



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 07:02 pm BST

PDB ID : 8P65  
EMDB ID : EMD-17461  
Title : Cytochrome bc1 complex (Bos taurus)  
Authors : Phillips, B.P.; Barra, I.M.C.C.; Meier, T.K.; Rimle, L.; von Ballmoos, C.  
Deposited on : 2023-05-25  
Resolution : 3.00 Å(reported)  
Based on initial model : 6FO2

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

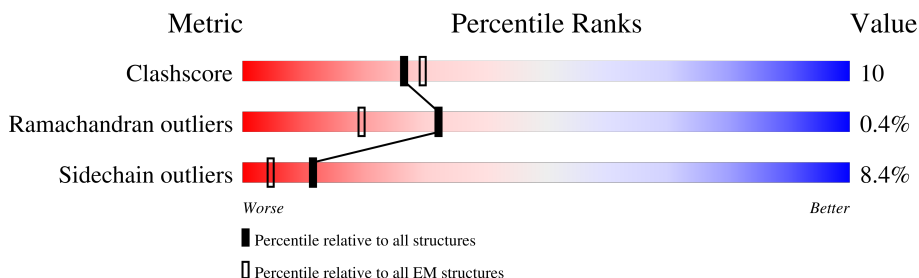
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	446	
1	N	446	
2	B	439	
2	O	439	
3	C	379	
3	P	379	
4	D	241	
4	Q	241	

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Mol	Chain	Length	Quality of chain
5	E	196	
5	R	196	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	78	
8	U	78	
9	I	54	
9	V	54	
10	J	64	
10	W	64	
11	K	49	
11	X	49	

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 33820 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	446	Total	C	N	O	S	0	0
			3457	2161	609	667	20		
1	N	446	Total	C	N	O	S	0	0
			3457	2161	609	667	20		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	439	Total	C	N	O	S	0	0
			3280	2063	580	630	7		
2	O	439	Total	C	N	O	S	0	0
			3280	2063	580	630	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	305	GLU	GLN	conflict	UNP P23004
O	305	GLU	GLN	conflict	UNP P23004

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	379	Total	C	N	O	S	0	0
			3010	2018	472	501	19		
3	P	379	Total	C	N	O	S	0	0
			3010	2018	472	501	19		

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	241	Total	C	N	O	S	0	0
			1918	1225	330	348	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	241	Total	C	N	O	S	0	0
			1918	1225	330	348	15		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		
5	R	196	Total	C	N	O	S	0	0
			1519	957	263	291	8		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	111	Total	C	N	O	S	0	0
			950	600	174	173	3		
6	S	111	Total	C	N	O	S	0	0
			950	600	174	173	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	57	ASP	ASN	conflict	UNP P00129
S	57	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	82	Total	C	N	O	S	0	0
			689	446	129	112	2		
7	T	82	Total	C	N	O	S	0	0
			689	446	129	112	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	78	Total	C	N	O	S	0	0
			638	384	111	138	5		
8	U	78	Total	C	N	O	S	0	0
			638	384	111	138	5		

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	54	Total	C	N	O	S	0	0
			383	239	71	71	2		
9	V	54	Total	C	N	O	S	0	0
			383	239	71	71	2		

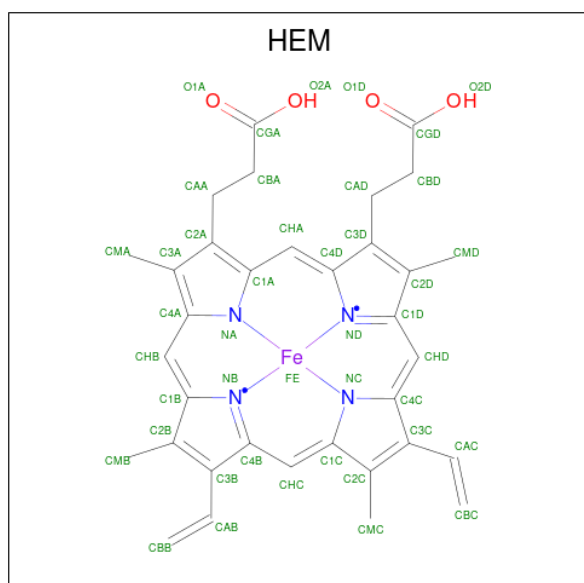
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	64	Total	C	N	O	S	0	0
			528	345	91	91	1		
10	W	64	Total	C	N	O	S	0	0
			528	345	91	91	1		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	49	Total	C	N	O	S	0	0
			405	270	72	62	1		
11	X	49	Total	C	N	O	S	0	0
			405	270	72	62	1		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



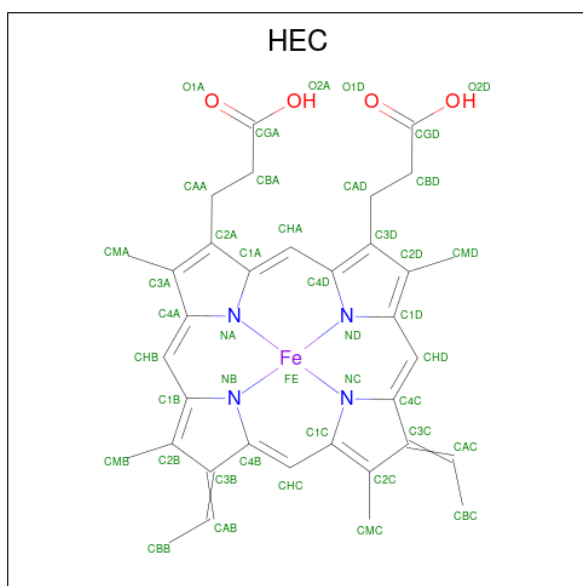
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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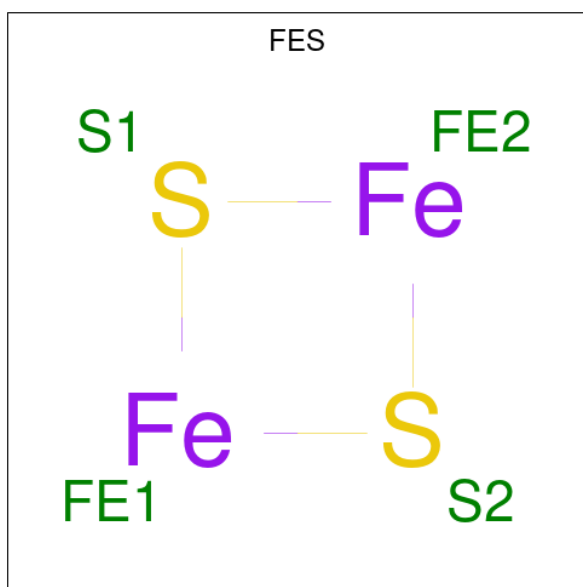
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 13 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ) (labeled as "Ligand of Interest" by depositor).

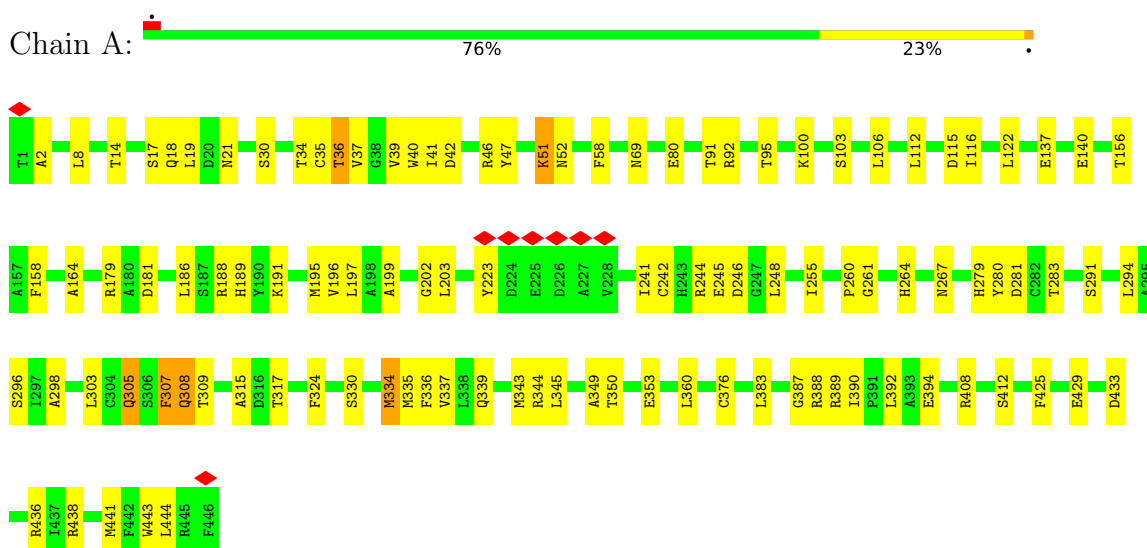


Mol	Chain	Residues	Atoms			AltConf
14	E	1	Total	Fe	S	0
			4	2	2	
14	R	1	Total	Fe	S	0
			4	2	2	

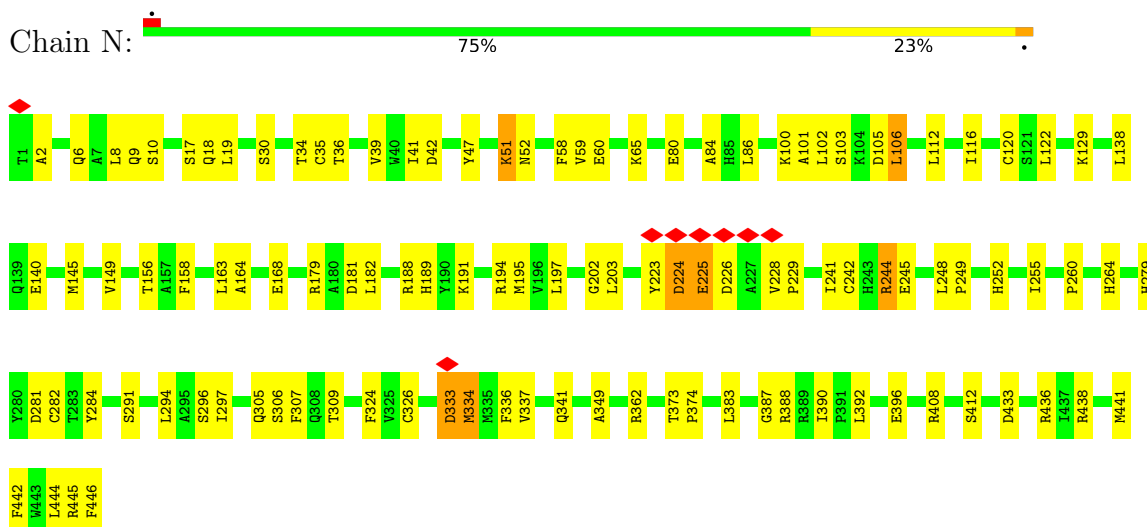
### 3 Residue-property plots

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.

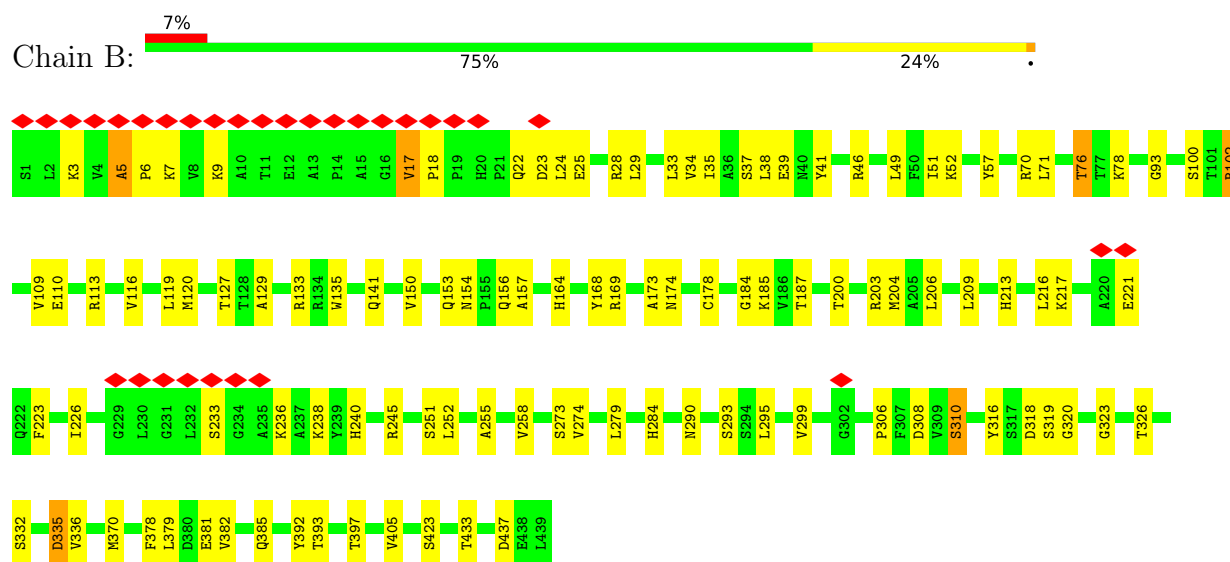
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



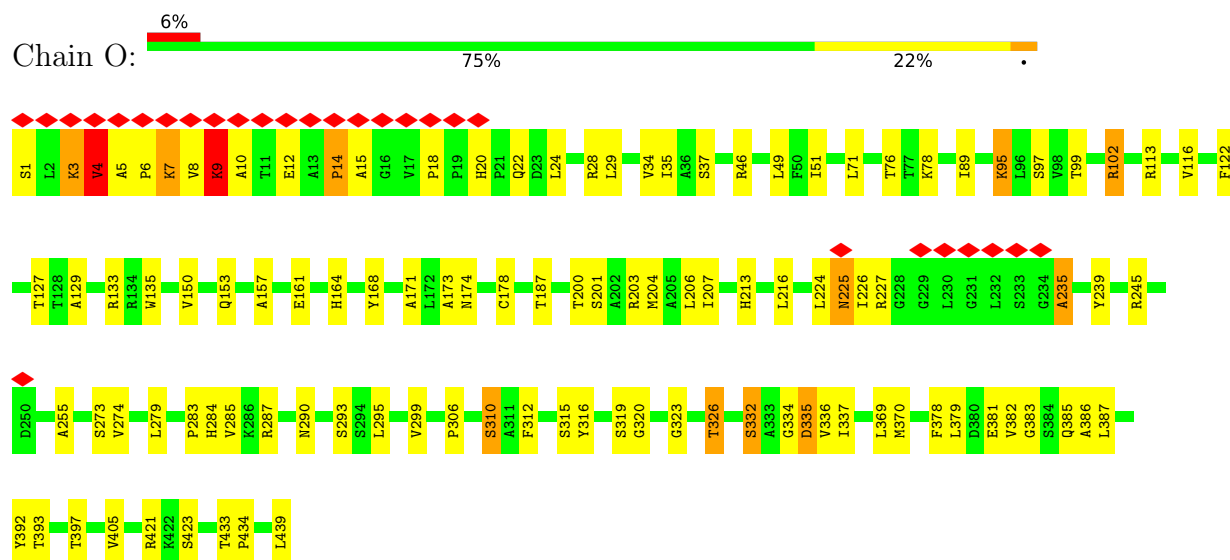
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



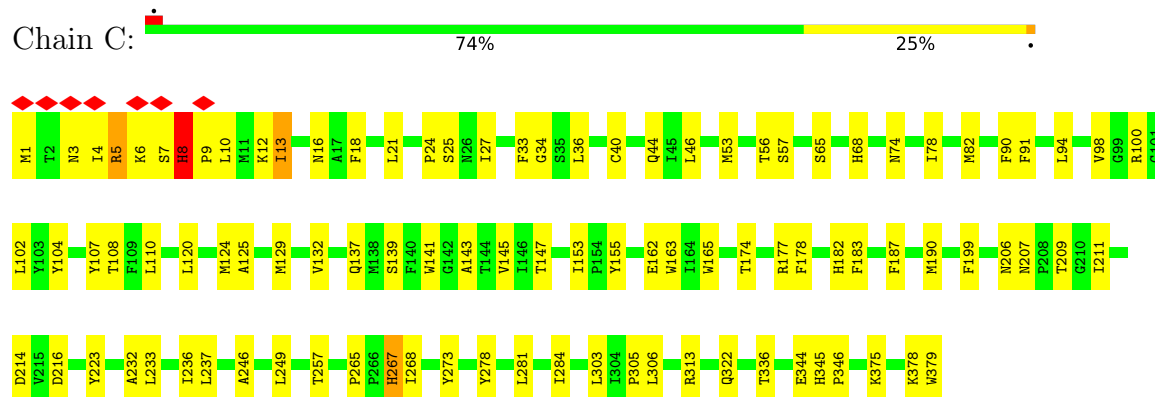
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial




• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

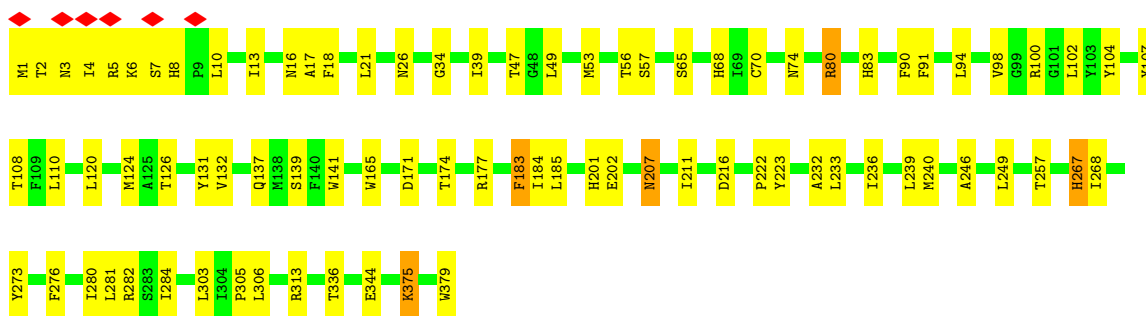


• Molecule 3: Cytochrome b




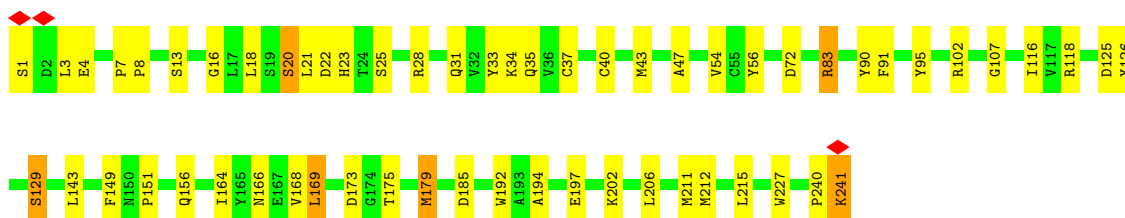
• Molecule 3: Cytochrome b

Chain P:  78% 21%




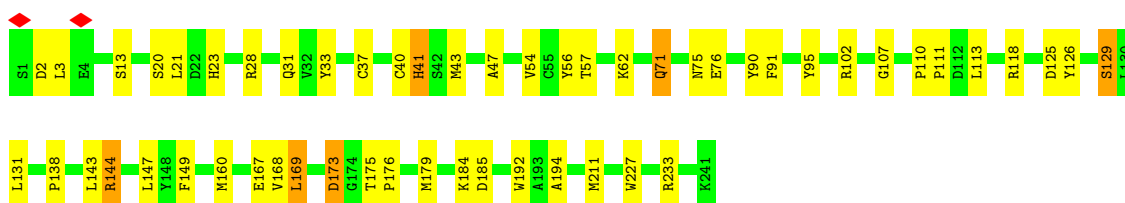
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  76% 22%



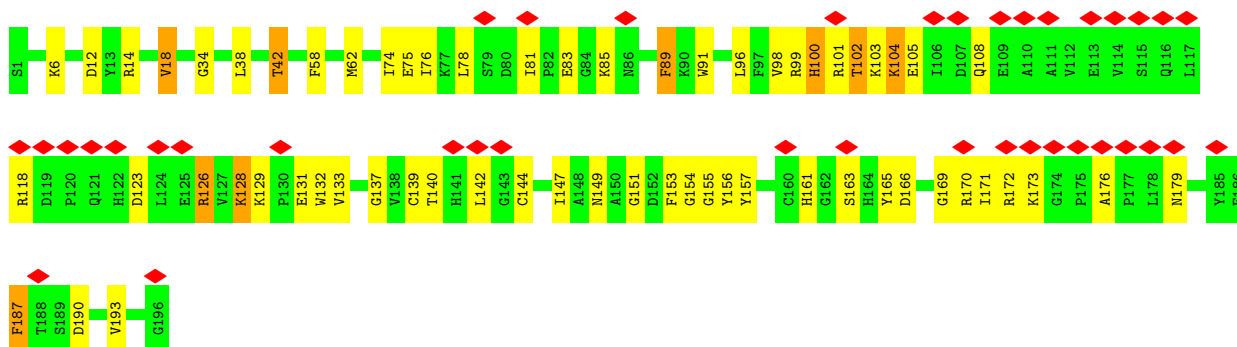
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:  78% 20%

