



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 12:41 PM JST

PDB ID : 8ZOW / pdb_00008zow
EMDB ID : EMD-60320
Title : Cryo-EM structure of Metyltetraprole-bound porcine bc1 complex
Authors : Wang, Y.X.; Sun, J.Y.; Cui, G.R.; Yang, G.F.
Deposited on : 2024-05-29
Resolution : 2.53 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:

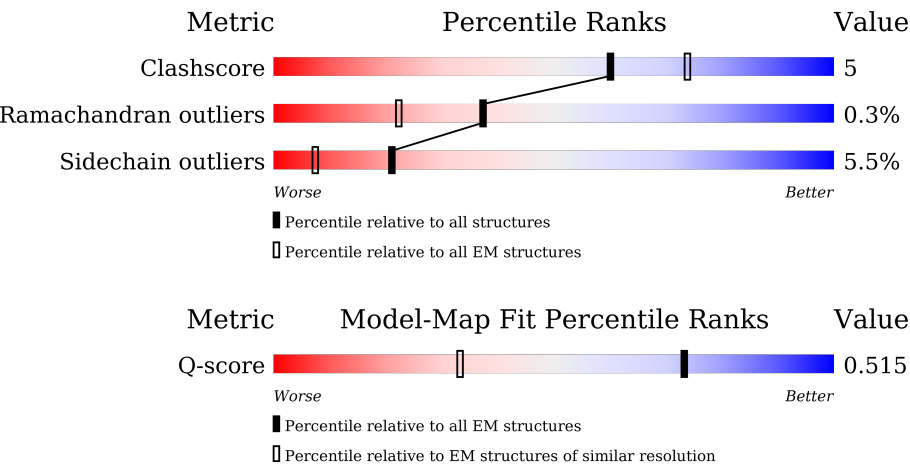
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7309 (2.03 - 3.03)

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

Mol	Chain	Length	Quality of chain
1	A	378	90%9%
1	a	378	92%7%
2	B	241	15% 89%10%
2	b	241	14% 82%14%

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Mol	Chain	Length	Quality of chain
3	C	196	
3	c	196	
4	D	446	
4	d	446	
5	E	418	
5	e	418	
6	F	64	
6	f	64	
7	G	106	
7	g	106	
8	H	79	
8	h	79	
9	I	62	
9	i	62	
10	J	52	
10	j	52	
11	K	57	
11	k	57	

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
16	HEC	B	401	X	-	-	-
16	HEC	b	401	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33477 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		
1	a	378	Total	C	N	O	S	0	0
			3017	2026	470	501	20		

- Molecule 2 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1920	1225	330	349	16		
2	b	239	Total	C	N	O	S	0	0
			1904	1214	327	347	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1502	946	261	288	7		
3	c	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	445	Total	C	N	O	S	0	0
			3452	2157	604	672	19		
4	d	446	Total	C	N	O	S	0	0
			3459	2161	605	674	19		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		
5	e	418	Total	C	N	O	S	0	0
			3134	1962	556	607	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	64	Total	C	N	O	S	0	0
			528	320	97	106	5		
6	f	64	Total	C	N	O	S	0	0
			528	320	97	106	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	106	Total	C	N	O	S	0	0
			921	589	162	168	2		
7	g	106	Total	C	N	O	S	0	0
			921	589	162	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	71	Total	C	N	O	S	0	0
			608	399	112	95	2		
8	h	79	Total	C	N	O	S	0	0
			666	434	122	108	2		

- Molecule 9 is a protein called Complex III subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	62	Total	C	N	O	0	0
			507	331	90	86		
9	i	62	Total	C	N	O	0	0
			507	331	90	86		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	49	Total	C	N	O	S	0	0
			405	269	71	63	2		

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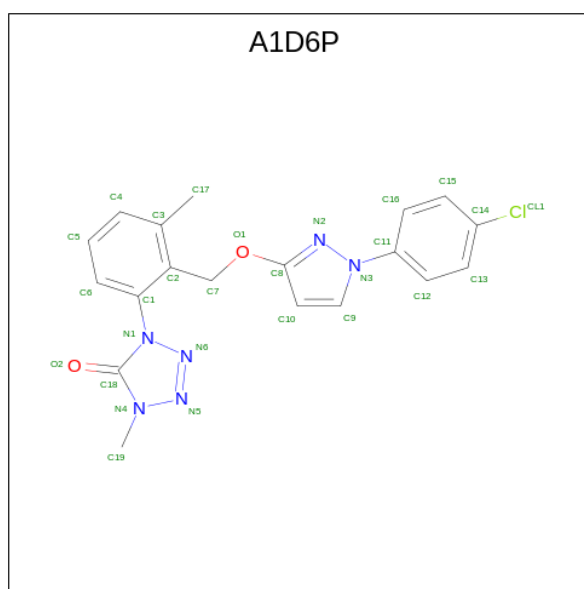
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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

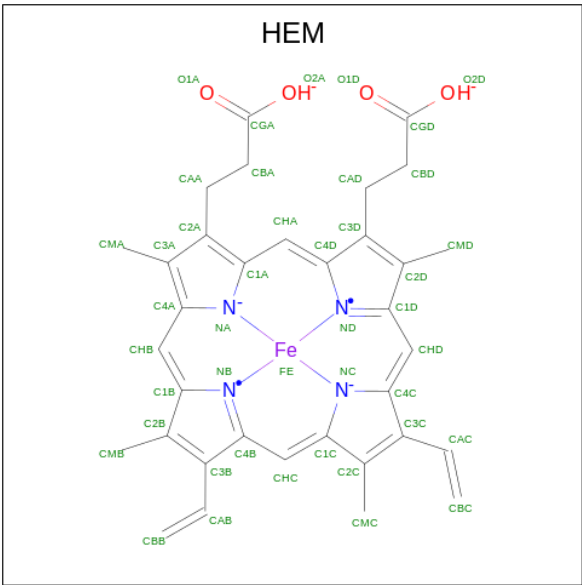
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	57	Total	C	N	O	S	0	0
			404	252	74	76	2		
11	k	57	Total	C	N	O	S	0	0
			404	252	74	76	2		

- Molecule 12 is 1-[2-[[1-(4-chlorophenyl)pyrazol-3-yl]oxymethyl]-3-methyl-phenyl]-4-methyl-1,2,3,4-tetrazol-5-one (CCD ID: A1D6P) (formula: C₁₉H₁₇ClN₆O₂) (labeled as "Ligand of Interest" by depositor).



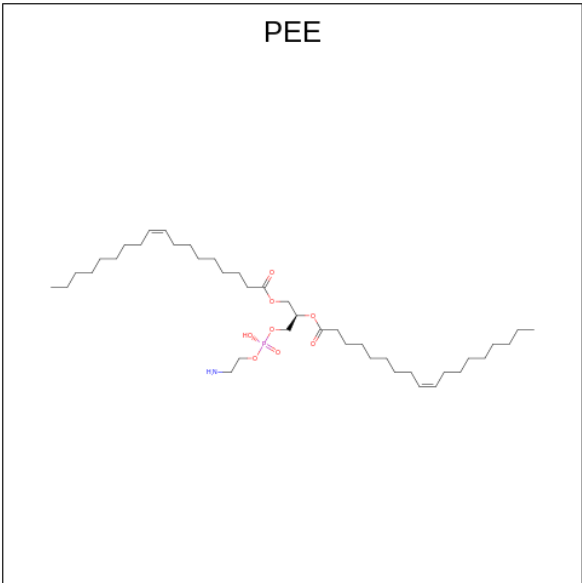
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
12	A	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
12	a	1	Total	C	Cl	N	O	0
			28	19	1	6	2	
12	a	1	Total	C	Cl	N	O	0
			28	19	1	6	2	

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



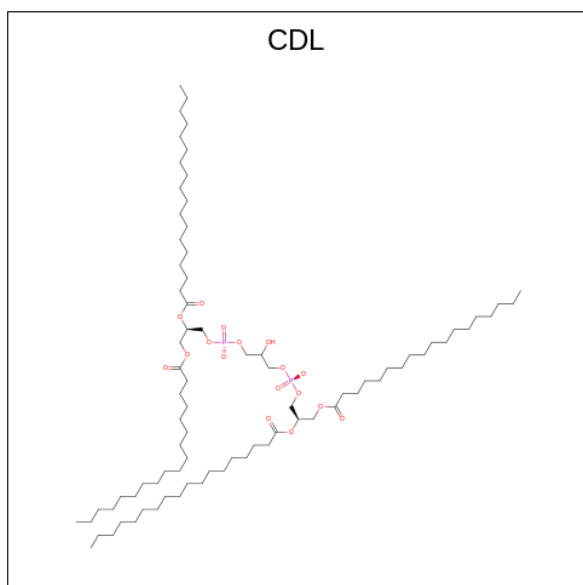
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
13	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 14 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



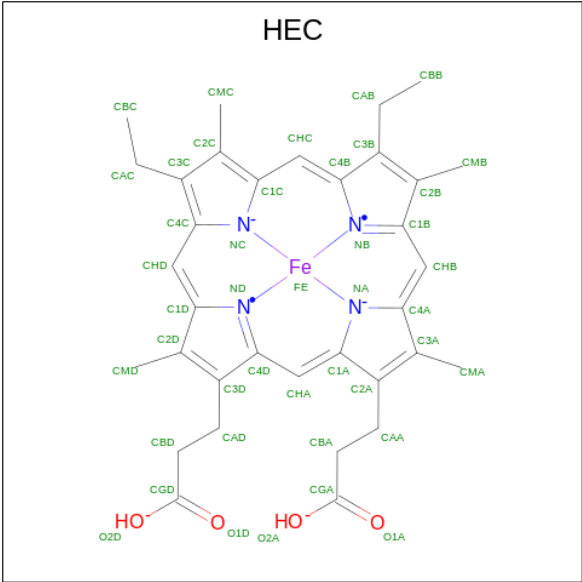
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
14	a	1	Total	C	N	O	P	0
			49	39	1	8	1	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



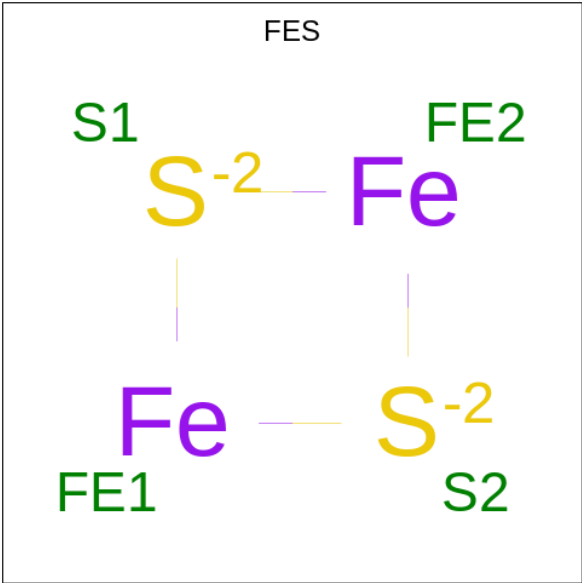
Mol	Chain	Residues	Atoms				AltConf
15	A	1	Total	C	O	P	0
			64	45	17	2	
15	a	1	Total	C	O	P	0
			64	45	17	2	

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
16	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
16	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).

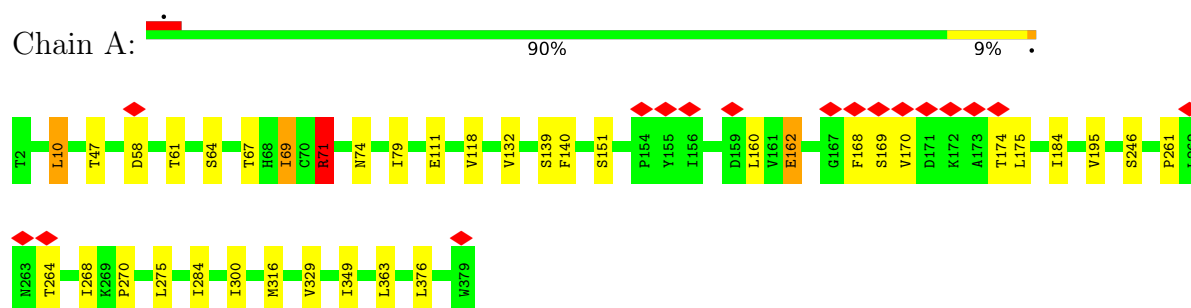


Mol	Chain	Residues	Atoms			AltConf
17	C	1	Total	Fe	S	0
			4	2	2	
17	c	1	Total	Fe	S	0
			4	2	2	

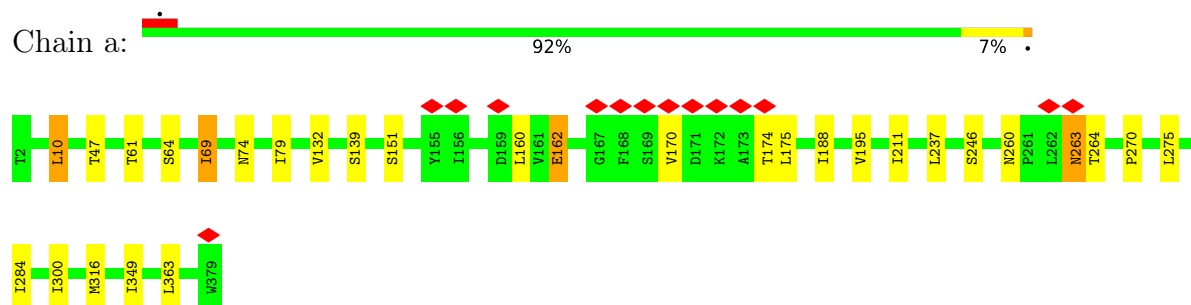
3 Residue-property plots [i](#)

