



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:33 PM EST

PDB ID : 7RJE
EMDB ID : EMD-24486
Title : Complex III2 from *Candida albicans*, Inz-5 bound
Authors : Di Trani, J.M.; Rubinstein, J.L.
Deposited on : 2021-07-20
Resolution : 3.30 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

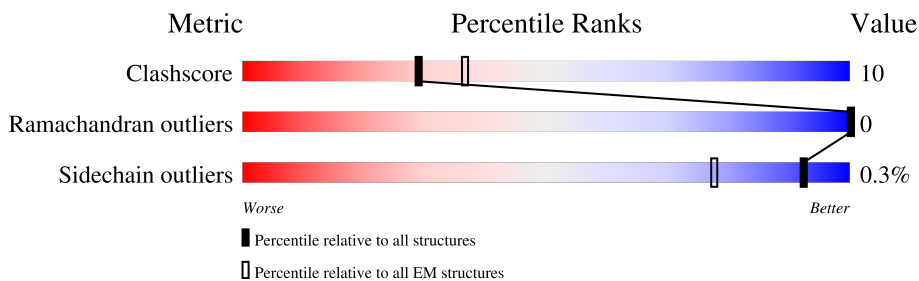
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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







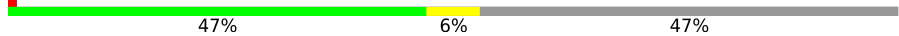
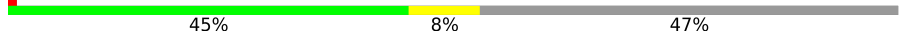
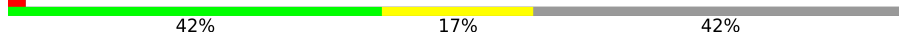
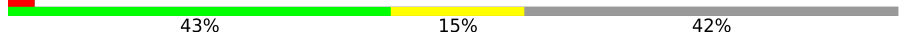


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	K	387	
1	T	387	
2	A	439	
2	E	439	
3	B	374	
3	L	374	
4	D	288	
4	N	288	

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Mol	Chain	Length	Quality of chain
5	G	127	 82% 14%
5	P	127	 83% 13%
6	F	95	 72% 21% 7%
6	O	95	 73% 20% 7%
7	H	135	 47% 6% 47%
7	Q	135	 45% 8% 47%
8	I	65	 42% 17% 42%
8	R	65	 43% 15% 42%
9	C	213	 60% 74% 11% 15%
9	M	213	 61% 74% 11% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	FES	M	301	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 57440 atoms, of which 28132 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.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	K	384	Total	C	H	N	O	S	0	0
			6146	2060	3088	478	503	17		
1	T	384	Total	C	H	N	O	S	0	0
			6146	2060	3088	478	503	17		

- Molecule 2 is a protein called Ubiquinol--cytochrome-c reductase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	A	417	Total	C	H	N	O	S	0	0
			6359	2012	3162	547	635	3		
2	E	417	Total	C	H	N	O	S	0	0
			6359	2012	3162	547	635	3		

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	B	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		
3	L	364	Total	C	H	N	O	S	0	0
			5392	1708	2692	443	548	1		

- Molecule 4 is a protein called Ubiquinol--cytochrome-c reductase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	243	Total	C	H	N	O	S	0	0
			3713	1215	1812	332	348	6		
4	N	243	Total	C	H	N	O	S	0	0
			3713	1215	1812	332	348	6		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	G	122	1978	629	1002	161	183	3	0	0
5	P	122	1978	629	1002	161	183	3	0	0

- Molecule 6 is a protein called Ubiquinol--cytochrome-c reductase subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	88	1410	472	687	124	126	1	0	0
6	O	88	1410	472	687	124	126	1	0	0

- Molecule 7 is a protein called Ubiquinol--cytochrome-c reductase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	H	72	1104	363	522	105	108	6	0	0
7	Q	72	1104	363	522	105	108	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	47	GLU	ASP	conflict	UNP A0A1D8PJT8
Q	47	GLU	ASP	conflict	UNP A0A1D8PJT8

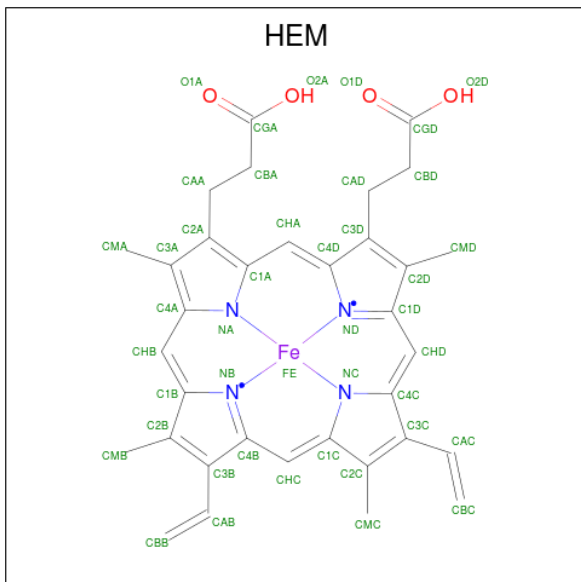
- Molecule 8 is a protein called Ubiquinol--cytochrome-c reductase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	H	N			O
8	I	38	613	211	300	53	49	0	0
8	R	38	613	211	300	53	49	0	0

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

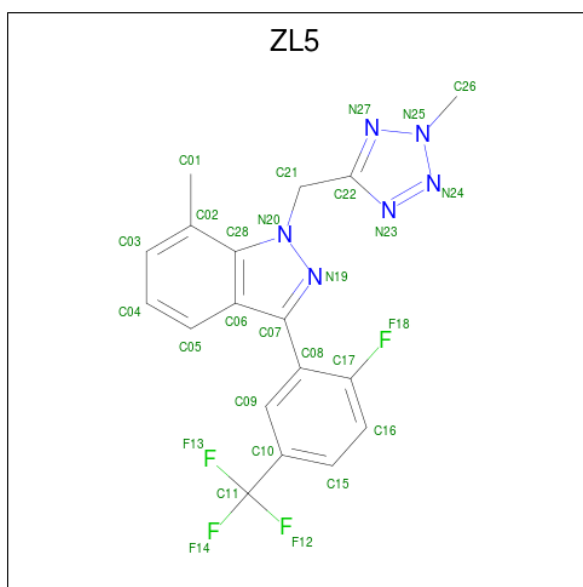
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	C	181	1740	638	697	193	210	2	0	0
9	M	181	1740	638	697	193	210	2	0	0

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



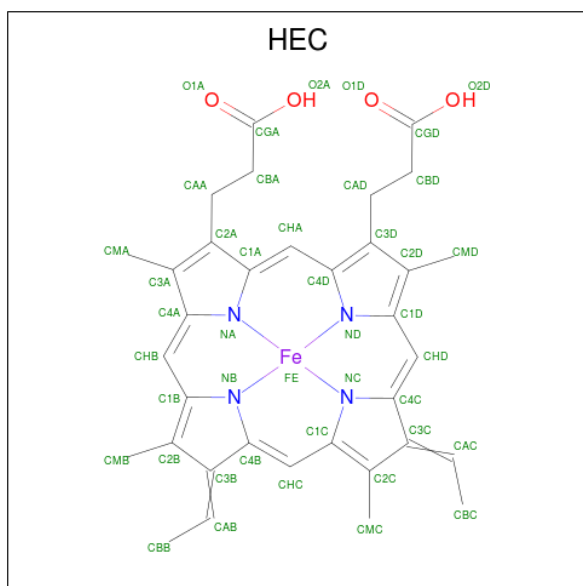
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Fe	H	N		O
10	K	1	Total	C	Fe	H	N	O	0
			146	68	2	60	8	8	
10	K	1	Total	C	Fe	H	N	O	0
			146	68	2	60	8	8	
10	T	1	Total	C	Fe	H	N	O	0
			146	68	2	60	8	8	
10	T	1	Total	C	Fe	H	N	O	0
			146	68	2	60	8	8	

- Molecule 11 is 3-[2-fluoro-5-(trifluoromethyl)phenyl]-7-methyl-1-[(2-methyl-2H-tetrazol-5-yl)methyl]-1H-indazole (three-letter code: ZL5) (formula: $C_{18}H_{14}F_4N_6$) (labeled as "Ligand of Interest" by depositor).



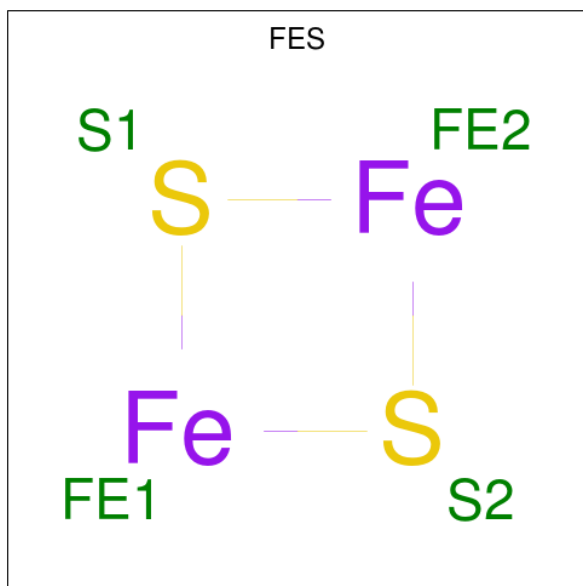
Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	H	N	
11	K	1	42	18	4	14	6	0
11	T	1	42	18	4	14	6	0

- Molecule 12 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
12	D	1	73	34	1	30	4	4	0
12	N	1	73	34	1	30	4	4	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).

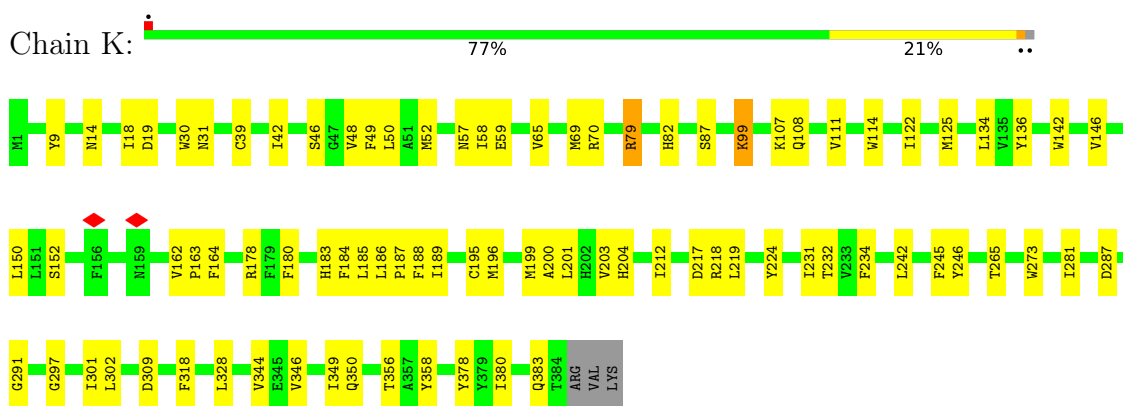


Mol	Chain	Residues	Atoms			AltConf
13	C	1	Total	Fe	S	0
			4	2	2	
13	M	1	Total	Fe	S	0
			4	2	2	

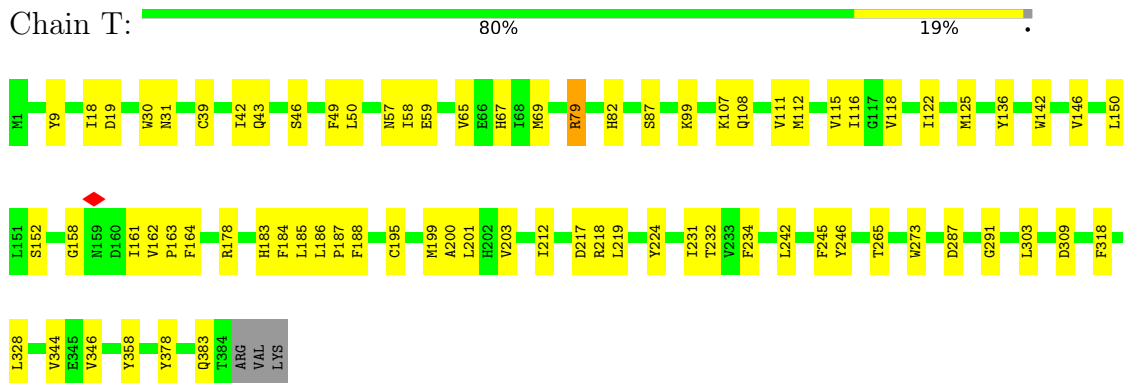
3 Residue-property plots

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.

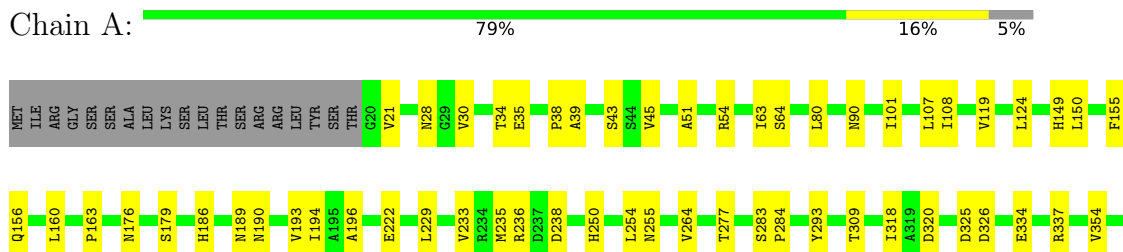
- Molecule 1: Cytochrome b

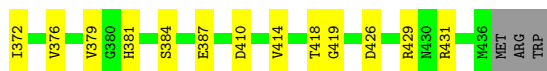


- Molecule 1: Cytochrome b



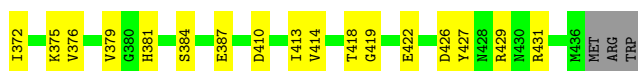
- Molecule 2: Ubiquinol--cytochrome-c reductase subunit





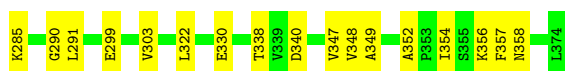
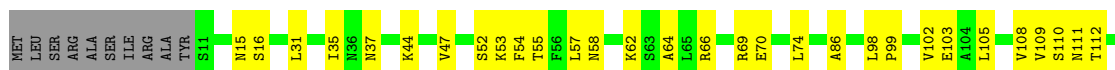
- Molecule 2: Ubiquinol--cytochrome-c reductase subunit

Chain E: 78% 17% 5%



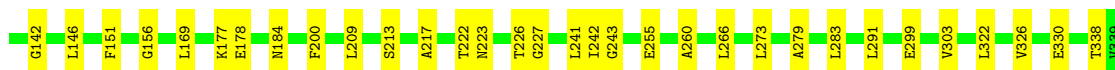
- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 76% 22% .



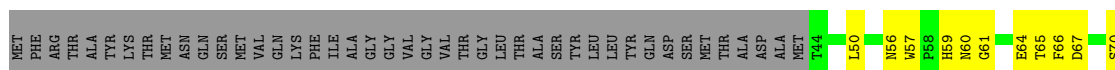
- Molecule 3: Cytochrome b-c1 complex subunit 2, mitochondrial

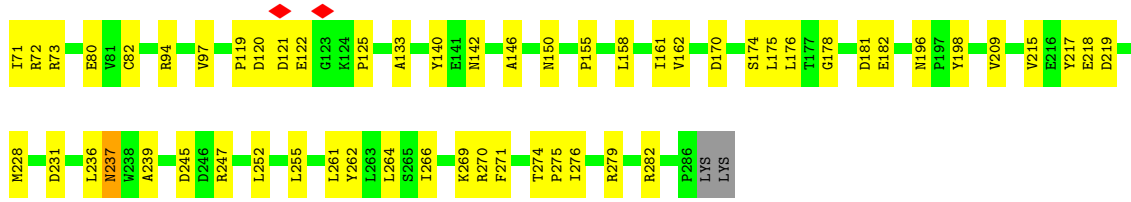
Chain L: 78% 19% .