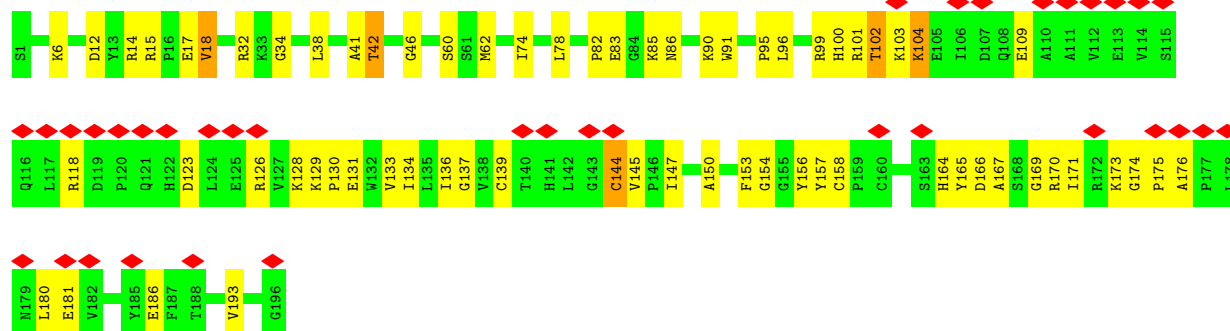


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

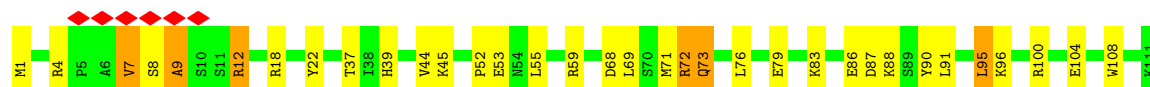
Chain E:  20% 68% 28% 5%



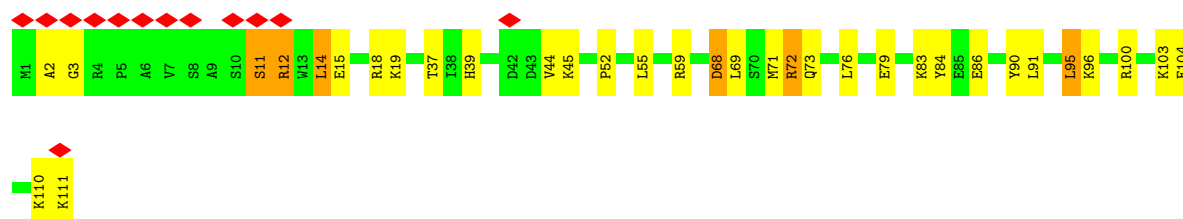
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



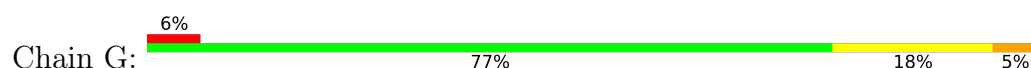
• Molecule 6: Cytochrome b-c1 complex subunit 7



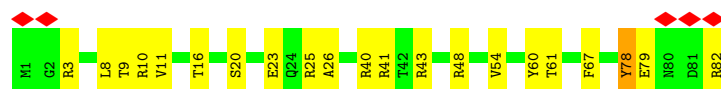
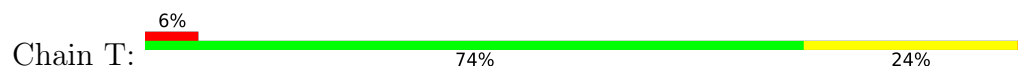
• Molecule 6: Cytochrome b-c1 complex subunit 7



• Molecule 7: Cytochrome b-c1 complex subunit 8

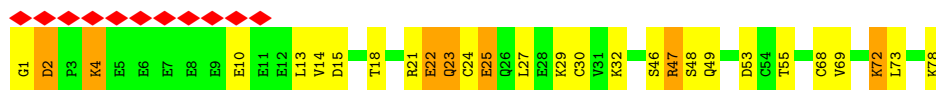


• Molecule 7: Cytochrome b-c1 complex subunit 8

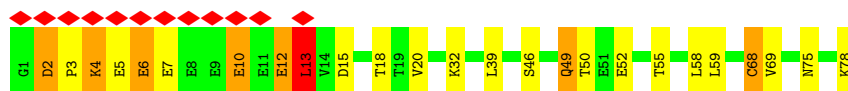


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

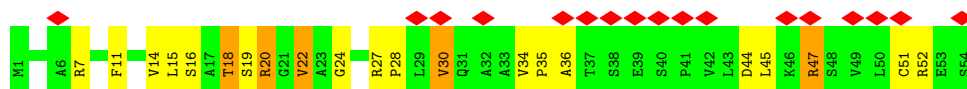




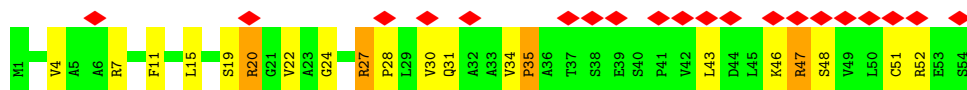
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



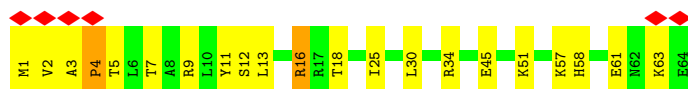
- Molecule 9: Cytochrome b-c1 complex subunit 9



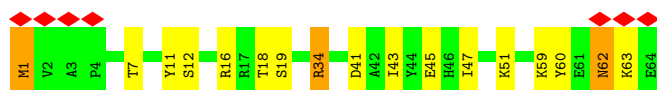
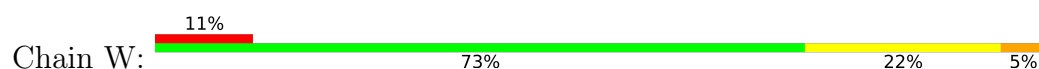
- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 10: Cytochrome b-c1 complex subunit 9



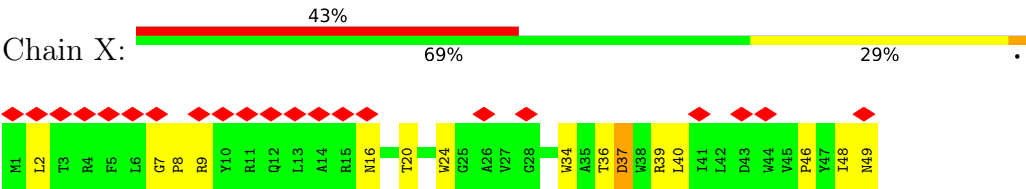
- Molecule 10: Cytochrome b-c1 complex subunit 9



- Molecule 11: Cytochrome b-c1 complex subunit 10



- Molecule 11: Cytochrome b-c1 complex subunit 10



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	140138	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CryoSPARC's own CTF correction	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	85000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	44.526	Depositor
Minimum map value	-22.986	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	438.6, 438.6, 438.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.462, 1.462, 1.462	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FES, HEC

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	0.27	0/3530	0.48	0/4792
1	N	0.27	0/3530	0.49	0/4792
2	B	0.26	0/3342	0.47	0/4537
2	O	0.27	0/3342	0.48	0/4537
3	C	0.27	0/3107	0.44	0/4252
3	P	0.27	0/3107	0.44	0/4252
4	D	0.27	0/1977	0.49	0/2684
4	Q	0.27	0/1977	0.47	0/2684
5	E	0.26	0/1553	0.49	0/2100
5	R	0.26	0/1553	0.50	0/2100
6	F	0.27	0/970	0.50	0/1301
6	S	0.26	0/970	0.53	0/1301
7	G	0.27	0/711	0.53	0/961
7	T	0.27	0/711	0.54	0/961
8	H	0.32	0/644	0.63	0/864
8	U	0.36	0/644	0.62	0/864
9	I	0.27	0/388	0.65	0/528
9	V	0.26	0/388	0.64	0/528
10	J	0.26	0/541	0.47	0/729
10	W	0.26	0/541	0.48	0/729
11	K	0.31	0/420	0.53	0/578
11	X	0.25	0/420	0.52	0/578
All	All	0.27	0/34366	0.49	0/46652

There are no bond length outliers.

There are no bond angle outliers.

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	3457	0	3356	58	0
1	N	3457	0	3356	63	0
2	B	3280	0	3276	79	0
2	O	3280	0	3276	81	0
3	C	3010	0	3077	56	0
3	P	3010	0	3077	50	0
4	D	1918	0	1870	36	0
4	Q	1918	0	1870	41	0
5	E	1519	0	1503	41	0
5	R	1519	0	1504	44	0
6	F	950	0	949	20	0
6	S	950	0	949	24	0
7	G	689	0	688	16	0
7	T	689	0	688	14	0
8	H	638	0	602	17	0
8	U	638	0	602	24	0
9	I	383	0	410	21	0
9	V	383	0	410	23	0
10	J	528	0	533	16	0
10	W	528	0	533	9	0
11	K	405	0	409	12	0
11	X	405	0	409	12	0
12	C	86	0	60	14	0
12	P	86	0	60	14	0
13	D	43	0	32	1	0
13	Q	43	0	32	7	0
14	E	4	0	0	0	0
14	R	4	0	0	1	0
All	All	33820	0	33531	659	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 10.