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

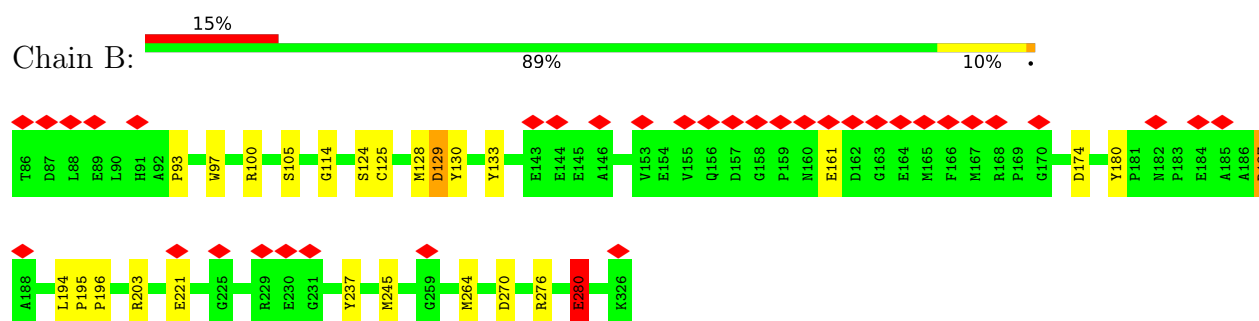
- Molecule 1: Cytochrome b



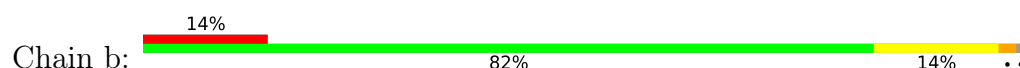
- Molecule 1: Cytochrome b

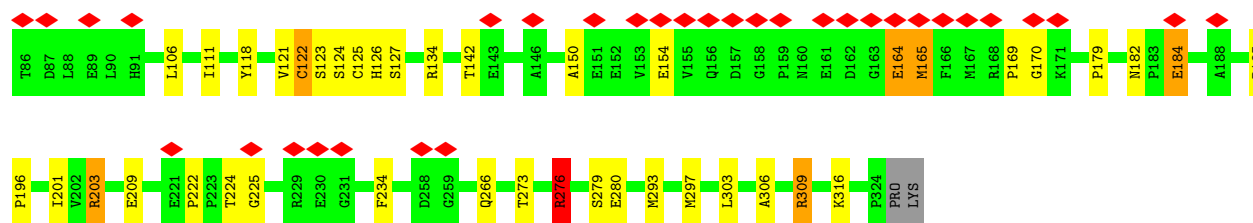


- Molecule 2: Cytochrome c1, heme protein, mitochondrial

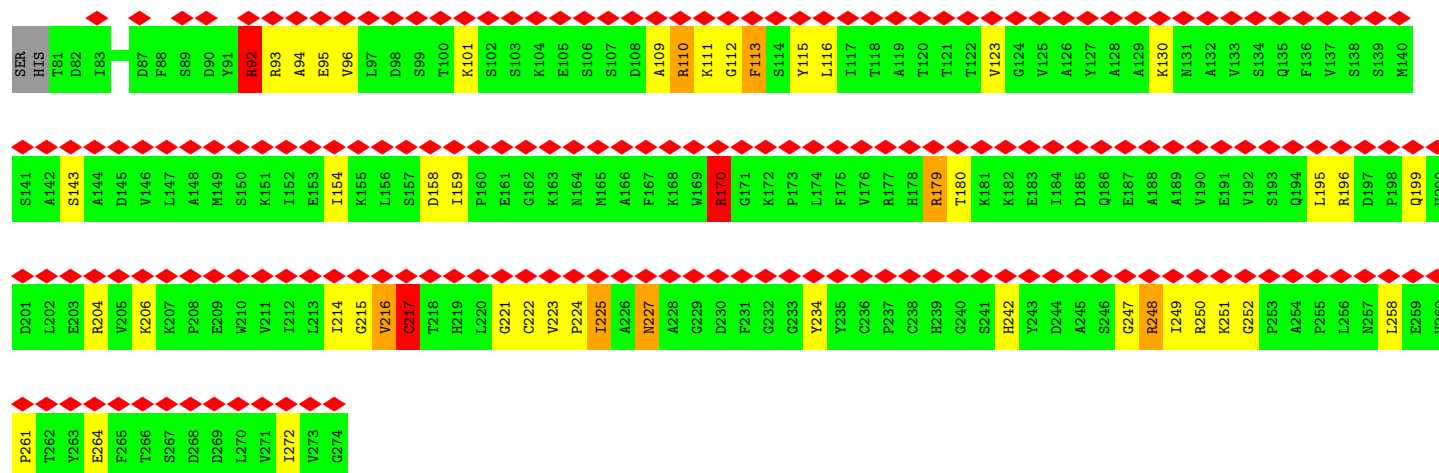
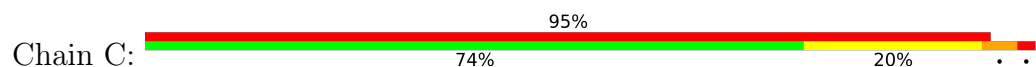


- Molecule 2: Cytochrome c1, heme protein, mitochondrial

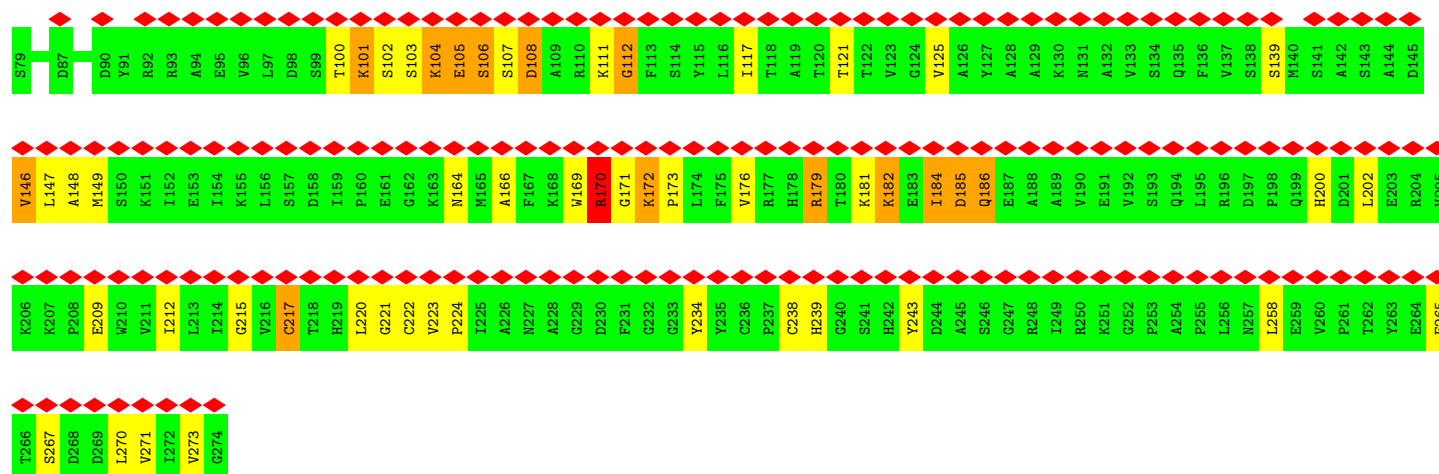




• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial

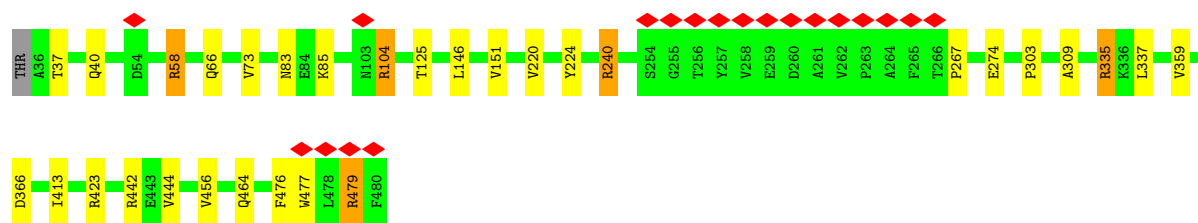


• Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



• Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial





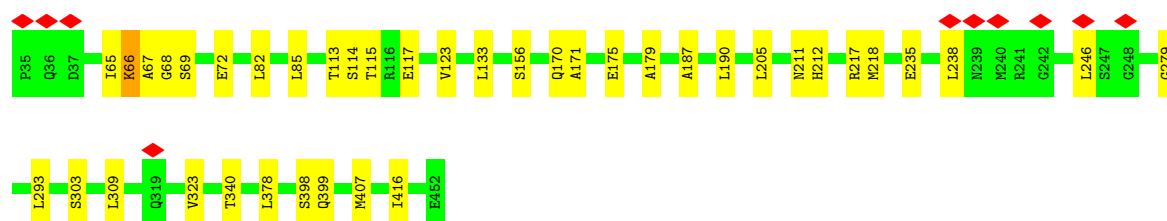
- Molecule 4: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain d: 93% 6% .



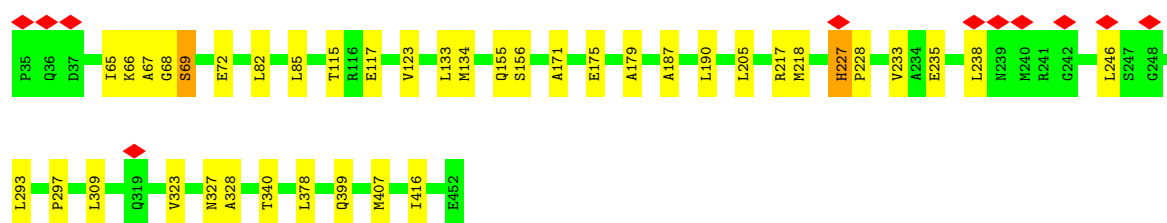
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain E: 90% 9% .



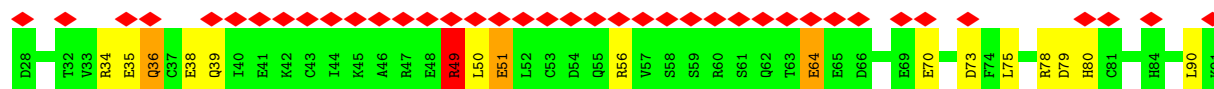
- Molecule 5: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain e: 90% 9% .

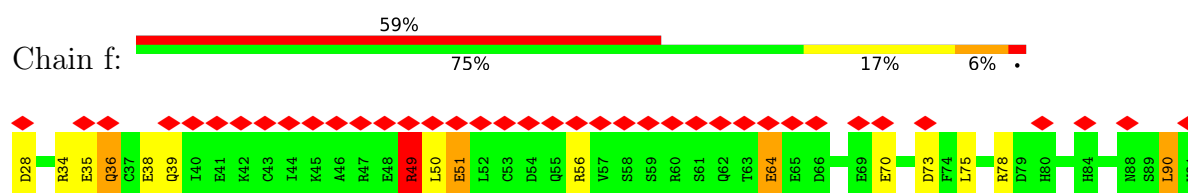


- Molecule 6: Cytochrome b-c1 complex subunit 6

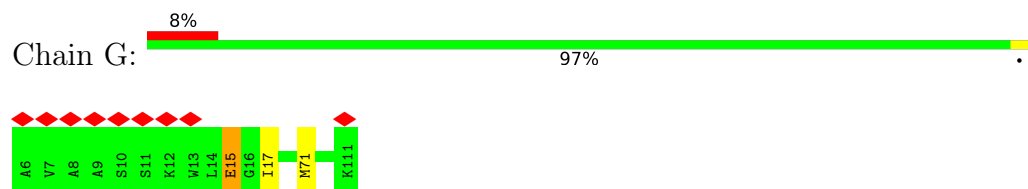
Chain F: 61% 73% 20% 5% .