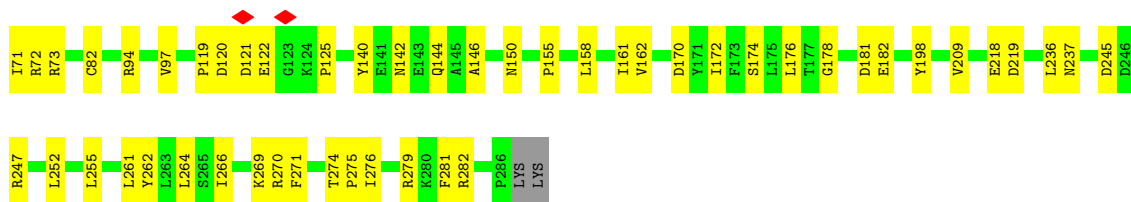
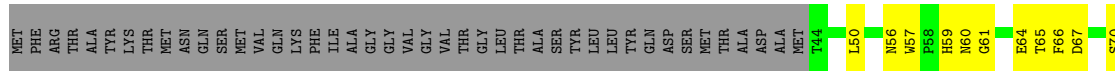
- Molecule 4: Ubiquinol--cytochrome-c reductase catalytic subunit

Chain D: 61% 23% 16%

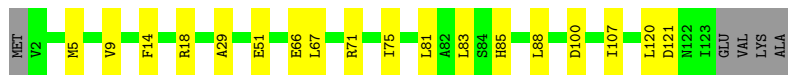
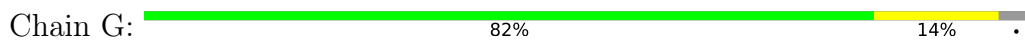




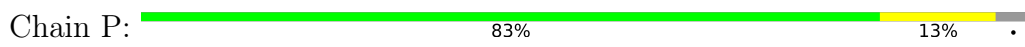
• Molecule 4: Ubiquinol--cytochrome-c reductase catalytic subunit



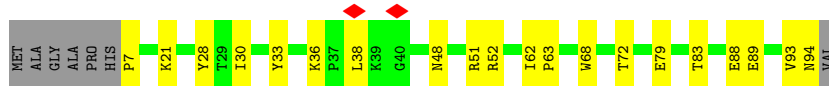
• Molecule 5: Cytochrome b-c1 complex subunit 7



• Molecule 5: Cytochrome b-c1 complex subunit 7



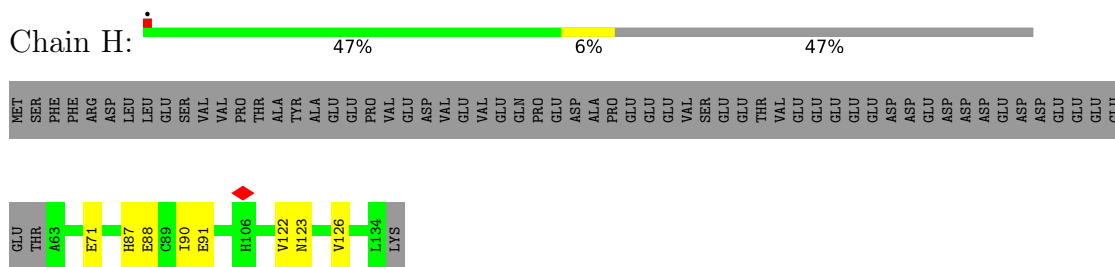
• Molecule 6: Ubiquinol--cytochrome-c reductase subunit 8



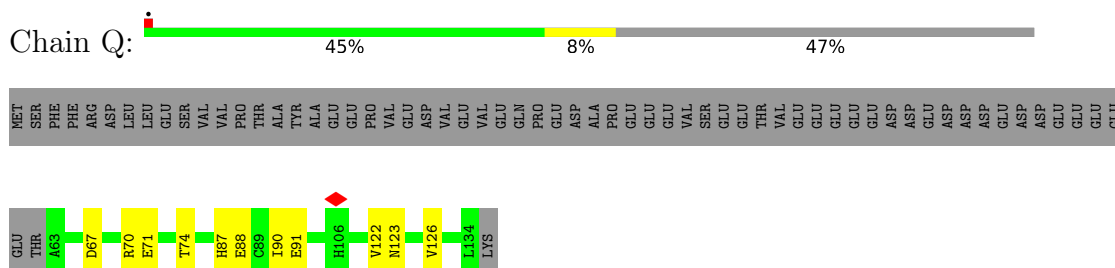
• Molecule 6: Ubiquinol--cytochrome-c reductase subunit 8



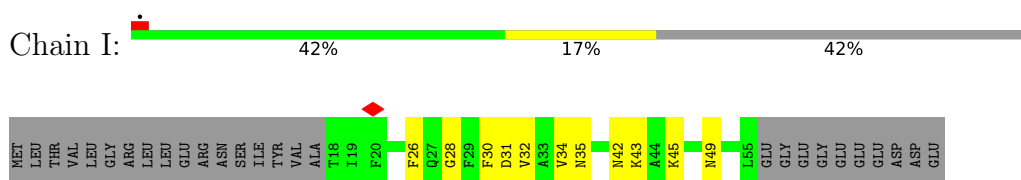
• Molecule 7: Ubiquinol--cytochrome-c reductase subunit 6



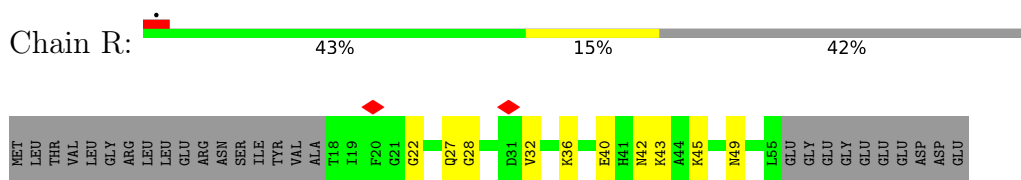
• Molecule 7: Ubiquinol--cytochrome-c reductase subunit 6



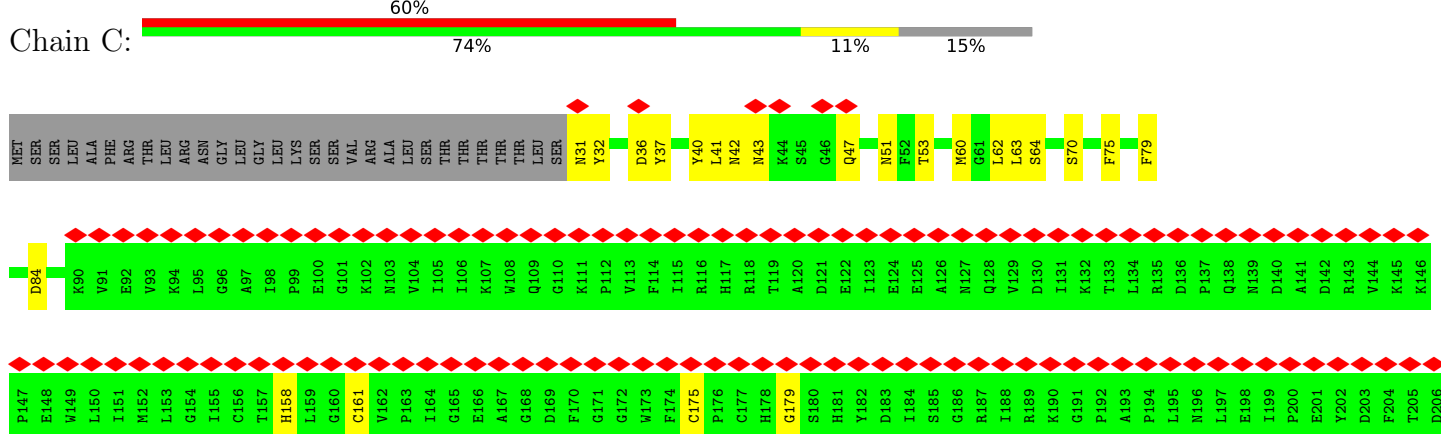
• Molecule 8: Ubiquinol--cytochrome-c reductase subunit 9

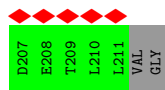


• Molecule 8: Ubiquinol--cytochrome-c reductase subunit 9

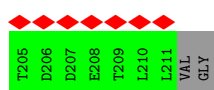
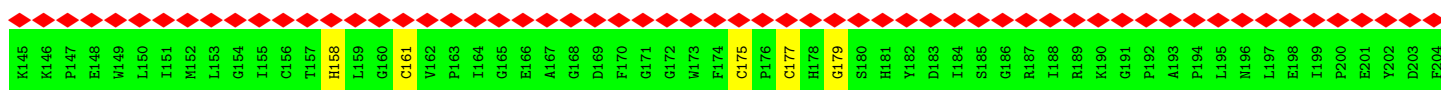
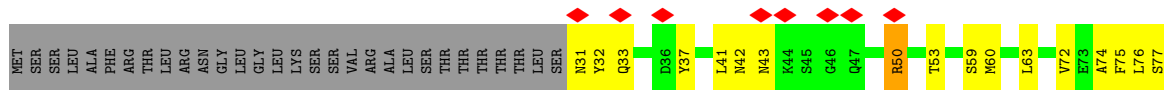
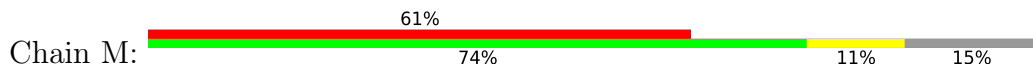


• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial





• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.718	Depositor
Minimum map value	-2.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.52	Depositor
Map size (Å)	296.63998, 296.63998, 296.63998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: FES, HEM, ZL5, 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	K	0.30	0/3161	0.46	0/4323
1	T	0.30	0/3161	0.46	0/4323
2	A	0.27	0/3253	0.45	0/4409
2	E	0.27	0/3253	0.45	0/4409
3	B	0.27	0/2748	0.48	2/3735 (0.1%)
3	L	0.27	0/2748	0.48	2/3735 (0.1%)
4	D	0.30	0/1961	0.50	2/2672 (0.1%)
4	N	0.28	0/1961	0.50	2/2672 (0.1%)
5	G	0.26	0/994	0.45	0/1346
5	P	0.26	0/994	0.45	0/1346
6	F	0.32	0/747	0.51	0/1018
6	O	0.30	0/747	0.50	0/1018
7	H	0.25	0/598	0.46	0/810
7	Q	0.26	0/598	0.47	0/810
8	I	0.24	0/324	0.36	0/435
8	R	0.25	0/324	0.36	0/435
9	C	0.28	0/1051	0.45	0/1441
9	M	0.27	0/1051	0.47	0/1441
All	All	0.28	0/29674	0.47	8/40378 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	217	ALA	CB-CA-C	7.22	120.93	110.10
3	L	217	ALA	CB-CA-C	7.21	120.92	110.10
4	N	119	PRO	N-CA-CB	5.95	110.44	103.30
4	D	125	PRO	N-CA-CB	5.92	110.41	103.30
4	N	125	PRO	N-CA-CB	5.92	110.41	103.30
4	D	119	PRO	N-CA-CB	5.82	110.28	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	217	ALA	N-CA-CB	5.50	117.81	110.10
3	B	217	ALA	N-CA-CB	5.46	117.75	110.10

There are no chirality outliers.

There are no planarity outliers.