All (659) 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)
5:R:158:CYS:HB3	14:R:201:FES:S1	2.04	0.98
4:Q:160:MET:SD	13:Q:301:HEC:ND	2.53	0.82
1:N:41:ILE:HG22	1:N:195:MET:HG2	1.62	0.81
1:A:41:ILE:HG22	1:A:195:MET:HG2	1.61	0.81
1:N:6:GLN:HG2	2:O:9:LYS:HB3	1.62	0.80
8:U:4:LYS:HB2	8:U:12:GLU:HA	1.64	0.80
4:D:168:VAL:HG13	4:D:169:LEU:HD23	1.63	0.79
4:Q:176:PRO:HB3	8:U:13:LEU:HD13	1.62	0.78
8:U:2:ASP:HB3	8:U:12:GLU:HB3	1.64	0.78
8:H:22:GLU:HA	8:H:25:GLU:HB2	1.68	0.76
4:Q:168:VAL:HG13	4:Q:169:LEU:HD23	1.65	0.76
5:E:170:ARG:HG2	5:E:179:ASN:HD21	1.52	0.75
3:C:13:ILE:O	3:C:16:ASN:ND2	2.20	0.74
1:N:6:GLN:HB3	2:O:10:ALA:HB2	1.68	0.73
6:S:2:ALA:HB1	6:S:18:ARG:HE	1.51	0.73
4:Q:160:MET:SD	13:Q:301:HEC:FE	1.80	0.73
8:H:48:SER:OG	8:H:49:GLN:OE1	2.06	0.73
3:P:7:SER:HB2	3:P:10:LEU:HD13	1.71	0.73
6:F:52:PRO:HG2	6:F:55:LEU:HB2	1.70	0.72
6:S:52:PRO:HG2	6:S:55:LEU:HB2	1.72	0.72
5:E:154:GLY:HA3	5:E:166:ASP:HA	1.72	0.71
9:I:20:ARG:HG3	9:I:47:ARG:HE	1.53	0.71
6:F:108:TRP:O	11:K:9:ARG:NH2	2.25	0.70
9:I:20:ARG:NH2	9:I:51:CYS:SG	2.64	0.70
1:A:245:GLU:HG3	1:A:248:LEU:HG	1.74	0.70
3:P:132:VAL:HA	3:P:139:SER:HB3	1.74	0.69
2:O:37:SER:HB3	2:O:216:LEU:HD12	1.74	0.69
1:A:244:ARG:NH1	1:A:429:GLU:OE1	2.26	0.68
3:P:375:LYS:O	6:S:18:ARG:NH2	2.25	0.68
8:H:49:GLN:OE1	8:H:49:GLN:N	2.26	0.68
3:C:107:TYR:HB2	3:C:305:PRO:HG3	1.76	0.68
5:E:166:ASP:OD1	5:E:170:ARG:N	2.27	0.68
2:B:78:LYS:HG3	2:B:129:ALA:HB1	1.75	0.67
9:V:20:ARG:NH2	9:V:48:SER:OG	2.28	0.67
2:B:46:ARG:NH1	2:B:110:GLU:OE1	2.27	0.67
9:I:28:PRO:HB3	2:O:310:SER:HB3	1.76	0.67
12:P:401:HEM:HMC1	12:P:401:HEM:HBC2	1.77	0.66
2:B:37:SER:OG	2:B:213:HIS:ND1	2.24	0.66
1:N:245:GLU:HG3	1:N:248:LEU:HG	1.77	0.66
1:A:444:LEU:HB2	10:J:18:THR:HG21	1.78	0.66
1:N:412:SER:O	10:W:16:ARG:NH1	2.29	0.66
8:U:4:LYS:HB2	8:U:12:GLU:CA	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:401:HEM:HBC2	12:C:401:HEM:HMC1	1.77	0.66
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.78	0.65
3:P:107:TYR:HB2	3:P:305:PRO:HG3	1.77	0.65
1:N:145:MET:SD	1:N:252:HIS:ND1	2.69	0.65
1:N:336:PHE:HB3	3:P:4:ILE:HD11	1.79	0.65
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.78	0.64
2:B:9:LYS:HE3	2:B:22:GLN:H	1.63	0.64
5:E:128:LYS:HG2	5:E:129:LYS:HG2	1.79	0.64
3:C:375:LYS:O	6:F:18:ARG:NH2	2.30	0.64
3:C:132:VAL:HA	3:C:139:SER:HB3	1.78	0.64
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.80	0.64
9:V:20:ARG:HD3	9:V:51:CYS:HA	1.80	0.64
2:B:273:SER:OG	9:V:7:ARG:NH2	2.31	0.63
1:N:444:LEU:HB2	10:W:18:THR:HG21	1.81	0.63
2:O:335:ASP:N	2:O:335:ASP:OD1	2.32	0.62
12:C:402:HEM:HBC2	12:C:402:HEM:HHD	1.81	0.62
4:Q:160:MET:SD	13:Q:301:HEC:NA	2.72	0.62
3:C:33:PHE:HA	3:C:36:LEU:HB2	1.82	0.62
1:N:122:LEU:O	1:N:179:ARG:NH2	2.33	0.62
1:A:137:GLU:HA	1:A:140:GLU:HB2	1.80	0.62
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.81	0.62
2:B:156:GLN:HG3	9:V:27:ARG:HE	1.64	0.62
3:P:13:ILE:O	3:P:16:ASN:ND2	2.25	0.62
2:B:7:LYS:HE2	2:B:382:VAL:HG21	1.81	0.62
3:C:207:ASN:ND2	3:C:209:THR:OG1	2.29	0.62
9:I:36:ALA:HB1	1:N:140:GLU:HG3	1.82	0.62
2:O:7:LYS:C	2:O:9:LYS:N	2.49	0.62
1:N:334:MET:HA	1:N:337:VAL:HG12	1.80	0.62
2:B:335:ASP:OD1	2:B:335:ASP:N	2.33	0.61
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.82	0.61
5:R:118:ARG:NH1	5:R:174:GLY:O	2.32	0.61
12:P:402:HEM:HBC2	12:P:402:HEM:HHD	1.82	0.61
4:Q:28:ARG:HH12	8:U:78:LYS:HE3	1.66	0.61
2:B:310:SER:HB3	9:V:28:PRO:HB3	1.81	0.61
4:D:28:ARG:NH1	4:D:185:ASP:OD1	2.34	0.61
10:W:1:MET:SD	10:W:12:SER:OG	2.59	0.61
2:B:245:ARG:NH1	2:B:433:THR:O	2.33	0.61
2:B:319:SER:OG	2:B:320:GLY:N	2.33	0.60
3:C:10:LEU:HG	3:C:12:LYS:H	1.65	0.60
2:O:164:HIS:NE2	2:O:316:TYR:OH	2.31	0.60
5:E:102:THR:OG1	5:E:103:LYS:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:82:ARG:NH1	8:H:46:SER:OG	2.34	0.60
3:P:108:THR:OG1	3:P:313:ARG:NH1	2.33	0.60
6:S:100:ARG:NH2	6:S:104:GLU:OE2	2.34	0.60
3:P:34:GLY:HA3	12:P:402:HEM:HBA2	1.83	0.60
2:B:381:GLU:OE2	2:B:385:GLN:NE2	2.35	0.60
5:R:109:GLU:O	5:R:170:ARG:NH1	2.35	0.60
1:A:334:MET:HA	1:A:337:VAL:HG12	1.83	0.60
1:N:60:GLU:OE2	2:O:287:ARG:NH1	2.31	0.60
2:B:5:ALA:HB3	2:B:6:PRO:HD3	1.83	0.60
4:Q:75:ASN:OD1	4:Q:76:GLU:N	2.35	0.59
5:R:166:ASP:OD1	5:R:170:ARG:N	2.29	0.59
2:B:279:LEU:HB3	2:B:295:LEU:HD13	1.84	0.59
9:I:34:VAL:HG13	2:O:287:ARG:HG2	1.83	0.59
5:R:15:ARG:HH21	5:R:32:ARG:HG2	1.67	0.59
2:O:51:ILE:HG23	2:O:204:MET:HG2	1.85	0.59
2:O:245:ARG:NH1	2:O:433:THR:O	2.35	0.59
6:S:59:ARG:NH2	6:S:90:TYR:OH	2.36	0.59
4:D:22:ASP:OD2	8:H:78:LYS:NZ	2.31	0.59
4:Q:28:ARG:NH1	4:Q:185:ASP:OD1	2.34	0.59
5:R:78:LEU:HD11	5:R:193:VAL:HG13	1.83	0.59
5:E:147:ILE:HD11	5:E:157:TYR:HB3	1.85	0.59
6:F:100:ARG:NH2	6:F:104:GLU:OE2	2.36	0.59
6:S:11:SER:O	6:S:11:SER:OG	2.19	0.59
1:A:412:SER:O	10:J:16:ARG:NH1	2.36	0.59
9:I:11:PHE:CD1	9:I:24:GLY:HA2	2.37	0.59
2:O:28:ARG:HG2	2:O:34:VAL:HG22	1.85	0.59
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.84	0.59
6:F:59:ARG:NH2	6:F:90:TYR:OH	2.35	0.58
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.85	0.58
2:O:37:SER:OG	2:O:213:HIS:ND1	2.32	0.58
1:A:137:GLU:N	1:A:137:GLU:OE1	2.35	0.58
6:F:44:VAL:HG22	6:F:95:LEU:HD11	1.85	0.58
2:O:381:GLU:OE2	2:O:385:GLN:NE2	2.37	0.58
7:T:78:TYR:OH	8:U:49:GLN:O	2.22	0.58
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.85	0.58
1:N:158:PHE:O	1:N:164:ALA:HB2	2.03	0.58
2:O:4:VAL:HG22	2:O:7:LYS:HB3	1.85	0.58
8:U:50:THR:HG22	8:U:52:GLU:H	1.69	0.58
8:U:55:THR:HA	8:U:58:LEU:HB3	1.84	0.57
3:C:34:GLY:HA3	12:C:402:HEM:HBA2	1.86	0.57
6:F:83:LYS:HB2	6:F:86:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:46:LYS:HE2	9:V:47:ARG:HH22	1.69	0.57
2:O:1:SER:HA	2:O:7:LYS:HE2	1.86	0.57
5:R:129:LYS:HG2	5:R:131:GLU:H	1.68	0.57
1:A:122:LEU:O	1:A:179:ARG:NH2	2.35	0.57
2:O:76:THR:HG21	2:O:133:ARG:HD2	1.87	0.57
11:K:18:VAL:O	11:K:22:SER:N	2.31	0.57
2:B:38:LEU:HD23	2:B:39:GLU:N	2.19	0.57
3:C:141:TRP:HB3	3:C:268:ILE:HD12	1.87	0.57
1:N:80:GLU:HG2	2:O:284:HIS:HB2	1.86	0.57
4:Q:118:ARG:HG3	4:Q:194:ALA:HB1	1.86	0.57
4:Q:125:ASP:O	4:Q:129:SER:OG	2.22	0.57
1:A:242:CYS:HB2	7:G:16:THR:HG22	1.87	0.57
4:D:31:GLN:OE1	4:D:56:TYR:OH	2.23	0.57
2:B:236:LYS:HE3	2:B:318:ASP:HB2	1.87	0.56
4:D:126:TYR:OH	13:D:301:HEC:O2A	2.22	0.56
4:D:125:ASP:O	4:D:129:SER:OG	2.22	0.56
6:F:73:GLN:O	7:G:40:ARG:NH1	2.37	0.56
9:I:16:SER:HB3	2:O:97:SER:HB3	1.86	0.56
2:O:200:THR:HG21	2:O:226:ILE:HB	1.87	0.56
10:W:59:LYS:NZ	10:W:60:TYR:OH	2.37	0.56
5:E:83:GLU:HA	5:E:100:HIS:HB3	1.87	0.56
9:I:44:ASP:HB2	1:N:249:PRO:HG2	1.88	0.56
1:N:260:PRO:HB2	1:N:264:HIS:HB3	1.86	0.56
5:R:154:GLY:HA3	5:R:166:ASP:HA	1.88	0.56
9:I:14:VAL:HB	9:I:22:VAL:HG22	1.87	0.56
1:A:158:PHE:O	1:A:164:ALA:HB2	2.06	0.56
2:B:28:ARG:HG2	2:B:34:VAL:HG22	1.88	0.56
2:B:141:GLN:HG2	2:B:184:GLY:HA2	1.87	0.56
12:P:402:HEM:HBB2	12:P:402:HEM:HMB1	1.88	0.56
6:S:111:LYS:HG2	11:X:2:LEU:H	1.71	0.55
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.88	0.55
7:T:20:SER:HB3	7:T:23:GLU:HG3	1.88	0.55
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.88	0.55
1:N:294:LEU:HB2	1:N:341:GLN:HG3	1.88	0.55
2:B:76:THR:HG21	2:B:133:ARG:HD2	1.87	0.55
3:C:98:VAL:HG22	12:C:402:HEM:HAC	1.89	0.55
10:J:61:GLU:OE1	10:J:63:LYS:NZ	2.39	0.55
3:P:98:VAL:HG22	12:P:402:HEM:HAC	1.87	0.55
2:O:78:LYS:HG3	2:O:129:ALA:HB1	1.88	0.55
2:B:3:LYS:HE3	2:B:9:LYS:HE2	1.89	0.55
1:A:444:LEU:HD13	11:X:24:TRP:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:184:LYS:HZ1	8:U:78:LYS:HG3	1.71	0.55
2:B:164:HIS:NE2	2:B:316:TYR:OH	2.32	0.55
5:R:147:ILE:HD12	5:R:150:ALA:HB3	1.89	0.55
5:E:139:CYS:SG	5:E:165:TYR:OH	2.62	0.55
3:C:322:GLN:OE1	7:G:48:ARG:NH2	2.39	0.54
5:E:151:GLY:H	5:E:155:GLY:HA2	1.72	0.54
12:P:401:HEM:HMB1	12:P:401:HEM:HBB2	1.89	0.54
4:D:16:GLY:O	4:D:202:LYS:NZ	2.40	0.54
9:I:20:ARG:NH1	9:I:52:ARG:H	2.05	0.54
12:C:402:HEM:HMB1	12:C:402:HEM:HBB2	1.87	0.54
2:O:102:ARG:NH2	2:O:174:ASN:O	2.40	0.54
5:R:86:ASN:ND2	5:R:156:TYR:OH	2.39	0.54
2:B:52:LYS:HB2	2:B:203:ARG:HB2	1.89	0.54
1:N:281:ASP:HA	1:N:306:SER:HA	1.89	0.54
2:O:102:ARG:NH1	2:O:161:GLU:OE2	2.40	0.54
2:O:274:VAL:HG11	2:O:405:VAL:HG11	1.89	0.54
9:I:15:LEU:HG	2:O:71:LEU:HD12	1.89	0.54
2:B:274:VAL:HG11	2:B:405:VAL:HG11	1.90	0.54
1:N:2:ALA:O	2:O:113:ARG:NE	2.40	0.54
2:O:225:ASN:H	2:O:226:ILE:HD12	1.73	0.54
2:B:102:ARG:NH2	2:B:174:ASN:O	2.41	0.54
3:C:199:PHE:HE1	3:P:10:LEU:HA	1.72	0.54
3:C:344:GLU:HG3	7:G:67:PHE:HE1	1.73	0.54
4:D:33:TYR:HA	4:D:37:CYS:SG	2.47	0.54
8:H:1:GLY:N	8:H:4:LYS:HD2	2.23	0.54
11:K:48:ILE:HA	10:W:34:ARG:HD2	1.89	0.54
8:U:20:VAL:HG12	8:U:69:VAL:HG12	1.90	0.54
2:B:57:TYR:HE2	2:B:203:ARG:HH12	1.56	0.53
3:C:56:THR:HG23	3:P:56:THR:HG23	1.90	0.53
2:B:157:ALA:HA	9:V:11:PHE:HE2	1.73	0.53
2:O:150:VAL:HA	2:O:153:GLN:HG3	1.89	0.53
5:R:171:ILE:HG21	5:R:176:ALA:HB3	1.90	0.53
3:C:145:VAL:HG12	5:E:142:LEU:HB3	1.91	0.53
2:O:29:LEU:HD21	2:O:35:ILE:HD12	1.90	0.53
3:C:4:ILE:HG23	3:C:6:LYS:H	1.73	0.53
3:P:2:THR:HG22	3:P:5:ARG:H	1.73	0.53
1:A:80:GLU:HG2	2:B:284:HIS:HB2	1.90	0.53
2:B:308:ASP:OD1	9:V:31:GLN:NE2	2.41	0.53
10:J:2:VAL:HG22	10:J:3:ALA:H	1.74	0.53
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.48	0.53
6:F:4:ARG:HB2	6:F:9:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:18:THR:HG21	2:O:95:LYS:HA	1.89	0.53
2:O:89:ILE:HG13	2:O:122:PHE:HD2	1.74	0.53
1:A:46:ARG:HH22	1:A:315:ALA:HB3	1.74	0.53
3:C:143:ALA:O	3:C:147:THR:OG1	2.20	0.53
5:R:102:THR:OG1	5:R:103:LYS:N	2.42	0.53
2:B:290:ASN:HB3	2:B:293:SER:HB3	1.90	0.53
4:D:31:GLN:O	4:D:35:GLN:NE2	2.39	0.53
1:A:37:VAL:HG23	1:A:199:ALA:HB2	1.89	0.52
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.91	0.52
1:A:281:ASP:OD2	9:V:48:SER:OG	2.25	0.52
4:D:23:HIS:ND1	4:D:54:VAL:O	2.40	0.52
3:P:100:ARG:HG3	3:P:104:TYR:HD2	1.74	0.52
5:R:139:CYS:N	5:R:144:CYS:O	2.42	0.52
1:N:362:ARG:NE	1:N:396:GLU:OE2	2.32	0.52
2:O:225:ASN:O	2:O:225:ASN:ND2	2.39	0.52
1:A:260:PRO:HB2	1:A:264:HIS:HB3	1.92	0.52
3:C:214:ASP:OD1	7:G:3:ARG:NH1	2.43	0.52
4:D:1:SER:HB3	8:H:55:THR:HG21	1.91	0.52
9:I:35:PRO:HB2	2:O:306:PRO:HB3	1.91	0.52
12:C:401:HEM:HBB2	12:C:401:HEM:HMB1	1.91	0.52
6:S:73:GLN:O	7:T:40:ARG:NH1	2.42	0.52
1:A:2:ALA:O	2:B:113:ARG:NE	2.41	0.52
1:N:51:LYS:HD2	1:N:52:ASN:HB3	1.92	0.52
1:N:65:LYS:NZ	2:O:287:ARG:O	2.33	0.52
1:N:6:GLN:HB3	2:O:10:ALA:CB	2.39	0.52
2:O:239:TYR:OH	2:O:421:ARG:O	2.27	0.52
4:Q:160:MET:SD	13:Q:301:HEC:NC	2.83	0.52
5:E:78:LEU:HD11	5:E:193:VAL:HG13	1.92	0.52
8:U:4:LYS:HD3	8:U:12:GLU:HA	1.92	0.52
8:H:15:ASP:HB3	8:H:18:THR:HG22	1.92	0.52
1:A:91:THR:OG1	1:A:92:ARG:N	2.43	0.51
4:D:13:SER:HB2	10:J:51:LYS:HE2	1.92	0.51
3:P:8:HIS:O	3:P:10:LEU:N	2.39	0.51
2:B:306:PRO:HB3	9:V:35:PRO:HB2	1.91	0.51
5:R:96:LEU:HA	5:R:136:ILE:HA	1.91	0.51
1:A:261:GLY:O	1:A:267:ASN:ND2	2.38	0.51
3:C:165:TRP:O	3:C:174:THR:OG1	2.26	0.51
3:C:267:HIS:O	3:C:267:HIS:ND1	2.33	0.51
4:D:72:ASP:HB2	4:D:83:ARG:HG2	1.93	0.51
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.92	0.51
6:S:44:VAL:HG22	6:S:95:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ASP:OD1	2:B:23:ASP:N	2.42	0.51
5:E:104:LYS:H	5:E:104:LYS:HD3	1.75	0.51
6:F:7:VAL:HG13	6:F:8:SER:H	1.76	0.51
9:I:19:SER:OG	9:I:20:ARG:N	2.44	0.51
1:N:39:VAL:HG22	1:N:197:LEU:HD12	1.92	0.51
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.93	0.51
5:E:81:ILE:HD11	5:E:85:LYS:HB3	1.93	0.51
5:E:100:HIS:ND1	5:E:131:GLU:O	2.39	0.51
1:A:39:VAL:HG22	1:A:197:LEU:HD12	1.93	0.51
3:C:100:ARG:HG3	3:C:104:TYR:HD2	1.76	0.51
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.93	0.51
2:O:14:PRO:HB3	2:O:20:HIS:CD2	2.46	0.51
5:R:186:GLU:N	5:R:186:GLU:OE1	2.43	0.51
6:S:83:LYS:HB2	6:S:86:GLU:HB2	1.93	0.51
9:V:43:LEU:HD23	9:V:46:LYS:HD3	1.93	0.51
2:O:34:VAL:HG11	2:O:386:ALA:HB1	1.93	0.51
2:O:207:ILE:HG13	2:O:383:GLY:HA2	1.92	0.51
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.93	0.51
6:S:2:ALA:O	6:S:14:LEU:HB2	2.10	0.51
10:J:3:ALA:HB1	10:J:4:PRO:HD2	1.94	0.50
6:S:3:GLY:H	6:S:18:ARG:NE	2.09	0.50
2:O:7:LYS:HB2	2:O:9:LYS:HG2	1.92	0.50
2:O:332:SER:O	2:O:332:SER:OG	2.29	0.50
4:Q:20:SER:OG	4:Q:21:LEU:N	2.43	0.50
4:Q:167:GLU:OE2	8:U:12:GLU:HG3	2.11	0.50
1:A:305:GLN:OE1	9:V:46:LYS:N	2.44	0.50
1:N:112:LEU:O	1:N:116:ILE:HG13	2.12	0.50
2:O:7:LYS:C	2:O:9:LYS:H	2.14	0.50
5:R:101:ARG:HE	5:R:133:VAL:HB	1.77	0.50
5:E:58:PHE:HZ	3:P:47:THR:HG22	1.77	0.50
5:R:123:ASP:OD2	5:R:170:ARG:NH1	2.45	0.50
2:B:49:LEU:HD13	2:B:206:LEU:HD13	1.92	0.50
5:R:129:LYS:HZ3	5:R:131:GLU:HB3	1.77	0.50
1:A:156:THR:HG21	1:A:241:ILE:HB	1.93	0.50
2:B:150:VAL:HG12	9:V:46:LYS:HA	1.93	0.50
2:B:221:GLU:N	2:B:221:GLU:OE1	2.42	0.50
1:N:433:ASP:OD2	3:P:223:TYR:OH	2.29	0.50
1:N:194:ARG:HD2	1:N:228:VAL:HG13	1.94	0.49
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.94	0.49
2:B:157:ALA:HA	9:V:11:PHE:CE2	2.47	0.49
5:E:153:PHE:HB2	5:E:172:ARG:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:6:GLN:HG2	2:O:9:LYS:CB	2.39	0.49
4:Q:31:GLN:OE1	4:Q:56:TYR:OH	2.28	0.49
1:A:69:ASN:ND2	1:A:115:ASP:OD1	2.39	0.49
2:B:255:ALA:HB3	2:B:326:THR:HG22	1.94	0.49
10:J:30:LEU:HD21	11:X:34:TRP:HB2	1.93	0.49
1:A:106:LEU:HD13	1:A:203:LEU:HD22	1.94	0.49
3:C:53:MET:HE1	5:R:62:MET:HG2	1.95	0.49
4:Q:184:LYS:NZ	8:U:78:LYS:HG3	2.27	0.49
5:R:165:TYR:HB3	5:R:169:GLY:HA2	1.95	0.49
3:C:108:THR:OG1	3:C:313:ARG:NH1	2.43	0.49
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.92	0.49
1:N:442:PHE:CD1	1:N:445:ARG:HB3	2.47	0.49
3:P:177:ARG:NH2	5:R:62:MET:O	2.43	0.49
8:U:3:PRO:HA	8:U:10:GLU:HB2	1.94	0.49
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.94	0.49
2:O:319:SER:OG	2:O:320:GLY:N	2.45	0.49
8:U:68:CYS:SG	8:U:69:VAL:N	2.85	0.49
7:G:19:LEU:HD22	7:G:23:GLU:HB2	1.95	0.49
1:N:349:ALA:H	1:N:408:ARG:HD3	1.78	0.49
8:U:4:LYS:C	8:U:10:GLU:HB3	2.32	0.49
9:V:51:CYS:SG	9:V:52:ARG:N	2.86	0.49
11:X:46:PRO:O	11:X:49:ASN:ND2	2.45	0.49
1:A:14:THR:OG1	1:A:389:ARG:HD3	2.13	0.49
3:C:120:LEU:O	3:C:124:MET:HG3	2.12	0.49
5:R:38:LEU:O	5:R:42:THR:OG1	2.27	0.49
11:X:7:GLY:N	11:X:8:PRO:HD3	2.28	0.49
2:B:46:ARG:HH21	2:B:209:LEU:HD12	1.77	0.49
2:O:255:ALA:HB3	2:O:326:THR:HG22	1.95	0.49
1:A:8:LEU:HD22	1:A:392:LEU:HB3	1.95	0.48
4:D:215:LEU:HD21	5:R:46:GLY:HA3	1.95	0.48
5:E:14:ARG:HG3	5:E:18:VAL:HG23	1.95	0.48
4:Q:233:ARG:NH1	6:S:68:ASP:OD1	2.31	0.48
7:G:81:ASP:OD1	7:G:81:ASP:N	2.46	0.48
1:N:8:LEU:HD22	1:N:392:LEU:HB3	1.96	0.48
5:E:96:LEU:HA	5:E:137:GLY:H	1.78	0.48
1:N:294:LEU:HD11	1:N:334:MET:SD	2.52	0.48
4:Q:3:LEU:HD23	4:Q:3:LEU:H	1.77	0.48
9:V:11:PHE:CD1	9:V:24:GLY:HA2	2.47	0.48
1:A:112:LEU:O	1:A:116:ILE:HG13	2.13	0.48
9:I:7:ARG:NH2	2:O:273:SER:OG	2.46	0.48
8:H:24:CYS:O	8:H:30:CYS:SG	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:LEU:HD12	2:B:33:LEU:HB3	1.96	0.48
4:D:28:ARG:HH12	8:H:78:LYS:HE3	1.79	0.48
8:H:24:CYS:SG	8:H:27:LEU:HB2	2.53	0.48
2:O:15:ALA:HB3	2:O:18:PRO:HG2	1.96	0.48
6:S:45:LYS:HD2	6:S:45:LYS:HA	1.65	0.48
4:Q:126:TYR:OH	13:Q:301:HEC:O2A	2.30	0.48
1:N:242:CYS:HB2	7:T:16:THR:HG22	1.96	0.48
2:O:49:LEU:HD23	2:O:127:THR:HG21	1.94	0.48
7:T:25:ARG:HH21	7:T:26:ALA:H	1.62	0.48
1:A:408:ARG:NH2	11:X:16:ASN:OD1	2.47	0.48
1:A:433:ASP:OD2	3:C:223:TYR:OH	2.31	0.48
4:D:3:LEU:HD12	4:D:4:GLU:H	1.79	0.48
4:D:18:LEU:HD22	4:D:206:LEU:HB2	1.96	0.48
4:D:173:ASP:N	4:D:173:ASP:OD1	2.43	0.48
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.96	0.48
7:T:82:ARG:O	8:U:46:SER:OG	2.30	0.48
1:A:307:PHE:HA	1:A:324:PHE:HA	1.96	0.48
3:C:5:ARG:O	3:C:5:ARG:NH2	2.35	0.48
3:P:344:GLU:HG3	7:T:67:PHE:HE1	1.79	0.47
5:R:126:ARG:HH22	5:R:170:ARG:HG3	1.79	0.47
2:O:5:ALA:HB3	2:O:6:PRO:HD3	1.95	0.47
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.49	0.47
4:Q:41:HIS:HD1	4:Q:113:LEU:HG	1.79	0.47
2:B:57:TYR:HA	2:B:233:SER:OG	2.15	0.47
5:E:38:LEU:O	5:E:42:THR:OG1	2.28	0.47
2:O:3:LYS:H	2:O:7:LYS:HD3	1.79	0.47
6:S:19:LYS:HZ2	6:S:84:TYR:HD2	1.63	0.47
10:J:45:GLU:N	10:J:45:GLU:OE1	2.48	0.47
2:O:49:LEU:HD13	2:O:206:LEU:HD13	1.96	0.47
3:P:3:ASN:O	3:P:6:LYS:HG2	2.15	0.47
3:P:120:LEU:O	3:P:124:MET:HG3	2.15	0.47
3:P:165:TRP:O	3:P:174:THR:OG1	2.30	0.47
1:A:308:GLN:HB2	9:V:52:ARG:HD3	1.97	0.47
4:D:166:ASN:OD1	4:D:179:MET:N	2.44	0.47
7:G:77:ALA:O	8:H:47:ARG:NH1	2.39	0.47
11:K:38:TRP:HA	11:K:38:TRP:CE3	2.49	0.47
1:N:334:MET:O	1:N:334:MET:HG3	2.14	0.47
3:P:80:ARG:HH21	3:P:80:ARG:HG3	1.78	0.47
1:A:336:PHE:O	3:C:1:MET:HB3	2.14	0.47
1:A:343:MET:SD	1:A:443:TRP:HB2	2.55	0.47
5:E:173:LYS:HE3	5:E:173:LYS:HB3	1.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:4:PRO:HA	10:J:9:ARG:NH2	2.29	0.47
6:F:69:LEU:HD11	6:F:76:LEU:HG	1.97	0.47
6:F:71:MET:HE3	6:F:72:ARG:HD3	1.97	0.47
3:P:232:ALA:O	3:P:236:ILE:HG12	2.15	0.47
11:K:1:MET:SD	11:K:1:MET:N	2.73	0.47
1:N:244:ARG:HG2	7:T:11:VAL:HG12	1.97	0.47
4:D:143:LEU:HD11	4:D:149:PHE:HB2	1.97	0.47
3:C:78:ILE:O	3:C:82:MET:HG2	2.15	0.46
2:B:71:LEU:HD12	9:V:15:LEU:HG	1.97	0.46
12:C:402:HEM:HBD1	12:C:402:HEM:HHA	1.97	0.46
6:F:91:LEU:HG	6:F:95:LEU:HD23	1.96	0.46
1:N:156:THR:HG21	1:N:241:ILE:HB	1.97	0.46
9:V:34:VAL:HB	9:V:35:PRO:HD3	1.97	0.46
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.50	0.46
2:B:295:LEU:O	2:B:299:VAL:HG23	2.15	0.46
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.50	0.46
2:O:7:LYS:O	2:O:8:VAL:C	2.53	0.46
3:P:4:ILE:H	3:P:4:ILE:HD12	1.79	0.46
2:B:7:LYS:HD3	2:B:24:LEU:HG	1.97	0.46
2:B:46:ARG:HD3	2:B:379:LEU:HD22	1.98	0.46
2:B:185:LYS:HA	2:B:185:LYS:HD3	1.77	0.46
6:F:45:LYS:HA	6:F:45:LYS:HD2	1.64	0.46
7:G:23:GLU:OE2	5:R:32:ARG:NH1	2.49	0.46
4:Q:173:ASP:OD1	4:Q:175:THR:HG23	2.15	0.46
2:O:14:PRO:HB3	2:O:20:HIS:HD2	1.80	0.46
3:C:7:SER:C	3:C:9:PRO:HD2	2.35	0.46
5:E:98:VAL:HG12	5:E:132:TRP:HZ3	1.81	0.46
6:F:53:GLU:OE2	7:G:10:ARG:NH1	2.49	0.46
7:G:60:TYR:O	7:G:64:THR:OG1	2.25	0.46
1:N:129:LYS:HA	1:N:129:LYS:HD3	1.68	0.46
6:S:111:LYS:H	11:X:9:ARG:HB2	1.81	0.46
3:C:53:MET:HB2	3:C:53:MET:HE2	1.70	0.46
5:E:165:TYR:HB3	5:E:169:GLY:HA2	1.97	0.46
1:N:19:LEU:HD23	1:N:19:LEU:HA	1.78	0.46
1:N:188:ARG:HD2	1:N:225:GLU:HG3	1.98	0.46
1:N:324:PHE:HE2	1:N:326:CYS:HG	1.64	0.46
2:B:24:LEU:HD22	2:B:25:GLU:H	1.79	0.46
2:B:332:SER:O	2:B:332:SER:OG	2.34	0.46
4:Q:23:HIS:ND1	4:Q:54:VAL:O	2.44	0.46
2:B:3:LYS:HG2	2:B:6:PRO:O	2.14	0.46
11:K:39:ARG:H	11:K:39:ARG:HG3	1.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.97	0.46
7:T:82:ARG:HH12	8:U:39:LEU:HB3	1.81	0.46
8:U:6:GLU:HG3	8:U:7:GLU:N	2.31	0.46
1:A:390:ILE:HG23	1:A:394:GLU:HG2	1.97	0.46
4:D:240:PRO:O	4:D:241:LYS:HD3	2.16	0.46
5:E:139:CYS:H	5:E:144:CYS:H	1.63	0.46
2:O:7:LYS:HD2	2:O:9:LYS:HZ2	1.80	0.46
1:A:21:ASN:OD1	1:A:21:ASN:N	2.40	0.45
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.84	0.45
8:H:1:GLY:H2	8:H:4:LYS:HD2	1.81	0.45
1:A:294:LEU:HD11	1:A:334:MET:SD	2.56	0.45
1:A:360:LEU:HD12	2:B:93:GLY:HA2	1.98	0.45
2:B:153:GLN:HE22	9:V:46:LYS:HB2	1.81	0.45
1:N:297:ILE:HD11	3:P:2:THR:OG1	2.15	0.45
4:Q:143:LEU:HD11	4:Q:149:PHE:HB2	1.98	0.45
2:B:3:LYS:HD3	2:B:7:LYS:HA	1.98	0.45
3:C:187:PHE:HZ	3:P:184:ILE:HD12	1.82	0.45
5:E:104:LYS:O	5:E:108:GLN:NE2	2.34	0.45
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.45
2:O:295:LEU:O	2:O:299:VAL:HG23	2.15	0.45
1:N:224:ASP:OD1	1:N:225:GLU:N	2.43	0.45
6:S:110:LYS:HB2	11:X:7:GLY:HA2	1.97	0.45
8:U:15:ASP:O	8:U:18:THR:OG1	2.33	0.45
9:V:47:ARG:O	9:V:47:ARG:NH2	2.45	0.45
2:B:29:LEU:HD21	2:B:35:ILE:HD12	1.99	0.45
4:D:102:ARG:NH2	4:D:107:GLY:O	2.49	0.45
10:J:57:LYS:HB3	10:J:57:LYS:HE3	1.84	0.45
5:R:104:LYS:HD3	5:R:104:LYS:H	1.82	0.45
1:N:9:GLN:NE2	2:O:7:LYS:HE3	2.32	0.45
2:O:200:THR:HG22	2:O:224:LEU:HD22	1.98	0.45
4:Q:54:VAL:HG11	4:Q:192:TRP:CE2	2.52	0.45
1:A:281:ASP:O	1:A:283:THR:N	2.49	0.45
9:I:45:LEU:HA	1:N:305:GLN:HE22	1.81	0.45
1:A:279:HIS:HB2	9:V:20:ARG:NH1	2.32	0.45
4:D:54:VAL:HG11	4:D:192:TRP:CE2	2.52	0.45
11:K:39:ARG:HD2	11:K:40:LEU:H	1.82	0.45
3:P:137:GLN:HG3	3:P:137:GLN:O	2.17	0.45
3:C:100:ARG:HH22	12:C:402:HEM:HBD2	1.81	0.45
3:C:345:HIS:ND1	3:C:346:PRO:HD3	2.32	0.45
2:O:171:ALA:HB2	2:O:235:ALA:H	1.82	0.45
6:S:91:LEU:HG	6:S:95:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:THR:HG22	2:B:397:THR:HB	1.99	0.44
12:C:401:HEM:O1D	12:C:401:HEM:HBA2	2.17	0.44
4:D:1:SER:HB2	4:D:156:GLN:HB2	1.99	0.44
5:E:99:ARG:HE	5:E:101:ARG:CZ	2.29	0.44
5:E:126:ARG:HH11	5:E:133:VAL:HB	1.82	0.44
3:P:183:PHE:CZ	12:P:401:HEM:HBC1	2.52	0.44
5:R:17:GLU:H	5:R:17:GLU:HG2	1.49	0.44
12:P:402:HEM:HBD1	12:P:402:HEM:HHA	1.98	0.44
2:B:258:VAL:HA	2:B:323:GLY:HA3	1.99	0.44
5:E:76:ILE:HG12	5:E:89:PHE:CZ	2.52	0.44
5:E:166:ASP:OD1	5:E:169:GLY:N	2.50	0.44
2:O:7:LYS:O	2:O:9:LYS:N	2.51	0.44
2:O:290:ASN:HB3	2:O:293:SER:HB3	1.99	0.44
2:O:312:PHE:N	2:O:323:GLY:O	2.45	0.44
3:P:70:CYS:SG	3:P:80:ARG:HD3	2.57	0.44
12:P:401:HEM:O1D	12:P:401:HEM:HBA2	2.17	0.44
4:Q:75:ASN:OD1	4:Q:76:GLU:HG3	2.17	0.44
5:R:14:ARG:HG3	5:R:18:VAL:HG23	1.99	0.44
2:B:3:LYS:HB2	2:B:38:LEU:HD21	1.98	0.44
3:C:183:PHE:CZ	12:C:401:HEM:HBC1	2.52	0.44
4:Q:138:PRO:HG3	8:U:55:THR:HB	2.00	0.44
2:B:17:VAL:HB	2:B:18:PRO:HD3	1.98	0.44
3:C:246:ALA:HB1	3:C:249:LEU:HB2	2.00	0.44
12:C:402:HEM:HBC2	12:C:402:HEM:CHD	2.45	0.44
4:D:116:ILE:HD12	4:D:116:ILE:HA	1.89	0.44
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.99	0.44
4:Q:144:ARG:HE	4:Q:147:LEU:HD22	1.83	0.44
1:A:383:LEU:HA	1:A:387:GLY:O	2.17	0.44
5:E:34:GLY:HA2	10:W:11:TYR:HB2	1.99	0.44
7:G:20:SER:HB3	7:G:23:GLU:HG3	2.00	0.44
3:P:26:ASN:HD21	3:P:207:ASN:HB2	1.83	0.44
3:C:129:MET:HE2	3:C:178:PHE:HA	1.99	0.44
3:P:91:PHE:HA	3:P:94:LEU:HB2	2.00	0.44
7:T:78:TYR:HD1	7:T:79:GLU:H	1.66	0.44
1:A:350:THR:HG21	11:X:9:ARG:HD3	1.99	0.44
3:C:137:GLN:HG3	3:C:265:PRO:HG3	1.98	0.44
5:E:101:ARG:CZ	5:E:101:ARG:HA	2.48	0.44
1:N:383:LEU:HA	1:N:387:GLY:O	2.17	0.44
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.00	0.44
3:P:17:ALA:HB1	3:P:201:HIS:CE1	2.53	0.44
12:P:402:HEM:HBC2	12:P:402:HEM:CHD	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:LYS:HD2	2:B:392:TYR:CG	2.53	0.43
3:C:163:TRP:O	3:C:177:ARG:NH1	2.41	0.43
8:U:13:LEU:H	8:U:13:LEU:HG	1.45	0.43
1:A:191:LYS:HE3	1:A:223:TYR:HB2	2.00	0.43
3:C:7:SER:O	3:C:8:HIS:HB2	2.17	0.43
5:E:171:ILE:HG21	5:E:176:ALA:HB3	2.00	0.43
6:F:88:LYS:HD3	6:F:88:LYS:HA	1.84	0.43
1:A:47:TYR:HB3	1:A:189:HIS:NE2	2.34	0.43
4:D:43:MET:O	4:D:91:PHE:HB2	2.18	0.43
1:N:84:ALA:HB2	1:N:101:ALA:HB2	1.99	0.43
2:O:387:LEU:HD23	2:O:387:LEU:HA	1.86	0.43
1:A:349:ALA:H	1:A:408:ARG:HD3	1.82	0.43
2:B:51:ILE:HG23	2:B:204:MET:HG2	2.01	0.43
9:I:30:VAL:HB	2:O:283:PRO:HG3	2.00	0.43
10:J:1:MET:HA	10:J:5:THR:HG21	2.00	0.43
11:K:33:VAL:HG22	11:K:38:TRP:HB2	2.00	0.43
2:O:24:LEU:HD21	2:O:382:VAL:HG21	2.00	0.43
4:Q:62:LYS:HB2	4:Q:62:LYS:HE2	1.82	0.43
3:C:177:ARG:NH2	5:E:62:MET:O	2.51	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.43
9:I:7:ARG:HG2	2:O:315:SER:OG	2.18	0.43
10:J:58:HIS:HA	10:J:63:LYS:HE2	2.01	0.43
8:U:4:LYS:HB2	8:U:12:GLU:N	2.33	0.43
10:W:41:ASP:O	10:W:45:GLU:HG3	2.19	0.43
1:A:36:THR:HG23	1:A:376:CYS:SG	2.58	0.43
6:F:12:ARG:O	6:F:12:ARG:HG2	2.19	0.43
1:N:138:LEU:HD21	1:N:168:GLU:HB2	1.99	0.43
1:N:145:MET:HB3	1:N:252:HIS:CG	2.53	0.43
5:R:147:ILE:HD11	5:R:157:TYR:HB3	2.01	0.43
6:S:96:LYS:HE3	6:S:96:LYS:HB3	1.90	0.43
1:A:51:LYS:HD2	1:A:52:ASN:HB3	1.99	0.43
2:B:3:LYS:HZ3	2:B:24:LEU:HD23	1.82	0.43
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.85	0.43
4:D:40:CYS:SG	4:D:95:TYR:OH	2.67	0.43
4:Q:71:GLN:HE21	4:Q:71:GLN:HB3	1.53	0.43
5:R:95:PRO:O	5:R:137:GLY:N	2.52	0.43
7:T:9:THR:OG1	7:T:10:ARG:N	2.52	0.43
1:A:330:SER:OG	1:A:330:SER:O	2.36	0.43
1:A:335:MET:O	1:A:339:GLN:HG3	2.18	0.43
2:B:7:LYS:HD2	2:B:392:TYR:CD1	2.53	0.43
2:B:18:PRO:HA	2:B:41:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ARG:HH12	12:C:402:HEM:HBD2	1.84	0.43
3:C:162:GLU:N	3:C:162:GLU:OE1	2.52	0.43
3:C:378:LYS:HE3	6:F:18:ARG:HD3	2.01	0.43
2:O:24:LEU:HD23	2:O:392:TYR:CD2	2.53	0.43
3:P:267:HIS:O	3:P:267:HIS:ND1	2.41	0.43
5:R:99:ARG:NH2	5:R:167:ALA:HA	2.34	0.43
7:T:43:ARG:HD2	7:T:43:ARG:O	2.19	0.43
3:C:24:PRO:HB2	3:C:27:ILE:HG12	1.99	0.43
6:F:22:TYR:OH	6:F:87:ASP:OD2	2.31	0.43
3:P:185:LEU:HD12	3:P:185:LEU:HA	1.83	0.43
7:T:78:TYR:HD1	7:T:79:GLU:N	2.17	0.43
8:U:55:THR:O	8:U:59:LEU:N	2.46	0.43
9:V:47:ARG:HH21	9:V:47:ARG:C	2.22	0.43
2:B:154:ASN:HD21	2:B:156:GLN:HG2	1.83	0.43
3:C:182:HIS:CD2	12:C:401:HEM:NC	2.86	0.43
5:E:62:MET:HG2	3:P:53:MET:HE1	2.00	0.43
1:N:9:GLN:OE1	2:O:9:LYS:HB2	2.19	0.43
2:O:89:ILE:HG13	2:O:122:PHE:CD2	2.54	0.42
1:N:102:LEU:HD22	2:O:369:LEU:HD12	2.01	0.42
3:P:240:MET:HE3	3:P:240:MET:HA	2.01	0.42
6:S:2:ALA:HB3	6:S:15:GLU:HA	2.01	0.42
2:B:7:LYS:HZ2	2:B:7:LYS:HG2	1.73	0.42
3:P:222:PRO:HG2	3:P:223:TYR:CD2	2.54	0.42
5:R:136:ILE:HG12	5:R:181:GLU:OE1	2.18	0.42
6:S:69:LEU:HD11	6:S:76:LEU:HG	2.01	0.42
2:B:252:LEU:HD23	2:B:252:LEU:HA	1.87	0.42
11:K:40:LEU:HG	11:K:41:ILE:HG12	2.00	0.42
3:P:246:ALA:HB1	3:P:249:LEU:HB2	2.00	0.42
4:Q:102:ARG:NH2	4:Q:107:GLY:O	2.50	0.42
5:R:174:GLY:HA2	5:R:175:PRO:HD3	1.87	0.42
1:A:388:ARG:NH1	1:A:394:GLU:OE2	2.53	0.42
3:C:40:CYS:O	3:C:44:GLN:HG2	2.18	0.42
3:C:232:ALA:O	3:C:236:ILE:HG12	2.19	0.42
4:D:20:SER:OG	4:D:21:LEU:N	2.53	0.42
4:D:164:ILE:HG22	4:D:179:MET:SD	2.59	0.42
5:E:128:LYS:HE2	5:E:129:LYS:HE3	2.02	0.42
6:S:71:MET:HE3	6:S:72:ARG:HD3	2.00	0.42
7:G:25:ARG:HH21	7:G:26:ALA:H	1.66	0.42
8:H:23:GLN:HE21	8:H:72:LYS:HD2	1.85	0.42
4:Q:131:LEU:HD11	13:Q:301:HEC:HMB2	2.01	0.42
3:P:120:LEU:HB2	12:P:402:HEM:HMC2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:14:LEU:HD12	6:S:15:GLU:N	2.35	0.42
3:C:141:TRP:O	3:C:268:ILE:HD11	2.20	0.42
7:G:82:ARG:HG3	8:H:47:ARG:HA	2.00	0.42
4:Q:43:MET:O	4:Q:91:PHE:HB2	2.19	0.42
2:B:236:LYS:HA	2:B:236:LYS:HD2	1.77	0.42
5:E:128:LYS:HE3	5:E:187:PHE:HE2	1.83	0.42
11:K:4:ARG:NH1	11:K:10:TYR:OH	2.51	0.42
1:N:336:PHE:HB3	3:P:4:ILE:CD1	2.49	0.42
9:I:7:ARG:HA	9:I:7:ARG:HD3	1.83	0.42
1:N:226:ASP:HB3	1:N:229:PRO:HB3	2.01	0.42
3:P:131:TYR:O	3:P:139:SER:OG	2.28	0.42
5:R:82:PRO:HG2	5:R:85:LYS:HD3	2.02	0.42
5:R:99:ARG:HH22	5:R:167:ALA:HA	1.84	0.42
10:J:34:ARG:HD3	11:X:48:ILE:HG23	2.02	0.41
1:N:47:TYR:HB3	1:N:189:HIS:NE2	2.34	0.41
3:P:83:HIS:HE1	12:P:401:HEM:NB	2.18	0.41
4:Q:41:HIS:CD2	4:Q:110:PRO:HB3	2.55	0.41
4:Q:111:PRO:HG2	13:Q:301:HEC:HAA1	2.02	0.41
5:E:74:ILE:HG12	5:E:91:TRP:CD1	2.55	0.41
1:N:388:ARG:NH2	1:N:390:ILE:HG12	2.35	0.41
5:R:74:ILE:HG12	5:R:91:TRP:CD1	2.55	0.41
1:A:246:ASP:OD2	7:G:11:VAL:N	2.48	0.41
2:B:200:THR:OG1	2:B:226:ILE:O	2.24	0.41
3:C:223:TYR:O	4:D:227:TRP:NE1	2.35	0.41
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.97	0.41
5:E:101:ARG:HH11	5:E:105:GLU:HG2	1.83	0.41
1:N:279:HIS:ND1	1:N:284:TYR:OH	2.38	0.41
10:W:43:ILE:O	10:W:47:ILE:HG13	2.21	0.41
11:X:36:THR:O	11:X:37:ASP:C	2.58	0.41
2:O:393:THR:HG22	2:O:397:THR:HB	2.03	0.41
3:P:141:TRP:O	3:P:268:ILE:HD11	2.21	0.41
5:R:101:ARG:HD2	5:R:130:PRO:O	2.20	0.41
1:A:103:SER:OG	1:A:202:GLY:O	2.27	0.41
2:B:378:PHE:O	2:B:382:VAL:HG12	2.21	0.41
1:N:86:LEU:HB3	2:O:285:VAL:HA	2.02	0.41
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.78	0.41
3:C:153:ILE:H	3:C:153:ILE:HG12	1.66	0.41
3:C:303:LEU:HD12	3:C:306:LEU:HD12	2.03	0.41
10:J:25:ILE:HD11	5:R:41:ALA:HA	2.03	0.41
6:S:3:GLY:H	6:S:18:ARG:HE	1.67	0.41
1:N:103:SER:OG	1:N:202:GLY:O	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:100:ARG:HH22	12:P:402:HEM:HBD2	1.84	0.41
4:Q:40:CYS:SG	4:Q:95:TYR:OH	2.74	0.41
7:T:25:ARG:HA	7:T:25:ARG:HD2	1.82	0.41
1:A:344:ARG:NH1	1:A:353:GLU:OE2	2.54	0.41
3:C:125:ALA:O	3:C:129:MET:HG3	2.21	0.41
1:N:59:VAL:HG23	1:N:182:LEU:HD22	2.03	0.41
2:O:157:ALA:O	2:O:161:GLU:HG2	2.20	0.41
4:Q:33:TYR:HD1	4:Q:37:CYS:HB2	1.86	0.41
3:C:120:LEU:HB2	12:C:402:HEM:HMC2	2.02	0.41
6:F:96:LYS:HE3	6:F:96:LYS:HB3	1.90	0.41
8:H:69:VAL:O	8:H:73:LEU:HB2	2.21	0.41
10:J:9:ARG:O	10:J:13:LEU:HB2	2.20	0.41
10:J:11:TYR:HB2	5:R:34:GLY:HA2	2.02	0.41
11:K:33:VAL:HG22	11:K:38:TRP:CB	2.51	0.41
11:K:38:TRP:CD1	11:K:40:LEU:HD21	2.56	0.41
1:N:163:LEU:HD12	1:N:163:LEU:HA	1.92	0.41
3:P:49:LEU:O	3:P:53:MET:HG3	2.21	0.41
3:P:303:LEU:HD12	3:P:306:LEU:HD12	2.02	0.41
5:R:166:ASP:OD1	5:R:169:GLY:N	2.53	0.41
5:R:180:LEU:HD23	5:R:181:GLU:N	2.36	0.41
11:X:36:THR:O	11:X:36:THR:OG1	2.33	0.41
3:C:91:PHE:HA	3:C:94:LEU:HB2	2.01	0.41
3:C:237:LEU:HB2	4:D:212:MET:SD	2.61	0.41
3:P:223:TYR:O	4:Q:227:TRP:NE1	2.37	0.41
1:A:40:TRP:HB2	1:A:196:VAL:HG13	2.02	0.40
2:B:3:LYS:CB	2:B:38:LEU:HD21	2.50	0.40
1:N:373:THR:HB	1:N:374:PRO:HD3	2.02	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.02	0.40
4:Q:13:SER:HB2	10:W:51:LYS:HE2	2.03	0.40
2:B:169:ARG:NE	2:B:240:HIS:HB2	2.36	0.40
8:H:24:CYS:HB2	8:H:68:CYS:HB2	2.04	0.40
1:N:333:ASP:O	3:P:4:ILE:HD13	2.21	0.40
1:A:260:PRO:HB2	1:A:264:HIS:CB	2.51	0.40
3:C:6:LYS:HB3	3:C:7:SER:H	1.60	0.40
5:E:187:PHE:CE1	5:E:193:VAL:HG12	2.56	0.40
1:N:106:LEU:HD13	1:N:203:LEU:HD22	2.03	0.40
1:N:191:LYS:O	1:N:195:MET:HG3	2.21	0.40
3:P:98:VAL:HG22	12:P:402:HEM:CAC	2.52	0.40
3:P:280:ILE:H	3:P:280:ILE:HG13	1.74	0.40
2:B:70:ARG:HH21	2:B:100:SER:HB3	1.86	0.40
2:B:238:LYS:HA	2:B:238:LYS:HD2	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:11:PHE:CE2	2:O:157:ALA:HA	2.56	0.40
2:O:378:PHE:O	2:O:382:VAL:HG12	2.22	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	444/446 (100%)	426 (96%)	18 (4%)	0	100	100
1	N	444/446 (100%)	424 (96%)	19 (4%)	1 (0%)	44	77
2	B	437/439 (100%)	413 (94%)	22 (5%)	2 (0%)	25	61
2	O	437/439 (100%)	408 (93%)	23 (5%)	6 (1%)	9	37
3	C	377/379 (100%)	357 (95%)	19 (5%)	1 (0%)	37	70
3	P	377/379 (100%)	362 (96%)	15 (4%)	0	100	100
4	D	239/241 (99%)	236 (99%)	3 (1%)	0	100	100
4	Q	239/241 (99%)	237 (99%)	2 (1%)	0	100	100
5	E	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
5	R	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
6	F	109/111 (98%)	103 (94%)	5 (5%)	1 (1%)	14	49
6	S	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	14	49
7	G	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
7	T	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
8	H	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	10	39
8	U	76/78 (97%)	68 (90%)	7 (9%)	1 (1%)	10	39
9	I	52/54 (96%)	37 (71%)	15 (29%)	0	100	100
9	V	52/54 (96%)	39 (75%)	13 (25%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	8	34
10	W	62/64 (97%)	58 (94%)	3 (5%)	1 (2%)	8	34
11	K	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
11	X	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
All	All	4234/4278 (99%)	3996 (94%)	222 (5%)	16 (0%)	32	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	VAL
3	C	8	HIS
10	J	4	PRO
1	N	224	ASP
2	O	4	VAL
2	O	201	SER
6	S	12	ARG
10	W	62	ASN
6	F	9	ALA
2	O	235	ALA
8	U	13	LEU
2	B	5	ALA
8	H	2	ASP
2	O	9	LYS
2	O	14	PRO
2	O	22	GLN