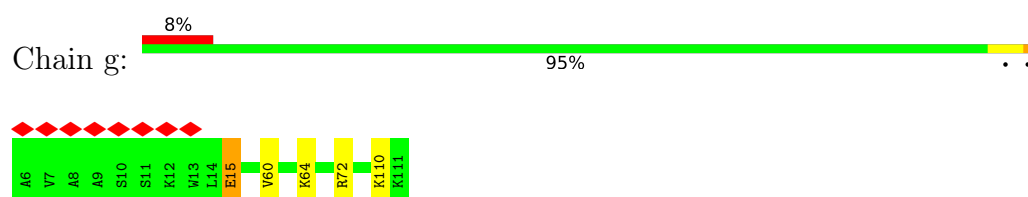
- Molecule 6: Cytochrome b-c1 complex subunit 6



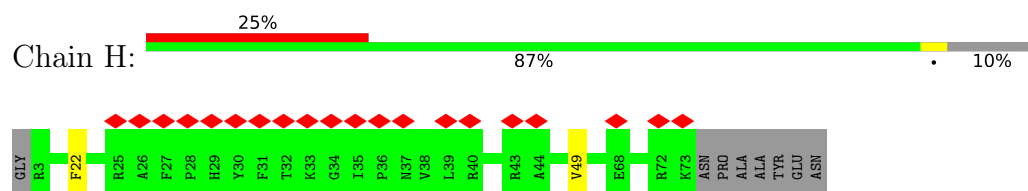
• Molecule 7: Cytochrome b-c1 complex subunit 7



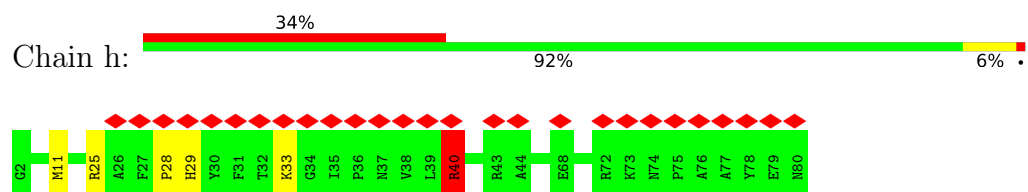
• Molecule 7: Cytochrome b-c1 complex subunit 7



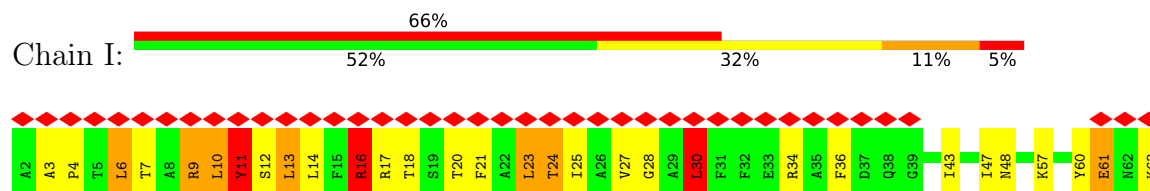
• Molecule 8: Cytochrome b-c1 complex subunit 8



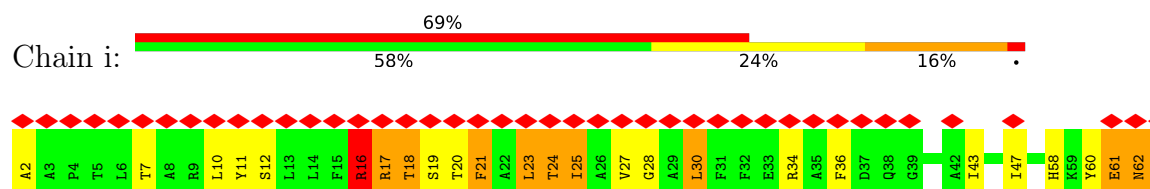
• Molecule 8: Cytochrome b-c1 complex subunit 8



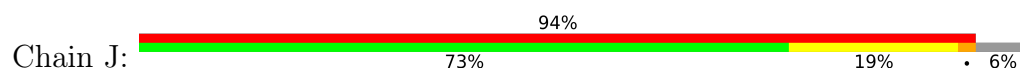
• Molecule 9: Complex III subunit 9



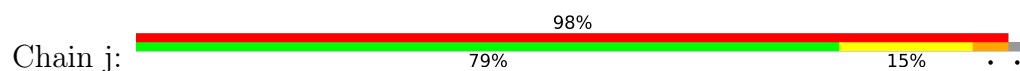
• Molecule 9: Complex III subunit 9



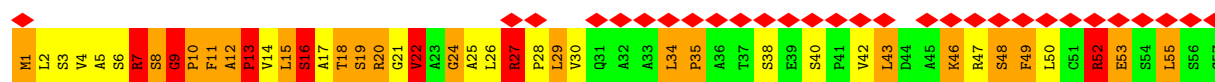
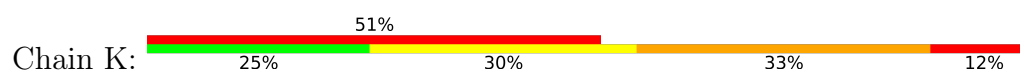
● Molecule 10: Cytochrome b-c1 complex subunit 10



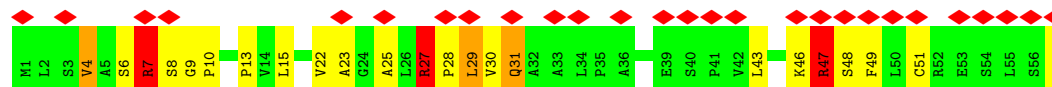
● Molecule 10: Cytochrome b-c1 complex subunit 10



● Molecule 11: Cytochrome b-c1 complex subunit Rieske, mitochondrial



● Molecule 11: 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	411418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.72	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.863	Depositor
Minimum map value	-5.367	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.223	Depositor
Recommended contour level	0.798	Depositor
Map size ($\text{\AA}$)	288.0, 288.0, 288.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, HEM, FES, HEC, A1D6P, CDL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/3115	0.66	3/4259 (0.1%)
1	a	0.42	0/3115	0.64	2/4259 (0.0%)
2	B	0.48	0/1978	0.79	6/2684 (0.2%)
2	b	0.55	1/1961 (0.1%)	0.89	8/2661 (0.3%)
3	C	0.59	1/1534 (0.1%)	0.88	6/2075 (0.3%)
3	c	0.51	1/1551 (0.1%)	0.90	2/2098 (0.1%)
4	D	0.42	0/3524	0.63	0/4783
4	d	0.48	2/3531 (0.1%)	0.72	6/4793 (0.1%)
5	E	0.45	2/3187 (0.1%)	0.63	1/4314 (0.0%)
5	e	0.48	2/3187 (0.1%)	0.67	4/4314 (0.1%)
6	F	0.35	0/534	0.91	6/714 (0.8%)
6	f	0.38	0/534	0.90	6/714 (0.8%)
7	G	0.39	0/941	0.64	1/1262 (0.1%)
7	g	0.39	0/941	0.64	1/1262 (0.1%)
8	H	0.38	0/628	0.71	0/848
8	h	0.34	0/688	0.75	0/931
9	I	0.66	0/520	1.17	3/701 (0.4%)
9	i	0.49	0/520	1.15	3/701 (0.4%)
10	J	0.40	0/420	0.87	1/576 (0.2%)
10	j	0.49	0/437	1.03	4/598 (0.7%)
11	K	1.42	4/410 (1.0%)	1.87	10/556 (1.8%)
11	k	0.73	0/410	1.34	3/556 (0.5%)
All	All	0.49	13/33666 (0.0%)	0.78	76/45659 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	b	0	4
3	C	0	6
3	c	0	1
4	D	0	5
6	F	0	1
6	f	0	1
8	h	0	1
9	I	0	4
9	i	0	3
10	J	0	1
11	K	0	3
11	k	0	4
All	All	0	37

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	217	CYS	C-N	13.54	1.52	1.33
2	b	121	VAL	C-N	9.97	1.49	1.33
4	d	351	THR	C-O	-9.46	1.13	1.23
5	e	67	ALA	C-O	-8.54	1.14	1.23
5	E	67	ALA	C-N	-8.49	1.25	1.32
5	E	66	LYS	C-N	7.83	1.40	1.33
11	K	10	PRO	C-O	-7.36	1.13	1.23
11	K	16	SER	C-O	-6.30	1.16	1.24
3	c	111	LYS	C-N	6.08	1.42	1.33
5	e	68	GLY	C-O	-5.92	1.16	1.23
4	d	451	ASP	C-O	-5.81	1.16	1.24
11	K	22	VAL	N-CA	5.37	1.52	1.46
11	K	12	ALA	C-O	-5.16	1.17	1.24

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	4	VAL	N-CA-CB	-11.65	99.39	112.21
9	i	19	SER	N-CA-C	-11.05	99.93	113.41
10	j	17	TRP	N-CA-C	-10.00	96.09	110.59
4	d	451	ASP	CA-CB-CG	9.42	122.02	112.60
11	K	16	SER	N-CA-C	9.21	124.14	108.02
11	K	11	PHE	CA-CB-CG	9.01	122.81	113.80
2	B	280	GLU	CB-CA-C	-8.65	100.43	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	162	GLU	CA-CB-CG	8.51	131.12	114.10
1	A	162	GLU	CA-CB-CG	8.49	131.08	114.10
11	K	16	SER	CB-CA-C	-8.49	97.07	110.74
2	b	276	ARG	N-CA-C	-8.38	101.79	112.93
11	K	7	ARG	N-CA-C	-7.81	94.17	110.80
11	k	31	GLN	N-CA-C	-7.77	103.75	113.23
9	I	12	SER	N-CA-C	-7.75	103.89	112.72
1	A	71	ARG	CB-CA-C	7.68	121.92	109.02
5	e	67	ALA	CA-C-O	-7.54	113.24	121.31
5	e	67	ALA	N-CA-C	-7.23	98.61	108.38
9	I	11	TYR	CB-CA-C	-7.02	98.31	110.17
3	c	170	ARG	N-CA-C	-7.00	104.69	113.23
9	I	30	LEU	CA-CB-CG	6.95	140.61	116.30
9	i	30	LEU	CA-CB-CG	6.93	140.56	116.30
1	a	162	GLU	CB-CG-CD	6.82	124.20	112.60
1	A	162	GLU	CB-CG-CD	6.82	124.19	112.60
4	d	351	THR	CB-CA-C	-6.71	97.66	113.02
11	K	11	PHE	N-CA-C	-6.66	101.56	110.55
10	j	24	TRP	N-CA-C	-6.63	96.68	110.80
3	C	112	GLY	N-CA-C	6.36	128.26	113.18
10	j	17	TRP	CA-C-O	-6.36	114.45	121.89
2	B	129	ASP	O-C-N	6.33	130.48	122.37
2	b	126	HIS	CA-C-O	-6.30	113.41	120.66
10	j	19	PRO	N-CA-C	-6.22	104.57	113.47
6	f	49	ARG	NE-CZ-NH2	6.16	124.75	119.20
7	g	15	GLU	CB-CG-CD	6.16	123.07	112.60
4	d	449	PHE	CA-C-O	-6.15	111.77	120.07
7	G	15	GLU	CB-CG-CD	6.14	123.03	112.60
6	F	49	ARG	NE-CZ-NH2	6.12	124.71	119.20
6	F	49	ARG	CG-CD-NE	6.11	125.45	112.00
6	f	49	ARG	CG-CD-NE	6.10	125.43	112.00
3	C	195	LEU	CA-C-N	6.06	133.12	121.54
3	C	195	LEU	C-N-CA	6.06	133.12	121.54
11	K	27	ARG	CB-CA-C	-6.03	98.30	110.17
3	C	113	PHE	N-CA-C	6.00	121.15	113.18
11	K	9	GLY	N-CA-C	5.93	124.44	112.34
6	F	49	ARG	CD-NE-CZ	5.91	132.67	124.40
6	f	49	ARG	CD-NE-CZ	5.89	132.65	124.40
2	b	126	HIS	CB-CA-C	5.80	120.84	109.35
10	J	22	SER	O-C-N	5.80	128.81	122.20
2	b	225	GLY	CA-C-N	-5.74	115.66	123.12
2	b	225	GLY	C-N-CA	-5.74	115.66	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	5	ALA	N-CA-C	-5.68	105.85	112.89
2	b	126	HIS	CA-C-N	5.63	132.11	121.81
2	b	126	HIS	C-N-CA	5.63	132.11	121.81
5	e	68	GLY	CA-C-N	5.53	128.46	120.38
5	e	68	GLY	C-N-CA	5.53	128.46	120.38
6	f	51	GLU	CA-CB-CG	5.52	125.15	114.10
4	d	449	PHE	CA-C-N	5.50	132.04	121.54
4	d	449	PHE	C-N-CA	5.50	132.04	121.54
6	F	51	GLU	CA-CB-CG	5.50	125.09	114.10
5	E	68	GLY	CA-C-O	-5.43	118.41	122.37
9	i	11	TYR	CA-CB-CG	5.36	123.54	113.90
2	B	129	ASP	CB-CA-C	-5.32	101.61	110.81
11	K	4	VAL	N-CA-C	-5.29	107.67	113.43
6	f	64	GLU	CB-CG-CD	5.27	121.56	112.60
3	C	94	ALA	CA-C-N	-5.26	113.11	122.42
3	C	94	ALA	C-N-CA	-5.26	113.11	122.42
6	F	64	GLU	CB-CG-CD	5.26	121.54	112.60
2	B	124	SER	N-CA-C	-5.24	107.06	113.50
3	c	112	GLY	N-CA-C	5.24	125.59	113.18
2	b	122	CYS	O-C-N	5.21	127.94	122.20
6	F	64	GLU	CA-CB-CG	5.18	124.47	114.10
6	f	64	GLU	CA-CB-CG	5.17	124.45	114.10
2	B	221	GLU	N-CA-C	-5.11	102.28	110.10
2	B	130	TYR	N-CA-C	-5.11	107.02	114.12
11	k	7	ARG	CA-C-N	-5.06	114.65	122.59
11	k	7	ARG	C-N-CA	-5.06	114.65	122.59
4	d	55	ASN	N-CA-C	-5.03	107.14	113.28

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	ARG	Sidechain
2	B	180	TYR	Peptide
2	B	187	ARG	Sidechain
3	C	110	ARG	Peptide
3	C	170	ARG	Sidechain
3	C	179	ARG	Sidechain
3	C	206	LYS	Peptide
3	C	248	ARG	Sidechain
3	C	92	ARG	Sidechain
4	D	104	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	D	240	ARG	Sidechain
4	D	335	ARG	Sidechain
4	D	479	ARG	Sidechain
4	D	58	ARG	Sidechain
6	F	34	ARG	Sidechain
9	I	16	ARG	Sidechain
9	I	24	THR	Peptide
9	I	36	PHE	Peptide
9	I	9	ARG	Sidechain
10	J	34	TRP	Peptide
11	K	27	ARG	Sidechain
11	K	52	ARG	Sidechain
11	K	7	ARG	Sidechain
2	b	203	ARG	Sidechain
2	b	273	THR	Peptide
2	b	276	ARG	Sidechain
2	b	309	ARG	Sidechain
3	c	170	ARG	Sidechain
6	f	34	ARG	Sidechain
8	h	40	ARG	Sidechain
9	i	16	ARG	Sidechain
9	i	24	THR	Peptide
9	i	36	PHE	Peptide
11	k	27	ARG	Sidechain
11	k	47	ARG	Sidechain
11	k	6	SER	Mainchain
11	k	7	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	3078	22	0
1	a	3017	0	3078	14	0
2	B	1920	0	1869	17	0
2	b	1904	0	1849	24	0
3	C	1502	0	1490	30	0
3	c	1518	0	1501	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3452	0	3343	16	0
4	d	3459	0	3350	16	0
5	E	3134	0	3112	25	0
5	e	3134	0	3112	21	0
6	F	528	0	510	8	0
6	f	528	0	510	5	0
7	G	921	0	917	2	0
7	g	921	0	917	5	0
8	H	608	0	616	2	0
8	h	666	0	663	5	0
9	I	507	0	509	11	0
9	i	507	0	509	12	0
10	J	405	0	405	9	0
10	j	421	0	418	4	0
11	K	404	0	425	48	0
11	k	404	0	425	19	0
12	A	56	0	0	0	0
12	a	56	0	0	0	0
13	A	86	0	60	0	0
13	a	86	0	60	0	0
14	A	45	0	67	4	0
14	a	49	0	75	3	0
15	A	64	0	72	2	0
15	a	64	0	72	2	0
16	B	43	0	32	5	0
16	b	43	0	32	4	0
17	C	4	0	0	0	0
17	c	4	0	0	0	0
All	All	33477	0	33076	300	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 5.