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	K	3058	3088	3088	76	0
1	T	3058	3088	3088	75	0
2	A	3197	3162	3167	72	0
2	E	3197	3162	3167	62	0
3	B	2700	2692	2685	57	0
3	L	2700	2692	2685	51	0
4	D	1901	1812	1798	64	0
4	N	1901	1812	1798	65	0
5	G	976	1002	1002	14	0
5	P	976	1002	1002	14	0
6	F	723	687	695	23	0
6	O	723	687	695	19	0
7	H	582	522	522	6	0
7	Q	582	522	522	6	0
8	I	313	300	302	8	0
8	R	313	300	302	7	0
9	C	1043	697	706	53	0
9	M	1043	697	706	67	0
10	K	86	60	60	19	0
10	T	86	60	60	17	0
11	K	28	14	0	0	0
11	T	28	14	0	0	0
12	D	43	30	32	10	0
12	N	43	30	32	10	0
13	C	4	0	0	1	0
13	M	4	0	0	4	0
All	All	29308	28132	28114	593	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 (593) 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)
2:A:149:HIS:CD2	9:M:31:ASN:HD22	1.44	1.32
2:A:410:ASP:OD2	9:M:50:ARG:NE	1.67	1.25
6:F:30:ILE:HD11	9:M:37:TYR:CG	1.72	1.25
6:O:30:ILE:HD11	9:C:37:TYR:CD1	1.73	1.23
9:M:158:HIS:O	13:M:301:FES:S2	1.97	1.21
6:O:30:ILE:HD11	9:C:37:TYR:CG	1.81	1.15
2:A:149:HIS:CD2	9:M:31:ASN:ND2	2.17	1.13
4:N:282:ARG:NH2	9:C:32:TYR:CZ	2.20	1.10
2:A:410:ASP:OD2	9:M:50:ARG:CD	2.00	1.08
2:E:163:PRO:HG3	9:C:31:ASN:N	1.68	1.07
6:O:36:LYS:NZ	9:C:41:LEU:O	1.89	1.06
1:T:67:HIS:CE1	9:C:84:ASP:OD2	2.09	1.05
8:R:27:GLN:NE2	9:C:70:SER:OG	1.90	1.03
9:C:158:HIS:CB	13:C:301:FES:S2	2.51	0.99
4:D:282:ARG:NH2	9:M:32:TYR:CZ	2.31	0.99
4:N:282:ARG:NE	9:C:32:TYR:CE2	2.33	0.96
2:A:163:PRO:HG3	9:M:31:ASN:N	1.81	0.96
4:N:282:ARG:CZ	9:C:32:TYR:CE2	2.48	0.95
2:A:410:ASP:OD2	9:M:50:ARG:HD2	1.67	0.95
4:N:261:LEU:CD1	9:C:63:LEU:HB3	1.97	0.94
4:D:261:LEU:HD11	9:M:63:LEU:HB3	1.50	0.94
4:N:261:LEU:HD11	9:C:63:LEU:HB3	1.49	0.93
6:O:30:ILE:CD1	9:C:37:TYR:CD1	2.50	0.93
4:D:282:ARG:CZ	9:M:32:TYR:CZ	2.53	0.92
3:B:58:ASN:ND2	3:B:118:GLU:OE1	2.03	0.91
2:A:410:ASP:CG	9:M:50:ARG:HE	1.72	0.91
1:T:318:PHE:O	1:T:378:TYR:OH	1.90	0.90
4:D:282:ARG:NE	9:M:32:TYR:CE2	2.39	0.89
2:A:149:HIS:CG	9:M:31:ASN:HD22	1.89	0.89
4:N:282:ARG:NH2	9:C:32:TYR:CE2	2.41	0.88
4:D:261:LEU:CD1	9:M:63:LEU:HB3	2.04	0.88
1:T:67:HIS:HE1	9:C:84:ASP:OD2	1.58	0.87
9:M:31:ASN:OD1	9:M:32:TYR:N	2.08	0.87
3:L:146:LEU:HD22	3:L:291:LEU:HD21	1.55	0.87
6:F:36:LYS:NZ	9:M:41:LEU:O	2.06	0.87
3:B:146:LEU:HD22	3:B:291:LEU:HD21	1.57	0.86
2:A:334:GLU:OE1	2:A:337:ARG:NH1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:401:HEM:HMC1	10:K:401:HEM:HBC2	1.57	0.86
4:N:282:ARG:CZ	9:C:32:TYR:CZ	2.58	0.86
10:T:401:HEM:HBC2	10:T:401:HEM:HMC1	1.58	0.86
2:E:334:GLU:OE1	2:E:337:ARG:NH1	2.07	0.86
1:K:318:PHE:O	1:K:378:TYR:OH	1.94	0.85
2:A:150:LEU:HD11	2:A:414:VAL:HG13	1.57	0.84
6:F:30:ILE:HD11	9:M:37:TYR:CD1	2.12	0.84
4:N:282:ARG:NE	9:C:32:TYR:HE2	1.73	0.84
2:E:150:LEU:HD11	2:E:414:VAL:HG13	1.60	0.83
4:D:282:ARG:CZ	9:M:32:TYR:CE2	2.62	0.83
3:B:57:LEU:O	3:B:64:ALA:HB2	1.80	0.82
2:A:229:LEU:CD1	9:M:41:LEU:HD11	2.09	0.82
4:D:176:LEU:HD21	12:D:301:HEC:HMB2	1.62	0.81
1:T:224:TYR:OH	2:E:426:ASP:OD1	1.98	0.81
2:A:229:LEU:HD13	9:M:41:LEU:HD11	1.63	0.80
4:N:176:LEU:HD21	12:N:301:HEC:HMB2	1.64	0.80
8:I:31:ASP:OD1	8:I:35:ASN:ND2	2.16	0.79
4:D:65:THR:OG1	4:D:245:ASP:OD1	2.01	0.78
1:K:185:LEU:HD12	1:T:188:PHE:CZ	2.19	0.78
4:N:65:THR:OG1	4:N:245:ASP:OD1	2.00	0.78
2:E:236:ARG:NH1	2:E:238:ASP:OD1	2.17	0.77
4:D:282:ARG:CZ	9:M:32:TYR:OH	2.32	0.77
2:E:229:LEU:HD13	9:C:41:LEU:HD11	1.66	0.77
2:A:236:ARG:NH1	2:A:238:ASP:OD1	2.17	0.77
2:E:149:HIS:NE2	9:C:31:ASN:ND2	2.33	0.77
2:E:45:VAL:HG23	2:E:101:ILE:HD11	1.65	0.76
10:K:402:HEM:HBC2	10:K:402:HEM:HHD	1.66	0.75
6:F:30:ILE:CD1	9:M:37:TYR:CD1	2.69	0.75
4:D:282:ARG:NE	9:M:32:TYR:HE2	1.85	0.75
2:A:45:VAL:HG23	2:A:101:ILE:HD11	1.66	0.75
3:B:178:GLU:OE1	3:B:215:ASN:N	2.19	0.75
6:O:48:ASN:OD1	6:O:51:ARG:NH2	2.18	0.75
10:T:402:HEM:HBC2	10:T:402:HEM:HHD	1.67	0.74
4:D:271:PHE:CZ	9:M:53:THR:HG21	2.23	0.74
1:K:196:MET:O	1:T:9:TYR:OH	2.06	0.74
5:G:14:PHE:O	5:G:18:ARG:NH1	2.22	0.73
6:F:30:ILE:CD1	9:M:37:TYR:CG	2.63	0.73
2:E:163:PRO:CG	9:C:31:ASN:N	2.52	0.73
2:E:149:HIS:CD2	9:C:31:ASN:ND2	2.57	0.72
1:T:217:ASP:OD2	4:N:279:ARG:NH2	2.23	0.72
6:F:30:ILE:HD11	9:M:37:TYR:CD2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:242:LEU:HD23	4:N:255:LEU:HD21	1.71	0.71
2:A:410:ASP:O	2:A:431:ARG:NH2	2.22	0.71
2:E:156:GLN:OE1	9:C:37:TYR:CD2	2.43	0.71
3:L:338:THR:HG23	3:L:340:ASP:OD1	1.90	0.71
2:A:21:VAL:HG22	2:A:35:GLU:OE1	1.89	0.71
2:A:384:SER:N	2:A:387:GLU:OE1	2.24	0.71
8:I:26:PHE:CE2	9:M:63:LEU:HD22	2.26	0.71
9:M:59:SER:O	9:M:63:LEU:HD23	1.91	0.70
1:K:217:ASP:OD2	4:D:279:ARG:NH2	2.23	0.70
1:T:344:VAL:HG23	1:T:344:VAL:O	1.91	0.70
6:F:7:PRO:N	2:E:293:TYR:HH	1.88	0.70
4:N:161:ILE:HG12	12:N:301:HEC:HMA3	1.74	0.70
4:D:271:PHE:HE2	9:M:53:THR:HG1	1.38	0.70
1:K:19:ASP:OD1	2:A:429:ARG:NH2	2.23	0.69
4:D:282:ARG:NH2	9:M:32:TYR:CE2	2.60	0.69
1:T:19:ASP:OD1	2:E:429:ARG:NH2	2.25	0.69
2:E:413:ILE:O	2:E:427:TYR:OH	2.07	0.69
1:K:183:HIS:NE2	10:K:401:HEM:NC	2.40	0.69
1:T:218:ARG:HG3	6:O:17:LEU:HD13	1.74	0.69
4:D:161:ILE:HG12	12:D:301:HEC:HMA3	1.75	0.68
2:E:384:SER:N	2:E:387:GLU:OE1	2.27	0.68
1:T:183:HIS:NE2	10:T:401:HEM:NC	2.42	0.68
9:M:177:CYS:CB	13:M:301:FES:S1	2.81	0.68
6:F:48:ASN:OD1	6:F:51:ARG:NH2	2.25	0.68
1:K:87:SER:HG	1:K:273:TRP:HE1	1.41	0.67
1:T:184:PHE:CE1	10:T:401:HEM:HBC1	2.29	0.67
3:L:109:VAL:HG11	3:L:209:LEU:HD11	1.78	0.66
1:T:87:SER:HG	1:T:273:TRP:HE1	1.42	0.65
2:A:63:ILE:HD11	2:A:179:SER:HB3	1.79	0.65
2:E:229:LEU:CD1	9:C:41:LEU:HD11	2.25	0.65
4:N:209:VAL:HG11	12:N:301:HEC:HMC2	1.78	0.65
1:T:164:PHE:HZ	9:M:76:LEU:HD12	1.62	0.65
4:D:271:PHE:CZ	9:M:53:THR:CG2	2.79	0.65
4:N:282:ARG:CZ	9:C:32:TYR:OH	2.44	0.65
1:T:178:ARG:NH2	9:M:79:PHE:O	2.29	0.65
2:A:149:HIS:NE2	9:M:31:ASN:ND2	2.39	0.64
4:D:209:VAL:HG11	12:D:301:HEC:HMC2	1.78	0.64
3:L:226:THR:OG1	3:L:356:LYS:O	2.16	0.64
4:N:261:LEU:HD11	9:C:63:LEU:CB	2.24	0.64
3:B:109:VAL:HG11	3:B:209:LEU:HD11	1.79	0.64
1:K:107:LYS:NZ	1:K:309:ASP:OD2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:67:HIS:ND1	9:C:84:ASP:OD2	2.30	0.63
10:T:401:HEM:HBC2	10:T:401:HEM:CMC	2.29	0.63
3:B:178:GLU:O	3:B:213:SER:OG	2.10	0.63
2:E:254:LEU:O	2:E:255:ASN:OD1	2.16	0.63
1:K:152:SER:HB3	1:K:162:VAL:HG21	1.81	0.63
1:K:30:TRP:NE1	10:K:402:HEM:O2D	2.32	0.62
1:T:112:MET:O	1:T:115:VAL:HG22	1.99	0.62
6:F:33:TYR:CE2	9:M:50:ARG:HG2	2.34	0.62
1:T:112:MET:O	1:T:116:ILE:HD12	1.99	0.62
3:L:178:GLU:O	3:L:213:SER:OG	2.11	0.62
1:T:107:LYS:NZ	1:T:309:ASP:OD2	2.31	0.62
2:A:149:HIS:CE1	9:M:31:ASN:HB2	2.33	0.62
2:A:254:LEU:O	2:A:255:ASN:OD1	2.17	0.62
5:P:51:GLU:OE2	5:P:71:ARG:NH1	2.31	0.62
1:T:231:ILE:HD11	4:N:269:LYS:CB	2.30	0.62
3:B:54:PHE:CE1	3:B:123:VAL:HG11	2.34	0.62
2:E:63:ILE:HD11	2:E:179:SER:HB3	1.80	0.61
5:P:58:THR:HG22	5:P:62:ARG:HD2	1.82	0.61
1:K:231:ILE:HD11	4:D:269:LYS:CB	2.31	0.61
2:A:229:LEU:CD1	9:M:41:LEU:CD1	2.77	0.61
1:T:152:SER:HB3	1:T:162:VAL:HG21	1.81	0.61
2:A:229:LEU:HD13	9:M:41:LEU:CD1	2.29	0.60
4:N:50:LEU:HD22	4:N:198:TYR:CE1	2.35	0.60
10:K:402:HEM:HBB2	10:K:402:HEM:HHC	1.82	0.60
3:L:58:ASN:ND2	3:L:118:GLU:OE1	2.34	0.60
2:A:293:TYR:HH	6:O:7:PRO:N	1.98	0.60
4:D:271:PHE:HZ	9:M:53:THR:HG21	1.64	0.60
7:Q:67:ASP:O	7:Q:71:GLU:OE1	2.20	0.60
1:K:344:VAL:O	1:K:344:VAL:HG23	2.01	0.60
3:L:299:GLU:O	3:L:303:VAL:HG23	2.01	0.59
4:D:261:LEU:HD11	9:M:63:LEU:CB	2.29	0.59
4:D:50:LEU:HD22	4:D:198:TYR:CE1	2.36	0.59
5:G:51:GLU:OE2	5:G:71:ARG:NH1	2.34	0.59
4:N:94:ARG:O	4:N:97:VAL:HG22	2.03	0.59
1:K:48:VAL:HG21	1:T:185:LEU:HD13	1.84	0.59
3:B:242:ILE:HG23	3:B:357:PHE:HB2	1.85	0.59
4:D:176:LEU:HD21	12:D:301:HEC:CMB	2.32	0.59
5:P:14:PHE:O	5:P:18:ARG:NH1	2.36	0.59
1:T:184:PHE:CZ	10:T:401:HEM:HBC1	2.38	0.59
10:T:401:HEM:HBB2	10:T:401:HEM:HMB1	1.84	0.58
4:N:270:ARG:O	4:N:274:THR:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:ILE:HD11	1:K:136:TYR:CZ	2.39	0.58
2:E:156:GLN:OE1	9:C:37:TYR:HD2	1.85	0.58
4:D:94:ARG:O	4:D:97:VAL:HG22	2.04	0.58
10:K:401:HEM:HMB1	10:K:401:HEM:HBB2	1.84	0.58
4:N:181:ASP:OD1	4:N:182:GLU:N	2.36	0.58
1:K:224:TYR:OH	2:A:426:ASP:OD1	2.16	0.58
3:B:299:GLU:O	3:B:303:VAL:HG23	2.03	0.58
1:K:185:LEU:HD12	1:T:188:PHE:HZ	1.68	0.58
4:D:56:ASN:OD1	4:D:56:ASN:O	2.21	0.58
6:F:68:TRP:O	6:F:72:THR:HG23	2.03	0.58
4:N:64:GLU:OE1	8:R:45:LYS:NZ	2.35	0.58
4:N:176:LEU:HD21	12:N:301:HEC:CMB	2.33	0.58
2:A:325:ASP:OD1	2:A:326:ASP:N	2.37	0.57
6:F:33:TYR:CE2	9:M:50:ARG:CG	2.87	0.57
7:Q:70:ARG:O	7:Q:74:THR:HG23	2.05	0.57
3:L:146:LEU:HD21	3:L:243:GLY:HA3	1.87	0.57
1:T:31:ASN:HB3	1:T:232:THR:HG21	1.87	0.57
1:T:142:TRP:CZ3	9:M:161:CYS:HA	2.40	0.57
3:B:338:THR:HG23	3:B:340:ASP:OD1	2.05	0.57
3:B:146:LEU:CD2	3:B:291:LEU:HD11	2.34	0.57
1:T:87:SER:OG	1:T:273:TRP:NE1	2.35	0.56
3:B:226:THR:OG1	3:B:356:LYS:O	2.23	0.56
1:T:30:TRP:NE1	10:T:402:HEM:O2D	2.37	0.56
4:N:56:ASN:OD1	4:N:56:ASN:O	2.23	0.56
10:T:402:HEM:HHC	10:T:402:HEM:HBB2	1.87	0.56
3:L:354:ILE:O	3:L:354:ILE:HG22	2.06	0.56
1:T:58:ILE:HD11	1:T:136:TYR:CZ	2.41	0.56
1:K:18:ILE:HG22	2:A:429:ARG:NH2	2.20	0.56
9:M:158:HIS:CB	13:M:301:FES:S2	2.93	0.56
1:T:164:PHE:CZ	9:M:76:LEU:HD12	2.41	0.56
5:P:5:MET:HG3	5:P:107:ILE:HG21	1.86	0.56
4:D:181:ASP:OD1	4:D:182:GLU:N	2.39	0.56
2:E:21:VAL:HG12	2:E:21:VAL:O	2.06	0.55
3:L:242:ILE:HG23	3:L:357:PHE:HB2	1.88	0.55
4:N:261:LEU:CD1	9:C:63:LEU:CB	2.81	0.55
2:A:156:GLN:OE1	9:M:37:TYR:HD2	1.90	0.55
6:O:68:TRP:O	6:O:72:THR:HG23	2.07	0.55
1:K:184:PHE:CE2	1:T:184:PHE:CD2	2.95	0.55
3:B:44:LYS:O	3:B:47:VAL:HG22	2.07	0.55
2:A:189:ASN:OD1	2:A:190:ASN:N	2.40	0.55
2:E:189:ASN:OD1	2:E:190:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:37:ASN:OD1	3:L:184:ASN:ND2	2.39	0.55
4:D:150:ASN:OD1	12:D:301:HEC:HBC2	2.07	0.55
6:F:30:ILE:HD11	9:M:37:TYR:CB	2.34	0.55
1:T:118:VAL:HG21	1:T:303:LEU:HD23	1.89	0.55
3:B:146:LEU:HD21	3:B:243:GLY:HA3	1.89	0.55
10:K:401:HEM:HBC2	10:K:401:HEM:CMC	2.34	0.54
3:B:354:ILE:HG22	3:B:354:ILE:O	2.06	0.54
1:T:195:CYS:O	1:T:199:MET:HG3	2.07	0.54
3:B:110:SER:O	3:B:111:ASN:OD1	2.25	0.54
5:G:5:MET:HG3	5:G:107:ILE:HG21	1.88	0.54
2:A:21:VAL:HG12	2:A:21:VAL:O	2.07	0.54
1:K:134:LEU:HD21	1:K:180:PHE:HA	1.88	0.54
4:D:282:ARG:NH1	9:M:32:TYR:OH	2.39	0.54
1:K:31:ASN:HB3	1:K:232:THR:HG21	1.90	0.54
1:T:18:ILE:HG22	2:E:429:ARG:NH2	2.22	0.54
4:D:155:PRO:HG3	12:D:301:HEC:HMD3	1.90	0.54
2:E:410:ASP:O	2:E:431:ARG:NH2	2.41	0.54
2:E:167:THR:HG21	9:C:31:ASN:O	2.08	0.54
3:L:110:SER:O	3:L:111:ASN:OD1	2.26	0.54
3:L:146:LEU:CD2	3:L:291:LEU:HD11	2.38	0.54
4:D:72:ARG:NE	4:D:218:GLU:OE2	2.38	0.53
4:D:270:ARG:O	4:D:274:THR:HG23	2.08	0.53
2:A:229:LEU:HD11	9:M:41:LEU:HD11	1.87	0.53
9:C:42:ASN:OD1	9:C:43:ASN:N	2.41	0.53
1:K:184:PHE:CE1	10:K:401:HEM:HBC1	2.43	0.53
6:O:93:VAL:HG13	6:O:94:ASN:OD1	2.09	0.53
6:F:93:VAL:HG13	6:F:94:ASN:OD1	2.09	0.53
4:N:72:ARG:NE	4:N:218:GLU:OE2	2.40	0.53
4:N:150:ASN:OD1	12:N:301:HEC:HBC2	2.09	0.53
1:T:57:ASN:OD1	1:T:59:GLU:N	2.40	0.53
4:N:155:PRO:HG3	12:N:301:HEC:HMD3	1.91	0.53
3:B:146:LEU:HD21	3:B:291:LEU:HD11	1.89	0.53
3:B:273:LEU:HD11	3:B:279:ALA:HB1	1.90	0.53
7:H:71:GLU:N	7:H:71:GLU:OE2	2.42	0.53
2:E:118:ILE:O	2:E:122:THR:OG1	2.16	0.53
9:M:74:ALA:O	9:M:77:SER:OG	2.27	0.53
1:K:69:MET:SD	1:K:79:ARG:HD2	2.49	0.53
3:B:15:ASN:O	3:B:16:SER:OG	2.24	0.52
1:T:231:ILE:HD11	4:N:269:LYS:HB3	1.90	0.52
4:D:121:ASP:CB	4:N:144:GLN:HG2	2.38	0.52
9:M:158:HIS:C	13:M:301:FES:S2	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:42:ASN:OD1	9:M:43:ASN:N	2.43	0.52
2:E:167:THR:O	2:E:171:VAL:HG23	2.10	0.52
1:K:346:VAL:O	1:K:350:GLN:OE1	2.27	0.52
9:C:47:GLN:OE1	9:C:51:ASN:ND2	2.43	0.52
1:T:69:MET:SD	1:T:79:ARG:HD2	2.50	0.51
10:T:401:HEM:HBB2	10:T:401:HEM:CMB	2.41	0.51
2:A:372:ILE:O	2:A:376:VAL:HG23	2.09	0.51
6:F:30:ILE:HD12	9:M:37:TYR:CD1	2.45	0.51
2:E:372:ILE:O	2:E:376:VAL:HG23	2.09	0.51
3:B:57:LEU:HB3	3:B:118:GLU:OE2	2.10	0.51
1:K:57:ASN:OD1	1:K:59:GLU:N	2.43	0.51
1:K:108:GLN:O	1:K:111:VAL:HG23	2.10	0.51
1:K:231:ILE:HD11	4:D:269:LYS:HB3	1.92	0.51
2:A:149:HIS:CE1	9:M:31:ASN:CB	2.93	0.51
3:L:119:PHE:HB2	3:L:169:LEU:HD12	1.92	0.51
1:K:65:VAL:HG13	10:K:401:HEM:O1D	2.10	0.51
4:D:60:ASN:OD1	4:D:61:GLY:N	2.43	0.51
1:K:185:LEU:HD21	1:K:189:ILE:HD11	1.93	0.51
1:K:195:CYS:O	1:K:199:MET:HG3	2.11	0.51
8:I:28:GLY:O	8:I:32:VAL:HG22	2.10	0.51
4:D:64:GLU:OE1	8:I:45:LYS:NZ	2.41	0.51
1:T:112:MET:SD	1:T:116:ILE:HD11	2.51	0.51
2:A:229:LEU:HD11	9:M:41:LEU:CD1	2.41	0.51
4:N:174:SER:O	4:N:178:GLY:N	2.43	0.51
1:T:108:GLN:O	1:T:111:VAL:HG23	2.11	0.50
4:D:174:SER:O	4:D:178:GLY:N	2.44	0.50
6:O:38:LEU:HD12	6:O:38:LEU:O	2.10	0.50
2:A:119:VAL:O	2:A:176:ASN:ND2	2.44	0.50
1:T:65:VAL:HG13	10:T:401:HEM:O1D	2.11	0.50
2:E:28:ASN:OD1	2:E:30:VAL:HG23	2.11	0.50
3:L:273:LEU:HD11	3:L:279:ALA:HB1	1.93	0.50
1:K:184:PHE:CD2	1:T:184:PHE:CD2	2.99	0.50
3:L:146:LEU:HD21	3:L:291:LEU:HD11	1.93	0.50
4:N:140:TYR:CD2	4:N:146:ALA:HB2	2.47	0.50
12:N:301:HEC:HBC2	12:N:301:HEC:HHD	1.93	0.50
12:D:301:HEC:HBC2	12:D:301:HEC:HHD	1.92	0.50
2:E:149:HIS:CE1	9:C:31:ASN:ND2	2.79	0.50
2:E:418:THR:HG23	2:E:419:GLY:N	2.27	0.50
6:F:38:LEU:HD12	6:F:38:LEU:O	2.11	0.50
4:N:264:LEU:HD23	9:C:60:MET:CA	2.41	0.50
8:R:43:LYS:O	8:R:49:ASN:ND2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:39:CYS:O	1:K:42:ILE:HG22	2.11	0.50
1:K:146:VAL:O	1:K:150:LEU:HD23	2.12	0.50
1:K:186:LEU:N	1:K:187:PRO:HD2	2.26	0.50
2:A:28:ASN:OD1	2:A:30:VAL:HG23	2.12	0.50
3:B:108:VAL:O	3:B:112:THR:OG1	2.28	0.50
1:T:234:PHE:CE1	4:N:261:LEU:HD23	2.47	0.50
2:A:156:GLN:OE1	9:M:37:TYR:CD2	2.64	0.50
2:A:418:THR:HG23	2:A:419:GLY:N	2.27	0.50
4:D:66:PHE:HB3	4:D:71:ILE:HD11	1.93	0.49
3:B:227:GLY:N	3:B:358:ASN:OD1	2.44	0.49
2:E:119:VAL:HG11	2:E:179:SER:OG	2.12	0.49
2:E:155:PHE:CE1	2:E:309:THR:HG21	2.47	0.49
2:E:278:ILE:HG22	2:E:278:ILE:O	2.13	0.49
1:K:234:PHE:CE1	4:D:261:LEU:HD23	2.47	0.49
1:T:212:ILE:HD12	5:P:75:ILE:HG23	1.95	0.49
5:G:81:LEU:HD21	5:G:88:LEU:HG	1.95	0.49
4:N:60:ASN:OD1	4:N:61:GLY:N	2.44	0.49
4:N:73:ARG:NH1	4:N:219:ASP:OD2	2.46	0.49
1:K:50:LEU:HD13	10:K:401:HEM:HBD1	1.94	0.49
3:B:122:ILE:O	3:B:122:ILE:HG22	2.13	0.49
1:K:178:ARG:NH2	9:C:79:PHE:O	2.46	0.48
1:K:200:ALA:O	1:K:203:VAL:HG12	2.13	0.48
1:K:231:ILE:HD11	4:D:269:LYS:HB2	1.95	0.48
10:K:401:HEM:HBB2	10:K:401:HEM:CMB	2.42	0.48
1:T:50:LEU:HD13	10:T:401:HEM:HBD1	1.95	0.48
10:K:402:HEM:HBB2	10:K:402:HEM:CHC	2.42	0.48
4:N:82:CYS:CA	12:N:301:HEC:HBB2	2.44	0.48
2:A:149:HIS:CE1	9:M:31:ASN:HD22	2.29	0.48
2:E:167:THR:CG2	9:C:31:ASN:O	2.61	0.48
2:E:255:ASN:HB3	2:E:379:VAL:HG12	1.95	0.48
4:N:146:ALA:O	4:N:150:ASN:N	2.46	0.48
1:K:70:ARG:NH1	4:D:239:ALA:O	2.36	0.48
1:T:79:ARG:NH1	10:T:401:HEM:O1A	2.47	0.48
1:T:344:VAL:O	1:T:344:VAL:CG2	2.61	0.48
4:D:57:TRP:NE1	4:D:170:ASP:OD1	2.41	0.48
1:K:184:PHE:HE1	10:K:401:HEM:HBC1	1.76	0.48
1:K:242:LEU:HD23	4:D:255:LEU:HD21	1.96	0.48
1:T:186:LEU:N	1:T:187:PRO:HD2	2.29	0.48
4:D:133:ALA:HB2	9:M:87:ALA:HB1	1.94	0.48
1:K:178:ARG:NH1	9:C:79:PHE:O	2.47	0.48
1:K:184:PHE:CE1	10:K:401:HEM:CBC	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:255:ASN:HB3	2:A:379:VAL:HG12	1.94	0.48
4:D:140:TYR:CD2	4:D:146:ALA:HB2	2.49	0.48
2:E:43:SER:OG	2:E:101:ILE:HD13	2.13	0.48
1:K:185:LEU:O	1:K:188:PHE:N	2.43	0.47
4:N:264:LEU:HD23	9:C:60:MET:N	2.29	0.47
2:A:238:ASP:HB2	6:F:21:LYS:HD2	1.96	0.47
2:E:222:GLU:OE1	2:E:222:GLU:N	2.45	0.47
4:N:57:TRP:NE1	4:N:170:ASP:OD1	2.41	0.47
5:P:56:MET:O	5:P:60:ILE:HG13	2.13	0.47
9:C:37:TYR:O	9:C:40:TYR:N	2.47	0.47
10:T:402:HEM:HBB2	10:T:402:HEM:CHC	2.44	0.47
7:Q:122:VAL:O	7:Q:126:VAL:HG13	2.14	0.47
2:A:119:VAL:HG11	2:A:179:SER:OG	2.13	0.47
1:T:118:VAL:HG11	1:T:303:LEU:HD21	1.95	0.47
9:M:175:CYS:O	9:M:179:GLY:N	2.47	0.47
1:K:52:MET:SD	9:M:79:PHE:CE2	3.08	0.47
1:T:231:ILE:HD11	4:N:269:LYS:HB2	1.97	0.47
2:A:155:PHE:CE1	2:A:309:THR:HG21	2.49	0.47
2:A:233:VAL:HG23	6:F:28:TYR:CE1	2.50	0.47
8:I:26:PHE:CD2	9:M:63:LEU:HD22	2.50	0.47
2:E:119:VAL:O	2:E:176:ASN:ND2	2.47	0.47
3:B:62:LYS:NZ	3:B:70:GLU:OE1	2.33	0.47
3:B:69:ARG:HG3	5:P:120:LEU:HD13	1.97	0.47
1:K:142:TRP:CZ3	9:C:161:CYS:HA	2.49	0.47
5:P:5:MET:HE3	5:P:9:VAL:HG23	1.96	0.47
1:T:46:SER:OG	1:T:82:HIS:ND1	2.44	0.47
1:T:346:VAL:HG11	6:O:93:VAL:HG21	1.97	0.47
4:D:82:CYS:CA	12:D:301:HEC:HBB2	2.45	0.47
6:F:33:TYR:HE2	9:M:50:ARG:HG2	1.79	0.46
3:L:37:ASN:O	3:L:42:THR:OG1	2.33	0.46
5:P:81:LEU:HD21	5:P:88:LEU:HG	1.97	0.46
1:K:212:ILE:HD12	5:G:75:ILE:HG23	1.98	0.46
3:B:31:LEU:HD22	3:B:105:LEU:CD1	2.45	0.46
7:Q:123:ASN:HA	7:Q:126:VAL:HG22	1.96	0.46
1:K:79:ARG:NH1	10:K:401:HEM:O1A	2.49	0.46
1:K:281:ILE:HG23	1:K:356:THR:HG21	1.98	0.46
2:A:277:THR:HG23	3:B:126:THR:HG21	1.96	0.46
7:H:88:GLU:HA	7:H:88:GLU:OE2	2.15	0.46
4:N:161:ILE:HG23	4:N:172:ILE:HD11	1.97	0.46
6:O:48:ASN:O	6:O:52:ARG:HG3	2.16	0.46
5:G:120:LEU:HD13	3:L:69:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:65:THR:HG22	8:R:42:ASN:OD1	2.16	0.46
5:G:66:GLU:HG2	5:G:67:LEU:N	2.31	0.46
2:E:164:THR:HG23	2:E:165:LEU:HG	1.97	0.46
3:L:31:LEU:HD22	3:L:105:LEU:CD1	2.46	0.46
1:K:346:VAL:O	1:K:349:ILE:HG12	2.15	0.46
4:D:65:THR:HG22	8:I:42:ASN:OD1	2.16	0.46
4:D:142:ASN:ND2	4:N:121:ASP:O	2.48	0.46
3:L:340:ASP:OD1	3:L:340:ASP:N	2.48	0.46
4:N:162:VAL:HG21	4:N:237:ASN:N	2.31	0.46
2:A:235:MET:O	2:A:236:ARG:C	2.55	0.46
5:G:85:HIS:O	6:F:48:ASN:ND2	2.45	0.46
3:L:53:LYS:NZ	3:L:130:GLU:OE1	2.44	0.46
4:D:120:ASP:O	4:D:122:GLU:N	2.49	0.45
4:D:215:VAL:HG22	4:D:228:MET:SD	2.56	0.45
7:H:122:VAL:O	7:H:126:VAL:HG13	2.16	0.45
3:L:88:ILE:HG21	3:L:340:ASP:HB2	1.97	0.45
1:K:134:LEU:HD21	1:K:180:PHE:CA	2.47	0.45
1:T:164:PHE:O	1:T:178:ARG:NH1	2.49	0.45
1:T:218:ARG:O	1:T:219:LEU:HD23	2.16	0.45
3:B:119:PHE:HB2	3:B:169:LEU:HD12	1.98	0.45
4:D:274:THR:OG1	4:D:275:PRO:HD3	2.15	0.45
2:E:233:VAL:O	2:E:233:VAL:HG13	2.17	0.45
4:N:271:PHE:CZ	9:C:53:THR:HG21	2.52	0.45
9:C:36:ASP:OD1	9:C:36:ASP:O	2.35	0.45
1:K:218:ARG:O	1:K:219:LEU:HD23	2.17	0.45
2:A:63:ILE:HD11	2:A:179:SER:CB	2.45	0.45
2:E:229:LEU:HD13	9:C:41:LEU:CD1	2.41	0.45
3:L:102:VAL:HG11	3:L:200:PHE:HB3	1.99	0.45
4:N:66:PHE:HB3	4:N:71:ILE:HD11	1.98	0.45
3:B:102:VAL:HG13	3:B:103:GLU:N	2.32	0.45
4:N:158:LEU:HB3	4:N:236:LEU:HD22	1.99	0.45
1:K:49:PHE:CE2	9:M:75:PHE:HB3	2.51	0.45
2:A:150:LEU:CD1	2:A:414:VAL:HG13	2.40	0.45
3:B:222:THR:HG23	3:B:223:ASN:N	2.32	0.45
1:K:184:PHE:CD1	10:K:401:HEM:CBC	3.00	0.45
2:E:149:HIS:CE1	9:C:31:ASN:CB	2.99	0.45
2:E:264:VAL:HA	2:E:354:VAL:HG21	1.99	0.45
3:L:55:THR:HG21	3:L:89:LEU:CD2	2.47	0.45
1:K:114:TRP:NE1	1:K:302:LEU:O	2.38	0.45
5:G:5:MET:HE3	5:G:9:VAL:HG23	1.97	0.45
6:F:88:GLU:HG2	6:F:89:GLU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:274:THR:OG1	4:N:275:PRO:HD3	2.17	0.45
9:M:33:GLN:O	9:M:33:GLN:HG2	2.17	0.45
2:E:80:LEU:HD12	3:L:266:LEU:HB3	2.00	0.44
3:L:54:PHE:CD2	3:L:123:VAL:HG21	2.52	0.44
1:T:116:ILE:HD12	1:T:116:ILE:H	1.82	0.44
2:E:80:LEU:CD1	3:L:266:LEU:HD22	2.47	0.44
3:B:54:PHE:HE1	3:B:123:VAL:HG11	1.79	0.44
3:L:122:ILE:O	3:L:122:ILE:HG22	2.16	0.44
3:B:102:VAL:HG11	3:B:200:PHE:HB3	2.00	0.44
7:H:123:ASN:HA	7:H:126:VAL:HG22	1.99	0.44
3:L:70:GLU:O	3:L:74:LEU:HD13	2.17	0.44
1:T:146:VAL:O	1:T:150:LEU:HD23	2.16	0.44
3:L:222:THR:HG23	3:L:223:ASN:N	2.31	0.44
1:T:265:THR:O	1:T:265:THR:HG23	2.16	0.44
3:L:55:THR:O	3:L:108:VAL:HG13	2.18	0.44
1:T:245:PHE:O	4:N:247:ARG:NH1	2.41	0.44
1:T:287:ASP:O	1:T:291:GLY:N	2.48	0.44
2:A:43:SER:OG	2:A:101:ILE:HD13	2.17	0.44
2:A:45:VAL:HG23	2:A:101:ILE:CD1	2.41	0.44
2:E:64:SER:O	2:E:90:ASN:ND2	2.51	0.44
12:D:301:HEC:CBB	12:D:301:HEC:HHC	2.48	0.44
8:I:30:PHE:O	8:I:34:VAL:HG23	2.17	0.44
2:E:51:ALA:HB2	2:E:186:HIS:CG	2.52	0.44
3:L:57:LEU:O	3:L:64:ALA:HB2	2.17	0.44
12:N:301:HEC:HHC	12:N:301:HEC:CBB	2.48	0.44
9:M:72:VAL:O	9:M:76:LEU:HD23	2.17	0.44
2:A:233:VAL:HG13	2:A:233:VAL:O	2.17	0.43
3:B:70:GLU:O	3:B:74:LEU:HD13	2.18	0.43
4:D:264:LEU:HD23	9:M:60:MET:CA	2.48	0.43
2:E:277:THR:HG23	3:L:126:THR:HG21	2.00	0.43
3:L:102:VAL:HG13	3:L:103:GLU:N	2.32	0.43
3:B:177:LYS:O	3:B:178:GLU:HB2	2.18	0.43
12:D:301:HEC:HBD1	12:D:301:HEC:HHA	1.99	0.43
2:E:229:LEU:CD1	9:C:41:LEU:CD1	2.95	0.43
1:K:142:TRP:O	1:K:146:VAL:HG23	2.18	0.43
1:T:43:GLN:NE2	1:T:82:HIS:O	2.45	0.43
1:T:200:ALA:O	1:T:203:VAL:HG12	2.18	0.43
3:B:340:ASP:OD1	3:B:340:ASP:N	2.51	0.43
3:B:348:VAL:O	3:B:349:ALA:HB3	2.18	0.43
6:F:48:ASN:O	6:F:52:ARG:HG3	2.16	0.43
7:H:88:GLU:O	7:H:91:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:VAL:HG23	2:E:101:ILE:CD1	2.41	0.43
2:E:138:VAL:HG13	2:E:144:SER:HB3	2.00	0.43
2:E:34:THR:HG22	2:E:196:ALA:HB3	1.99	0.43
2:E:168:THR:O	2:E:172:GLU:OE1	2.36	0.43
3:L:177:LYS:O	3:L:178:GLU:HB2	2.18	0.43
8:R:28:GLY:O	8:R:32:VAL:HG13	2.19	0.43
1:K:46:SER:OG	1:K:82:HIS:ND1	2.43	0.43
4:D:73:ARG:NH1	4:D:219:ASP:OD2	2.51	0.43
6:O:88:GLU:OE2	6:O:88:GLU:N	2.48	0.43
2:A:64:SER:O	2:A:90:ASN:ND2	2.52	0.43
2:E:107:LEU:C	2:E:107:LEU:HD23	2.39	0.43
3:L:98:LEU:HD22	3:L:200:PHE:CD2	2.53	0.43
4:N:142:ASN:C	4:N:142:ASN:OD1	2.57	0.43
3:L:151:PHE:O	3:L:156:GLY:HA3	2.18	0.43
3:L:227:GLY:N	3:L:358:ASN:OD1	2.51	0.43
5:P:100:ASP:OD1	5:P:100:ASP:N	2.52	0.43
3:L:255:GLU:HG2	3:L:283:LEU:HD23	2.01	0.43
4:N:276:ILE:CG2	5:P:83:LEU:HD11	2.49	0.43
1:K:164:PHE:O	1:K:178:ARG:NH1	2.52	0.43
2:A:80:LEU:CD1	3:B:266:LEU:HD22	2.49	0.43
4:D:158:LEU:HB3	4:D:236:LEU:HD22	1.99	0.43
3:L:109:VAL:CG1	3:L:209:LEU:HD11	2.48	0.43
9:C:37:TYR:HD1	9:C:40:TYR:HD2	1.66	0.43
2:E:375:LYS:O	2:E:379:VAL:HG22	2.19	0.43
3:L:330:GLU:HG3	3:L:347:VAL:HG21	1.99	0.43
2:A:318:ILE:HG22	2:A:320:ASP:H	1.84	0.42
5:G:121:ASP:OD2	5:G:121:ASP:C	2.57	0.42
4:N:120:ASP:O	4:N:122:GLU:N	2.51	0.42
2:A:264:VAL:HA	2:A:354:VAL:HG21	2.00	0.42
1:K:245:PHE:O	4:D:247:ARG:NH1	2.42	0.42
1:K:265:THR:HG23	1:K:265:THR:O	2.17	0.42
1:K:287:ASP:O	1:K:291:GLY:N	2.48	0.42
1:K:328:LEU:HD22	1:K:358:TYR:CZ	2.53	0.42
2:E:149:HIS:CE1	9:C:31:ASN:HB2	2.54	0.42
4:N:162:VAL:HG21	4:N:237:ASN:HA	2.02	0.42
8:R:22:GLY:HA3	9:C:62:LEU:HD13	2.00	0.42
2:A:193:VAL:HG22	2:A:194:ILE:N	2.34	0.42
2:A:222:GLU:OE1	2:A:222:GLU:N	2.47	0.42
4:N:67:ASP:O	4:N:70:SER:N	2.52	0.42
7:Q:87:HIS:HA	7:Q:90:ILE:HG12	2.01	0.42
8:R:36:LYS:O	8:R:40:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:108:GLN:HA	1:T:111:VAL:HG23	2.01	0.42
1:T:328:LEU:HD22	1:T:358:TYR:CZ	2.55	0.42
3:B:98:LEU:HD22	3:B:200:PHE:CD2	2.54	0.42
8:I:43:LYS:O	8:I:49:ASN:ND2	2.40	0.42
4:N:162:VAL:HG21	4:N:236:LEU:C	2.40	0.42
1:K:185:LEU:HD21	1:K:189:ILE:CD1	2.49	0.42
1:T:122:ILE:O	1:T:125:MET:HG2	2.19	0.42
3:B:246:VAL:HG22	3:B:290:GLY:C	2.39	0.42
4:N:281:PHE:CE1	6:O:27:GLN:HG2	2.55	0.42
3:B:117:HIS:CG	5:P:62:ARG:NH1	2.88	0.42
3:B:283:LEU:O	3:B:285:LYS:NZ	2.47	0.42
6:O:73:ARG:HG3	6:O:73:ARG:HH11	1.84	0.42
7:Q:88:GLU:O	7:Q:91:GLU:HG3	2.19	0.42
1:T:184:PHE:CE1	10:T:401:HEM:CBC	3.00	0.42
3:B:53:LYS:HB2	3:B:123:VAL:HG13	2.00	0.42
2:E:325:ASP:OD2	2:E:326:ASP:N	2.52	0.42
2:A:51:ALA:HB2	2:A:186:HIS:CG	2.54	0.42
3:B:37:ASN:OD1	3:B:184:ASN:ND2	2.45	0.42
3:B:35:ILE:O	3:B:86:ALA:HB1	2.20	0.42
3:B:98:LEU:N	3:B:99:PRO:HD2	2.35	0.42
4:N:261:LEU:HD21	9:C:64:SER:HA	2.01	0.42
4:N:264:LEU:HD22	9:C:63:LEU:HD12	2.02	0.42
3:L:57:LEU:O	3:L:58:ASN:CG	2.58	0.41
3:L:260:ALA:HB2	3:L:322:LEU:HD12	2.01	0.41
1:K:14:ASN:OD1	1:K:19:ASP:OD2	2.38	0.41
1:K:18:ILE:HG22	2:A:429:ARG:HH22	1.85	0.41
1:K:297:GLY:O	1:K:301:ILE:HG12	2.20	0.41
4:D:67:ASP:O	4:D:70:SER:N	2.53	0.41
4:D:276:ILE:CG2	5:G:83:LEU:HD11	2.50	0.41
4:N:271:PHE:CE2	9:C:53:THR:OG1	2.64	0.41
1:K:246:TYR:OH	4:D:252:LEU:N	2.53	0.41
1:T:246:TYR:CE2	4:N:255:LEU:HD11	2.56	0.41
2:A:80:LEU:HD23	2:A:80:LEU:O	2.20	0.41
3:L:124:LEU:HB2	3:L:125:PRO:HD3	2.01	0.41
3:L:348:VAL:O	3:L:349:ALA:HB3	2.19	0.41
2:A:80:LEU:HD12	3:B:266:LEU:HB3	2.01	0.41
3:B:52:SER:O	3:B:55:THR:HG22	2.20	0.41
5:P:51:GLU:OE2	5:P:71:ARG:NH2	2.54	0.41
1:K:99:LYS:NZ	10:K:402:HEM:O2A	2.46	0.41
1:K:201:LEU:HD12	10:K:402:HEM:CHA	2.51	0.41
6:O:62:ILE:HB	6:O:63:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:ILE:O	1:K:125:MET:HG2	2.20	0.41
1:K:380:ILE:HG23	5:G:29:ALA:CB	2.50	0.41
1:T:49:PHE:CE2	9:C:75:PHE:HB3	2.56	0.41
2:A:34:THR:HG22	2:A:196:ALA:HB3	2.01	0.41
2:A:124:LEU:HD12	2:A:176:ASN:OD1	2.21	0.41
4:D:217:TYR:OH	4:D:231:ASP:OD2	2.29	0.41
2:E:38:PRO:O	2:E:39:ALA:HB3	2.21	0.41
2:E:422:GLU:OE2	6:O:17:LEU:HB2	2.20	0.41
3:L:98:LEU:N	3:L:99:PRO:HD2	2.35	0.41
6:O:62:ILE:O	6:O:65:VAL:HG12	2.20	0.41
6:O:92:ARG:HG2	6:O:92:ARG:HH11	1.85	0.41
1:K:224:TYR:CE2	2:A:426:ASP:OD1	2.74	0.41
2:A:38:PRO:O	2:A:39:ALA:HB3	2.21	0.41
2:A:250:HIS:NE2	2:A:309:THR:HG23	2.36	0.41
4:D:146:ALA:O	4:D:150:ASN:N	2.51	0.41
1:K:162:VAL:HB	1:K:163:PRO:HD3	2.03	0.41
1:T:39:CYS:O	1:T:42:ILE:HG22	2.21	0.41
1:T:65:VAL:O	1:T:69:MET:HG2	2.21	0.41
5:G:100:ASP:N	5:G:100:ASP:OD1	2.50	0.41
2:E:80:LEU:HD12	3:L:266:LEU:HD22	2.02	0.41
1:T:162:VAL:HB	1:T:163:PRO:HD3	2.03	0.41
1:T:201:LEU:HD12	10:T:402:HEM:CHA	2.51	0.41
3:B:31:LEU:HD22	3:B:105:LEU:HD12	2.03	0.41
3:B:169:LEU:HD23	3:B:169:LEU:C	2.41	0.41
3:B:255:GLU:HG2	3:B:283:LEU:HD23	2.03	0.41
3:B:330:GLU:HG3	3:B:347:VAL:HG21	2.02	0.41
4:D:262:TYR:O	4:D:266:ILE:HG12	2.21	0.41
7:H:87:HIS:HA	7:H:90:ILE:HG12	2.01	0.41
3:L:66:ARG:NH1	3:L:66:ARG:HG3	2.36	0.41
3:L:142:GLY:HA3	3:L:241:LEU:HD13	2.03	0.41
3:L:326:VAL:CG2	3:L:349:ALA:HB2	2.51	0.41
4:N:262:TYR:O	4:N:266:ILE:HG12	2.20	0.41
3:B:260:ALA:HB2	3:B:322:LEU:HD12	2.02	0.41
4:D:59:HIS:HB3	4:D:66:PHE:HA	2.02	0.41
4:D:276:ILE:HG21	5:G:83:LEU:HD11	2.03	0.41
6:F:79:GLU:O	6:F:83:THR:HG23	2.20	0.41
1:K:9:TYR:OH	1:T:200:ALA:HB2	2.20	0.40
1:T:79:ARG:NH2	10:T:401:HEM:O1A	2.55	0.40
2:A:54:ARG:HE	2:A:160:LEU:HD13	1.86	0.40
2:A:107:LEU:HD23	2:A:108:ILE:N	2.36	0.40
3:B:151:PHE:O	3:B:156:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:379:VAL:HG23	2:E:381:HIS:O	2.21	0.40
9:C:175:CYS:O	9:C:179:GLY:N	2.54	0.40
1:K:203:VAL:HG13	1:K:204:HIS:N	2.35	0.40
1:T:246:TYR:OH	4:N:252:LEU:N	2.54	0.40
2:A:379:VAL:HG23	2:A:381:HIS:O	2.22	0.40
4:D:162:VAL:HG21	4:D:237:ASN:N	2.36	0.40
6:F:62:ILE:HB	6:F:63:PRO:HD3	2.03	0.40
3:B:254:TYR:CE1	3:B:352:ALA:HB1	2.56	0.40
4:N:59:HIS:HB3	4:N:66:PHE:HA	2.02	0.40
12:N:301:HEC:HHA	12:N:301:HEC:HBD1	2.02	0.40
10:K:401:HEM:HBA2	10:K:401:HEM:HHA	2.03	0.40
1:T:158:GLY:HA2	1:T:161:ILE:HG22	2.03	0.40
2:A:107:LEU:HD23	2:A:107:LEU:C	2.41	0.40
2:A:283:SER:N	2:A:284:PRO:CD	2.85	0.40
4:D:80:GLU:OE1	4:D:215:VAL:HG12	2.21	0.40
4:D:175:LEU:HD12	4:D:196:ASN:ND2	2.37	0.40
2:E:193:VAL:HG22	2:E:194:ILE:N	2.36	0.40
3:L:98:LEU:C	3:L:98:LEU:HD23	2.41	0.40
1:K:178:ARG:HD3	9:C:79:PHE:CD1	2.56	0.40
3:B:66:ARG:HA	5:P:120:LEU:HD11	2.04	0.40
3:B:163:GLU:OE2	3:B:163:GLU:HA	2.21	0.40
3:B:177:LYS:C	3:B:179:GLN:H	2.25	0.40
4:N:94:ARG:HB3	4:N:94:ARG:CZ	2.51	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	K	382/387 (99%)	367 (96%)	15 (4%)	0	100 100
1	T	382/387 (99%)	368 (96%)	14 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	415/439 (94%)	401 (97%)	14 (3%)	0	100	100
2	E	415/439 (94%)	401 (97%)	14 (3%)	0	100	100
3	B	362/374 (97%)	345 (95%)	17 (5%)	0	100	100
3	L	362/374 (97%)	342 (94%)	20 (6%)	0	100	100
4	D	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
4	N	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
5	G	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
5	P	120/127 (94%)	119 (99%)	1 (1%)	0	100	100
6	F	86/95 (90%)	83 (96%)	3 (4%)	0	100	100
6	O	86/95 (90%)	84 (98%)	2 (2%)	0	100	100
7	H	70/135 (52%)	70 (100%)	0	0	100	100
7	Q	70/135 (52%)	70 (100%)	0	0	100	100
8	I	36/65 (55%)	36 (100%)	0	0	100	100
8	R	36/65 (55%)	36 (100%)	0	0	100	100
9	C	179/213 (84%)	170 (95%)	9 (5%)	0	100	100
9	M	179/213 (84%)	171 (96%)	8 (4%)	0	100	100
All	All	3782/4246 (89%)	3649 (96%)	133 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	332/338 (98%)	329 (99%)	3 (1%)	78	87
1	T	332/338 (98%)	329 (99%)	3 (1%)	78	87
2	A	344/365 (94%)	344 (100%)	0	100	100
2	E	344/365 (94%)	343 (100%)	1 (0%)	92	96
3	B	295/307 (96%)	295 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	295/307 (96%)	295 (100%)	0	100	100
4	D	192/237 (81%)	191 (100%)	1 (0%)	88	93
4	N	192/237 (81%)	192 (100%)	0	100	100
5	G	106/110 (96%)	106 (100%)	0	100	100
5	P	106/110 (96%)	106 (100%)	0	100	100
6	F	72/80 (90%)	72 (100%)	0	100	100
6	O	72/80 (90%)	72 (100%)	0	100	100
7	H	62/128 (48%)	62 (100%)	0	100	100
7	Q	62/128 (48%)	62 (100%)	0	100	100
8	I	29/53 (55%)	29 (100%)	0	100	100
8	R	29/53 (55%)	29 (100%)	0	100	100
9	C	48/176 (27%)	48 (100%)	0	100	100
9	M	48/176 (27%)	47 (98%)	1 (2%)	53	75
All	All	2960/3588 (82%)	2951 (100%)	9 (0%)	92	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	79	ARG
1	K	99	LYS
1	K	383	GLN
1	T	79	ARG
1	T	99	LYS
1	T	383	GLN
4	D	237	ASN
2	E	291	GLN
9	M	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	173	ASN
1	T	67	HIS
1	T	173	ASN
2	A	149	HIS
2	A	291	GLN