### 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	370/370 (100%)	341 (92%)	29 (8%)	10	36
1	N	370/370 (100%)	339 (92%)	31 (8%)	9	33
2	B	343/343 (100%)	330 (96%)	13 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	343/343 (100%)	322 (94%)	21 (6%)	15	46
3	C	327/327 (100%)	298 (91%)	29 (9%)	8	31
3	P	327/327 (100%)	296 (90%)	31 (10%)	7	28
4	D	206/206 (100%)	195 (95%)	11 (5%)	19	51
4	Q	206/206 (100%)	196 (95%)	10 (5%)	21	54
5	E	168/168 (100%)	149 (89%)	19 (11%)	4	21
5	R	168/168 (100%)	153 (91%)	15 (9%)	8	31
6	F	99/99 (100%)	89 (90%)	10 (10%)	6	25
6	S	99/99 (100%)	89 (90%)	10 (10%)	6	25
7	G	72/72 (100%)	66 (92%)	6 (8%)	9	34
7	T	72/72 (100%)	64 (89%)	8 (11%)	5	21
8	H	74/74 (100%)	60 (81%)	14 (19%)	1	7
8	U	74/74 (100%)	63 (85%)	11 (15%)	2	12
9	I	42/42 (100%)	36 (86%)	6 (14%)	2	13
9	V	42/42 (100%)	34 (81%)	8 (19%)	1	7
10	J	54/54 (100%)	51 (94%)	3 (6%)	17	49
10	W	54/54 (100%)	48 (89%)	6 (11%)	5	21
11	K	40/40 (100%)	33 (82%)	7 (18%)	1	8
11	X	40/40 (100%)	36 (90%)	4 (10%)	6	25
All	All	3590/3590 (100%)	3288 (92%)	302 (8%)	11	33

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	18	GLN
1	A	30	SER
1	A	34	THR
1	A	35	CYS
1	A	36	THR
1	A	42	ASP
1	A	51	LYS
1	A	58	PHE
1	A	95	THR
1	A	100	LYS