All (300) 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:B:125:CYS:SG	16:B:401:HEC:HBC3	1.86	1.16
1:A:169:SER:HB2	3:c:171:GLY:HA3	1.45	0.95
2:b:125:CYS:SG	16:b:401:HEC:CAC	2.55	0.95
5:e:328:ALA:HA	11:k:8:SER:HB2	1.46	0.94
2:B:125:CYS:SG	16:B:401:HEC:CBC	2.54	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:125:CYS:SG	16:b:401:HEC:CBC	2.63	0.87
3:C:93:ARG:HB2	3:C:96:VAL:HG22	1.59	0.85
11:K:16:SER:HB2	11:K:19:SER:H	1.42	0.85
5:E:114:SER:O	11:K:13:PRO:HD2	1.77	0.84
2:B:125:CYS:SG	16:B:401:HEC:CAC	2.66	0.83
3:c:217:CYS:HB2	3:c:221:GLY:H	1.44	0.82
11:K:24:GLY:HA2	11:K:27:ARG:HG2	1.62	0.80
11:K:20:ARG:HB2	11:K:47:ARG:HH21	1.46	0.80
2:B:125:CYS:HG	16:B:401:HEC:HBC3	1.44	0.80
11:k:13:PRO:HA	11:k:23:ALA:HA	1.63	0.79
5:E:171:ALA:HA	11:K:11:PHE:CE1	2.18	0.79
3:c:146:VAL:HG22	3:c:149:MET:HG2	1.69	0.73
3:C:196:ARG:HH22	3:C:252:GLY:HA2	1.55	0.72
11:k:23:ALA:HB3	11:k:27:ARG:NH2	2.04	0.71
3:C:115:TYR:CD1	9:I:11:TYR:HB2	2.26	0.70
5:E:171:ALA:HA	11:K:11:PHE:HE1	1.56	0.70
11:k:23:ALA:HB3	11:k:27:ARG:HH21	1.57	0.70
3:c:103:SER:HB2	4:d:269:ARG:HB2	1.74	0.69
2:b:125:CYS:SG	16:b:401:HEC:HBC3	2.33	0.69
11:k:22:VAL:HA	11:k:47:ARG:HH22	1.58	0.68
11:K:20:ARG:HD3	11:K:52:ARG:HG3	1.76	0.67
9:i:20:THR:HA	9:i:23:LEU:HB2	1.76	0.67
5:e:327:ASN:O	11:k:8:SER:HA	1.94	0.67
11:K:11:PHE:CZ	11:K:27:ARG:HB3	2.31	0.66
4:D:104:ARG:HH21	4:D:146:LEU:HD23	1.60	0.65
9:I:10:LEU:HG	9:I:13:LEU:HD11	1.78	0.65
3:C:217:CYS:HB2	3:C:222:CYS:O	1.96	0.65
11:K:9:GLY:H	11:K:26:LEU:HD22	1.62	0.65
7:g:64:LYS:HD2	8:h:11:MET:HE1	1.79	0.64
1:A:10:LEU:HD21	1:a:195:VAL:HG13	1.80	0.64
3:C:196:ARG:HD2	3:C:250:ARG:HA	1.79	0.63
11:K:22:VAL:HG13	11:K:47:ARG:NH1	2.13	0.63
11:K:20:ARG:CZ	11:K:52:ARG:HB2	2.29	0.62
10:j:14:ALA:HA	10:j:17:TRP:HB3	1.81	0.62
4:D:359:VAL:HG21	11:K:46:LYS:HG3	1.81	0.62
11:K:8:SER:HB3	11:K:26:LEU:HD13	1.80	0.62
4:D:274:GLU:HG3	4:D:456:VAL:HB	1.82	0.62
3:C:110:ARG:HB3	3:C:111:LYS:HG3	1.82	0.62
2:B:93:PRO:HG3	6:F:79:ASP:HB3	1.81	0.61
5:E:211:ASN:HB3	5:E:246:LEU:HG	1.82	0.61
9:i:18:THR:HA	9:i:21:PHE:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:50:LEU:HB3	11:K:53:GLU:HB2	1.83	0.61
2:b:306:ALA:HB3	3:c:117:ILE:HG21	1.82	0.61
2:B:245:MET:HB2	16:B:401:HEC:C1D	2.31	0.61
11:K:27:ARG:H	11:K:28:PRO:HD3	1.65	0.60
11:K:12:ALA:CB	11:K:25:ALA:HB2	2.32	0.60
5:e:85:LEU:HA	11:k:15:LEU:HD22	1.85	0.59
9:i:16:ARG:HH21	9:i:17:ARG:HA	1.67	0.59
11:K:20:ARG:HB2	11:K:47:ARG:NH2	2.18	0.59
4:d:303:PRO:HB2	4:d:444:VAL:HG11	1.86	0.58
11:K:20:ARG:H	11:K:20:ARG:NH2	2.01	0.58
4:d:339:GLN:HB3	11:k:46:LYS:HB3	1.85	0.57
4:D:83:ASN:HD21	4:D:85:LYS:HG2	1.69	0.57
11:K:20:ARG:HE	11:K:48:SER:HA	1.69	0.57
5:e:115:THR:HG23	5:e:117:GLU:H	1.69	0.57
1:A:316:MET:HA	14:A:405:PEE:H11	1.87	0.57
2:B:276:ARG:HH21	2:B:280:GLU:HG3	1.70	0.57
3:c:200:HIS:HD2	3:c:202:LEU:HB2	1.69	0.57
1:a:316:MET:HA	14:a:405:PEE:H11	1.86	0.56
4:D:73:VAL:HG11	4:D:151:VAL:HG11	1.87	0.56
4:d:399:LEU:HB3	11:k:57:GLY:HA3	1.88	0.56
9:i:58:HIS:HA	9:i:61:GLU:HB2	1.86	0.56
5:E:115:THR:HG23	5:E:117:GLU:H	1.69	0.56
3:C:199:GLN:HB3	3:C:204:ARG:HD3	1.86	0.56
3:c:112:GLY:H	9:i:7:THR:HG22	1.71	0.56
2:b:134:ARG:HD2	3:c:148:ALA:H	1.70	0.56
4:D:303:PRO:HB2	4:D:444:VAL:HG11	1.87	0.56
11:K:16:SER:C	11:K:18:THR:H	2.14	0.56
5:E:85:LEU:HD23	11:K:15:LEU:HG	1.88	0.56
11:K:20:ARG:HB3	11:K:47:ARG:HB2	1.88	0.55
4:d:274:GLU:HG3	4:d:456:VAL:HB	1.88	0.55
1:A:329:VAL:HG22	14:A:405:PEE:H33	1.88	0.55
3:c:101:LYS:HE3	9:i:2:ALA:HB3	1.87	0.55
1:A:74:ASN:HB2	3:C:143:SER:HB2	1.87	0.55
1:A:195:VAL:HG13	1:a:10:LEU:HD21	1.89	0.55
3:C:109:ALA:HA	9:I:6:LEU:HB3	1.88	0.55
5:E:170:GLN:NE2	11:K:27:ARG:O	2.37	0.55
5:E:113:THR:HG23	11:K:14:VAL:HG22	1.89	0.55
4:d:359:VAL:HG11	11:k:46:LYS:HE3	1.87	0.55
10:J:24:TRP:HA	10:J:27:VAL:HG13	1.88	0.54
7:g:60:VAL:HG12	8:h:11:MET:HE3	1.88	0.54
3:C:224:PRO:HB2	3:C:234:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:73:VAL:HG11	4:d:151:VAL:HG11	1.89	0.54
10:j:33:VAL:HG11	10:j:41:ILE:HD13	1.90	0.54
11:K:11:PHE:CE2	11:K:27:ARG:HB3	2.44	0.53
2:b:316:LYS:HA	7:g:72:ARG:HE	1.73	0.53
3:c:217:CYS:HB2	3:c:221:GLY:N	2.20	0.53
3:c:224:PRO:HG2	3:c:234:TYR:HB3	1.90	0.53
9:I:57:LYS:O	9:I:61:GLU:HG2	2.09	0.52
3:C:115:TYR:CG	9:I:11:TYR:HB2	2.45	0.52
4:D:335:ARG:HE	4:D:337:LEU:HD11	1.73	0.52
5:e:66:LYS:HB2	5:e:217:ARG:HB3	1.91	0.52
3:C:216:VAL:HG12	3:C:221:GLY:HA2	1.91	0.52
3:c:265:PHE:HE1	3:c:271:VAL:HG13	1.74	0.52
10:J:21:ALA:HA	10:J:24:TRP:NE1	2.25	0.52
5:E:66:LYS:HB2	5:E:217:ARG:HB3	1.91	0.52
3:C:92:ARG:HE	3:C:96:VAL:HG23	1.75	0.51
11:K:28:PRO:O	11:K:29:LEU:C	2.53	0.51
3:c:169:TRP:CD1	3:c:170:ARG:H	2.28	0.51
3:c:217:CYS:SG	3:c:222:CYS:HB3	2.51	0.51
4:D:476:PHE:HB2	9:I:16:ARG:HH21	1.76	0.50
2:b:182:ASN:ND2	2:b:184:GLU:HB2	2.26	0.50
4:D:366:ASP:HB3	4:D:464:GLN:HE21	1.76	0.50
4:d:279:ASP:H	4:d:460:GLY:HA3	1.76	0.50
5:e:399:GLN:HE22	5:e:407:MET:H	1.60	0.50
5:E:399:GLN:HE22	5:E:407:MET:H	1.60	0.49
11:K:9:GLY:O	11:K:10:PRO:C	2.54	0.49
5:e:297:PRO:HB3	11:k:31:GLN:HG2	1.94	0.49
1:A:67:THR:O	1:A:71:ARG:HG2	2.12	0.49
11:k:4:VAL:HG13	11:k:10:PRO:HD2	1.94	0.49
3:c:146:VAL:HG13	3:c:149:MET:HE3	1.94	0.49
11:k:10:PRO:O	11:k:25:ALA:HB3	2.12	0.49
11:K:12:ALA:HB2	11:K:25:ALA:HB2	1.93	0.49
10:J:8:PRO:HD2	7:g:110:LYS:HB3	1.95	0.49
3:c:179:ARG:HG3	3:c:209:GLU:HA	1.95	0.48
9:I:3:ALA:N	9:I:4:PRO:HD2	2.27	0.48
5:e:323:VAL:HG23	5:e:340:THR:HG22	1.95	0.48
3:C:225:ILE:HG13	3:C:227:ASN:HD21	1.77	0.48
5:E:323:VAL:HG23	5:E:340:THR:HG22	1.95	0.48
2:b:164:GLU:HB2	2:b:165:MET:HE2	1.95	0.48
11:K:12:ALA:HB3	11:K:25:ALA:HB2	1.95	0.48
6:f:50:LEU:HD13	6:f:70:GLU:HB3	1.95	0.48
2:B:97:TRP:HB2	2:B:100:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:47:THR:HG23	1:a:79:ILE:HG23	1.96	0.48
3:c:179:ARG:O	3:c:182:LYS:HB2	2.14	0.48
11:K:27:ARG:H	11:K:28:PRO:CD	2.26	0.48
3:c:101:LYS:HE3	9:i:2:ALA:CB	2.43	0.48
3:c:101:LYS:HZ1	3:c:105:GLU:HG3	1.77	0.48
1:A:300:ILE:HD11	1:A:363:LEU:HG	1.96	0.47
6:F:50:LEU:HD13	6:F:70:GLU:HB3	1.95	0.47
3:C:247:GLY:HA2	3:C:258:LEU:HD21	1.95	0.47
11:K:8:SER:O	11:K:10:PRO:HD2	2.14	0.47
11:K:20:ARG:NH2	11:K:52:ARG:HB2	2.28	0.47
9:i:24:THR:HA	9:i:28:GLY:H	1.79	0.47
5:E:171:ALA:O	5:E:175:GLU:HG2	2.14	0.47
9:I:24:THR:HA	9:I:28:GLY:H	1.79	0.47
3:c:100:THR:OG1	4:d:266:THR:OG1	2.25	0.47
5:e:190:LEU:HD13	11:k:13:PRO:HD3	1.97	0.47
5:E:123:VAL:HG22	5:E:133:LEU:HD23	1.97	0.47
1:a:74:ASN:HB3	3:c:139:SER:HA	1.96	0.47
15:a:406:CDL:HA62	15:a:406:CDL:H121	1.97	0.47
3:c:182:LYS:C	3:c:184:ILE:H	2.23	0.47
5:e:171:ALA:O	5:e:175:GLU:HG2	2.14	0.47
1:A:111:GLU:HG3	15:A:406:CDL:HA31	1.97	0.47
2:b:303:LEU:HB3	3:c:121:THR:OG1	2.15	0.47
3:c:172:LYS:HB3	3:c:215:GLY:HA3	1.97	0.47
5:E:190:LEU:HD13	11:K:13:PRO:HD3	1.96	0.47
10:J:21:ALA:HA	10:J:24:TRP:CD1	2.50	0.47
11:K:27:ARG:N	11:K:28:PRO:CD	2.78	0.47
14:A:405:PEE:H48	8:H:49:VAL:HG11	1.97	0.47
2:b:106:LEU:HB3	2:b:111:ILE:HD11	1.97	0.47
11:K:24:GLY:O	11:K:25:ALA:C	2.57	0.46
1:a:300:ILE:HD11	1:a:363:LEU:HG	1.96	0.46
1:A:58:ASP:HB3	1:A:61:THR:OG1	2.15	0.46
1:a:270:PRO:HG2	1:a:275:LEU:HD23	1.96	0.46
10:j:17:TRP:O	10:j:18:ILE:HB	2.15	0.46
11:k:9:GLY:N	11:k:10:PRO:HD3	2.30	0.46
1:A:47:THR:HG23	1:A:79:ILE:HG23	1.96	0.46
5:E:69:SER:O	5:E:72:GLU:HG2	2.16	0.46
5:e:123:VAL:HG22	5:e:133:LEU:HD23	1.97	0.46
1:A:268:ILE:HG13	3:c:220:LEU:HD11	1.96	0.46
11:k:29:LEU:HD13	11:k:29:LEU:HA	1.73	0.46
2:B:105:SER:HB2	9:I:48:ASN:ND2	2.30	0.46
3:C:92:ARG:HH11	3:C:96:VAL:HB	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:PRO:HG2	1:A:275:LEU:HD23	1.96	0.46
4:d:70:THR:HG21	4:d:407:THR:HA	1.98	0.46
4:D:309:ALA:HB2	11:K:55:LEU:HD11	1.97	0.46
4:D:413:ILE:HG12	4:D:423:ARG:HD2	1.97	0.46
3:c:176:VAL:HA	3:c:212:ILE:HG22	1.96	0.46
6:f:49:ARG:HD3	6:f:49:ARG:HA	1.64	0.46
3:C:93:ARG:HH12	3:C:111:LYS:HD3	1.81	0.46
6:F:49:ARG:HA	6:F:49:ARG:HD3	1.64	0.46