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Mol	Chain	Res	Type
4	N	237	ASN
8	R	27	GLN
9	C	31	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	HEC	D	301	4	32,50,50	2.26	4 (12%)	24,82,82	1.38	2 (8%)
13	FES	M	301	9	0,4,4	-	-	-		
11	ZL5	K	403	-	25,31,31	4.64	11 (44%)	30,47,47	1.55	5 (16%)
10	HEM	T	402	1	41,50,50	1.54	3 (7%)	45,82,82	1.35	7 (15%)
11	ZL5	T	403	-	25,31,31	4.64	11 (44%)	30,47,47	1.54	5 (16%)
12	HEC	N	301	4	32,50,50	2.27	4 (12%)	24,82,82	1.38	2 (8%)
13	FES	C	301	9	0,4,4	-	-	-		
10	HEM	T	401	1	41,50,50	1.45	3 (7%)	45,82,82	1.27	2 (4%)
10	HEM	K	402	1	41,50,50	1.53	3 (7%)	45,82,82	1.35	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEM	K	401	1	41,50,50	1.45	3 (7%)	45,82,82	1.26	5 (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
12	HEC	D	301	4	-	2/10/54/54	-
13	FES	M	301	9	-	-	0/1/1/1
11	ZL5	K	403	-	-	2/12/14/14	0/4/4/4
10	HEM	T	402	1	-	4/12/54/54	-
11	ZL5	T	403	-	-	2/12/14/14	0/4/4/4
12	HEC	N	301	4	-	2/10/54/54	-
13	FES	C	301	9	-	-	0/1/1/1
10	HEM	T	401	1	-	3/12/54/54	-
10	HEM	K	402	1	-	1/12/54/54	-
10	HEM	K	401	1	-	5/12/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	403	ZL5	C07-N19	-13.62	1.23	1.35
11	K	403	ZL5	C07-N19	-13.62	1.23	1.35
11	T	403	ZL5	C08-C17	10.04	1.53	1.39
11	K	403	ZL5	C08-C17	10.03	1.53	1.39
11	T	403	ZL5	C09-C10	8.14	1.52	1.39
11	K	403	ZL5	C09-C10	8.06	1.52	1.39
11	K	403	ZL5	C16-C15	7.76	1.52	1.38
11	T	403	ZL5	C16-C15	7.68	1.52	1.38
12	N	301	HEC	C2B-C3B	-6.97	1.33	1.40
12	D	301	HEC	C2B-C3B	-6.82	1.33	1.40
12	D	301	HEC	C3C-C2C	-6.55	1.33	1.40
12	N	301	HEC	C3C-C2C	-6.49	1.34	1.40
10	K	402	HEM	C3C-C2C	-5.07	1.33	1.40
10	T	402	HEM	C3C-C2C	-5.02	1.33	1.40
11	K	403	ZL5	C09-C08	-4.75	1.31	1.39
11	K	403	ZL5	C15-C10	-4.73	1.31	1.39
11	T	403	ZL5	C09-C08	-4.68	1.32	1.39
11	T	403	ZL5	C15-C10	-4.67	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	401	HEM	C3C-C2C	-4.49	1.34	1.40
11	K	403	ZL5	N19-N20	-4.44	1.32	1.37
10	T	401	HEM	C3C-C2C	-4.43	1.34	1.40
11	T	403	ZL5	N19-N20	-4.27	1.32	1.37
12	N	301	HEC	CBB-CAB	-4.25	1.33	1.49
12	D	301	HEC	CBB-CAB	-4.19	1.33	1.49
12	D	301	HEC	CBC-CAC	-4.09	1.34	1.49
12	N	301	HEC	CBC-CAC	-4.07	1.34	1.49
11	K	403	ZL5	C06-C28	3.71	1.48	1.41
11	T	403	ZL5	C06-C28	3.67	1.48	1.41
10	T	402	HEM	C3C-CAC	3.54	1.55	1.47
11	T	403	ZL5	C22-N23	3.49	1.36	1.33
10	K	402	HEM	C3C-CAC	3.48	1.54	1.47
11	K	403	ZL5	C22-N23	3.45	1.36	1.33
11	T	403	ZL5	C08-C07	3.41	1.53	1.49
10	T	401	HEM	C3C-CAC	3.33	1.54	1.47
11	K	403	ZL5	C08-C07	3.29	1.53	1.49
10	K	401	HEM	C3C-CAC	3.13	1.54	1.47
11	K	403	ZL5	C16-C17	-2.85	1.31	1.37
11	T	403	ZL5	C16-C17	-2.85	1.31	1.37
10	K	402	HEM	CAB-C3B	2.82	1.55	1.47
10	T	402	HEM	CAB-C3B	2.80	1.55	1.47
10	T	401	HEM	CAB-C3B	2.78	1.55	1.47
10	K	401	HEM	CAB-C3B	2.76	1.54	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	403	ZL5	C22-N23-N24	4.19	108.56	104.33
11	K	403	ZL5	C22-N23-N24	4.18	108.55	104.33
10	K	402	HEM	C4D-ND-C1D	2.92	108.09	105.07
10	T	402	HEM	C4D-ND-C1D	2.83	108.00	105.07
11	K	403	ZL5	C26-N25-N24	2.82	126.19	122.66
11	T	403	ZL5	C26-N25-N24	2.78	126.15	122.66
10	T	402	HEM	C1B-NB-C4B	2.67	107.83	105.07
10	K	402	HEM	C1B-NB-C4B	2.64	107.81	105.07
10	T	401	HEM	C4D-ND-C1D	2.63	107.79	105.07
11	K	403	ZL5	C16-C17-C08	-2.57	120.16	123.30
10	T	402	HEM	CHC-C4B-C3B	2.54	128.46	124.57
10	T	402	HEM	C3B-C2B-C1B	2.51	108.35	106.49
11	T	403	ZL5	C16-C17-C08	-2.50	120.25	123.30
11	K	403	ZL5	C09-C08-C17	2.46	119.58	116.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	401	HEM	C4D-ND-C1D	2.46	107.61	105.07
10	K	402	HEM	C3B-C2B-C1B	2.45	108.30	106.49
11	T	403	ZL5	C09-C08-C17	2.38	119.47	116.15
10	K	402	HEM	CBD-CAD-C3D	-2.32	106.17	112.63
12	D	301	HEC	CMC-C2C-C1C	-2.31	124.91	128.46
10	K	402	HEM	CHC-C4B-C3B	2.29	128.07	124.57
12	N	301	HEC	CMB-C2B-C1B	-2.28	124.96	128.46
12	D	301	HEC	CMB-C2B-C1B	-2.28	124.97	128.46
12	N	301	HEC	CMC-C2C-C1C	-2.21	125.06	128.46
10	K	401	HEM	C2C-C3C-C4C	2.18	108.42	106.90
11	K	403	ZL5	C08-C07-N19	-2.16	117.08	120.78
11	T	403	ZL5	C08-C07-N19	-2.15	117.10	120.78
10	K	402	HEM	CBA-CAA-C2A	-2.14	108.97	112.62
10	T	401	HEM	C1B-NB-C4B	2.13	107.28	105.07
10	K	402	HEM	C3D-C4D-ND	-2.11	107.81	110.17
10	T	402	HEM	CBD-CAD-C3D	-2.11	106.78	112.63
10	K	401	HEM	C1B-NB-C4B	2.10	107.25	105.07
10	T	402	HEM	CBA-CAA-C2A	-2.09	109.06	112.62
10	K	401	HEM	CMC-C2C-C3C	2.08	128.56	124.68
10	T	402	HEM	C3D-C4D-ND	-2.07	107.86	110.17
10	K	401	HEM	C4C-CHD-C1D	2.02	125.22	122.56