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Mol	Chain	Res	Type
1	A	181	ASP
1	A	186	LEU
1	A	188	ARG
1	A	255	ILE
1	A	280	TYR
1	A	291	SER
1	A	296	SER
1	A	305	GLN
1	A	307	PHE
1	A	308	GLN
1	A	309	THR
1	A	317	THR
1	A	334	MET
1	A	345	LEU
1	A	425	PHE
1	A	436	ARG
1	A	438	ARG
1	A	441	MET
2	B	76	THR
2	B	102	ARG
2	B	116	VAL
2	B	120	MET
2	B	178	CYS
2	B	187	THR
2	B	223	PHE
2	B	251	SER
2	B	310	SER
2	B	335	ASP
2	B	370	MET
2	B	423	SER
2	B	437	ASP
3	C	3	ASN
3	C	5	ARG
3	C	8	HIS
3	C	13	ILE
3	C	18	PHE
3	C	21	LEU
3	C	25	SER
3	C	46	LEU
3	C	57	SER
3	C	65	SER
3	C	68	HIS

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Mol	Chain	Res	Type
3	C	74	ASN
3	C	90	PHE
3	C	102	LEU
3	C	110	LEU
3	C	155	TYR
3	C	190	MET
3	C	206	ASN
3	C	211	ILE
3	C	216	ASP
3	C	233	LEU
3	C	257	THR
3	C	267	HIS
3	C	273	TYR
3	C	278	TYR
3	C	281	LEU
3	C	284	ILE
3	C	336	THR
3	C	379	TRP
4	D	20	SER
4	D	25	SER
4	D	34	LYS
4	D	83	ARG
4	D	129	SER
4	D	169	LEU
4	D	175	THR
4	D	179	MET
4	D	197	GLU
4	D	211	MET
4	D	241	LYS
5	E	6	LYS
5	E	12	ASP
5	E	18	VAL
5	E	42	THR
5	E	75	GLU
5	E	89	PHE
5	E	100	HIS
5	E	102	THR
5	E	104	LYS
5	E	118	ARG
5	E	123	ASP
5	E	126	ARG
5	E	128	LYS

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Mol	Chain	Res	Type
5	E	140	THR
5	E	149	ASN
5	E	161	HIS
5	E	163	SER
5	E	187	PHE
5	E	190	ASP
6	F	1	MET
6	F	7	VAL
6	F	12	ARG
6	F	37	THR
6	F	39	HIS
6	F	68	ASP
6	F	72	ARG
6	F	73	GLN
6	F	79	GLU
6	F	95	LEU
7	G	48	ARG
7	G	54	VAL
7	G	60	TYR
7	G	78	TYR
7	G	81	ASP
7	G	82	ARG
8	H	2	ASP
8	H	4	LYS
8	H	10	GLU
8	H	13	LEU
8	H	14	VAL
8	H	21	ARG
8	H	22	GLU
8	H	23	GLN
8	H	25	GLU
8	H	29	LYS
8	H	32	LYS
8	H	47	ARG
8	H	53	ASP
8	H	72	LYS
9	I	18	THR
9	I	20	ARG
9	I	22	VAL
9	I	27	ARG
9	I	30	VAL
9	I	47	ARG

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Mol	Chain	Res	Type
10	J	7	THR
10	J	12	SER
10	J	16	ARG
11	K	1	MET
11	K	17	TRP
11	K	20	THR
11	K	38	TRP
11	K	39	ARG
11	K	45	VAL
11	K	47	TYR
1	N	10	SER
1	N	17	SER
1	N	18	GLN
1	N	30	SER
1	N	34	THR
1	N	35	CYS
1	N	36	THR
1	N	42	ASP
1	N	51	LYS
1	N	58	PHE
1	N	100	LYS
1	N	105	ASP
1	N	106	LEU
1	N	120	CYS
1	N	149	VAL
1	N	181	ASP
1	N	223	TYR
1	N	225	GLU
1	N	244	ARG
1	N	255	ILE
1	N	282	CYS
1	N	291	SER
1	N	296	SER
1	N	307	PHE
1	N	309	THR
1	N	333	ASP
1	N	334	MET
1	N	436	ARG
1	N	438	ARG
1	N	441	MET
1	N	446	PHE
2	O	3	LYS

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Mol	Chain	Res	Type
2	O	4	VAL
2	O	7	LYS
2	O	9	LYS
2	O	12	GLU
2	O	95	LYS
2	O	99	THR
2	O	102	ARG
2	O	116	VAL
2	O	178	CYS
2	O	187	THR
2	O	203	ARG
2	O	225	ASN
2	O	227	ARG
2	O	310	SER
2	O	326	THR
2	O	332	SER
2	O	335	ASP
2	O	370	MET
2	O	423	SER
2	O	439	LEU
3	P	1	MET
3	P	18	PHE
3	P	21	LEU
3	P	39	ILE
3	P	57	SER
3	P	65	SER
3	P	68	HIS
3	P	74	ASN
3	P	80	ARG
3	P	90	PHE
3	P	102	LEU
3	P	110	LEU
3	P	126	THR
3	P	171	ASP
3	P	183	PHE
3	P	202	GLU
3	P	207	ASN
3	P	211	ILE
3	P	216	ASP
3	P	233	LEU
3	P	239	LEU
3	P	257	THR

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Mol	Chain	Res	Type
3	P	267	HIS
3	P	273	TYR
3	P	276	PHE
3	P	281	LEU
3	P	282	ARG
3	P	284	ILE
3	P	336	THR
3	P	375	LYS
3	P	379	TRP
4	Q	2	ASP
4	Q	41	HIS
4	Q	57	THR
4	Q	71	GLN
4	Q	129	SER
4	Q	144	ARG
4	Q	169	LEU
4	Q	173	ASP
4	Q	179	MET
4	Q	211	MET
5	R	6	LYS
5	R	12	ASP
5	R	18	VAL
5	R	42	THR
5	R	60	SER
5	R	90	LYS
5	R	102	THR
5	R	104	LYS
5	R	128	LYS
5	R	134	ILE
5	R	144	CYS
5	R	145	VAL
5	R	153	PHE
5	R	164	HIS
5	R	173	LYS
6	S	11	SER
6	S	12	ARG
6	S	14	LEU
6	S	37	THR
6	S	39	HIS
6	S	68	ASP
6	S	72	ARG
6	S	79	GLU

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Mol	Chain	Res	Type
6	S	95	LEU
6	S	103	LYS
7	T	3	ARG
7	T	8	LEU
7	T	41	ARG
7	T	48	ARG
7	T	54	VAL
7	T	60	TYR
7	T	61	THR
7	T	78	TYR
8	U	2	ASP
8	U	4	LYS
8	U	5	GLU
8	U	6	GLU
8	U	10	GLU
8	U	12	GLU
8	U	13	LEU
8	U	32	LYS
8	U	49	GLN
8	U	68	CYS
8	U	75	ASN
9	V	4	VAL
9	V	19	SER
9	V	20	ARG
9	V	22	VAL
9	V	27	ARG
9	V	30	VAL
9	V	35	PRO
9	V	47	ARG
10	W	1	MET
10	W	7	THR
10	W	19	SER
10	W	34	ARG
10	W	62	ASN
10	W	63	LYS
11	X	20	THR
11	X	37	ASP
11	X	39	ARG
11	X	40	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	31	ASN
3	C	44	GLN
8	H	23	GLN
2	O	20	HIS
2	O	22	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](#)

8 ligands are modelled in this entry.

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$
12	HEM	C	401	3	41,50,50	1.45	3 (7%)	45,82,82	1.39	8 (17%)
14	FES	E	201	5	0,4,4	-	-	-		
13	HEC	D	301	4	32,50,50	2.20	3 (9%)	24,82,82	1.55	5 (20%)
12	HEM	P	402	3	41,50,50	1.52	4 (9%)	45,82,82	1.44	7 (15%)
13	HEC	Q	301	4	32,50,50	2.21	3 (9%)	24,82,82	1.53	4 (16%)
12	HEM	C	402	3	41,50,50	1.52	3 (7%)	45,82,82	1.41	8 (17%)
14	FES	R	201	5	0,4,4	-	-	-		
12	HEM	P	401	3	41,50,50	1.46	3 (7%)	45,82,82	1.42	8 (17%)

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
12	HEM	C	401	3	-	1/12/54/54	-
14	FES	E	201	5	-	-	0/1/1/1
13	HEC	D	301	4	-	0/10/54/54	-
12	HEM	P	402	3	-	5/12/54/54	-
13	HEC	Q	301	4	-	0/10/54/54	-
12	HEM	C	402	3	-	6/12/54/54	-
14	FES	R	201	5	-	-	0/1/1/1
12	HEM	P	401	3	-	1/12/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	301	HEC	C3C-C2C	-6.54	1.33	1.40
13	Q	301	HEC	C3C-C2C	-6.50	1.34	1.40
13	D	301	HEC	C2B-C3B	-6.46	1.34	1.40
13	Q	301	HEC	C2B-C3B	-6.43	1.34	1.40
13	Q	301	HEC	C3D-C2D	5.46	1.53	1.37
13	D	301	HEC	C3D-C2D	5.44	1.53	1.37
12	C	402	HEM	C3C-C2C	-4.99	1.33	1.40
12	P	402	HEM	C3C-C2C	-4.94	1.33	1.40
12	P	401	HEM	C3C-C2C	-4.12	1.34	1.40
12	C	401	HEM	C3C-C2C	-4.04	1.34	1.40
12	P	401	HEM	C3C-CAC	3.61	1.55	1.47
12	C	401	HEM	C3C-CAC	3.57	1.55	1.47
12	C	402	HEM	C3C-CAC	3.37	1.54	1.47
12	P	402	HEM	C3C-CAC	3.34	1.54	1.47
12	P	401	HEM	CAB-C3B	2.98	1.55	1.47
12	C	402	HEM	CAB-C3B	2.98	1.55	1.47
12	C	401	HEM	CAB-C3B	2.97	1.55	1.47
12	P	402	HEM	CAB-C3B	2.94	1.55	1.47
12	P	402	HEM	FE-ND	2.02	2.06	1.96

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	401	HEM	C4B-CHC-C1C	2.85	126.33	122.56
12	P	401	HEM	C4B-CHC-C1C	2.84	126.31	122.56
13	D	301	HEC	CMC-C2C-C1C	-2.80	124.16	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	301	HEC	CMC-C2C-C1C	-2.75	124.23	128.46
12	C	402	HEM	C4D-ND-C1D	2.75	107.92	105.07
12	P	402	HEM	C4D-ND-C1D	2.74	107.90	105.07
12	P	402	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
12	P	402	HEM	CAD-C3D-C4D	2.71	129.40	124.66
12	P	401	HEM	C4D-ND-C1D	2.71	107.87	105.07
12	C	401	HEM	C4D-ND-C1D	2.70	107.86	105.07
13	Q	301	HEC	CMB-C2B-C1B	-2.69	124.33	128.46
13	D	301	HEC	CMB-C2B-C1B	-2.57	124.52	128.46
12	P	402	HEM	CAD-C3D-C2D	-2.55	123.12	127.88
13	D	301	HEC	C1D-C2D-C3D	-2.52	105.24	107.00
12	P	401	HEM	C1B-NB-C4B	2.52	107.68	105.07
12	C	402	HEM	CAD-C3D-C4D	2.48	129.00	124.66
12	C	401	HEM	C1B-NB-C4B	2.48	107.64	105.07
12	P	401	HEM	CAD-CBD-CGD	-2.47	108.28	113.60
12	C	402	HEM	CAD-C3D-C2D	-2.46	123.29	127.88
12	C	401	HEM	CAD-CBD-CGD	-2.39	108.45	113.60
12	C	402	HEM	CBA-CAA-C2A	-2.38	108.55	112.62
12	P	401	HEM	C4C-CHD-C1D	2.37	125.68	122.56
13	Q	301	HEC	C1D-C2D-C3D	-2.34	105.37	107.00
12	P	402	HEM	CMA-C3A-C4A	-2.34	124.87	128.46
12	C	401	HEM	C4C-CHD-C1D	2.32	125.62	122.56
12	C	402	HEM	CMA-C3A-C4A	-2.32	124.91	128.46
12	P	401	HEM	C4A-C3A-C2A	2.28	108.58	107.00
12	P	402	HEM	C1B-NB-C4B	2.25	107.40	105.07
13	D	301	HEC	CAA-CBA-CGA	-2.21	107.55	113.76
12	C	402	HEM	C1B-NB-C4B	2.18	107.33	105.07
12	C	401	HEM	CMC-C2C-C3C	2.17	128.73	124.68
12	C	402	HEM	C4B-CHC-C1C	2.14	125.38	122.56
12	P	402	HEM	C4B-CHC-C1C	2.13	125.38	122.56
12	P	401	HEM	CMC-C2C-C3C	2.12	128.65	124.68
12	P	401	HEM	C3D-C4D-ND	-2.12	107.81	110.17
12	C	401	HEM	C3D-C4D-ND	-2.09	107.84	110.17
12	C	401	HEM	C4A-C3A-C2A	2.08	108.44	107.00
13	Q	301	HEC	CAA-CBA-CGA	-2.07	107.95	113.76
13	D	301	HEC	CBD-CAD-C3D	-2.05	109.13	112.62
12	C	402	HEM	C3D-C4D-ND	-2.04	107.90	110.17

There are no chirality outliers.

All (13) torsion outliers are listed below:

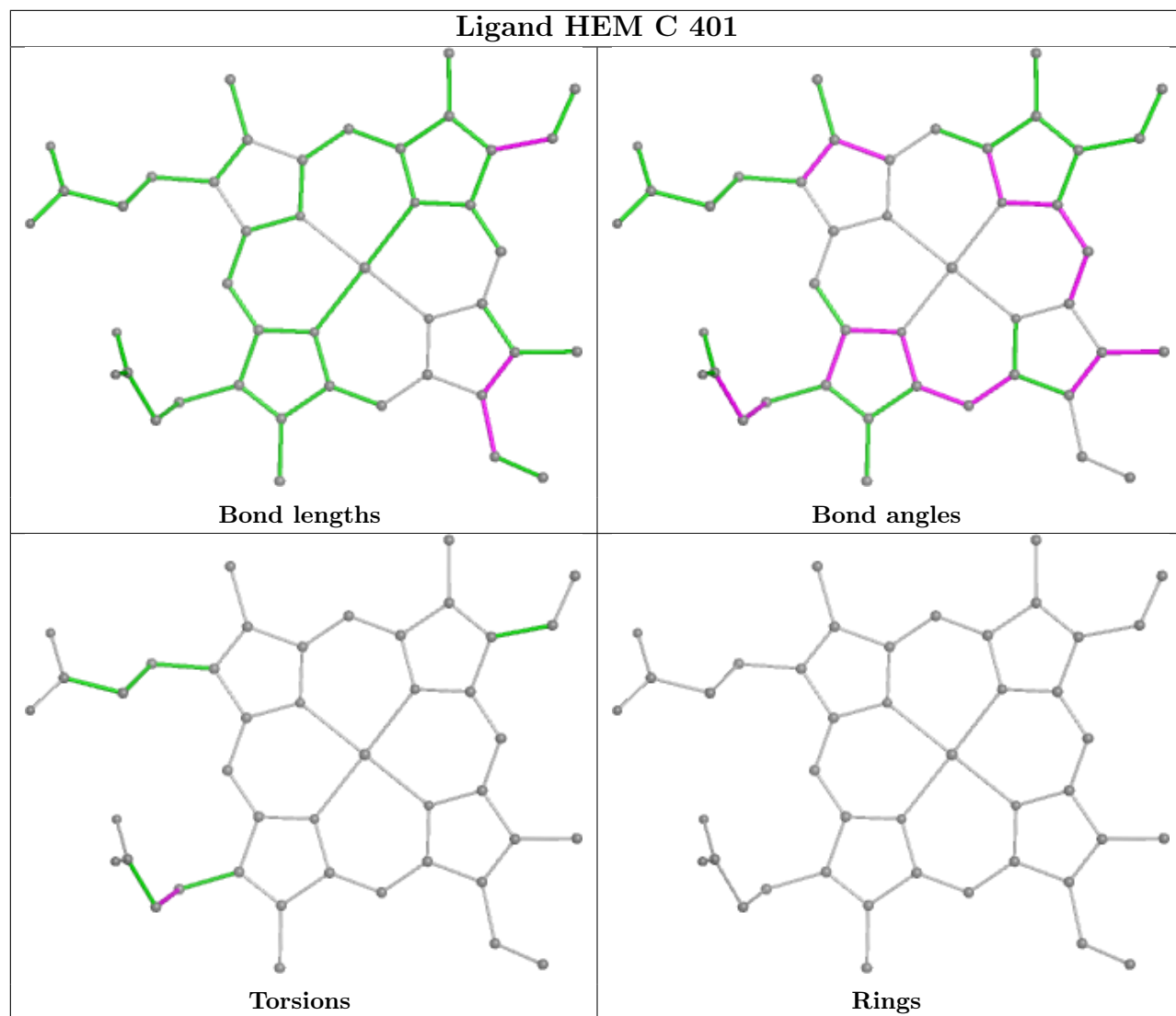
Mol	Chain	Res	Type	Atoms
12	P	402	HEM	C2A-CAA-CBA-CGA
12	C	402	HEM	C4D-C3D-CAD-CBD
12	P	402	HEM	C4D-C3D-CAD-CBD
12	C	402	HEM	C2A-CAA-CBA-CGA
12	P	402	HEM	C2D-C3D-CAD-CBD
12	C	402	HEM	C2D-C3D-CAD-CBD
12	P	401	HEM	C3D-CAD-CBD-CGD
12	C	401	HEM	C3D-CAD-CBD-CGD
12	C	402	HEM	CAD-CBD-CGD-O2D
12	C	402	HEM	CAD-CBD-CGD-O1D
12	C	402	HEM	CAA-CBA-CGA-O2A
12	P	402	HEM	CAA-CBA-CGA-O1A
12	P	402	HEM	CAA-CBA-CGA-O2A

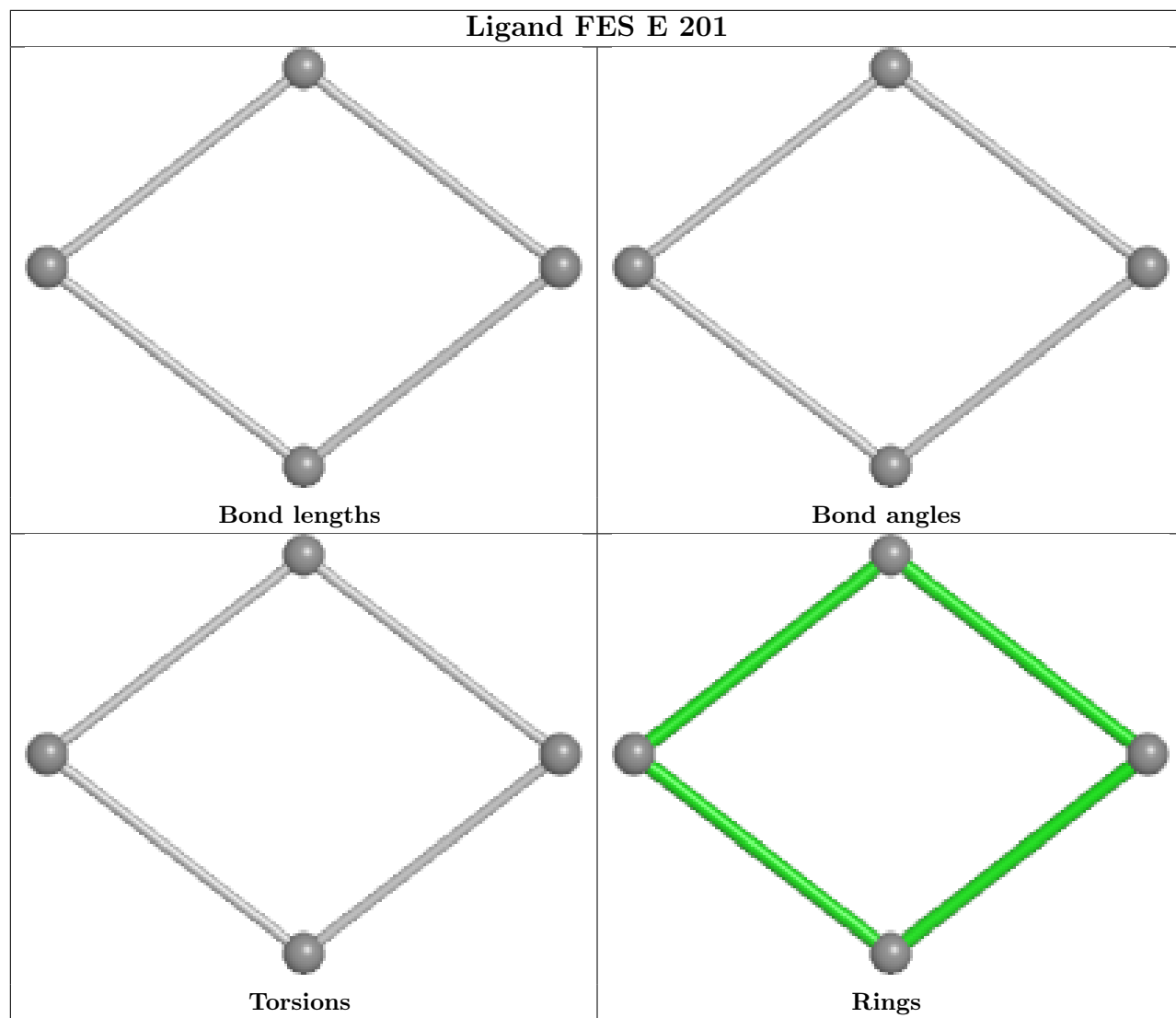
There are no ring outliers.