3:c:234:TYR:HB2	3:c:243:TYR:HB2	1.98	0.46
10:j:17:TRP:CE2	10:j:21:ALA:HB2	2.51	0.46
1:a:237:LEU:HB2	2:b:297:MET:HE2	1.98	0.45
9:i:58:HIS:HB2	9:i:62:ASN:HD21	1.81	0.45
2:B:93:PRO:HB3	6:F:80:HIS:CD2	2.50	0.45
11:K:34:LEU:HD12	11:K:34:LEU:HA	1.77	0.45
5:E:179:ALA:HA	5:E:187:ALA:HB1	1.99	0.45
6:F:75:LEU:HD22	6:F:78:ARG:HH21	1.82	0.45
9:I:30:LEU:HD11	10:J:31:GLY:HA2	1.99	0.45
2:B:161:GLU:HB3	2:b:182:ASN:HD21	1.81	0.45
3:C:214:ILE:HG23	3:C:261:PRO:HD3	1.98	0.45
14:a:405:PEE:H19	14:a:405:PEE:H26	1.70	0.45
5:e:179:ALA:HA	5:e:187:ALA:HB1	1.99	0.45
10:J:4:ARG:H	10:J:4:ARG:HG2	1.61	0.45
1:a:69:ILE:H	1:a:69:ILE:HG12	1.44	0.45
3:c:166:ALA:HA	3:c:173:PRO:HB3	1.98	0.45
9:i:63:LYS:HB3	9:i:63:LYS:HE3	1.37	0.45
3:C:115:TYR:HE2	8:H:22:PHE:CE2	2.35	0.44
4:d:55:ASN:HD21	4:d:251:SER:HA	1.82	0.44
3:C:113:PHE:HA	3:C:116:LEU:HD12	1.99	0.44
10:J:18:ILE:HA	10:J:21:ALA:HB3	1.99	0.44
11:K:20:ARG:HB3	11:K:47:ARG:HE	1.83	0.44
6:f:75:LEU:HD22	6:f:78:ARG:HH21	1.82	0.44
4:d:460:GLY:HA2	4:d:462:ILE:HG12	1.99	0.44
4:D:309:ALA:HA	11:K:55:LEU:HD21	2.00	0.44
1:a:211:ILE:H	1:a:211:ILE:HG13	1.67	0.44
3:C:130:LYS:NZ	10:J:34:TRP:HE1	2.16	0.44
3:C:158:ASP:HB2	3:C:159:ILE:HG12	2.00	0.44
3:c:179:ARG:H	3:c:179:ARG:HG2	1.40	0.44
11:K:20:ARG:CD	11:K:52:ARG:HG3	2.47	0.43
3:c:243:TYR:CD2	3:c:258:LEU:HD11	2.53	0.43
7:G:71:MET:HE2	7:G:71:MET:HB3	1.83	0.43
3:c:267:SER:HB2	3:c:270:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:4:VAL:HA	11:k:8:SER:OG	2.18	0.43
3:C:216:VAL:HA	3:C:223:VAL:HG22	1.99	0.43
4:D:37:THR:HG23	4:D:40:GLN:H	1.84	0.43
5:E:212:HIS:CE1	5:E:246:LEU:HB2	2.54	0.43
1:A:168:PHE:HA	3:c:170:ARG:HH12	1.82	0.43
11:K:15:LEU:HD22	11:K:15:LEU:HA	1.63	0.43
11:K:34:LEU:O	11:K:35:PRO:C	2.62	0.43
6:f:36:GLN:HA	6:f:39:GLN:HE21	1.83	0.43
1:a:260:ASN:HB3	1:a:263:ASN:HD21	1.82	0.43
5:e:227:HIS:CD2	5:e:228:PRO:HD3	2.54	0.43
1:A:376:LEU:HD21	7:G:17:ILE:HG22	2.01	0.43
5:E:279:GLY:HA2	11:K:1:MET:HE2	2.00	0.43
3:C:170:ARG:HA	3:C:170:ARG:HD3	1.58	0.43
4:d:52:GLN:HE21	4:d:56:GLY:HA2	1.84	0.43
5:e:65:ILE:HG12	5:e:218:MET:HG2	2.01	0.43
2:B:93:PRO:HB3	6:F:80:HIS:HD2	1.84	0.42
3:C:242:HIS:HB2	3:C:251:LYS:HE3	2.00	0.42
4:D:442:ARG:HH22	10:J:15:ARG:HH22	1.66	0.42
1:a:174:THR:HG22	1:a:175:LEU:HD23	2.02	0.42
8:h:29:HIS:HB3	8:h:33:LYS:HD2	2.01	0.42
8:h:40:ARG:HE	8:h:40:ARG:HB2	1.64	0.42
1:A:261:PRO:HG3	3:c:172:LYS:HG2	2.01	0.42
3:C:101:LYS:HD3	4:D:267:PRO:HG2	2.02	0.42
5:E:398:SER:OG	11:K:3:SER:HB3	2.19	0.42
6:F:36:GLN:HA	6:F:39:GLN:HE21	1.83	0.42
11:K:21:GLY:O	11:K:47:ARG:NE	2.53	0.42
2:b:222:PRO:HG3	2:b:234:PHE:HB2	2.02	0.42
2:b:293:MET:HE3	2:b:293:MET:HB3	1.91	0.42
4:d:220:VAL:HG13	4:d:224:TYR:HD2	1.85	0.42
4:d:413:ILE:HG12	4:d:423:ARG:HD2	2.01	0.42
5:E:171:ALA:CA	11:K:11:PHE:HE1	2.28	0.42
11:k:48:SER:HB2	11:k:51:CYS:HA	2.02	0.42
1:A:174:THR:HG22	1:A:175:LEU:HD23	2.02	0.42
2:B:237:TYR:OH	6:F:79:ASP:OD2	2.27	0.42
3:C:92:ARG:HA	3:C:92:ARG:HD2	1.64	0.42
1:a:132:VAL:HA	1:a:139:SER:HB3	2.02	0.42
5:e:69:SER:O	5:e:72:GLU:HG2	2.20	0.42
5:E:293:LEU:HB3	5:E:309:LEU:HG	2.02	0.42
11:K:43:LEU:HD22	11:K:43:LEU:HA	1.89	0.42
2:b:122:CYS:C	2:b:124:SER:H	2.28	0.41
2:b:201:ILE:HG12	16:b:401:HEC:HMA1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:266:GLN:HA	6:f:90:LEU:HD21	2.02	0.41
3:c:185:ASP:O	3:c:186:GLN:C	2.62	0.41
5:e:155:GLN:HE21	5:e:155:GLN:HB3	1.69	0.41
2:B:114:GLY:HA2	2:B:270:ASP:HB3	2.02	0.41
1:a:188:ILE:HG12	15:a:406:CDL:H151	2.01	0.41
2:b:164:GLU:O	2:b:165:MET:C	2.62	0.41
1:A:69:ILE:H	1:A:69:ILE:HG12	1.44	0.41
5:E:65:ILE:HG12	5:E:218:MET:HG2	2.01	0.41
2:b:195:PRO:HA	2:b:196:PRO:HD3	1.86	0.41
3:c:104:LYS:C	3:c:106:SER:N	2.77	0.41
3:c:146:VAL:HG22	3:c:149:MET:CG	2.43	0.41
4:d:477:TRP:HD1	4:d:480:PHE:H	1.66	0.41
2:b:316:LYS:HD3	7:g:72:ARG:HG2	2.03	0.41
3:c:112:GLY:N	9:i:7:THR:HG22	2.33	0.41
5:E:82:LEU:HD23	5:E:205:LEU:HD11	2.02	0.41
2:b:124:SER:O	2:b:179:PRO:HB2	2.21	0.41
2:B:133:TYR:HD2	2:B:174:ASP:HB3	1.85	0.41
2:B:195:PRO:HA	2:B:196:PRO:HD3	1.84	0.41
2:b:154:GLU:HA	2:b:169:PRO:HA	2.02	0.41
3:c:184:ILE:H	3:c:184:ILE:HG12	1.70	0.41
2:B:194:LEU:HD12	2:B:195:PRO:HD2	2.03	0.41
4:D:220:VAL:HG13	4:D:224:TYR:HD2	1.86	0.41
3:c:121:THR:HG22	3:c:125:VAL:HG23	2.02	0.41
3:c:107:SER:O	3:c:108:ASP:C	2.62	0.41
1:A:132:VAL:HA	1:A:139:SER:HB3	2.02	0.41
5:E:378:LEU:HG	5:E:416:ILE:HD13	2.02	0.41
2:b:150:ALA:HB1	2:b:170:GLY:HA3	2.03	0.41
3:c:217:CYS:HB2	3:c:222:CYS:H	1.86	0.41
1:A:140:PHE:HZ	3:c:172:LYS:HD3	1.86	0.41
3:C:214:ILE:HD12	3:C:216:VAL:HG23	2.02	0.41
9:I:20:THR:HA	9:I:23:LEU:HB2	2.03	0.41
5:e:82:LEU:HD23	5:e:205:LEU:HD11	2.02	0.41
1:A:184:ILE:HD13	1:A:184:ILE:HA	1.96	0.40
14:A:405:PEE:H30	14:A:405:PEE:H35	1.79	0.40
3:c:170:ARG:HA	3:c:170:ARG:HD2	1.29	0.40
5:e:293:LEU:HB3	5:e:309:LEU:HG	2.02	0.40
11:k:43:LEU:HG	11:k:46:LYS:HD3	2.03	0.40
14:a:405:PEE:H50	14:a:405:PEE:H56	1.90	0.40
5:e:378:LEU:HG	5:e:416:ILE:HD13	2.02	0.40
5:E:246:LEU:HD23	5:E:246:LEU:HA	1.87	0.40
11:K:29:LEU:HD13	11:K:29:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:118:TYR:CD1	2:b:122:CYS:SG	3.13	0.40
5:e:134:MET:SD	5:e:233:VAL:HG21	2.62	0.40
5:e:246:LEU:HD23	5:e:246:LEU:HA	1.85	0.40
8:h:25:ARG:HE	8:h:28:PRO:HA	1.86	0.40
1:A:118:VAL:HG21	15:A:406:CDL:H141	2.04	0.40
3:C:215:GLY:HA3	3:C:223:VAL:HG13	2.02	0.40
3:C:264:GLU:HB3	3:C:272:ILE:HB	2.04	0.40
9:i:25:ILE:H	9:i:25:ILE:HG12	1.51	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	A	376/378 (100%)	362 (96%)	14 (4%)	0	100	100
1	a	376/378 (100%)	363 (96%)	13 (4%)	0	100	100
2	B	239/241 (99%)	225 (94%)	13 (5%)	1 (0%)	30	47
2	b	237/241 (98%)	213 (90%)	24 (10%)	0	100	100
3	C	192/196 (98%)	163 (85%)	29 (15%)	0	100	100
3	c	194/196 (99%)	153 (79%)	41 (21%)	0	100	100
4	D	443/446 (99%)	423 (96%)	20 (4%)	0	100	100
4	d	444/446 (100%)	421 (95%)	23 (5%)	0	100	100
5	E	416/418 (100%)	399 (96%)	17 (4%)	0	100	100
5	e	416/418 (100%)	398 (96%)	18 (4%)	0	100	100
6	F	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
6	f	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
7	G	104/106 (98%)	99 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
8	H	69/79 (87%)	61 (88%)	8 (12%)	0	100	100
8	h	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
9	I	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
9	i	60/62 (97%)	49 (82%)	11 (18%)	0	100	100
10	J	47/52 (90%)	42 (89%)	5 (11%)	0	100	100
10	j	49/52 (94%)	42 (86%)	6 (12%)	1 (2%)	6	9
11	K	55/57 (96%)	37 (67%)	10 (18%)	8 (14%)	0	0
11	k	55/57 (96%)	43 (78%)	10 (18%)	2 (4%)	2	3
All	All	4137/4198 (98%)	3826 (92%)	299 (7%)	12 (0%)	37	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	7	ARG
11	K	8	SER
10	j	18	ILE
11	k	27	ARG
11	K	9	GLY
11	K	17	ALA
11	K	49	PHE
2	B	128	MET
11	K	24	GLY
11	K	27	ARG
11	K	13	PRO
11	k	28	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	319 (96%)	12 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	331/331 (100%)	318 (96%)	13 (4%)	28	52
2	B	206/206 (100%)	201 (98%)	5 (2%)	43	69
2	b	204/206 (99%)	191 (94%)	13 (6%)	16	31
3	C	164/166 (99%)	151 (92%)	13 (8%)	11	22
3	c	166/166 (100%)	144 (87%)	22 (13%)	4	7
4	D	371/372 (100%)	365 (98%)	6 (2%)	55	78
4	d	372/372 (100%)	366 (98%)	6 (2%)	55	78
5	E	327/328 (100%)	323 (99%)	4 (1%)	63	82
5	e	327/328 (100%)	322 (98%)	5 (2%)	57	79
6	F	61/61 (100%)	52 (85%)	9 (15%)	3	5
6	f	61/61 (100%)	51 (84%)	10 (16%)	2	4
7	G	95/95 (100%)	94 (99%)	1 (1%)	65	83
7	g	95/95 (100%)	94 (99%)	1 (1%)	65	83
8	H	65/70 (93%)	65 (100%)	0	100	100
8	h	70/70 (100%)	69 (99%)	1 (1%)	59	80
9	I	50/50 (100%)	29 (58%)	21 (42%)	0	0
9	i	50/50 (100%)	33 (66%)	17 (34%)	0	0
10	J	40/42 (95%)	39 (98%)	1 (2%)	42	67
10	j	41/42 (98%)	39 (95%)	2 (5%)	22	43
11	K	44/44 (100%)	18 (41%)	26 (59%)	0	0
11	k	44/44 (100%)	38 (86%)	6 (14%)	3	7
All	All	3515/3530 (100%)	3321 (94%)	194 (6%)	21	38