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	K	401	HEM	C3D-CAD-CBD-CGD
10	T	401	HEM	C3D-CAD-CBD-CGD
10	K	401	HEM	C2D-C3D-CAD-CBD
10	T	401	HEM	C2D-C3D-CAD-CBD
10	K	401	HEM	C4D-C3D-CAD-CBD
10	T	401	HEM	C4D-C3D-CAD-CBD
10	K	402	HEM	C4B-C3B-CAB-CBB
10	T	402	HEM	C4B-C3B-CAB-CBB
11	K	403	ZL5	N20-C21-C22-N23
11	K	403	ZL5	N20-C21-C22-N27
11	T	403	ZL5	N20-C21-C22-N23
11	T	403	ZL5	N20-C21-C22-N27
10	K	401	HEM	C1A-C2A-CAA-CBA
10	T	402	HEM	C2A-CAA-CBA-CGA
12	D	301	HEC	CAA-CBA-CGA-O2A
10	T	402	HEM	CAA-CBA-CGA-O1A

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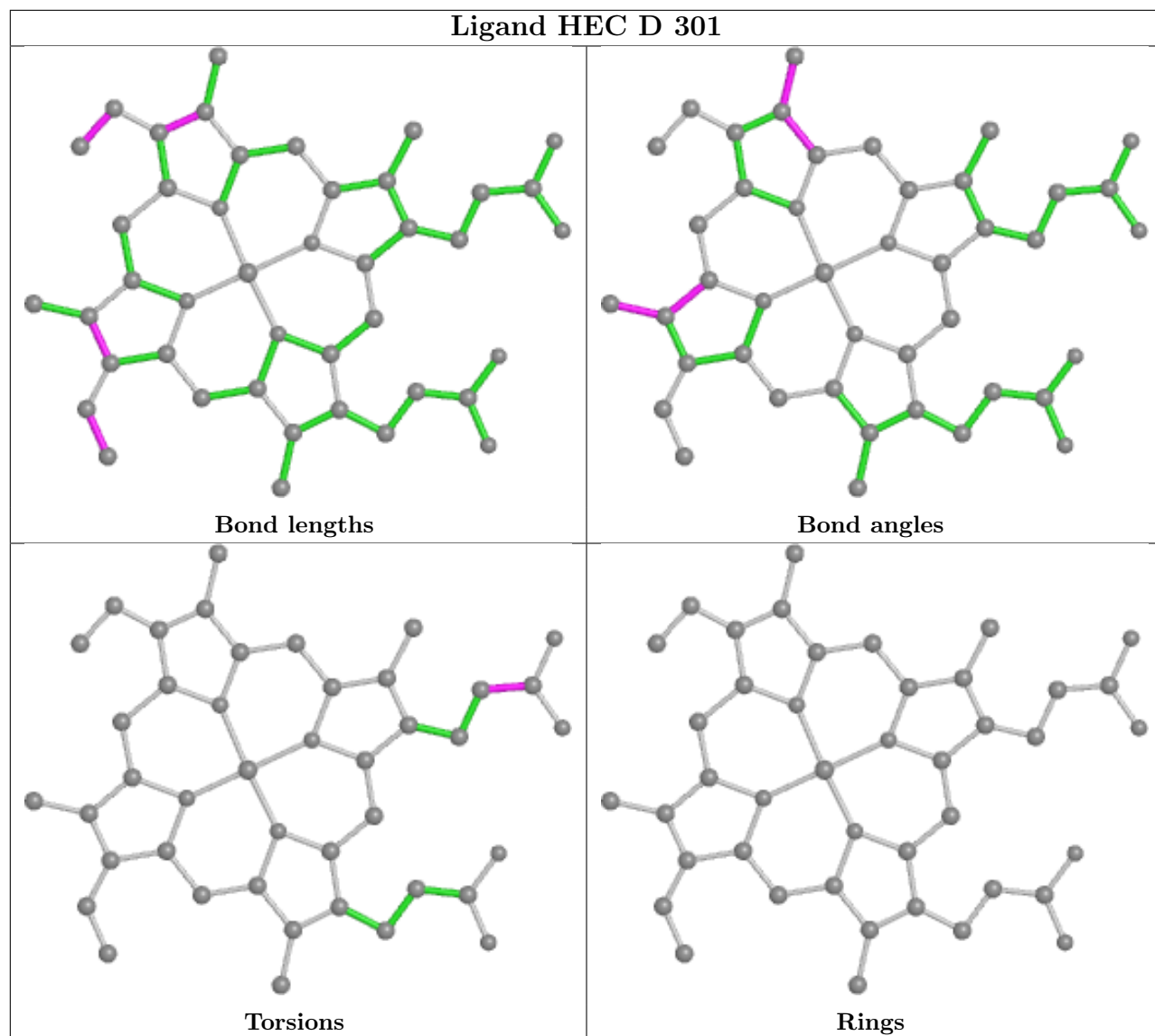
Mol	Chain	Res	Type	Atoms
12	D	301	HEC	CAA-CBA-CGA-O1A
12	N	301	HEC	CAA-CBA-CGA-O2A
10	T	402	HEM	CAA-CBA-CGA-O2A
12	N	301	HEC	CAA-CBA-CGA-O1A
10	K	401	HEM	CAD-CBD-CGD-O2D

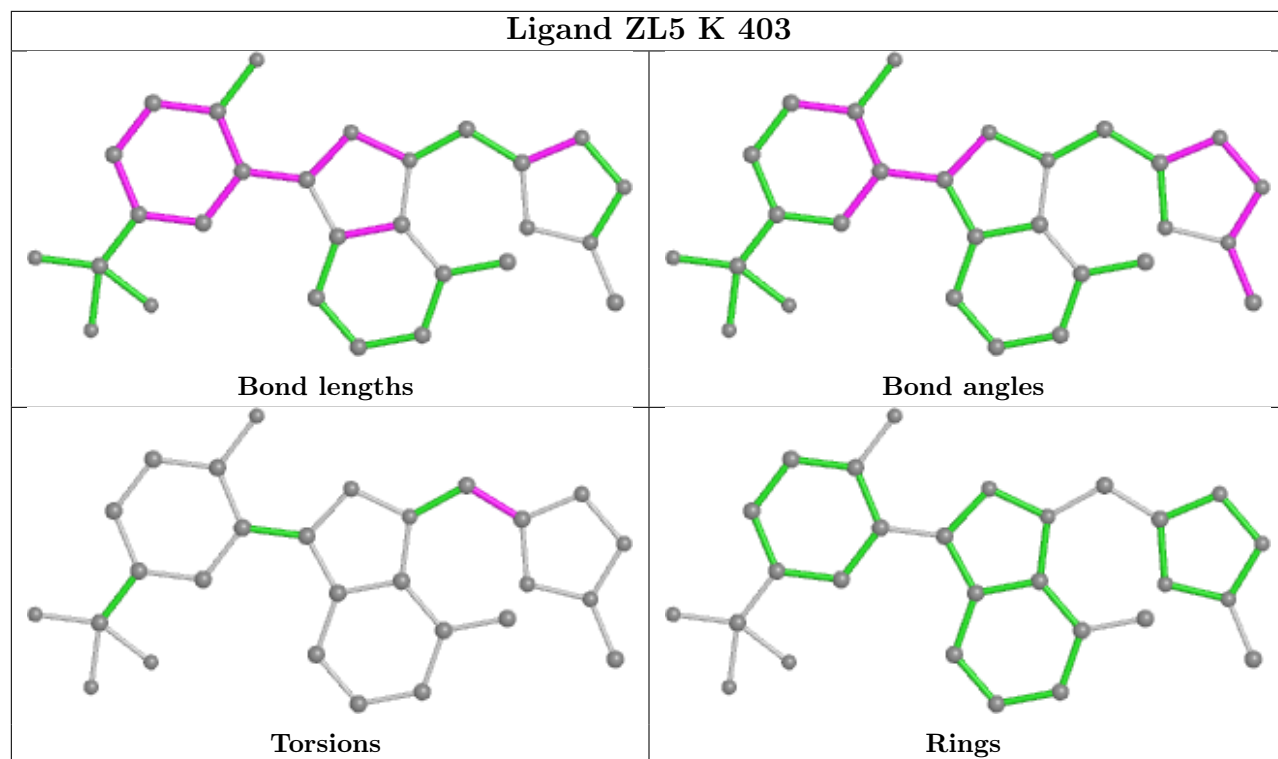
There are no ring outliers.

