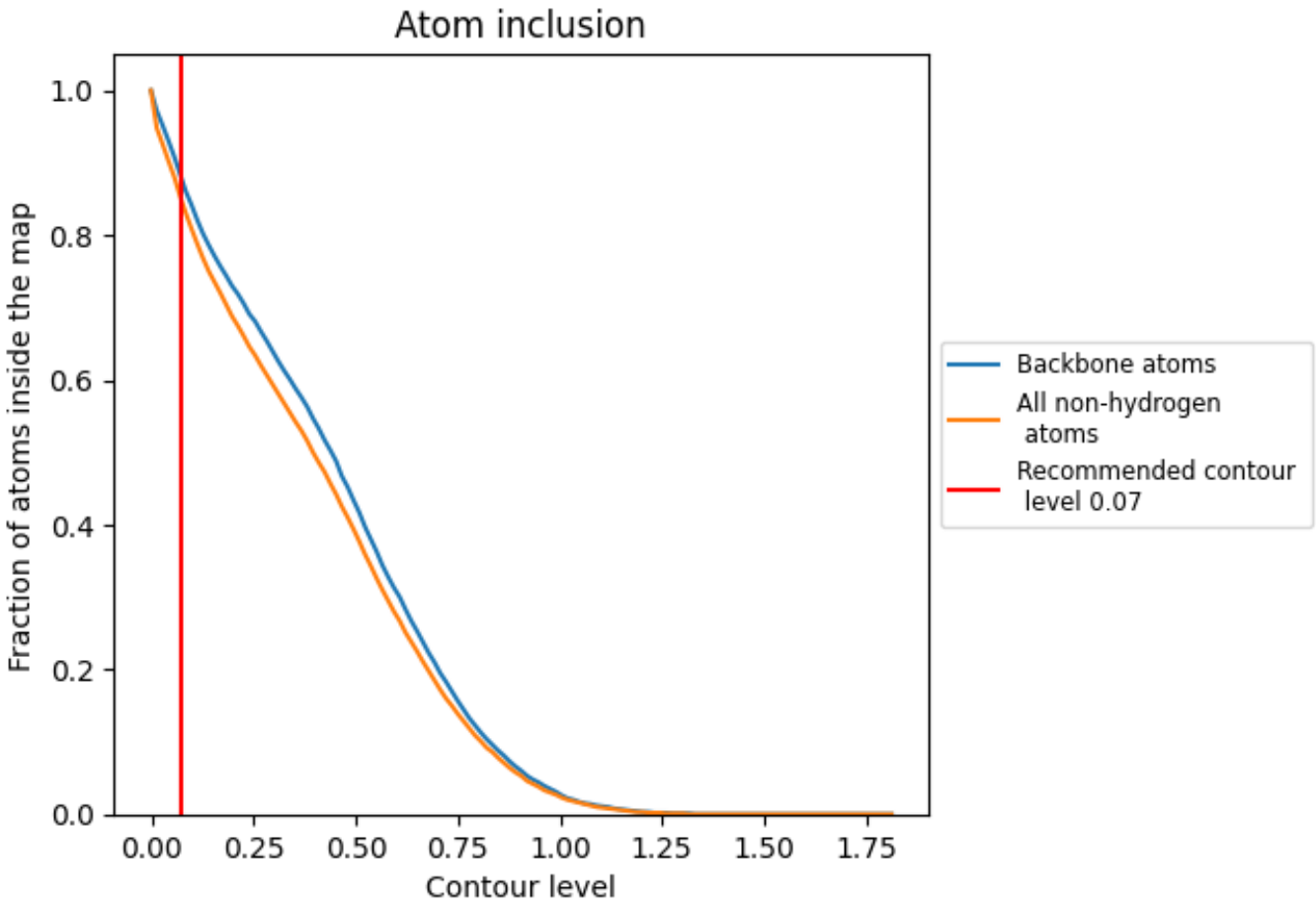
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.4860
A	0.7160	0.3890
a	0.9250	0.5300
b	0.8660	0.4870
c	0.8510	0.4910
d	0.8860	0.5090
e	0.8500	0.4960
f	0.8690	0.5040
g	0.8970	0.5180
h	0.8700	0.5100
i	0.8270	0.4860