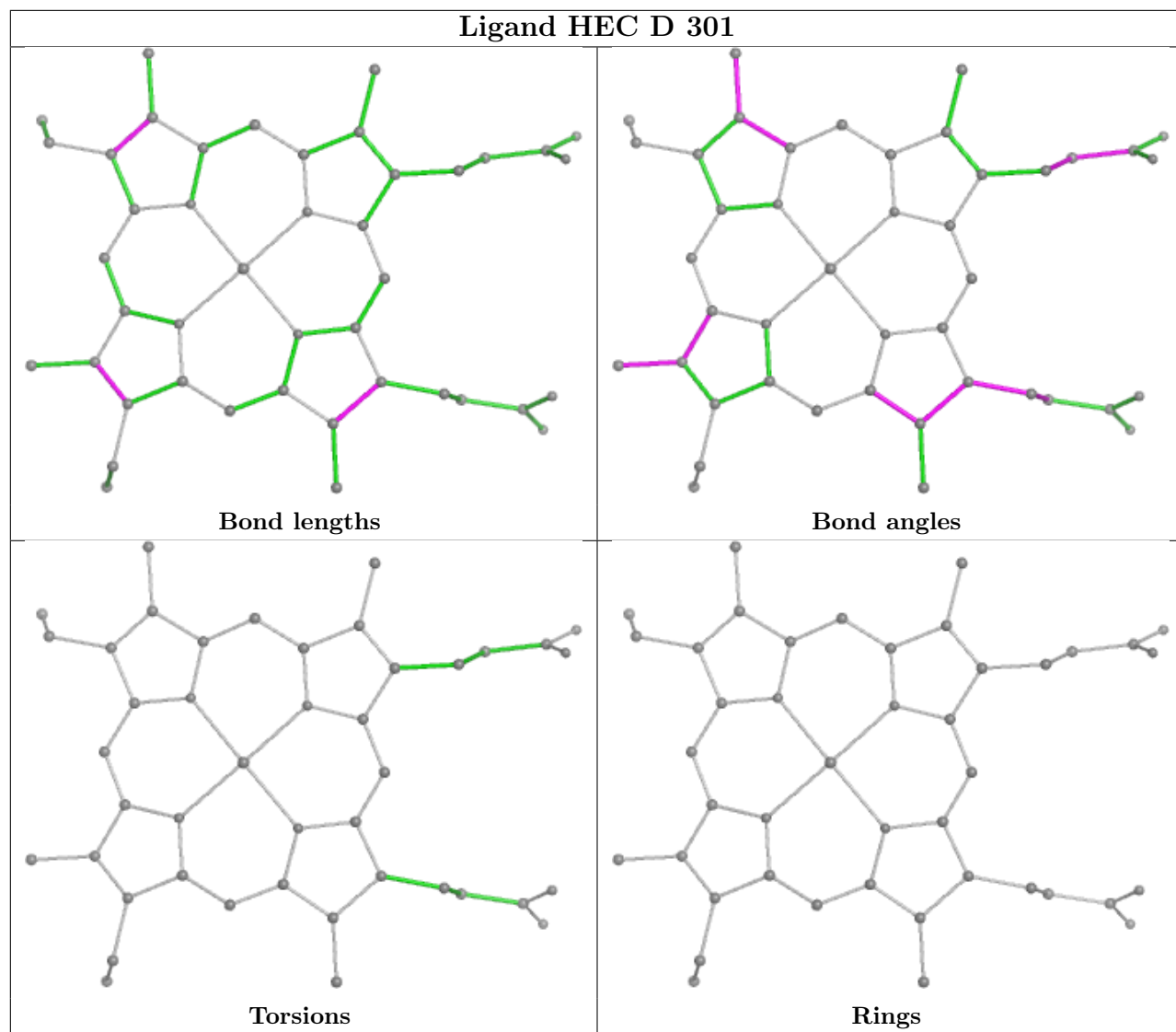
7 monomers are involved in 37 short contacts:

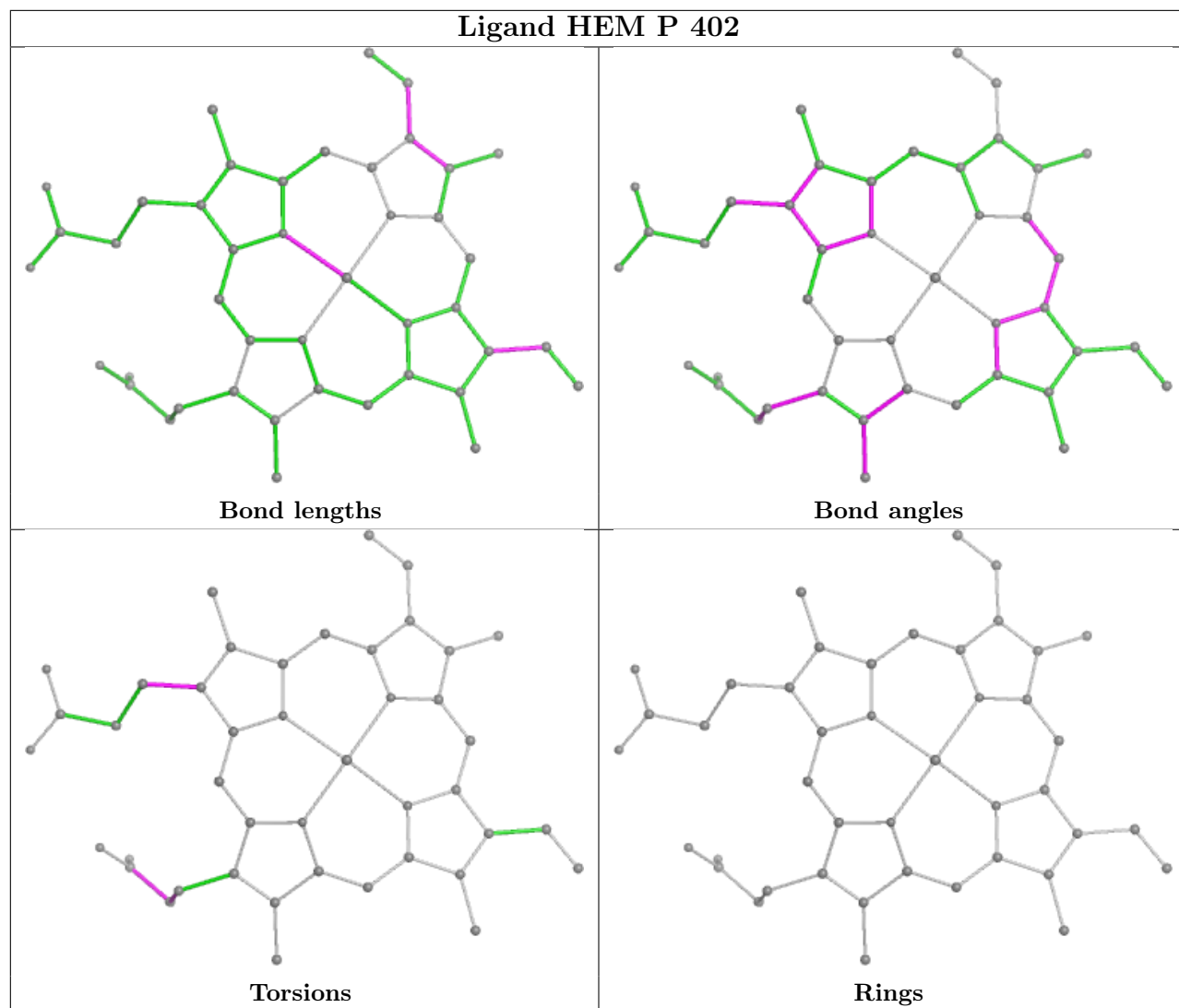
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	401	HEM	5	0
13	D	301	HEC	1	0
12	P	402	HEM	9	0
13	Q	301	HEC	7	0
12	C	402	HEM	9	0
14	R	201	FES	1	0
12	P	401	HEM	5	0

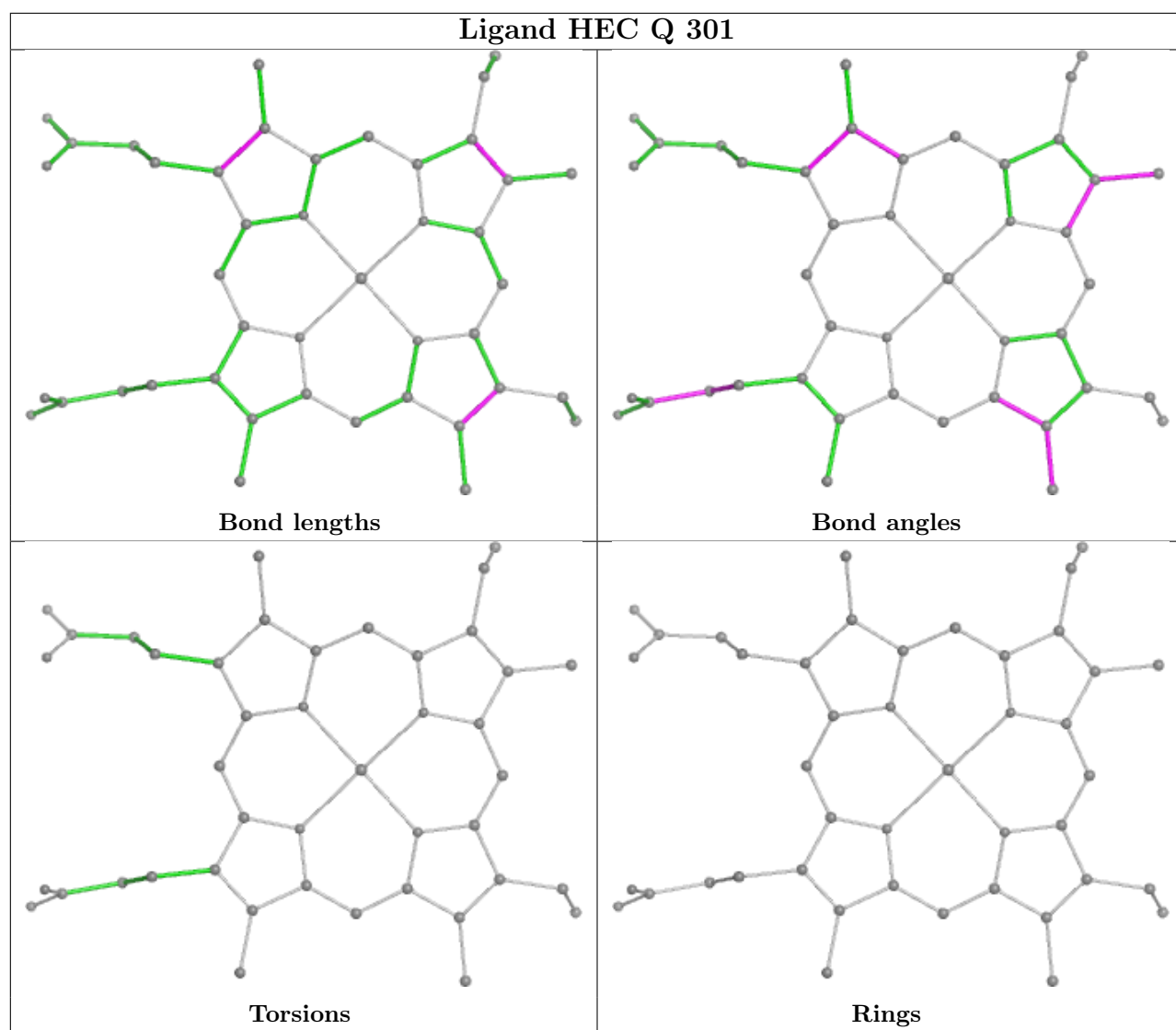
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

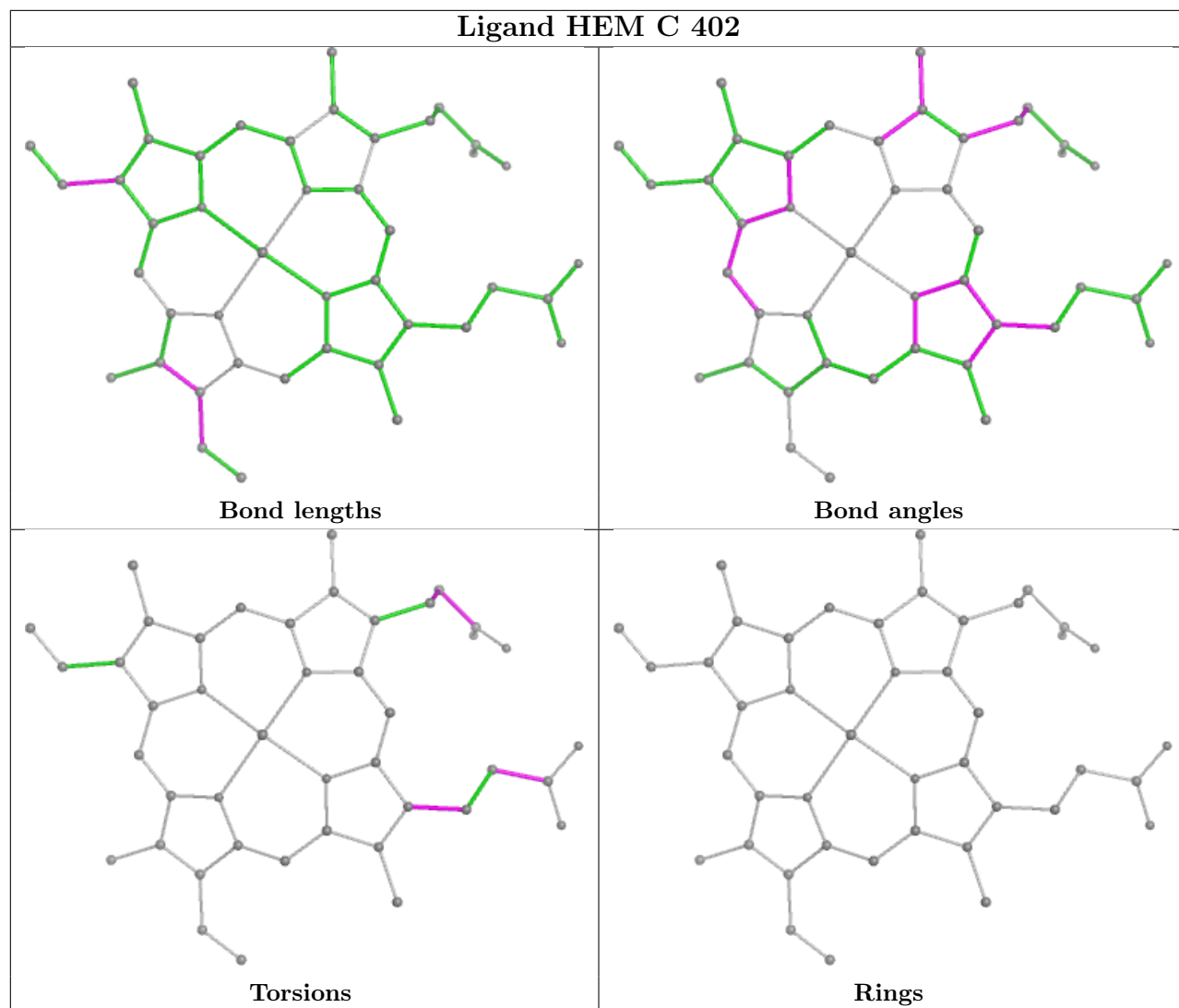


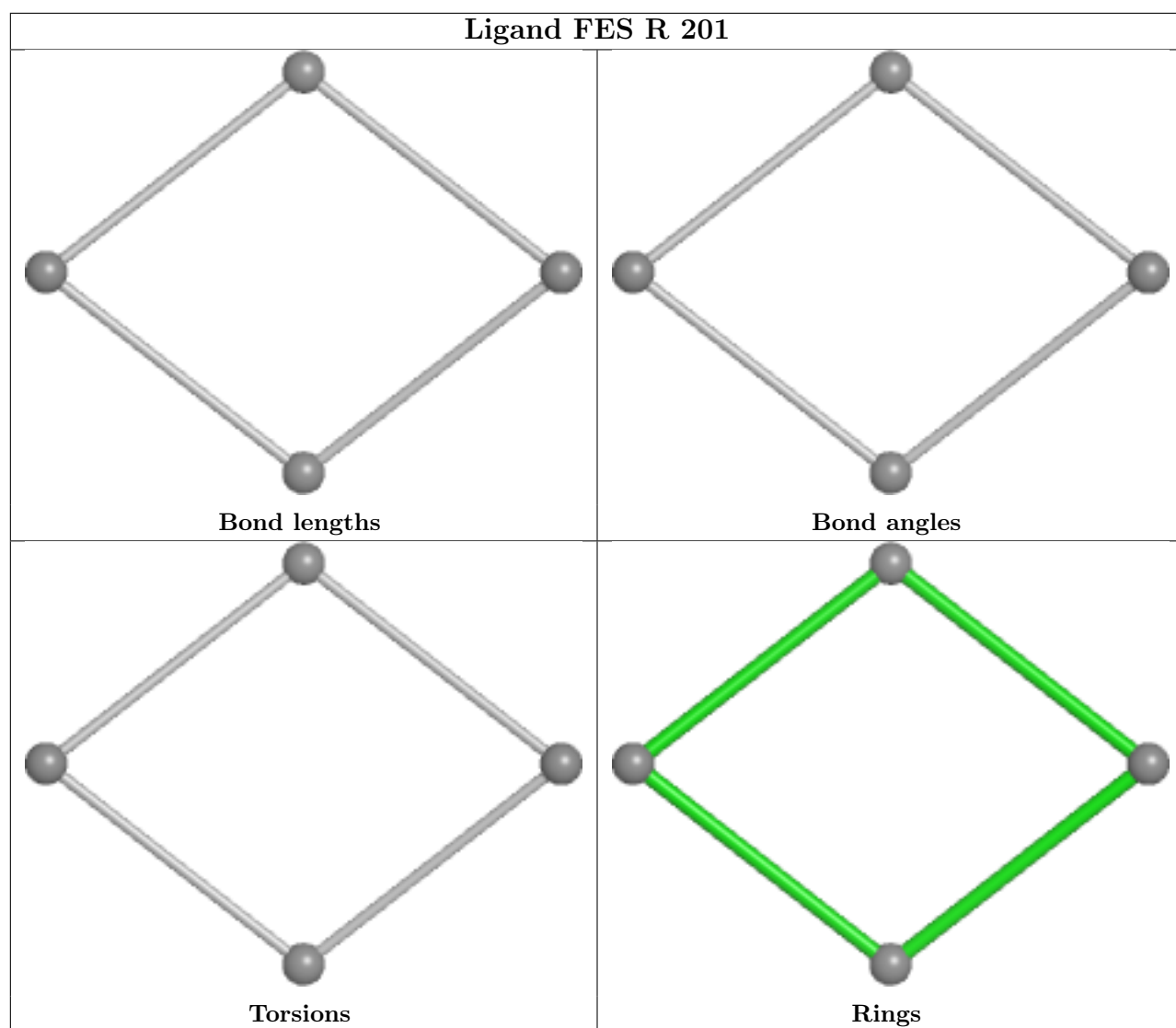


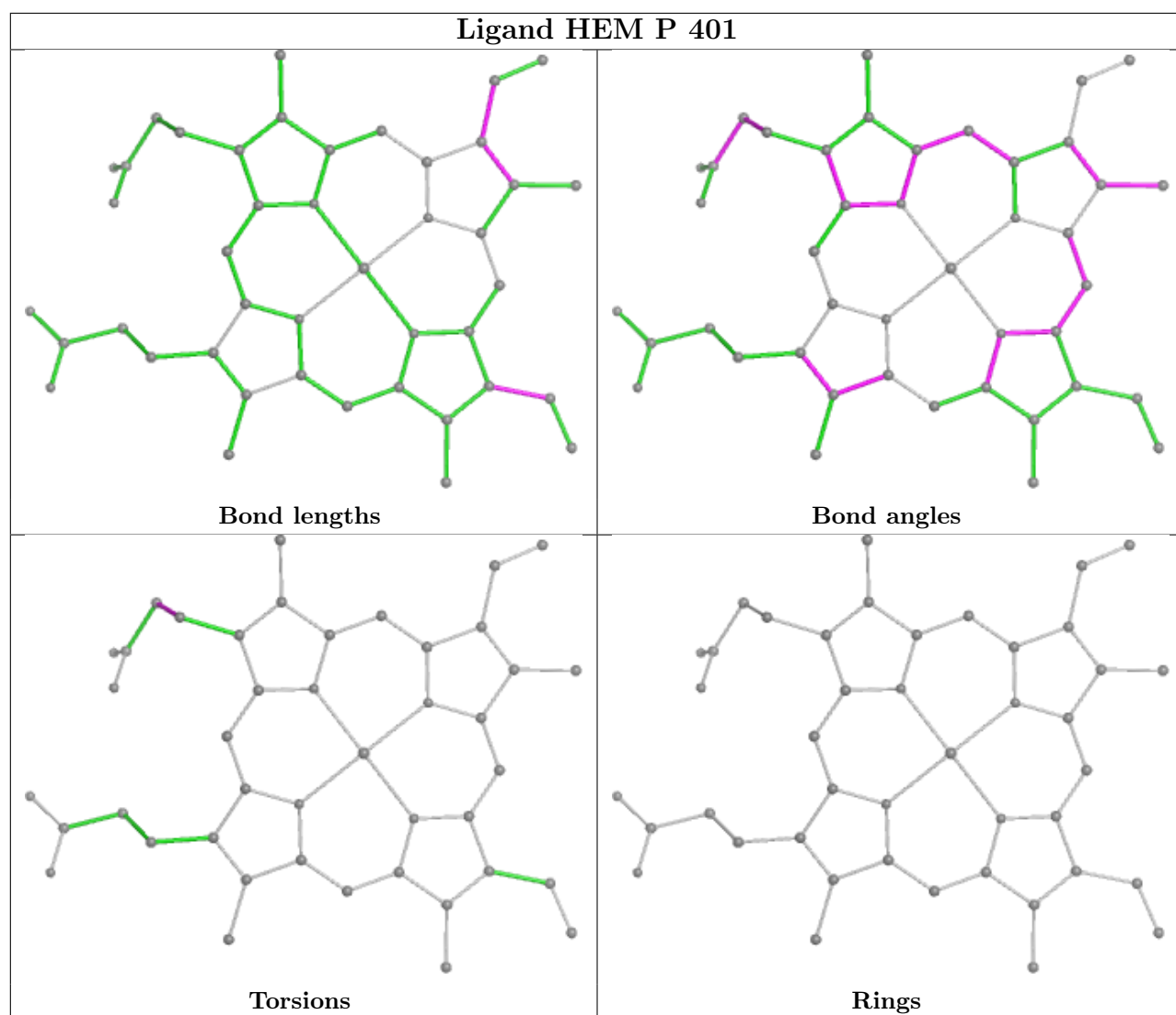












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

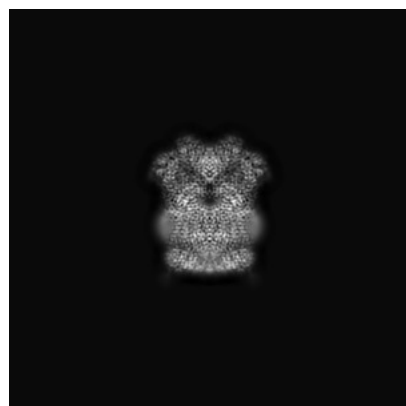
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17461. These allow visual inspection of the internal detail of the map and identification of artifacts.