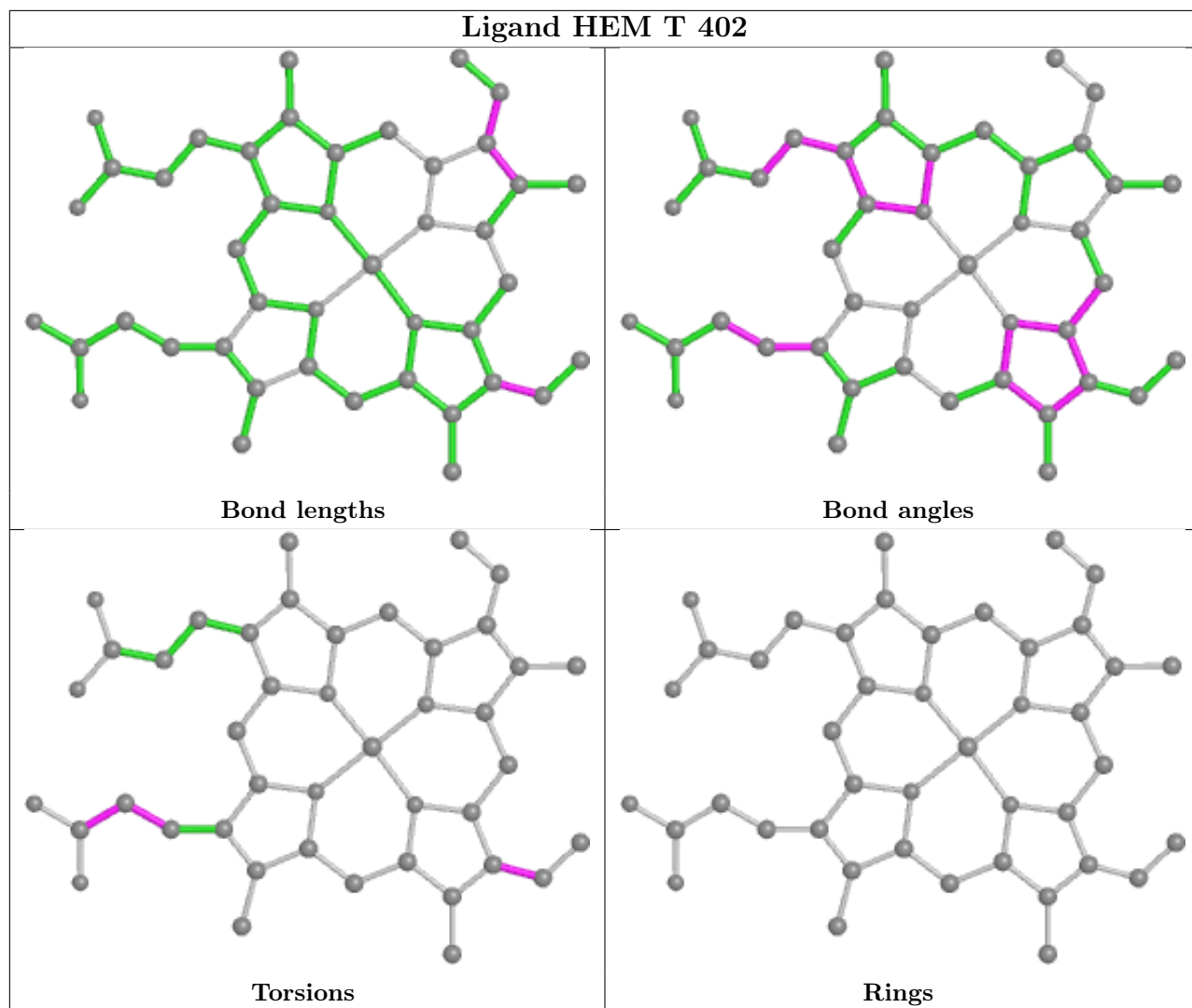
8 monomers are involved in 61 short contacts:

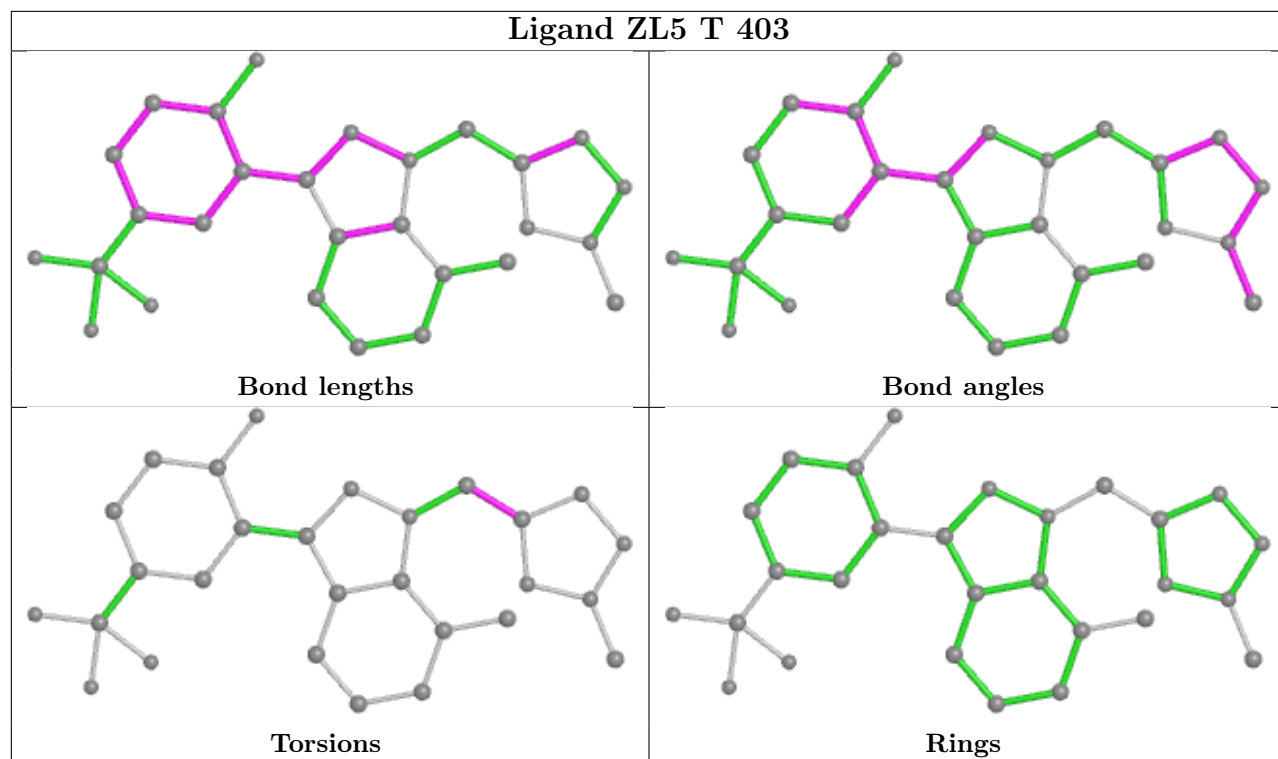
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	301	HEC	10	0
13	M	301	FES	4	0
10	T	402	HEM	5	0
12	N	301	HEC	10	0
13	C	301	FES	1	0
10	T	401	HEM	12	0
10	K	402	HEM	6	0
10	K	401	HEM	13	0

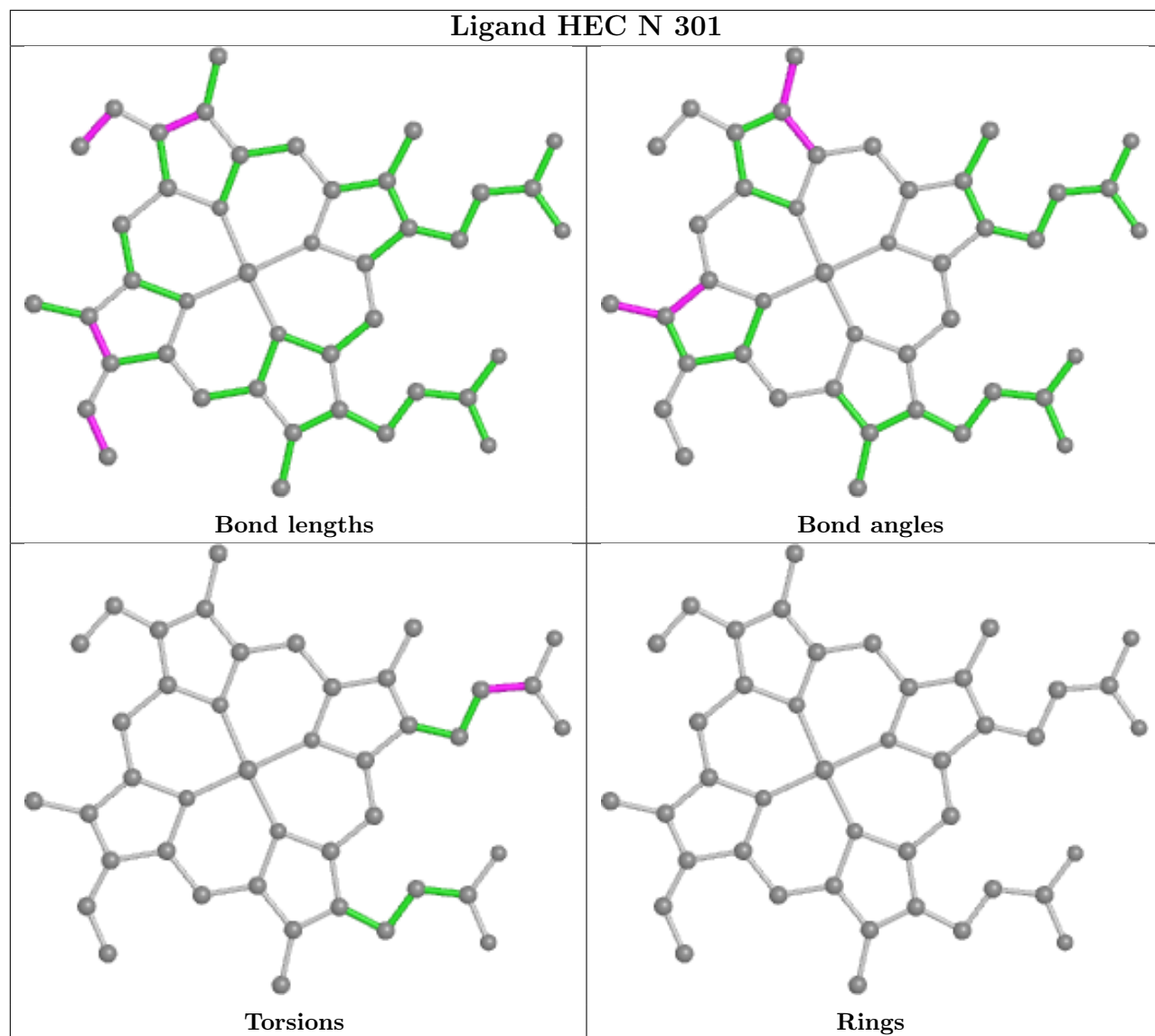
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