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	64	SER
1	A	69	ILE
1	A	71	ARG
1	A	151	SER
1	A	160	LEU
1	A	162	GLU
1	A	170	VAL
1	A	246	SER

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Mol	Chain	Res	Type
1	A	264	THR
1	A	284	ILE
1	A	349	ILE
2	B	129	ASP
2	B	187	ARG
2	B	203	ARG
2	B	264	MET
2	B	280	GLU
3	C	92	ARG
3	C	95	GLU
3	C	123	VAL
3	C	154	ILE
3	C	170	ARG
3	C	179	ARG
3	C	180	THR
3	C	216	VAL
3	C	217	CYS
3	C	225	ILE
3	C	227	ASN
3	C	248	ARG
3	C	249	ILE
4	D	58	ARG
4	D	66	GLN
4	D	125	THR
4	D	240	ARG
4	D	477	TRP
4	D	479	ARG
5	E	156	SER
5	E	235	GLU
5	E	238	LEU
5	E	303	SER
6	F	35	GLU
6	F	36	GLN
6	F	38	GLU
6	F	49	ARG
6	F	51	GLU
6	F	56	ARG
6	F	64	GLU
6	F	73	ASP
6	F	90	LEU
7	G	15	GLU
9	I	6	LEU

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Mol	Chain	Res	Type
9	I	7	THR
9	I	9	ARG
9	I	10	LEU
9	I	11	TYR
9	I	13	LEU
9	I	14	LEU
9	I	16	ARG
9	I	17	ARG
9	I	18	THR
9	I	21	PHE
9	I	23	LEU
9	I	25	ILE
9	I	27	VAL
9	I	30	LEU
9	I	34	ARG
9	I	43	ILE
9	I	47	ILE
9	I	60	TYR
9	I	61	GLU
9	I	63	LYS
10	J	48	ILE
11	K	1	MET
11	K	2	LEU
11	K	6	SER
11	K	7	ARG
11	K	13	PRO
11	K	15	LEU
11	K	16	SER
11	K	18	THR
11	K	19	SER
11	K	20	ARG
11	K	22	VAL
11	K	27	ARG
11	K	29	LEU
11	K	30	VAL
11	K	34	LEU
11	K	35	PRO
11	K	38	SER
11	K	40	SER
11	K	42	VAL
11	K	43	LEU
11	K	46	LYS

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Mol	Chain	Res	Type
11	K	48	SER
11	K	49	PHE
11	K	52	ARG
11	K	53	GLU
11	K	55	LEU
1	a	10	LEU
1	a	61	THR
1	a	64	SER
1	a	69	ILE
1	a	151	SER
1	a	160	LEU
1	a	162	GLU
1	a	170	VAL
1	a	246	SER
1	a	263	ASN
1	a	264	THR
1	a	284	ILE
1	a	349	ILE
2	b	123	SER
2	b	127	SER
2	b	142	THR
2	b	164	GLU
2	b	165	MET
2	b	184	GLU
2	b	203	ARG
2	b	209	GLU
2	b	224	THR
2	b	276	ARG
2	b	279	SER
2	b	280	GLU
2	b	309	ARG
3	c	101	LYS
3	c	102	SER
3	c	104	LYS
3	c	105	GLU
3	c	106	SER
3	c	108	ASP
3	c	146	VAL
3	c	147	LEU
3	c	164	ASN
3	c	170	ARG
3	c	172	LYS

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Mol	Chain	Res	Type
3	c	179	ARG
3	c	181	LYS
3	c	182	LYS
3	c	184	ILE
3	c	185	ASP
3	c	186	GLN
3	c	217	CYS
3	c	223	VAL
3	c	238	CYS
3	c	239	HIS
3	c	273	VAL
4	d	37	THR
4	d	70	THR
4	d	71	VAL
4	d	262	VAL
4	d	351	THR
4	d	477	TRP
5	e	69	SER
5	e	156	SER
5	e	227	HIS
5	e	235	GLU
5	e	238	LEU
6	f	28	ASP
6	f	35	GLU
6	f	36	GLN
6	f	38	GLU
6	f	49	ARG
6	f	51	GLU
6	f	56	ARG
6	f	64	GLU
6	f	73	ASP
6	f	90	LEU
7	g	15	GLU
8	h	40	ARG
9	i	10	LEU
9	i	12	SER
9	i	16	ARG
9	i	17	ARG
9	i	18	THR
9	i	21	PHE
9	i	23	LEU
9	i	25	ILE

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Mol	Chain	Res	Type
9	i	27	VAL
9	i	30	LEU
9	i	34	ARG
9	i	43	ILE
9	i	47	ILE
9	i	60	TYR
9	i	61	GLU
9	i	62	ASN
9	i	63	LYS
10	j	20	THR
10	j	36	THR
11	k	4	VAL
11	k	7	ARG
11	k	29	LEU
11	k	30	VAL
11	k	47	ARG
11	k	49	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	207	ASN
2	B	190	ASN
2	B	206	HIS
3	C	164	ASN
3	C	219	HIS
4	D	83	ASN
4	D	87	ASN
4	D	153	ASN
4	D	160	GLN
4	D	193	GLN
4	D	222	GLN
4	D	305	GLN
4	D	464	GLN
5	E	75	ASN
5	E	155	GLN
5	E	206	HIS
5	E	212	HIS
5	E	290	GLN
5	E	298	HIS
5	E	399	GLN

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Mol	Chain	Res	Type
5	E	415	GLN
6	F	39	GLN
6	F	62	GLN
6	F	80	HIS
8	H	13	HIS
10	J	16	ASN
11	K	31	GLN
1	a	148	ASN
2	b	182	ASN
2	b	190	ASN
2	b	310	HIS
3	c	131	ASN
3	c	178	HIS
3	c	200	HIS
3	c	239	HIS
4	d	40	GLN
4	d	55	ASN
4	d	87	ASN
4	d	128	HIS
4	d	193	GLN
4	d	286	HIS
4	d	305	GLN
4	d	345	ASN
4	d	464	GLN
4	d	469	ASN
5	e	75	ASN
5	e	155	GLN
5	e	206	HIS
5	e	227	HIS
5	e	290	GLN
5	e	399	GLN
5	e	415	GLN
6	f	39	GLN
6	f	62	GLN
8	h	65	GLN
11	k	31	GLN

5.3.3 RNA ⓘ

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](#)

16 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	$\# Z > 2$
13	HEM	a	404	1	50,50,50	1.58	7 (14%)	66,82,82	1.40	10 (15%)
16	HEC	b	401	2	50,50,50	2.86	26 (52%)	68,82,82	2.50	26 (38%)
17	FES	c	301	3	0,4,4	-	-	-	-	-
12	A1D6P	a	402	-	31,31,31	1.70	7 (22%)	34,44,44	1.92	6 (17%)
15	CDL	A	406	-	63,63,99	1.08	8 (12%)	69,75,111	1.14	4 (5%)
12	A1D6P	a	401	-	31,31,31	1.65	5 (16%)	34,44,44	1.92	4 (11%)
14	PEE	a	405	-	48,48,50	1.49	5 (10%)	51,53,55	1.31	4 (7%)
13	HEM	A	404	1	50,50,50	1.62	7 (14%)	66,82,82	1.94	19 (28%)
17	FES	C	301	-	0,4,4	-	-	-	-	-
13	HEM	A	403	1	50,50,50	1.62	7 (14%)	66,82,82	1.36	10 (15%)
12	A1D6P	A	402	-	31,31,31	1.71	7 (22%)	34,44,44	1.91	6 (17%)
16	HEC	B	401	2	50,50,50	2.76	28 (56%)	68,82,82	2.62	32 (47%)
12	A1D6P	A	401	-	31,31,31	1.65	6 (19%)	34,44,44	1.92	4 (11%)
15	CDL	a	406	-	63,63,99	1.10	8 (12%)	69,75,111	1.17	4 (5%)
13	HEM	a	403	1	50,50,50	1.53	6 (12%)	66,82,82	1.62	17 (25%)
14	PEE	A	405	-	44,44,50	1.54	5 (11%)	46,49,55	1.38	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HEM	a	404	1	-	2/14/54/54	-
16	HEC	b	401	2	1/1/3/7	8/14/54/54	-
17	FES	c	301	3	-	-	0/1/1/1
12	A1D6P	a	402	-	-	2/13/13/13	0/4/4/4
15	CDL	A	406	-	-	44/74/74/110	-
12	A1D6P	a	401	-	-	2/13/13/13	0/4/4/4
14	PEE	a	405	-	-	26/52/52/54	-
13	HEM	A	404	1	-	4/14/54/54	-
17	FES	C	301	-	-	-	0/1/1/1
12	A1D6P	A	402	-	-	2/13/13/13	0/4/4/4
13	HEM	A	403	1	-	2/14/54/54	-
16	HEC	B	401	2	1/1/3/7	8/14/54/54	-
12	A1D6P	A	401	-	-	2/13/13/13	0/4/4/4
15	CDL	a	406	-	-	37/74/74/110	-
13	HEM	a	403	1	-	6/14/54/54	-
14	PEE	A	405	-	-	28/48/48/54	-