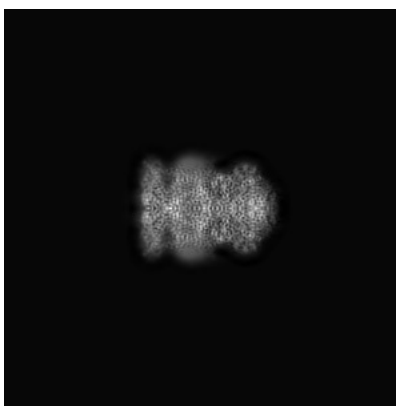
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

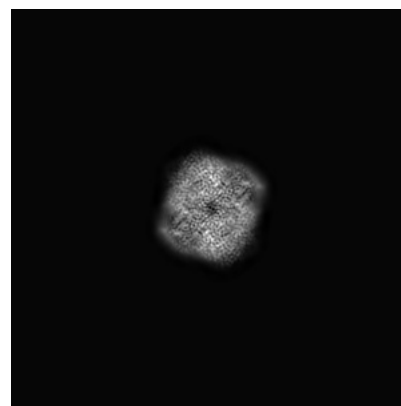
#### 6.1.1 Primary map



X

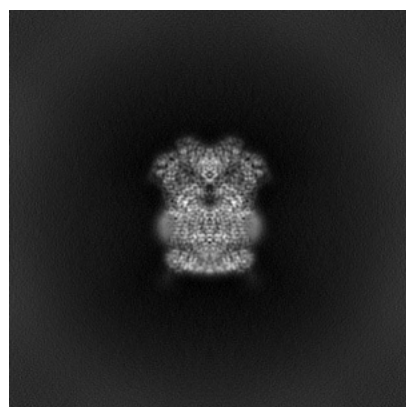


Y

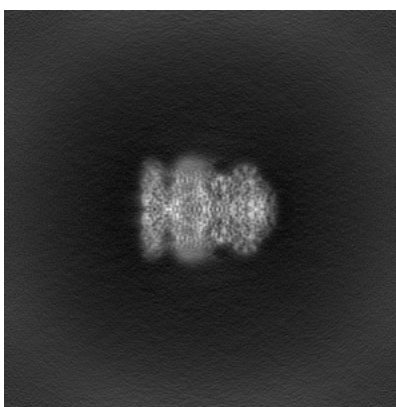


Z

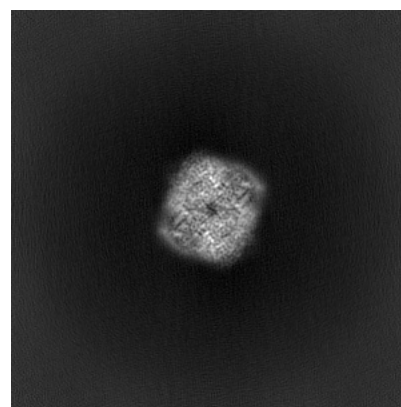
#### 6.1.2 Raw map



X



Y

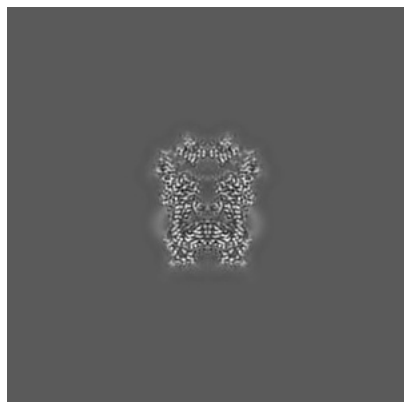


Z

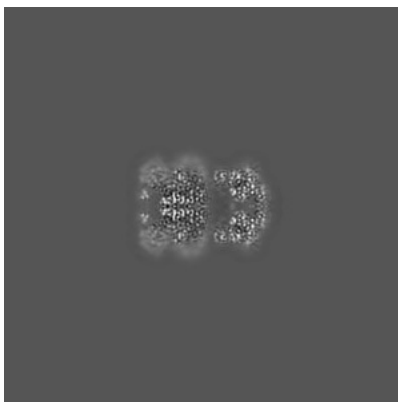
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

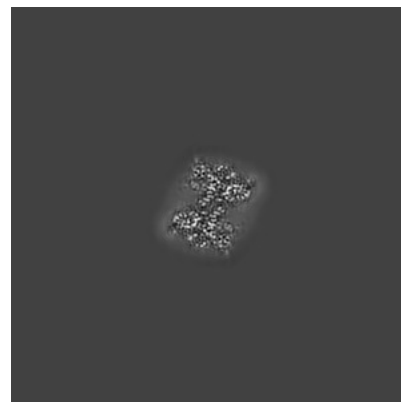
### 6.2.1 Primary map



X Index: 150

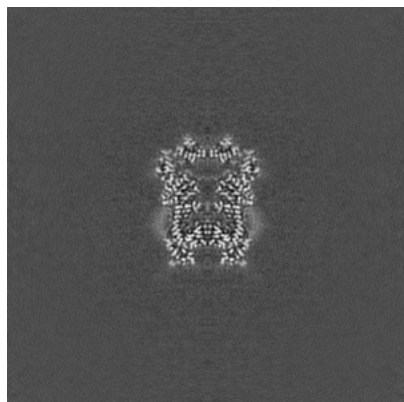


Y Index: 150

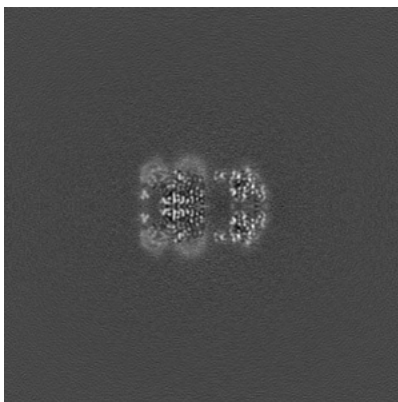


Z Index: 150

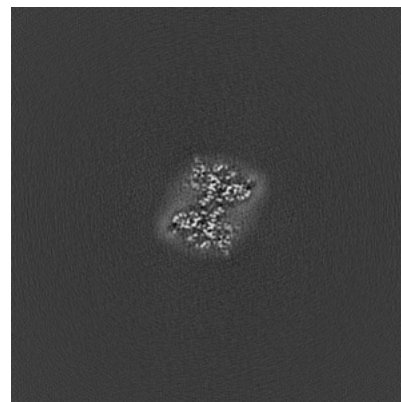
### 6.2.2 Raw map



X Index: 150



Y Index: 150

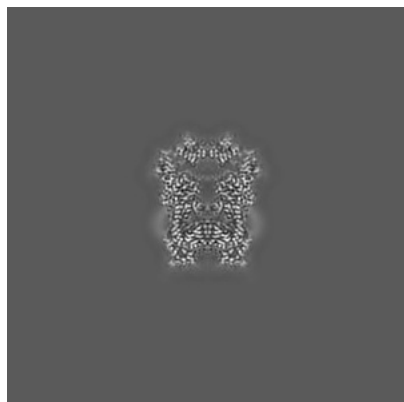


Z Index: 150

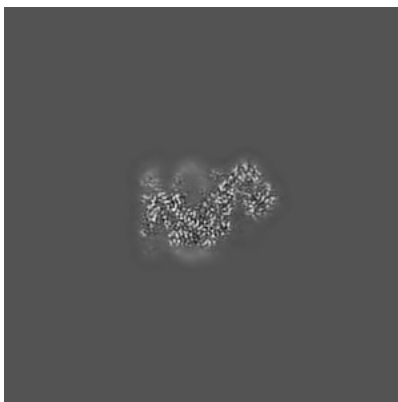
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

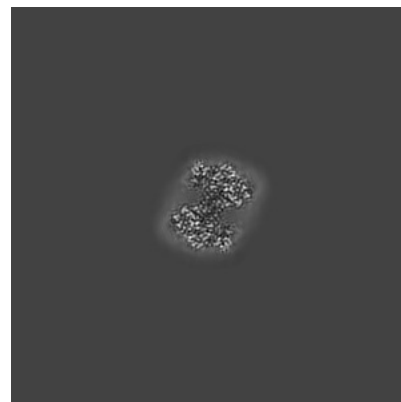
### 6.3.1 Primary map



X Index: 150

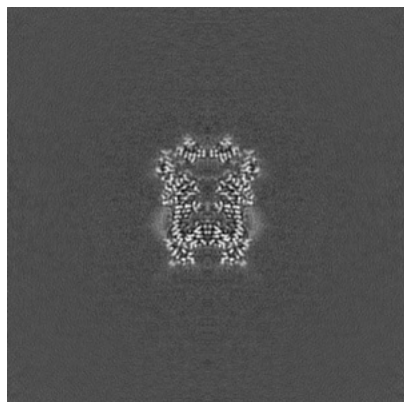


Y Index: 139

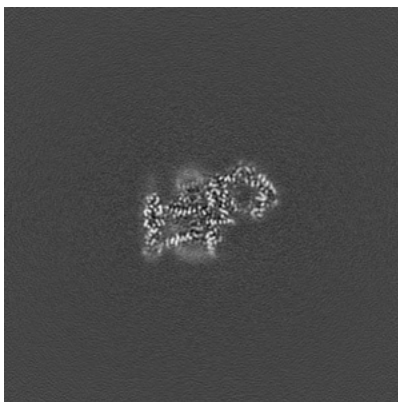


Z Index: 147

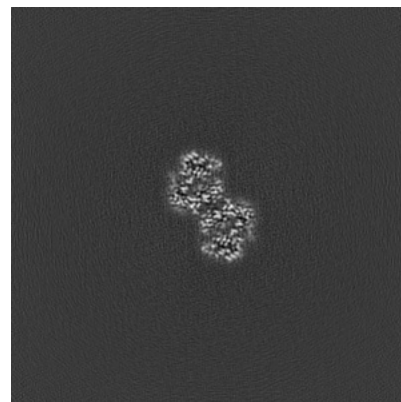
### 6.3.2 Raw map



X Index: 150



Y Index: 132

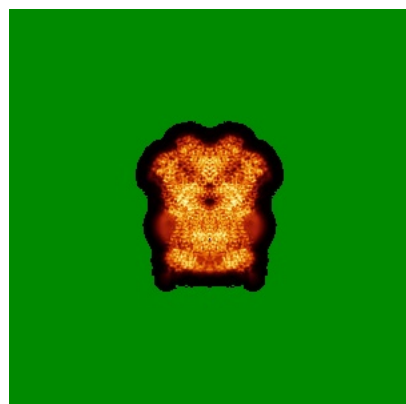


Z Index: 186

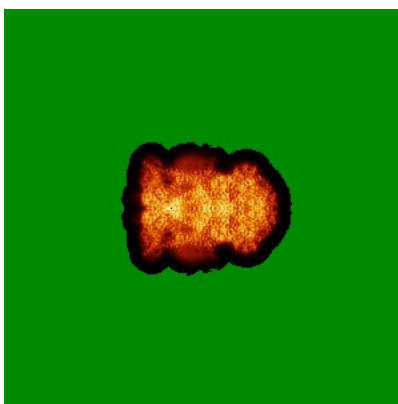
The images above show the largest variance slices of the map in three orthogonal directions.

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

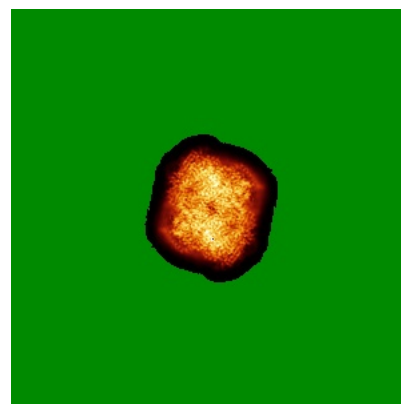
### 6.4.1 Primary map



X

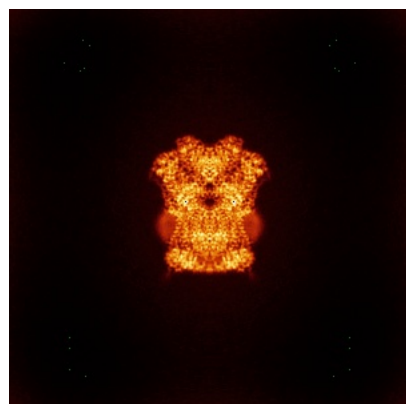


Y

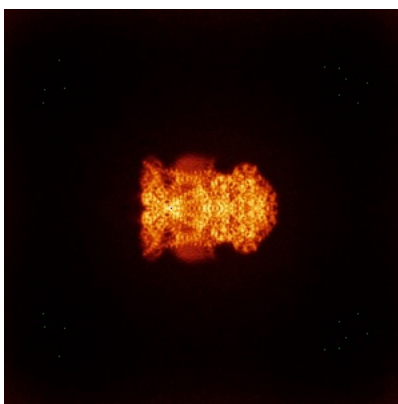


Z

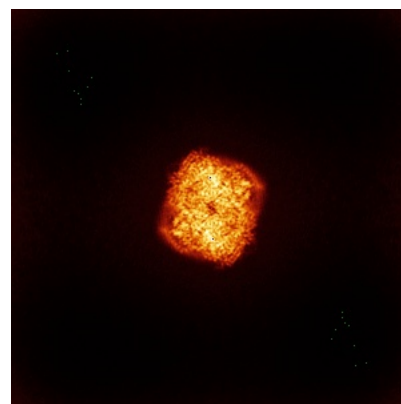
### 6.4.2 Raw map



X



Y

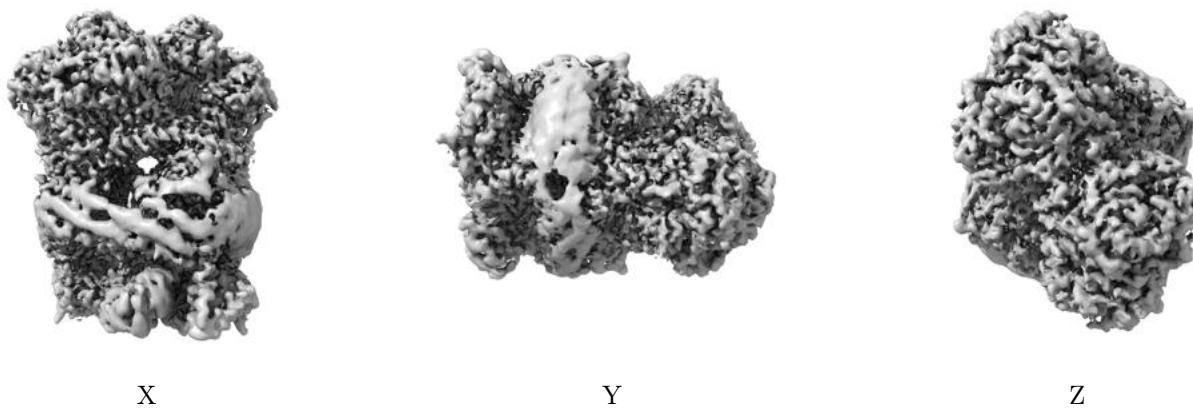


Z

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.

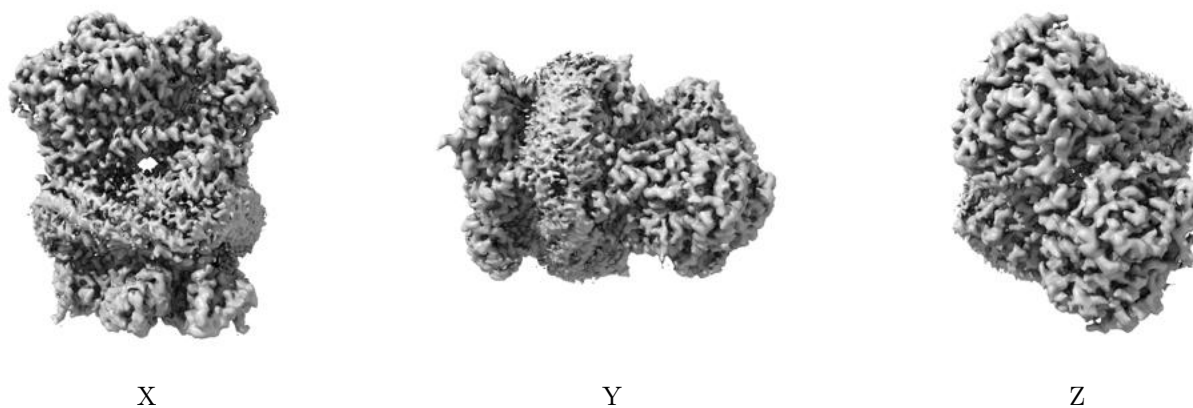
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.5. 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.

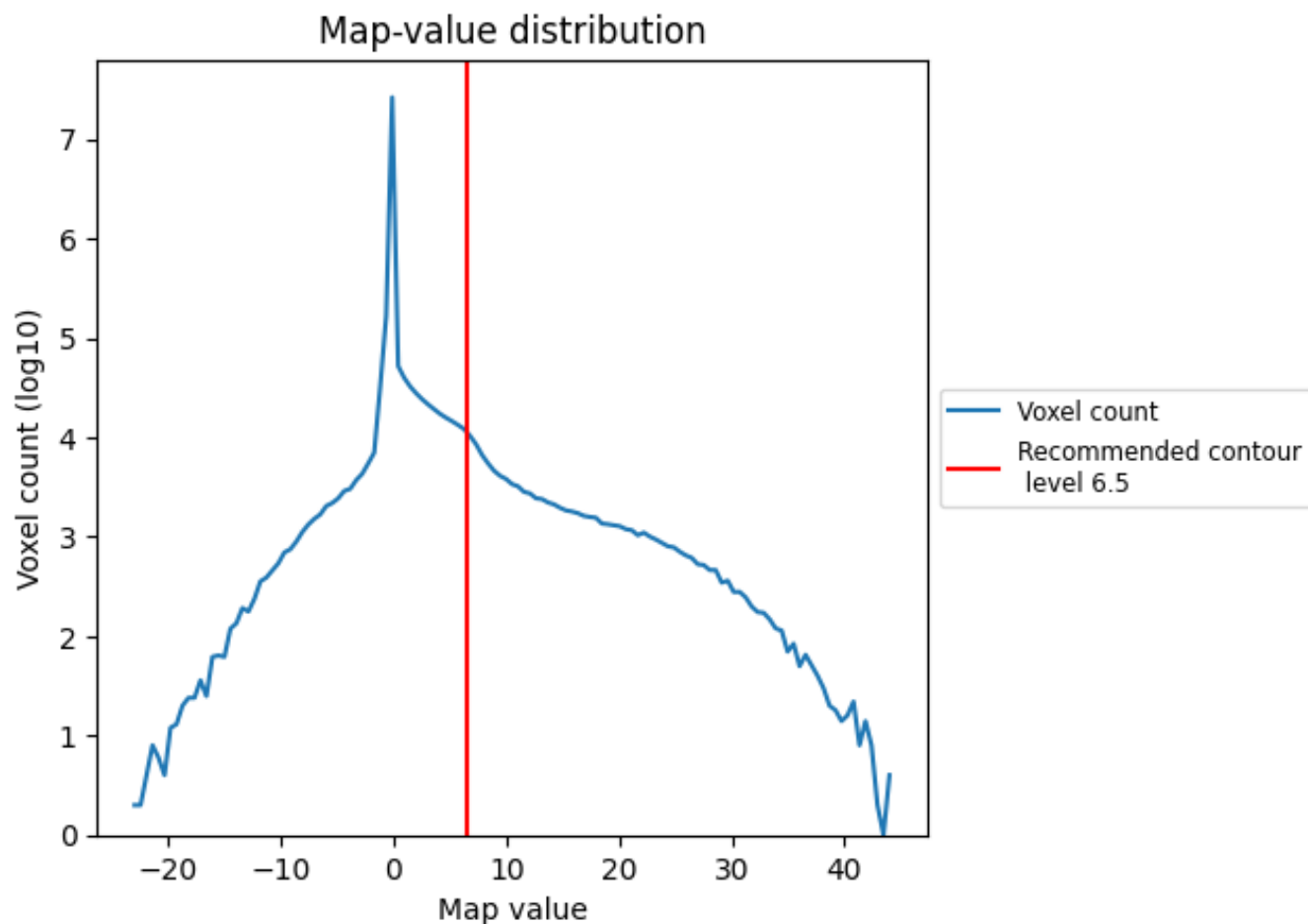
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