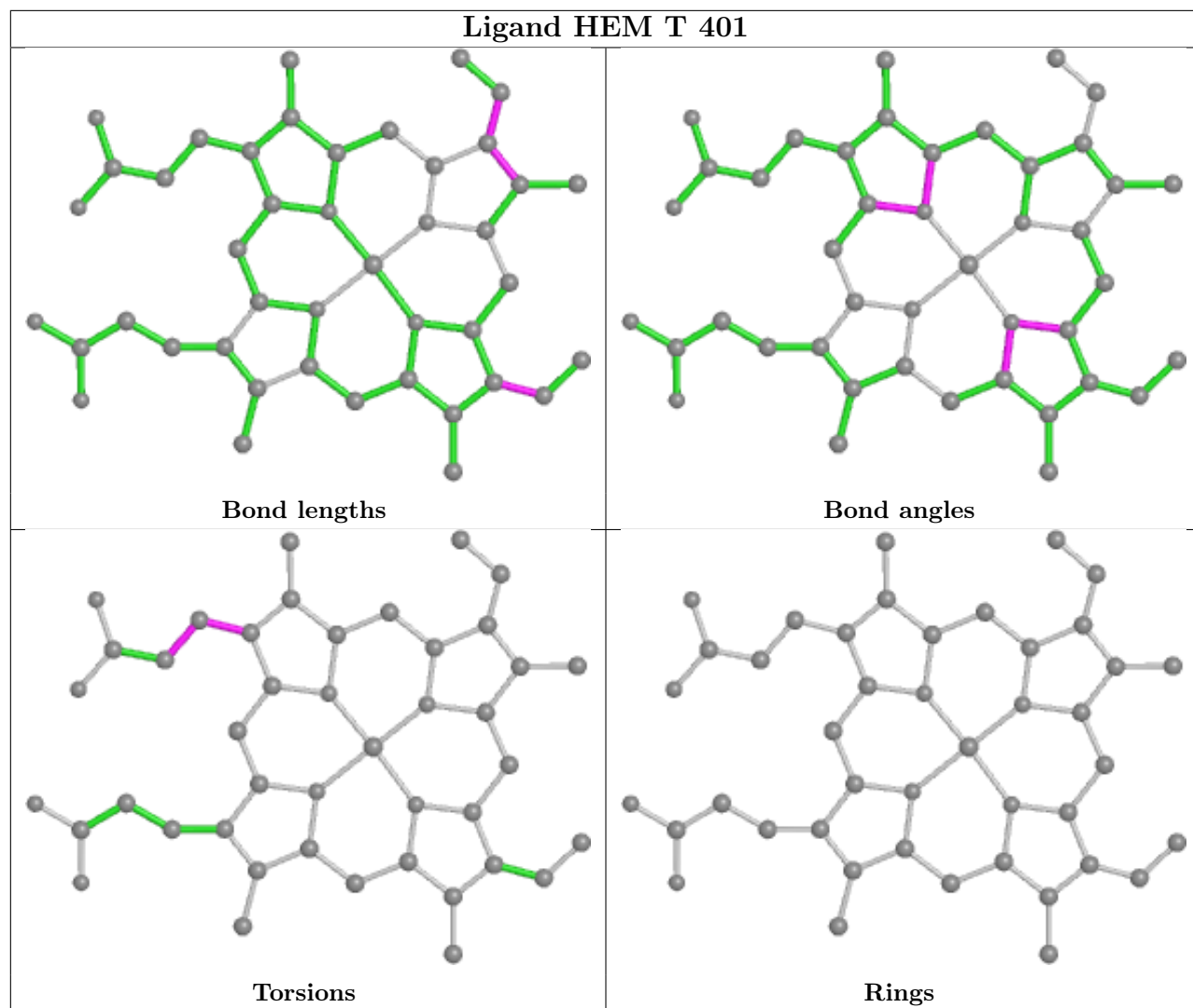


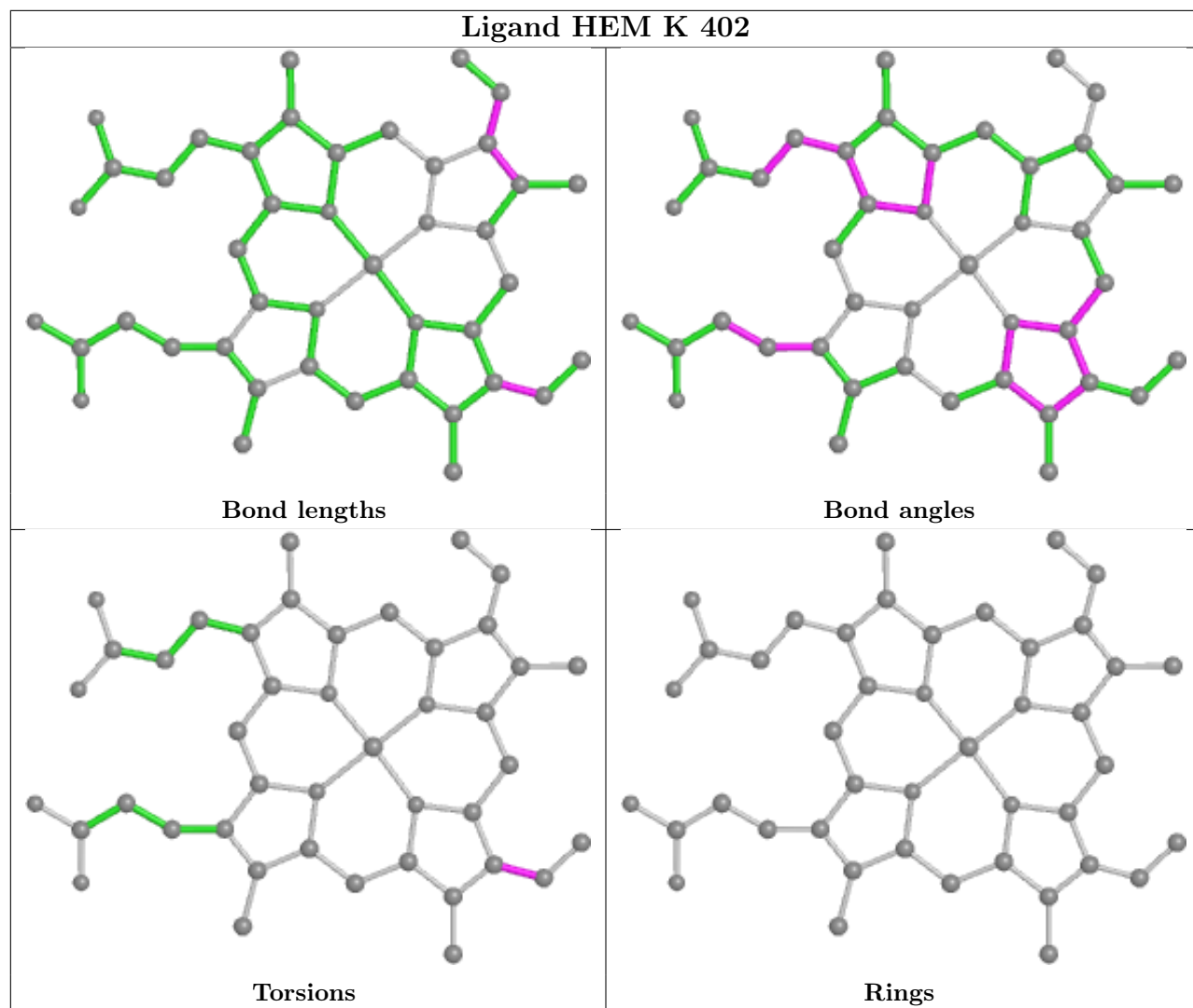


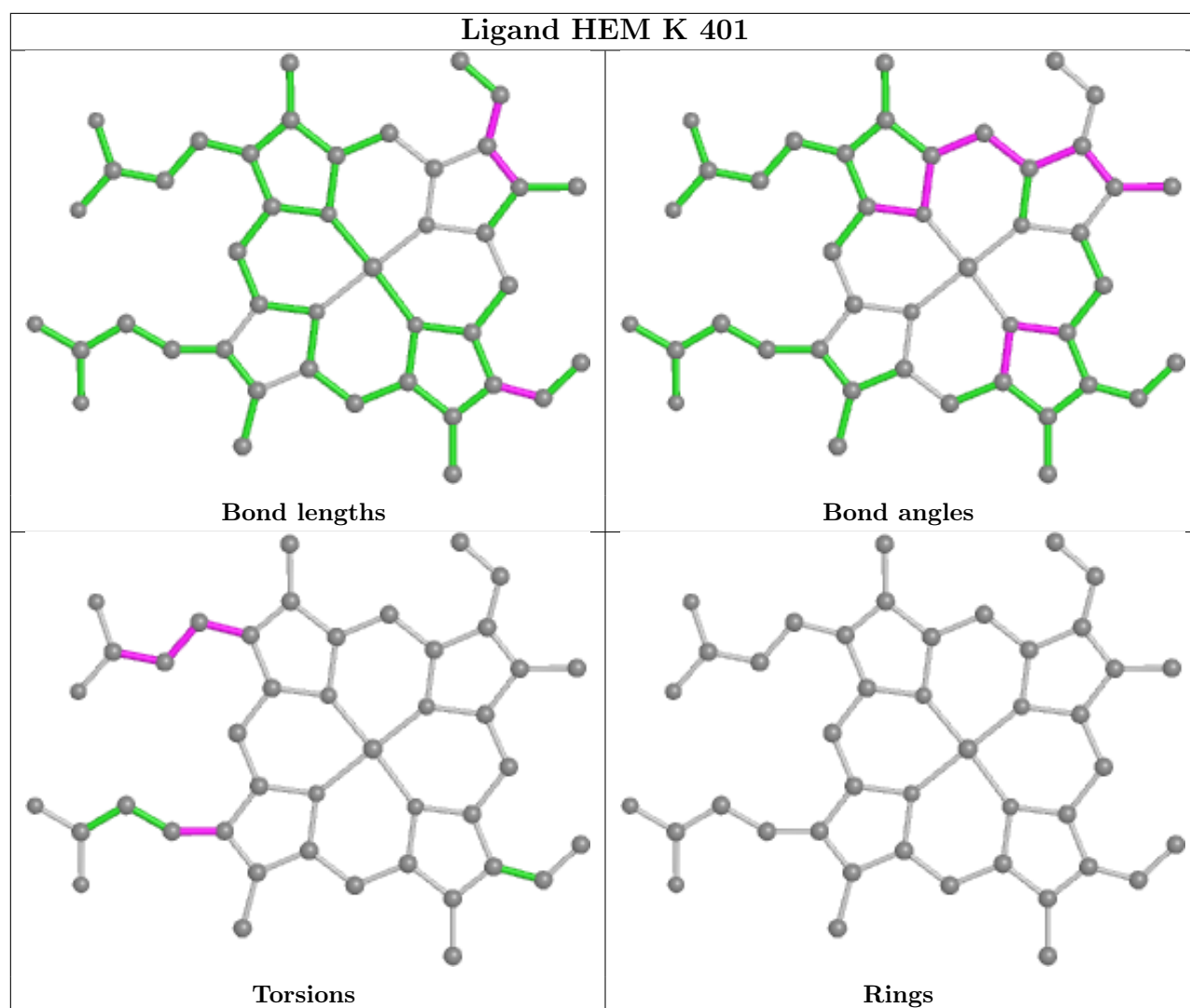












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

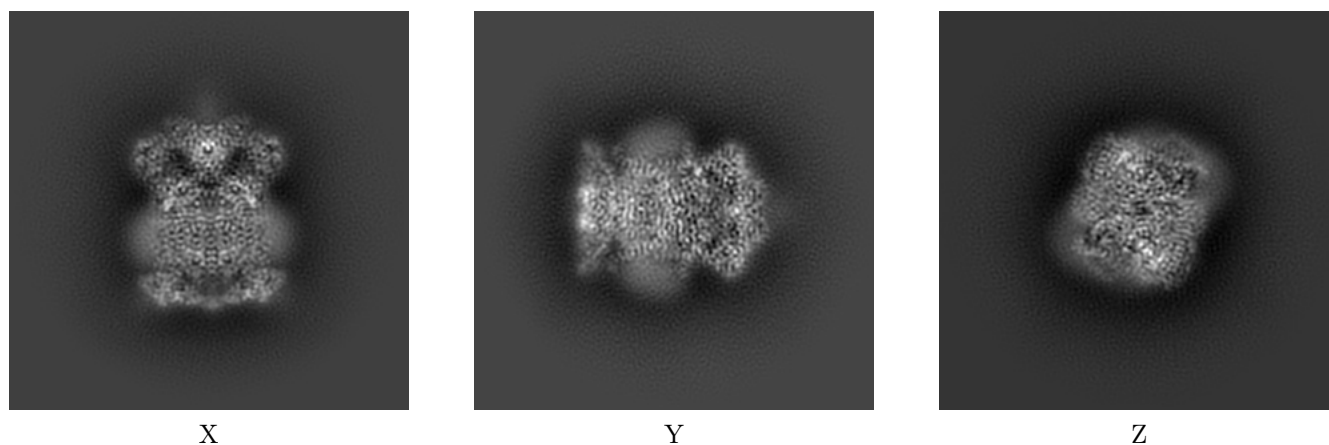
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24486. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

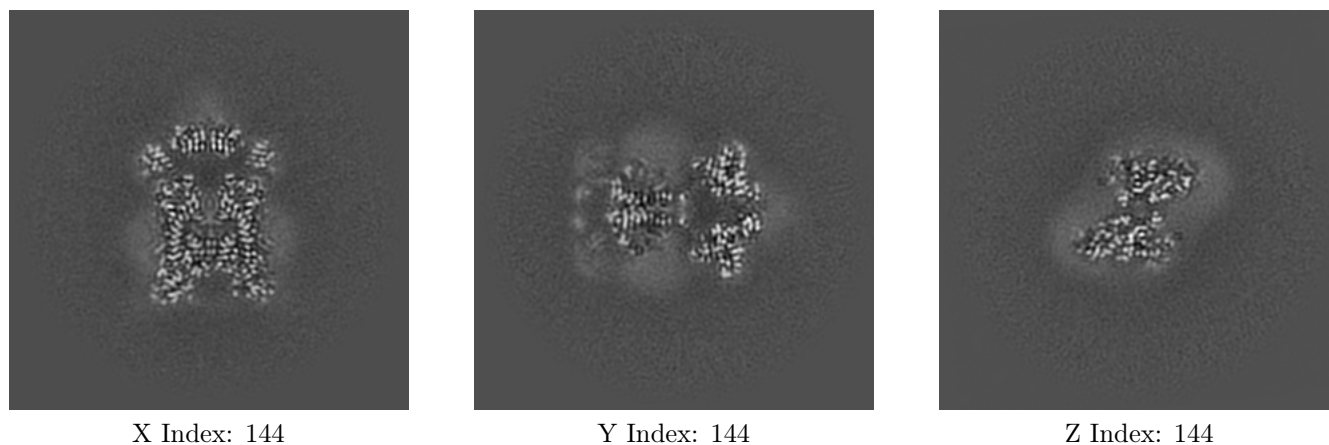
6.1.1 Primary map



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

6.2 Central slices [i](#)

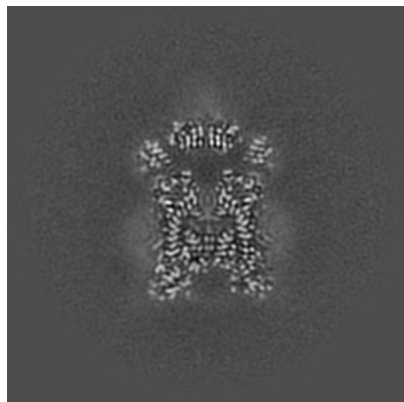
6.2.1 Primary map



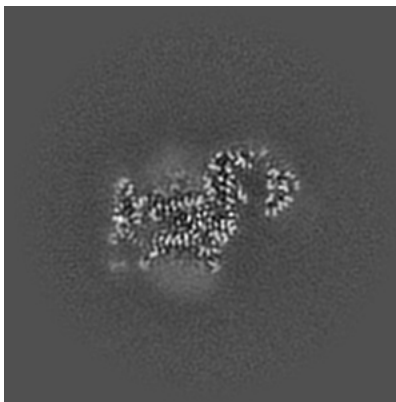
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

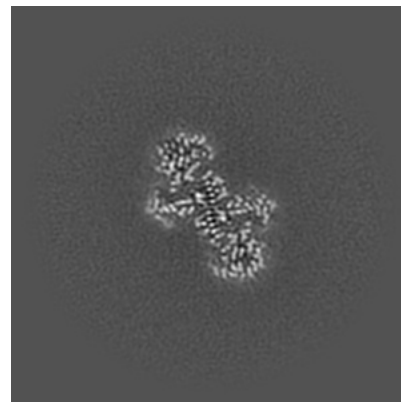
6.3.1 Primary map



X Index: 144



Y Index: 122

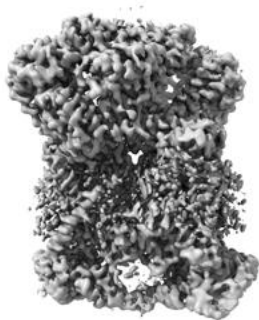


Z Index: 191

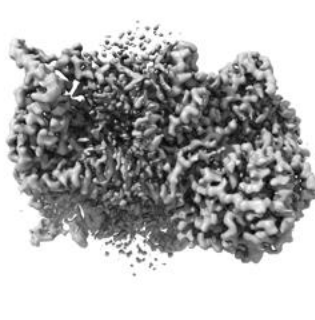
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

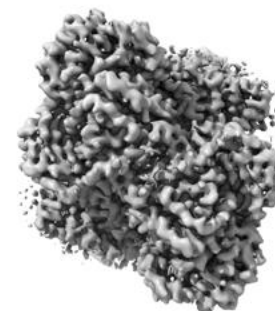
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

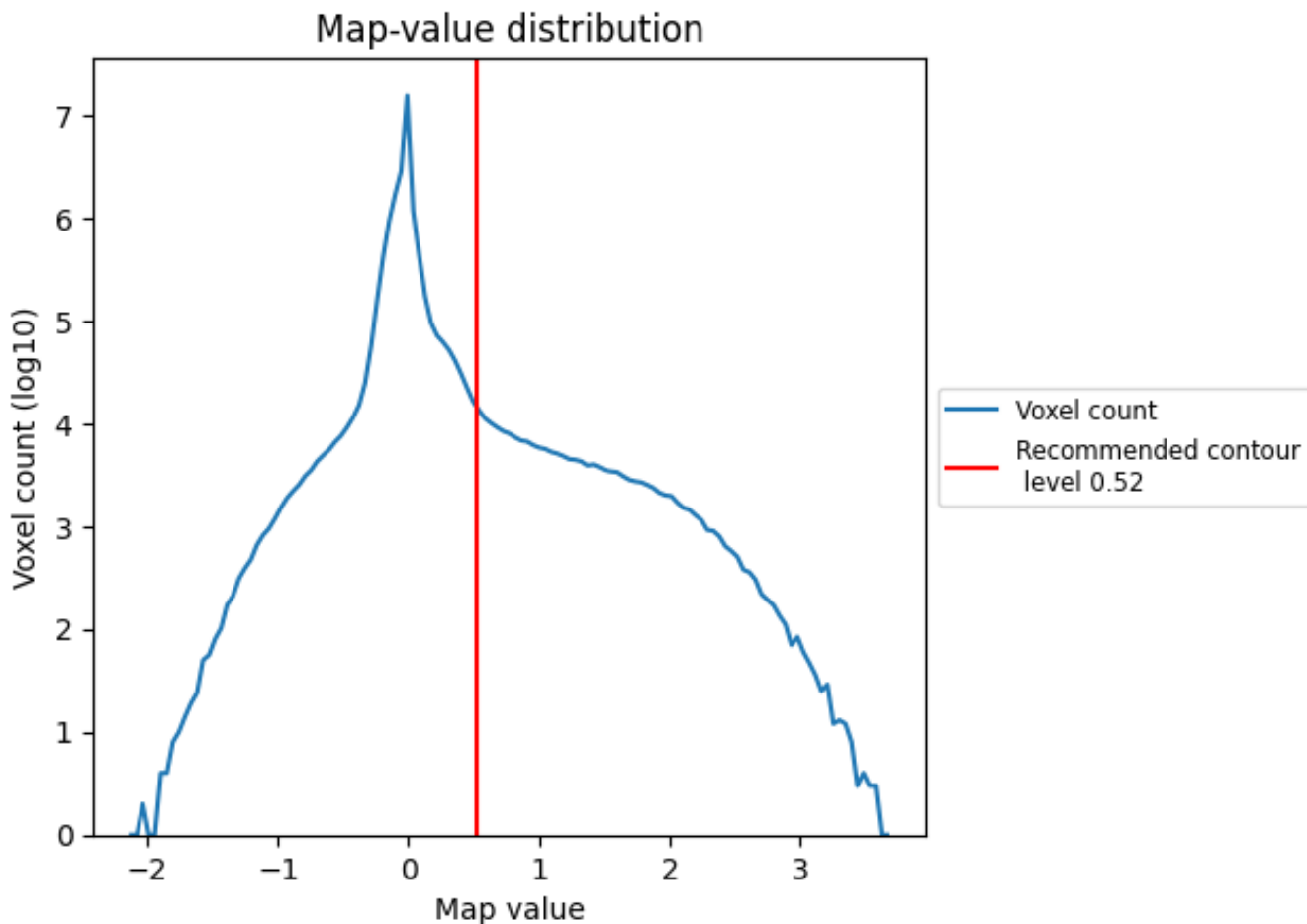
6.5 Mask visualisation

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

7 Map analysis [i](#)

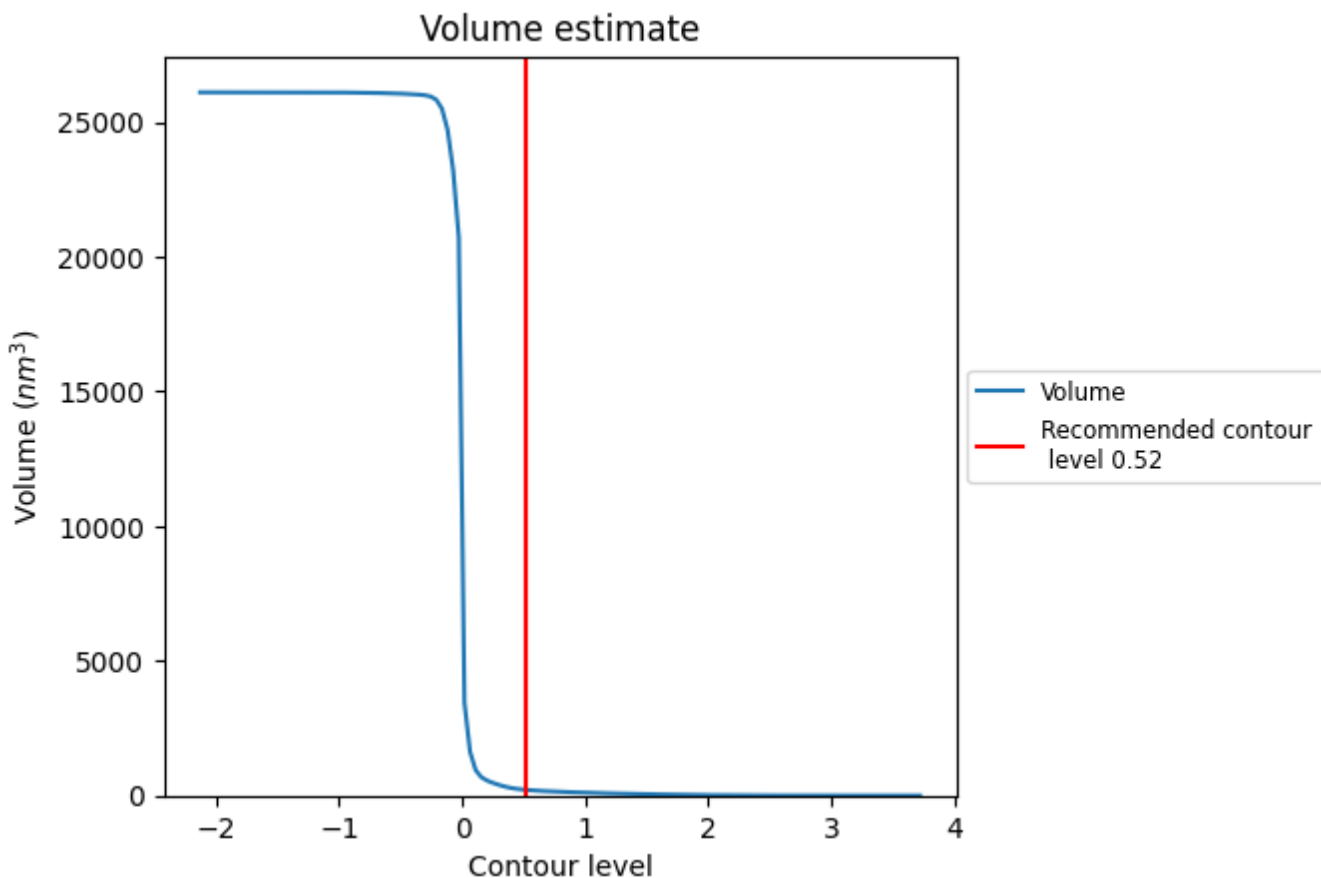
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