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	403	HEM	FE-ND	5.76	2.12	1.94
13	A	404	HEM	FE-ND	5.67	2.12	1.94
13	a	404	HEM	FE-ND	5.46	2.11	1.94
13	a	403	HEM	FE-ND	5.31	2.11	1.94
13	A	404	HEM	FE-NB	5.30	2.11	1.94
16	b	401	HEC	C2A-C3A	5.13	1.47	1.36
16	B	401	HEC	C3B-C2B	5.01	1.47	1.36
16	b	401	HEC	C3D-C2D	4.99	1.47	1.36
16	b	401	HEC	FE-NB	4.92	2.10	1.94
16	b	401	HEC	CHC-C4B	4.90	1.48	1.38
16	B	401	HEC	CHA-C1A	4.88	1.47	1.38
16	b	401	HEC	FE-ND	4.87	2.09	1.94
16	B	401	HEC	FE-NB	4.86	2.09	1.94
16	B	401	HEC	FE-ND	4.75	2.09	1.94
16	B	401	HEC	FE-NC	4.74	2.11	1.95
16	b	401	HEC	C3B-C2B	4.74	1.46	1.36
12	A	402	A1D6P	O1-C8	4.73	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	402	A1D6P	O1-C8	4.64	1.40	1.35
16	b	401	HEC	CHA-C1A	4.63	1.47	1.38
16	B	401	HEC	C3D-C2D	4.63	1.46	1.36
16	b	401	HEC	CHD-C1D	4.62	1.47	1.38
16	b	401	HEC	CHB-C4A	4.61	1.47	1.38
13	a	403	HEM	FE-NB	4.60	2.09	1.94
16	B	401	HEC	CHB-C4A	4.60	1.47	1.38
16	B	401	HEC	FE-NA	4.59	2.10	1.95
16	B	401	HEC	C2A-C3A	4.59	1.46	1.36
12	A	401	A1D6P	O1-C8	4.49	1.40	1.35
12	a	401	A1D6P	O1-C8	4.46	1.40	1.35
14	a	405	PEE	C39-C38	4.40	1.57	1.31
13	A	403	HEM	FE-NC	4.38	2.10	1.95
14	A	405	PEE	C39-C38	4.32	1.56	1.31
16	b	401	HEC	FE-NA	4.22	2.09	1.95
16	B	401	HEC	CHD-C1D	4.20	1.47	1.38
16	b	401	HEC	FE-NC	4.18	2.09	1.95
14	A	405	PEE	C18-C19	4.16	1.55	1.31
14	a	405	PEE	C18-C19	4.16	1.55	1.31
13	a	404	HEM	FE-NA	4.03	2.08	1.95
16	b	401	HEC	CHD-C4C	4.00	1.48	1.39
13	a	404	HEM	FE-NC	3.95	2.08	1.95
12	a	401	A1D6P	N3-N2	-3.91	1.32	1.37
13	A	403	HEM	FE-NA	3.91	2.08	1.95
12	A	401	A1D6P	N3-N2	-3.89	1.32	1.37
16	B	401	HEC	CHA-C4D	3.87	1.48	1.39
12	A	402	A1D6P	N3-N2	-3.86	1.32	1.37
16	b	401	HEC	CHC-C1C	3.85	1.48	1.39
12	a	402	A1D6P	N3-N2	-3.84	1.32	1.37
16	B	401	HEC	CHC-C4B	3.79	1.46	1.38
16	b	401	HEC	CHA-C4D	3.71	1.47	1.39
16	B	401	HEC	CHB-C1B	3.70	1.47	1.39
16	b	401	HEC	C3C-C2C	3.57	1.48	1.38
16	b	401	HEC	CHB-C1B	3.45	1.47	1.39
14	a	405	PEE	O3-C30	3.36	1.43	1.33
16	B	401	HEC	CHD-C4C	3.35	1.46	1.39
14	A	405	PEE	O3-C30	3.28	1.42	1.33
12	a	401	A1D6P	C9-N3	-3.21	1.31	1.35
16	b	401	HEC	C1D-ND	-3.19	1.34	1.40
12	A	401	A1D6P	C9-N3	-3.16	1.31	1.35
13	a	404	HEM	CAB-C3B	3.16	1.56	1.47
13	a	404	HEM	CAC-C3C	3.15	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	403	HEM	CAB-C3B	3.14	1.56	1.47
13	A	403	HEM	CAC-C3C	3.11	1.55	1.47
12	A	402	A1D6P	C9-N3	-3.10	1.31	1.35
12	a	402	A1D6P	C9-N3	-3.05	1.31	1.35
16	B	401	HEC	C3C-C2C	3.03	1.46	1.38
16	B	401	HEC	C1D-ND	-3.03	1.35	1.40
14	A	405	PEE	O2-C10	3.02	1.42	1.34
16	B	401	HEC	C4B-NB	-3.00	1.35	1.40
16	B	401	HEC	CHC-C1C	2.97	1.46	1.39
14	a	405	PEE	O2-C10	2.90	1.42	1.34
16	b	401	HEC	C4B-NB	-2.86	1.35	1.40
16	B	401	HEC	C1A-NA	-2.80	1.34	1.39
16	b	401	HEC	C4B-C3B	2.79	1.49	1.45
13	a	403	HEM	CAC-C3C	2.76	1.54	1.47
16	b	401	HEC	C4A-NA	-2.75	1.34	1.39
13	a	403	HEM	CAB-C3B	2.72	1.54	1.47
13	A	404	HEM	CAB-C3B	2.67	1.54	1.47
13	A	404	HEM	CAC-C3C	2.62	1.54	1.47
15	A	406	CDL	OB8-CB7	2.61	1.41	1.33
16	b	401	HEC	C1A-NA	-2.56	1.34	1.39
15	a	406	CDL	OA6-CA4	-2.54	1.40	1.46
14	a	405	PEE	O2-C2	-2.51	1.40	1.46
15	A	406	CDL	OA6-CA4	-2.50	1.40	1.46
12	a	401	A1D6P	O1-C7	-2.49	1.40	1.45
16	b	401	HEC	C1C-C2C	2.49	1.49	1.43
16	b	401	HEC	C4C-NC	-2.48	1.35	1.39
12	A	401	A1D6P	O1-C7	-2.48	1.40	1.45
12	A	402	A1D6P	O1-C7	-2.46	1.40	1.45
12	A	402	A1D6P	O2-C18	-2.44	1.18	1.22
16	B	401	HEC	C4A-NA	-2.44	1.35	1.39
16	B	401	HEC	C4C-NC	-2.43	1.35	1.39
15	a	406	CDL	OA6-CA5	2.43	1.41	1.34
12	A	401	A1D6P	O2-C18	-2.43	1.18	1.22
12	a	402	A1D6P	O1-C7	-2.42	1.40	1.45
12	a	402	A1D6P	O2-C18	-2.41	1.18	1.22
15	A	406	CDL	OA8-CA7	2.39	1.40	1.33
15	a	406	CDL	OA8-CA7	2.38	1.40	1.33
12	a	401	A1D6P	O2-C18	-2.37	1.18	1.22
15	a	406	CDL	OB8-CB7	2.35	1.40	1.33
15	a	406	CDL	OB6-CB4	-2.33	1.40	1.46
16	b	401	HEC	C1C-NC	-2.33	1.35	1.39
14	A	405	PEE	O2-C2	-2.32	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	406	CDL	OA8-CA6	-2.29	1.39	1.45
13	A	404	HEM	C3B-C2B	-2.24	1.32	1.37
15	A	406	CDL	OB6-CB4	-2.24	1.41	1.46
16	B	401	HEC	C1C-NC	-2.22	1.35	1.39
15	a	406	CDL	OB8-CB6	-2.22	1.40	1.45
15	a	406	CDL	OB6-CB5	2.22	1.40	1.34
15	A	406	CDL	OA6-CA5	2.20	1.40	1.34
16	b	401	HEC	C1D-C2D	2.19	1.48	1.44
12	a	402	A1D6P	C1-N1	2.18	1.46	1.43
13	A	404	HEM	C2A-C3A	-2.18	1.33	1.38
16	B	401	HEC	C1A-C2A	2.18	1.49	1.45
13	a	403	HEM	C3B-C2B	-2.15	1.32	1.37
12	A	402	A1D6P	C1-N1	2.14	1.46	1.43
15	a	406	CDL	OA8-CA6	-2.14	1.40	1.45
16	B	401	HEC	C4D-ND	-2.14	1.34	1.38
15	A	406	CDL	OB8-CB6	-2.11	1.40	1.45
15	A	406	CDL	OB6-CB5	2.09	1.40	1.34
13	a	403	HEM	C2A-C3A	-2.08	1.33	1.38
13	A	403	HEM	CMB-C2B	2.07	1.55	1.50
16	B	401	HEC	O2D-CGD	-2.06	1.23	1.30
16	B	401	HEC	C1B-C2B	2.06	1.48	1.44
13	A	404	HEM	CAD-C3D	2.05	1.56	1.51
12	A	402	A1D6P	C9-C10	2.05	1.42	1.37
16	b	401	HEC	C4D-C3D	2.05	1.48	1.45
13	A	403	HEM	CMD-C2D	2.04	1.55	1.50
13	a	404	HEM	C2A-C3A	-2.03	1.33	1.38
12	a	402	A1D6P	C9-C10	2.03	1.42	1.37
13	a	404	HEM	CMB-C2B	2.01	1.55	1.50
12	A	401	A1D6P	C9-C10	2.01	1.41	1.37
16	B	401	HEC	C4A-C3A	2.01	1.49	1.45
16	B	401	HEC	O2A-CGA	-2.00	1.24	1.30