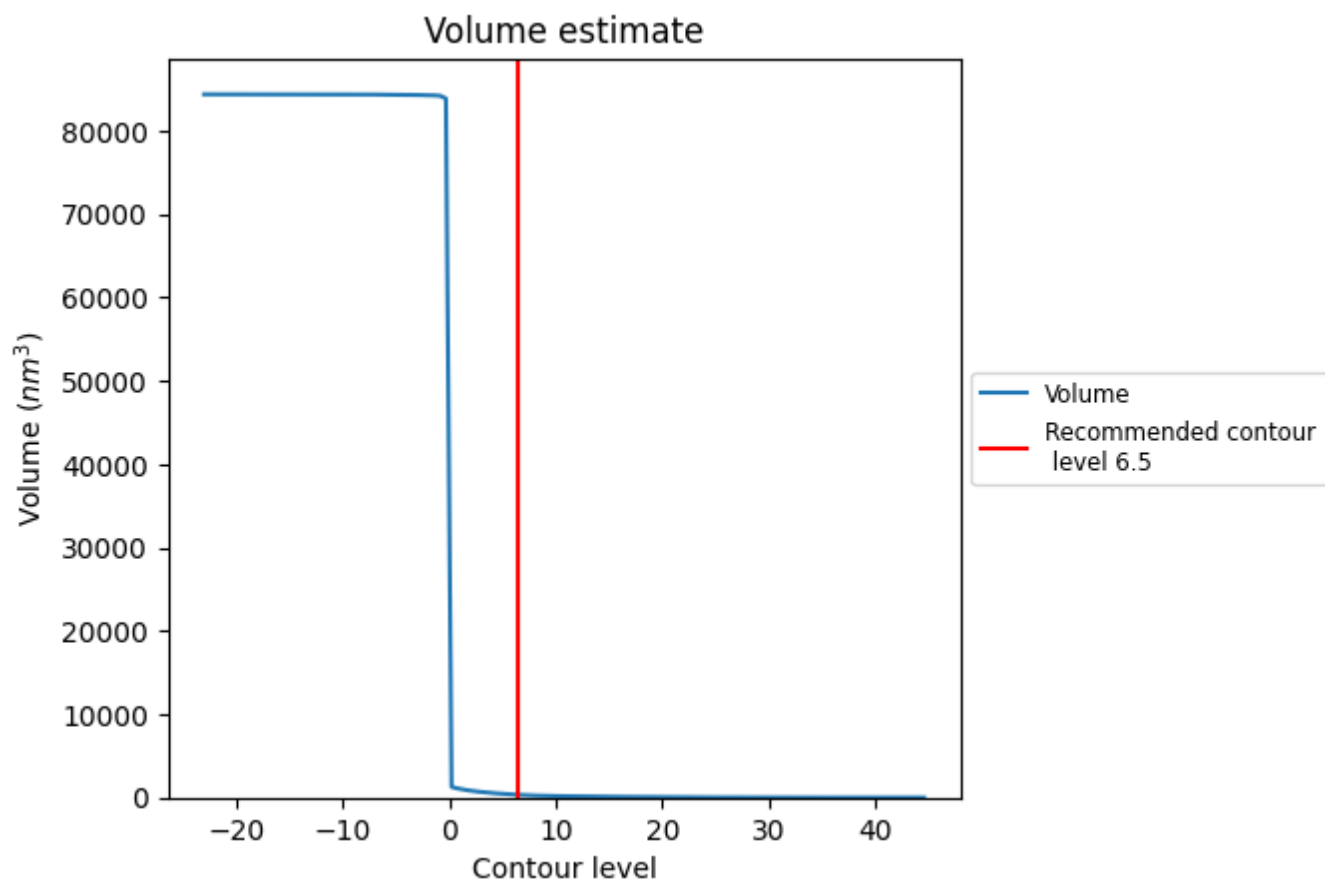
This section contains the results of statistical analysis of the map.

### 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.

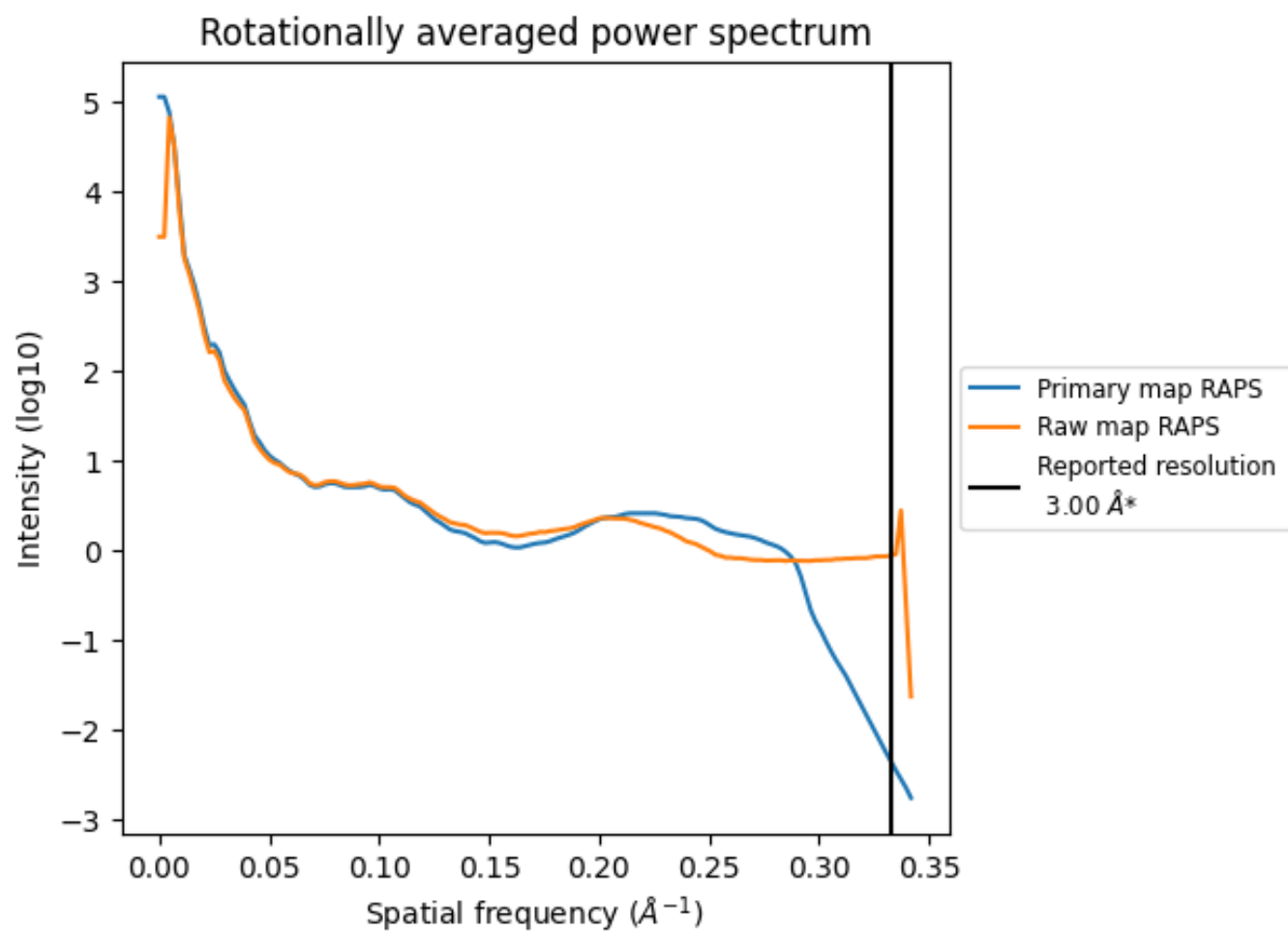
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 326  $\text{nm}^3$ ; this corresponds to an approximate mass of 295 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 ⓘ

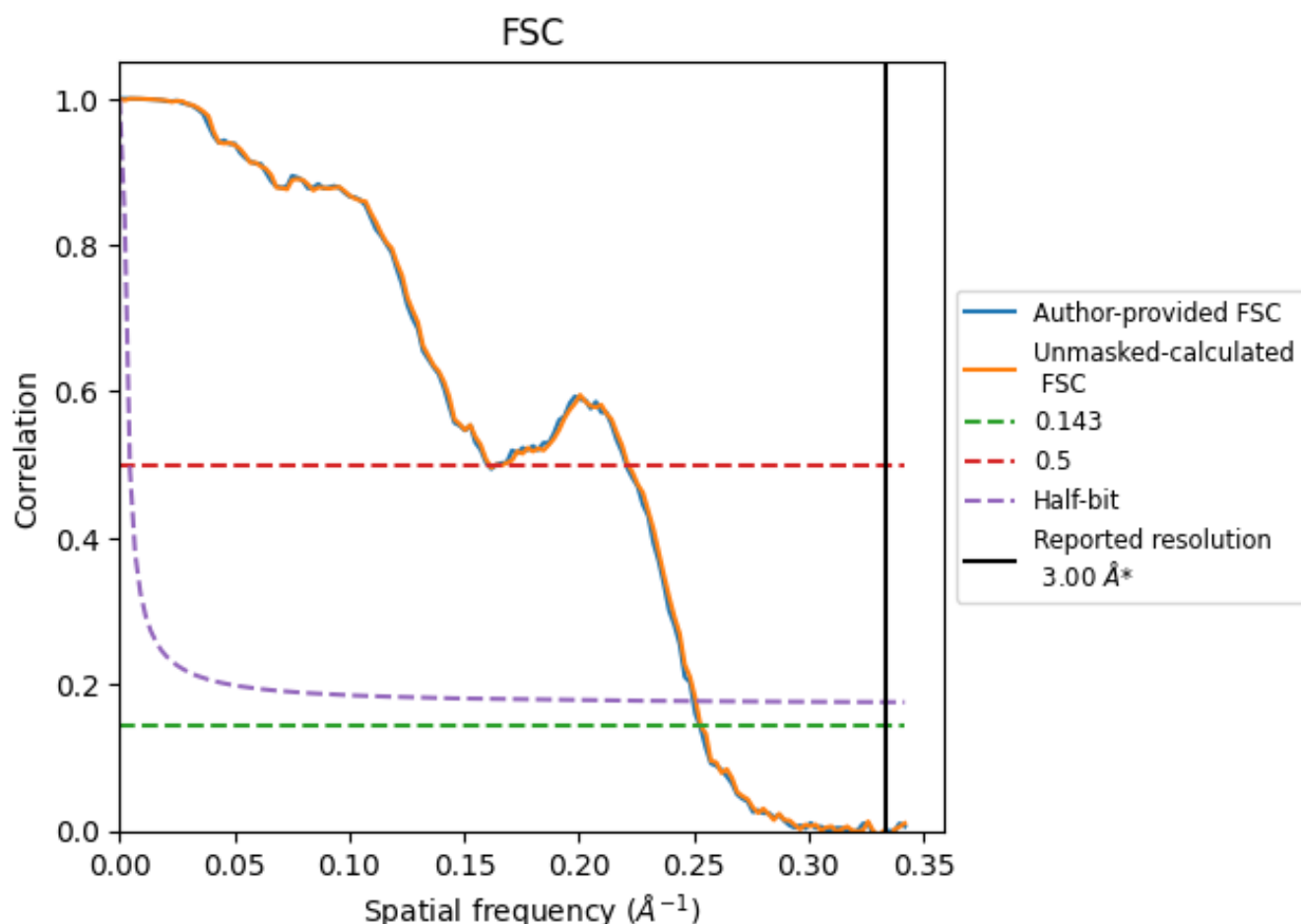


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.96	6.23	4.00
Unmasked-calculated*	3.95	6.21	3.98

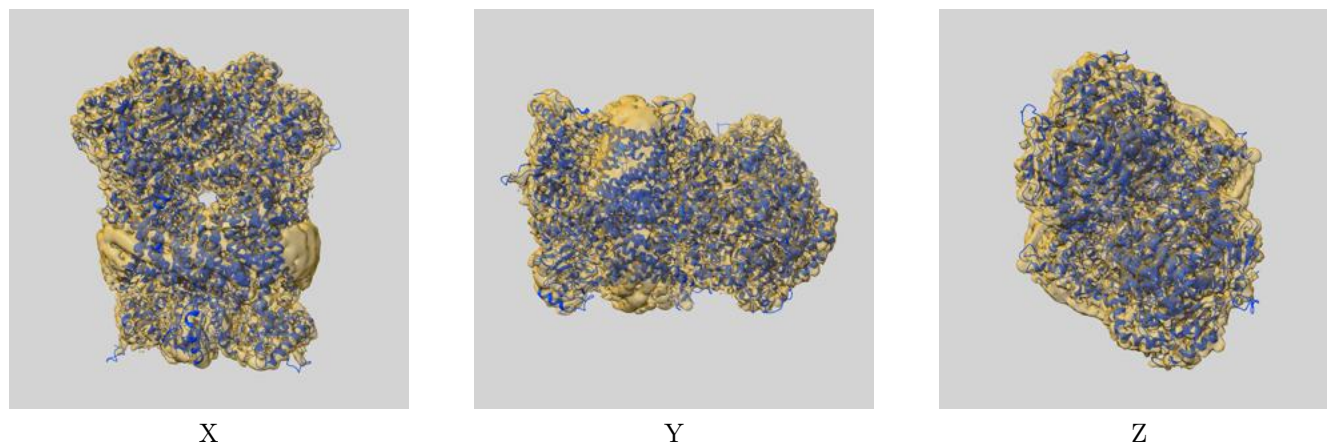
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.96 differs from the reported value 3.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.95 differs from the reported value 3.0 by more than 10 %

## 9 Map-model fit [i](#)

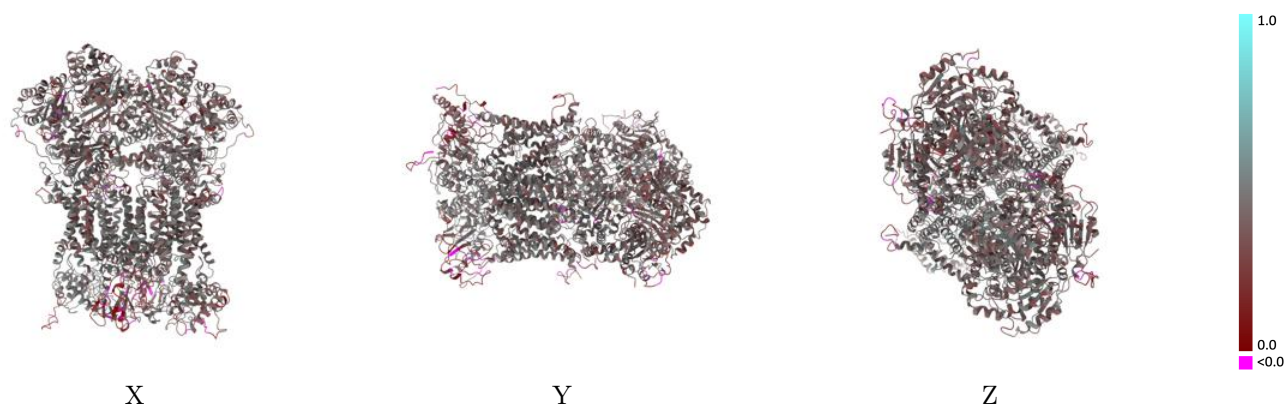
This section contains information regarding the fit between EMDB map EMD-17461 and PDB model 8P65. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



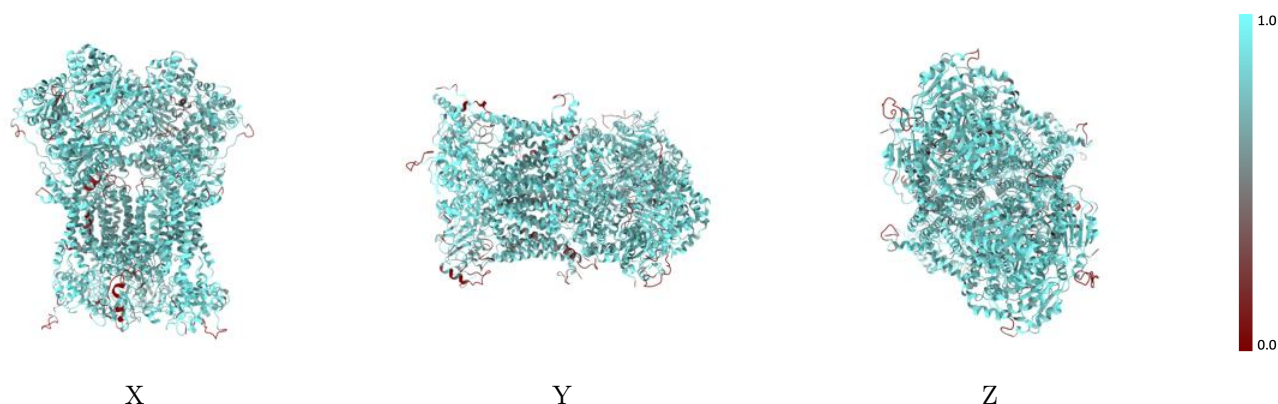
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



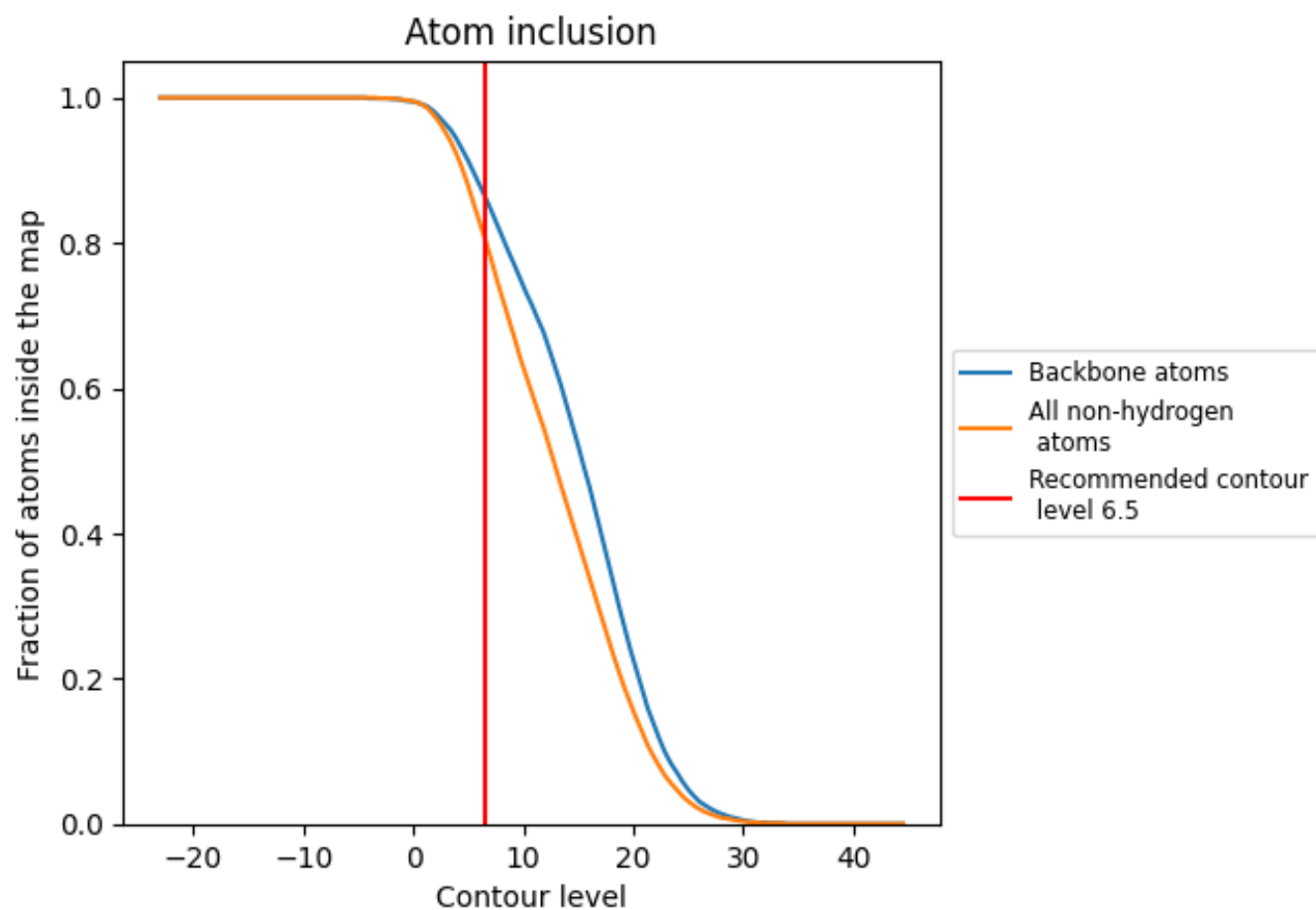
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 81% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.3920
A	 0.8410	 0.3990
B	 0.8120	 0.3870
C	 0.8460	 0.4270
D	 0.8860	 0.4290
E	 0.6830	 0.2810
F	 0.8220	 0.3890
G	 0.8520	 0.4040
H	 0.7090	 0.3120
I	 0.5520	 0.2740
J	 0.8240	 0.3910
K	 0.4590	 0.2860
N	 0.8560	 0.4170
O	 0.8140	 0.3910
P	 0.8530	 0.4440
Q	 0.8950	 0.4510
R	 0.6590	 0.2700
S	 0.8000	 0.4010
T	 0.8450	 0.4170
U	 0.7480	 0.3700
V	 0.5010	 0.2840
W	 0.8200	 0.4200
X	 0.4690	 0.3040