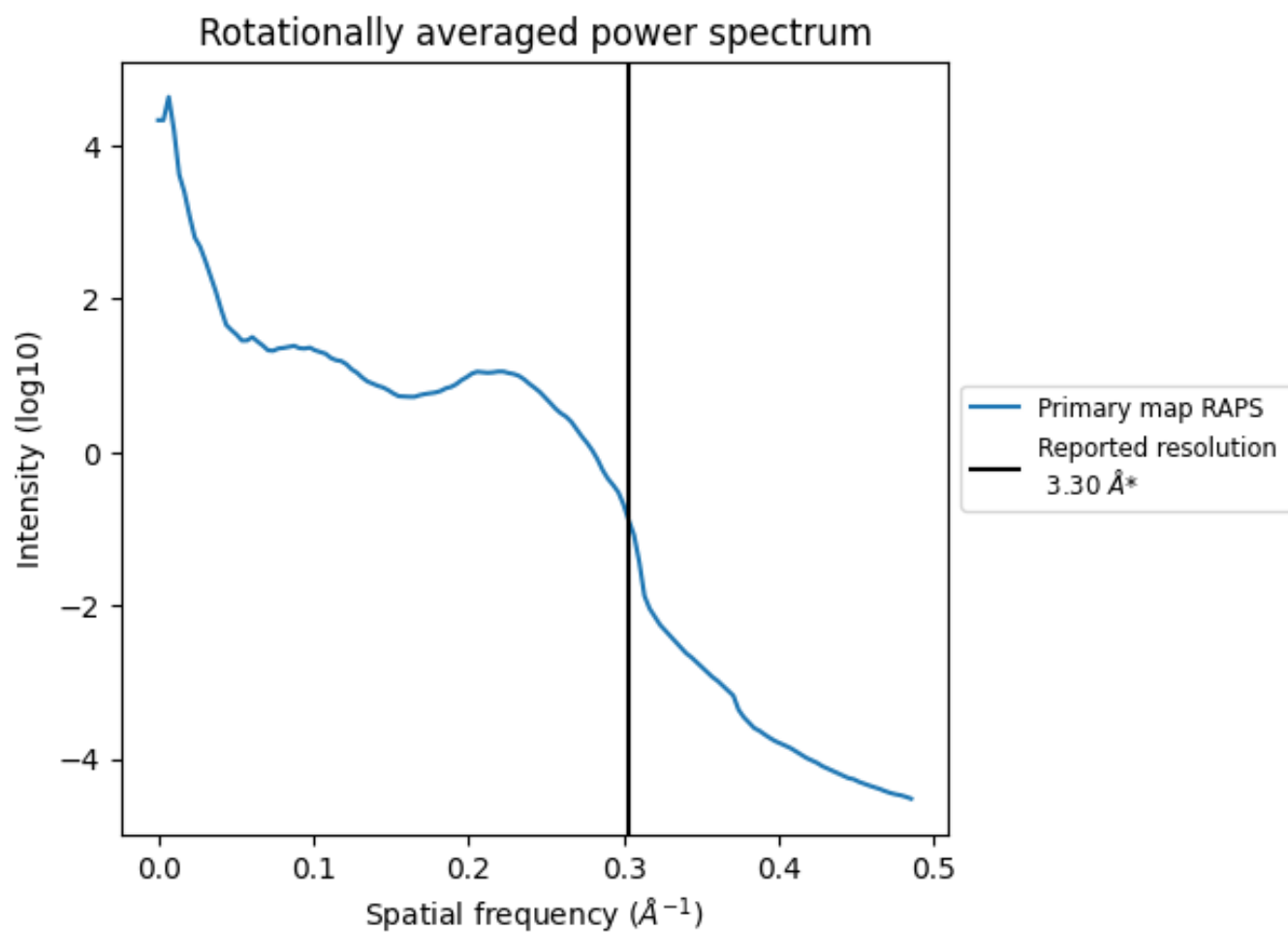
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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](#)

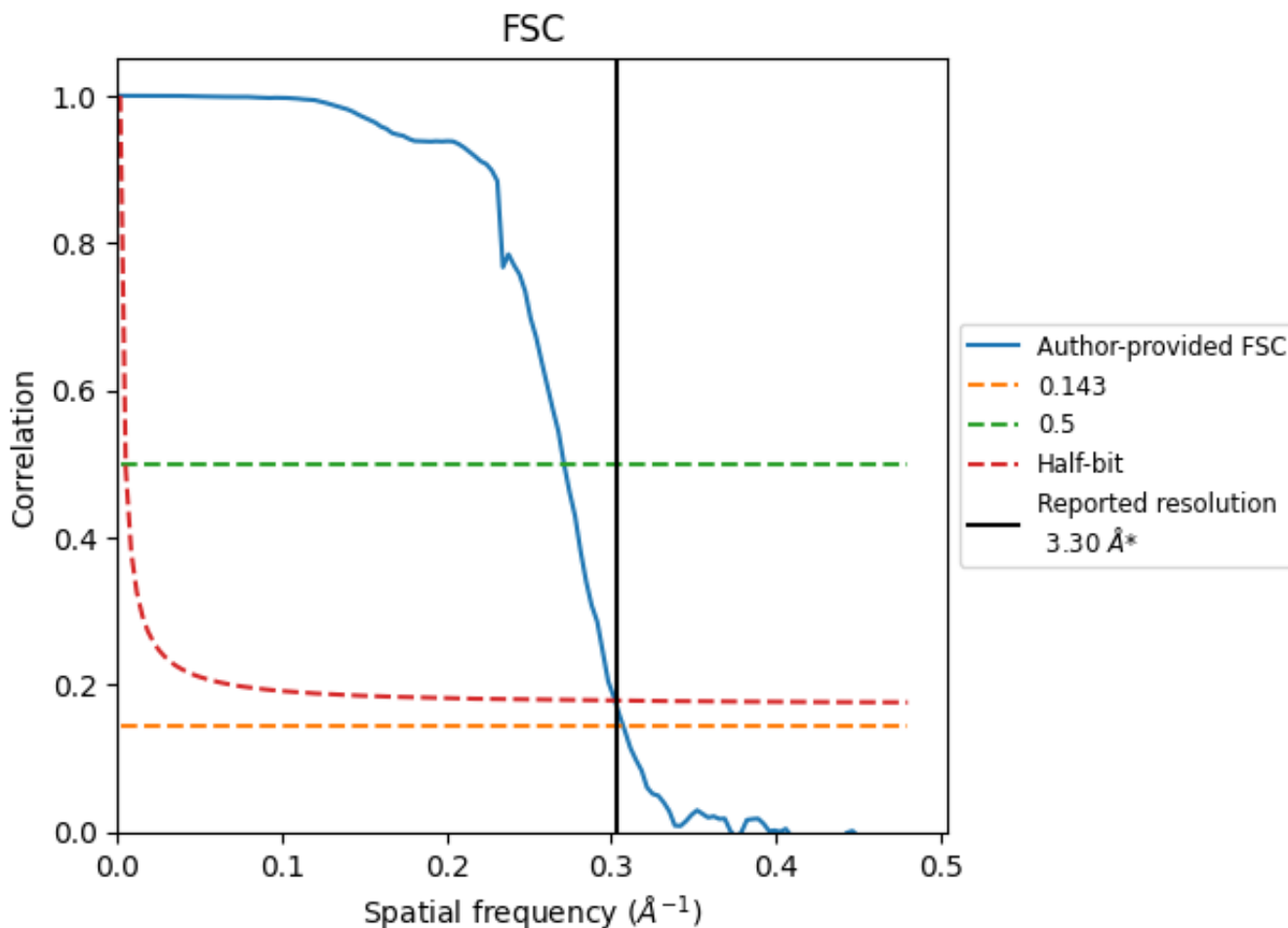


*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

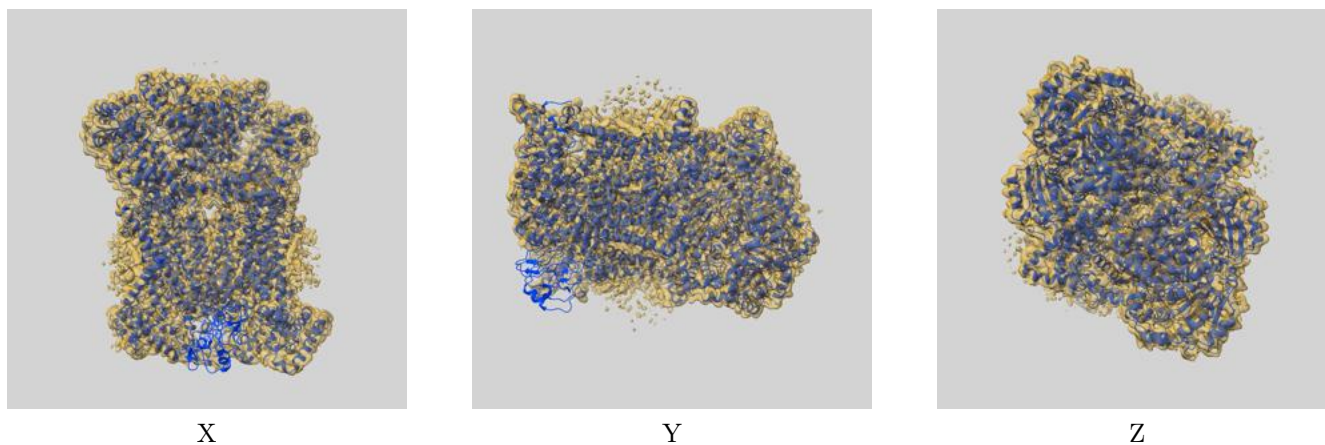
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.68	3.31
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

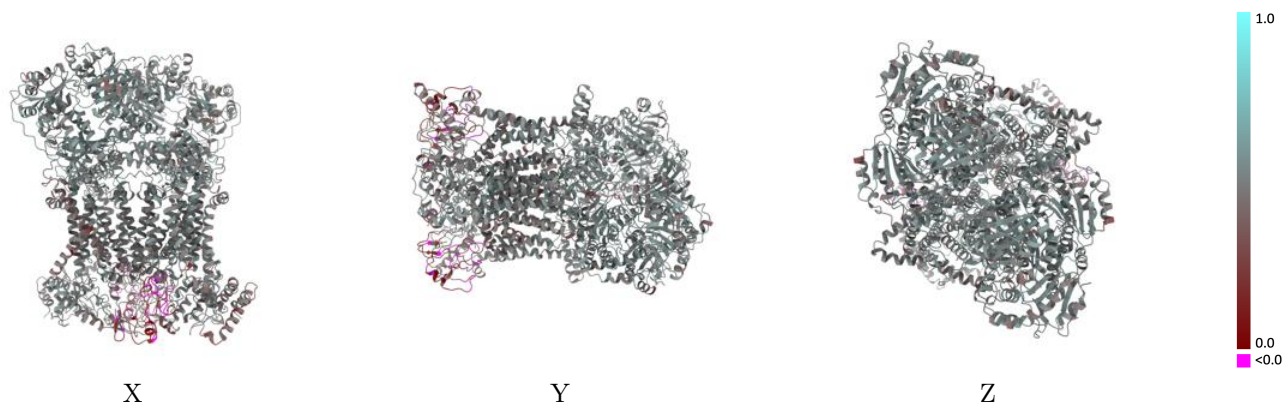
This section contains information regarding the fit between EMDB map EMD-24486 and PDB model 7RJE. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



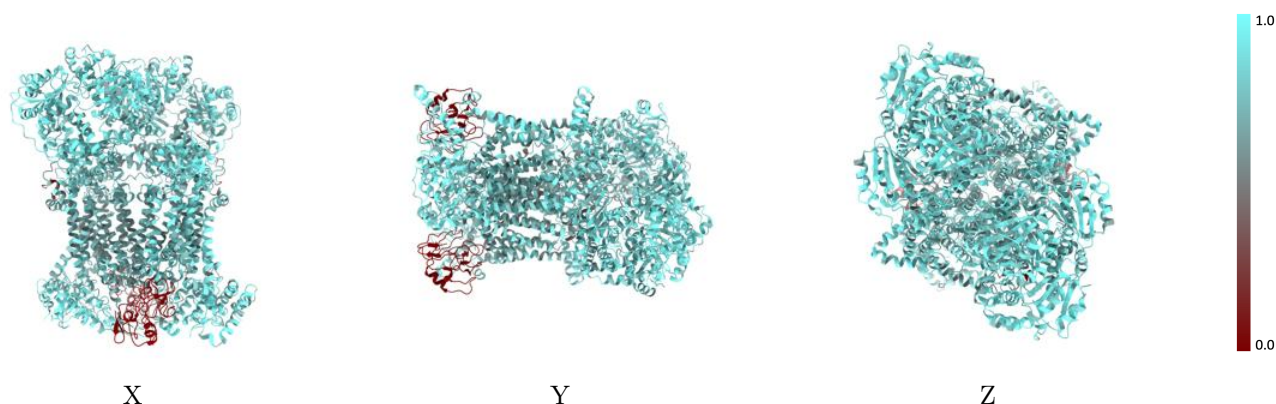
The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



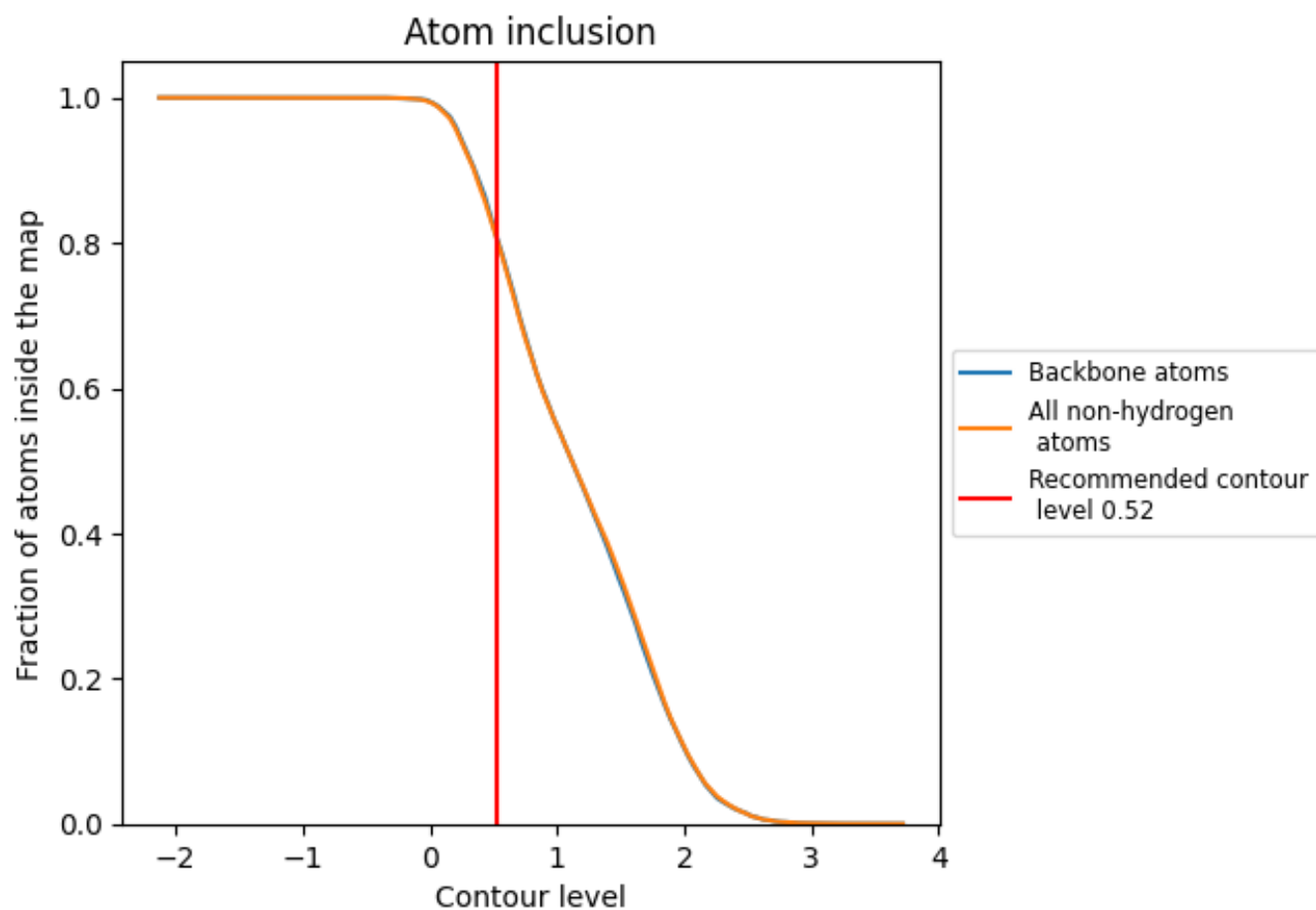
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.52).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% 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 (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8085	 0.4860
A	 0.8735	 0.5170
B	 0.8723	 0.5130
C	 0.2815	 0.2890
D	 0.8654	 0.4920
E	 0.8735	 0.5150
F	 0.8083	 0.4760
G	 0.8460	 0.5090
H	 0.8290	 0.4320
I	 0.8000	 0.4520
K	 0.8135	 0.5000
L	 0.8716	 0.5140
M	 0.2680	 0.2890
N	 0.8738	 0.4940
O	 0.8212	 0.4810
P	 0.8366	 0.5060
Q	 0.8237	 0.4260
R	 0.8097	 0.4550
T	 0.8189	 0.5020