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	402	A1D6P	C10-C8-N2	-7.59	107.77	113.53
12	A	402	A1D6P	C10-C8-N2	-7.54	107.80	113.53
12	a	401	A1D6P	C10-C8-N2	-7.19	108.07	113.53
12	A	401	A1D6P	C10-C8-N2	-7.16	108.09	113.53
16	b	401	HEC	CAB-C3B-C4B	5.89	132.45	124.81
13	A	404	HEM	CAD-C3D-C4D	5.85	134.88	124.66
16	B	401	HEC	C1B-C2B-C3B	-5.75	100.91	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	401	HEC	C1B-C2B-C3B	-5.62	101.05	106.96
16	B	401	HEC	C1C-C2C-C3C	-5.52	100.37	106.83
16	B	401	HEC	C2B-C1B-NB	5.29	116.22	109.88
16	b	401	HEC	C2B-C1B-NB	5.19	116.10	109.88
13	A	404	HEM	CAD-C3D-C2D	-5.18	118.23	127.88
16	B	401	HEC	C2A-C1A-NA	5.16	115.34	110.32
16	b	401	HEC	C1C-C2C-C3C	-5.14	100.81	106.83
14	A	405	PEE	O2-C10-C11	4.96	122.20	111.50
16	b	401	HEC	C2A-C1A-NA	4.90	115.09	110.32
16	b	401	HEC	C3D-C4D-ND	4.78	114.99	110.36
16	B	401	HEC	C2D-C1D-ND	4.75	115.46	109.84
16	B	401	HEC	C1D-C2D-C3D	-4.63	102.08	106.96
14	a	405	PEE	O2-C10-C11	4.63	121.47	111.50
16	b	401	HEC	CBC-CAC-C3C	4.49	124.82	112.43
16	B	401	HEC	C2C-C1C-NC	4.44	116.83	110.08
16	b	401	HEC	CBB-CAB-C3B	4.35	124.43	112.43
15	a	406	CDL	OB6-CB5-C51	4.35	120.87	111.50
15	a	406	CDL	OA6-CA5-C11	4.31	120.79	111.50
16	B	401	HEC	C3D-C4D-ND	4.20	114.42	110.36
16	b	401	HEC	C2D-C1D-ND	4.19	114.81	109.84
16	B	401	HEC	CBC-CAC-C3C	4.16	123.90	112.43
12	A	401	A1D6P	C19-N4-N5	4.12	128.46	121.14
16	B	401	HEC	CBB-CAB-C3B	4.11	123.78	112.43
12	a	401	A1D6P	C19-N4-N5	4.09	128.41	121.14
16	b	401	HEC	C1D-C2D-C3D	-3.84	102.92	106.96
15	A	406	CDL	OA6-CA5-C11	3.81	119.72	111.50
16	B	401	HEC	C4A-C3A-C2A	-3.81	101.38	106.94
13	a	404	HEM	C1B-NB-C4B	3.75	108.94	105.07
16	B	401	HEC	C3A-C4A-NA	3.71	116.54	109.69
13	A	403	HEM	C1B-NB-C4B	3.70	108.89	105.07
14	A	405	PEE	C3-C2-C1	-3.69	103.06	111.79
12	a	401	A1D6P	C1-N1-N6	3.65	126.99	120.39
16	b	401	HEC	C2C-C1C-NC	3.64	115.62	110.08
12	A	401	A1D6P	C1-N1-N6	3.63	126.94	120.39
16	B	401	HEC	CBD-CAD-C3D	-3.59	102.65	112.63
16	b	401	HEC	C1A-C2A-C3A	-3.58	102.46	107.13
16	B	401	HEC	C3B-C4B-NB	3.52	114.09	110.17
15	A	406	CDL	OB6-CB5-C51	3.51	119.06	111.50
16	B	401	HEC	C3C-C4C-NC	3.51	114.07	110.15
13	a	403	HEM	C1B-NB-C4B	3.47	108.65	105.07
12	A	401	A1D6P	C11-N3-N2	3.41	124.17	119.96
13	A	403	HEM	C4D-ND-C1D	3.37	108.55	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	401	A1D6P	C11-N3-N2	3.36	124.11	119.96
13	A	404	HEM	CHA-C4D-C3D	3.32	131.56	125.33
13	A	404	HEM	CHD-C4C-NC	3.32	128.03	124.44
13	a	404	HEM	C4D-ND-C1D	3.30	108.48	105.07
16	B	401	HEC	CHA-C1A-NA	-3.23	120.95	124.44
13	A	404	HEM	C1B-NB-C4B	3.17	108.35	105.07
13	a	404	HEM	C4C-NC-C1C	3.15	108.44	105.35
13	A	403	HEM	C4C-NC-C1C	3.14	108.42	105.35
13	A	404	HEM	C4D-ND-C1D	3.12	108.30	105.07
16	b	401	HEC	CAB-C3B-C2B	-3.11	122.21	127.53
16	B	401	HEC	CAA-CBA-CGA	-3.10	106.93	113.60
16	B	401	HEC	CMC-C2C-C3C	3.09	132.29	125.61
13	a	403	HEM	C2A-C1A-NA	-3.09	106.69	110.15
16	B	401	HEC	CAD-CBD-CGD	-3.07	106.99	113.60
13	a	403	HEM	CHD-C4C-NC	3.07	127.76	124.44
13	A	404	HEM	C2A-C1A-NA	-3.06	106.73	110.15
12	a	402	A1D6P	C11-N3-N2	3.03	123.70	119.96
16	b	401	HEC	CMC-C2C-C3C	3.01	132.13	125.61
13	a	403	HEM	C4A-NA-C1A	3.01	108.29	105.35
12	A	402	A1D6P	C1-N1-N6	3.00	125.80	120.39
12	A	402	A1D6P	C11-N3-N2	3.00	123.66	119.96
12	a	402	A1D6P	C1-N1-N6	2.99	125.79	120.39
13	A	403	HEM	CMB-C2B-C1B	-2.98	120.50	125.04
13	a	404	HEM	C4A-NA-C1A	2.98	108.26	105.35
16	b	401	HEC	C3A-C4A-NA	2.94	115.11	109.69
13	a	403	HEM	C3B-C2B-C1B	2.93	108.66	106.49
13	A	403	HEM	C4A-NA-C1A	2.93	108.22	105.35
13	a	403	HEM	CBA-CAA-C2A	-2.93	104.50	112.63
16	b	401	HEC	CMB-C2B-C1B	2.92	129.49	125.04
13	A	404	HEM	C3B-C2B-C1B	2.91	108.65	106.49
15	A	406	CDL	OB8-CB7-C71	2.90	121.00	111.91
16	B	401	HEC	CHB-C4A-NA	-2.90	121.31	124.44
13	A	404	HEM	C4A-NA-C1A	2.88	108.17	105.35
16	b	401	HEC	C4D-C3D-C2D	-2.86	102.73	106.90
13	a	404	HEM	CMB-C2B-C1B	-2.85	120.70	125.04
13	A	404	HEM	CHA-C4D-ND	-2.83	120.89	124.37
16	b	401	HEC	CHC-C4B-NB	-2.81	120.91	124.37
13	a	403	HEM	C4D-ND-C1D	2.80	107.97	105.07
16	b	401	HEC	C4A-C3A-C2A	-2.78	102.88	106.94
16	B	401	HEC	CMA-C3A-C4A	2.78	129.62	124.71
16	B	401	HEC	CHB-C1B-C2B	-2.75	120.68	124.98
16	B	401	HEC	CAC-C3C-C2C	2.74	131.25	126.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	401	HEC	C1A-C2A-C3A	-2.72	103.58	107.13
16	b	401	HEC	C3C-C4C-NC	2.66	113.12	110.15
12	a	402	A1D6P	C9-N3-N2	-2.63	109.58	111.71
13	A	404	HEM	CBD-CAD-C3D	2.62	119.91	112.63
15	A	406	CDL	OA8-CA7-C31	2.62	120.14	111.91
13	A	404	HEM	CAB-C3B-C2B	-2.62	119.97	128.60
15	a	406	CDL	OB8-CB7-C71	2.61	120.11	111.91
16	B	401	HEC	CHC-C1C-C2C	-2.61	119.86	127.24
12	A	402	A1D6P	C9-N3-N2	-2.58	109.62	111.71
16	b	401	HEC	CMD-C2D-C1D	2.57	128.95	125.04
13	a	403	HEM	CAD-CBD-CGD	-2.57	108.08	113.60
14	a	405	PEE	O3-C30-C31	2.55	119.92	111.91
15	a	406	CDL	OA8-CA7-C31	2.55	119.91	111.91
14	a	405	PEE	C3-C2-C1	-2.53	105.80	111.79
16	b	401	HEC	CAA-CBA-CGA	-2.51	108.20	113.60
13	a	403	HEM	CAB-C3B-C2B	-2.50	120.35	128.60
16	B	401	HEC	CMD-C2D-C1D	2.47	128.81	125.04
12	a	402	A1D6P	C19-N4-N5	2.47	125.53	121.14
12	A	402	A1D6P	C19-N4-N5	2.46	125.51	121.14
16	B	401	HEC	CAA-C2A-C1A	2.46	129.53	124.89
13	A	404	HEM	CAC-C3C-C4C	-2.45	118.98	124.90
16	b	401	HEC	CAC-C3C-C2C	2.44	130.77	126.86
13	A	404	HEM	CHC-C4B-C3B	2.41	130.32	125.13
13	a	403	HEM	CAC-C3C-C4C	-2.41	119.07	124.90
16	b	401	HEC	CAD-C3D-C4D	2.41	128.86	124.66
16	B	401	HEC	CMB-C2B-C3B	2.40	132.64	126.12
13	a	403	HEM	CHC-C4B-C3B	2.40	130.30	125.13
13	A	404	HEM	C3D-C4D-ND	-2.35	107.55	110.17
13	a	403	HEM	CHC-C1C-NC	2.33	126.96	124.44
16	b	401	HEC	CHB-C1B-C2B	-2.31	121.36	124.98
13	a	404	HEM	C3B-C2B-C1B	2.31	108.20	106.49
13	a	403	HEM	C4C-NC-C1C	2.30	107.61	105.35
13	A	404	HEM	C4C-NC-C1C	2.29	107.59	105.35
13	A	404	HEM	CHC-C1C-NC	2.29	126.92	124.44
12	a	402	A1D6P	O1-C7-C2	2.28	111.33	107.69
13	A	403	HEM	C3B-C2B-C1B	2.27	108.17	106.49
16	B	401	HEC	C4A-NA-C1A	-2.26	103.13	105.35
12	A	402	A1D6P	O1-C7-C2	2.26	111.30	107.69
13	A	404	HEM	CHB-C4A-NA	2.24	127.97	123.85
16	B	401	HEC	CAD-C3D-C4D	2.21	128.52	124.66
13	A	403	HEM	C3D-C4D-ND	-2.20	107.71	110.17
14	A	405	PEE	O3-C30-C31	2.18	118.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	403	HEM	C2A-C1A-NA	-2.17	107.72	110.15
13	a	403	HEM	C3D-C4D-ND	-2.16	107.76	110.17
13	a	404	HEM	C2A-C1A-NA	-2.15	107.74	110.15
16	B	401	HEC	C4D-C3D-C2D	-2.15	103.77	106.90
13	A	404	HEM	C1D-C2D-C3D	2.14	109.20	106.96
13	a	404	HEM	CAC-C3C-C4C	-2.12	119.78	124.90
13	a	403	HEM	CHB-C4A-NA	2.11	127.73	123.85
13	a	403	HEM	CAD-C3D-C2D	-2.10	123.96	127.88
13	a	404	HEM	C3D-C4D-ND	-2.10	107.83	110.17
14	a	405	PEE	C17-C18-C19	-2.08	108.74	124.73
16	B	401	HEC	CBA-CAA-C2A	-2.07	106.88	112.63
13	a	404	HEM	CHB-C1B-NB	2.06	126.92	124.37
14	A	405	PEE	C12-C11-C10	-2.04	106.19	113.62
16	b	401	HEC	C3B-C4B-NB	2.02	112.42	110.17
13	A	403	HEM	CHB-C1B-NB	2.02	126.86	124.37
14	A	405	PEE	C17-C18-C19	-2.02	109.26	124.73
13	a	403	HEM	CHA-C1A-NA	2.00	127.53	123.85
13	A	403	HEM	C2D-C1D-ND	-2.00	107.48	109.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	B	401	HEC	NA
16	b	401	HEC	NA

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	401	A1D6P	C10-C8-O1-C7
12	A	402	A1D6P	C10-C8-O1-C7
12	A	402	A1D6P	N2-C8-O1-C7
12	a	401	A1D6P	C10-C8-O1-C7
12	a	402	A1D6P	C10-C8-O1-C7
12	a	402	A1D6P	N2-C8-O1-C7
13	A	404	HEM	C2D-C3D-CAD-CBD
13	A	404	HEM	C4D-C3D-CAD-CBD
14	A	405	PEE	C1-O3P-P-O4P
14	A	405	PEE	C4-O4P-P-O1P
14	A	405	PEE	C5-C4-O4P-P
14	A	405	PEE	O4P-C4-C5-N
14	a	405	PEE	C1-O3P-P-O1P
14	a	405	PEE	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
14	a	405	PEE	C5-C4-O4P-P
14	a	405	PEE	O4P-C4-C5-N
15	A	406	CDL	CB2-OB2-PB2-OB3
15	A	406	CDL	CB2-OB2-PB2-OB4
15	A	406	CDL	CB2-OB2-PB2-OB5
15	A	406	CDL	OB9-CB7-OB8-CB6
15	A	406	CDL	C71-CB7-OB8-CB6
15	a	406	CDL	CA2-OA2-PA1-OA3
15	a	406	CDL	CA2-OA2-PA1-OA5
15	a	406	CDL	CA3-OA5-PA1-OA2
15	a	406	CDL	CA3-OA5-PA1-OA3
15	a	406	CDL	CA3-OA5-PA1-OA4
15	a	406	CDL	OB6-CB4-CB6-OB8
15	a	406	CDL	OB7-CB5-OB6-CB4
16	b	401	HEC	C2B-C3B-CAB-CBB
16	b	401	HEC	C4B-C3B-CAB-CBB
15	A	406	CDL	OA9-CA7-OA8-CA6
15	a	406	CDL	OB9-CB7-OB8-CB6
15	a	406	CDL	C71-CB7-OB8-CB6
16	B	401	HEC	C2B-C3B-CAB-CBB
16	B	401	HEC	C4B-C3B-CAB-CBB
14	a	405	PEE	O5-C30-O3-C3
16	B	401	HEC	C4C-C3C-CAC-CBC
16	b	401	HEC	C4C-C3C-CAC-CBC
16	B	401	HEC	C2C-C3C-CAC-CBC
16	b	401	HEC	C2C-C3C-CAC-CBC
15	A	406	CDL	OB7-CB5-OB6-CB4
14	a	405	PEE	C31-C30-O3-C3
15	A	406	CDL	C31-CA7-OA8-CA6
15	a	406	CDL	C51-CB5-OB6-CB4
14	A	405	PEE	C14-C15-C16-C17
14	A	405	PEE	C37-C38-C39-C40
15	A	406	CDL	O1-C1-CA2-OA2
15	A	406	CDL	O1-C1-CB2-OB2
15	A	406	CDL	C11-CA5-OA6-CA4
15	A	406	CDL	C51-CB5-OB6-CB4
16	b	401	HEC	C3D-CAD-CBD-CGD
15	A	406	CDL	CB2-C1-CA2-OA2
15	A	406	CDL	OA7-CA5-OA6-CA4
14	a	405	PEE	C14-C15-C16-C17
15	A	406	CDL	CA7-C31-C32-C33
15	A	406	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	a	405	PEE	C17-C18-C19-C20
14	A	405	PEE	C4-O4P-P-O3P
14	a	405	PEE	C4-O4P-P-O3P
15	A	406	CDL	CA2-C1-CB2-OB2
15	a	406	CDL	C31-CA7-OA8-CA6
15	A	406	CDL	C31-C32-C33-C34
15	a	406	CDL	C11-CA5-OA6-CA4
14	A	405	PEE	C21-C22-C23-C24
14	a	405	PEE	C12-C13-C14-C15
15	a	406	CDL	C11-C12-C13-C14
15	a	406	CDL	C52-C53-C54-C55
14	A	405	PEE	C33-C34-C35-C36
15	a	406	CDL	OA7-CA5-OA6-CA4
15	A	406	CDL	CB5-C51-C52-C53
15	a	406	CDL	C72-C73-C74-C75
14	a	405	PEE	C22-C23-C24-C25
15	a	406	CDL	OA9-CA7-OA8-CA6
15	A	406	CDL	C54-C55-C56-C57
14	A	405	PEE	C12-C13-C14-C15
14	A	405	PEE	C30-C31-C32-C33
14	A	405	PEE	C11-C10-O2-C2
14	a	405	PEE	C11-C10-O2-C2
14	A	405	PEE	O3P-C1-C2-O2
15	A	406	CDL	OA5-CA3-CA4-OA6
15	A	406	CDL	C74-C75-C76-C77
14	A	405	PEE	O4-C10-O2-C2
14	a	405	PEE	O4-C10-O2-C2
14	A	405	PEE	O3P-C1-C2-C3
15	A	406	CDL	OA5-CA3-CA4-CA6
15	A	406	CDL	OB5-CB3-CB4-CB6
15	a	406	CDL	CA4-CA6-OA8-CA7
15	A	406	CDL	CA3-CA4-CA6-OA8
15	a	406	CDL	CB3-CB4-CB6-OB8
15	A	406	CDL	C72-C73-C74-C75
14	a	405	PEE	C42-C43-C44-C45
15	A	406	CDL	CB6-CB4-OB6-CB5
15	A	406	CDL	C33-C34-C35-C36
14	A	405	PEE	C13-C14-C15-C16
15	A	406	CDL	C51-C52-C53-C54
14	a	405	PEE	C37-C38-C39-C40
14	a	405	PEE	C23-C24-C25-C26
15	a	406	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
15	A	406	CDL	C1-CB2-OB2-PB2
13	a	403	HEM	C3D-CAD-CBD-CGD
14	A	405	PEE	C1-C2-C3-O3
14	a	405	PEE	C33-C34-C35-C36
14	A	405	PEE	C10-C11-C12-C13
15	a	406	CDL	OB5-CB3-CB4-OB6
15	a	406	CDL	CB7-C71-C72-C73
15	A	406	CDL	OA6-CA4-CA6-OA8
15	A	406	CDL	OB6-CB4-CB6-OB8
15	a	406	CDL	CA4-CA3-OA5-PA1
14	A	405	PEE	C38-C39-C40-C41
14	a	405	PEE	C11-C12-C13-C14
14	A	405	PEE	C16-C17-C18-C19
14	A	405	PEE	C2-C1-O3P-P
13	A	404	HEM	C4B-C3B-CAB-CBB
14	A	405	PEE	O2-C2-C3-O3
15	a	406	CDL	CA5-C11-C12-C13
15	A	406	CDL	CA3-OA5-PA1-OA2
14	a	405	PEE	C4-O4P-P-O2P
15	a	406	CDL	C14-C15-C16-C17
15	A	406	CDL	OB5-CB3-CB4-OB6
15	a	406	CDL	C12-C13-C14-C15
15	a	406	CDL	C71-C72-C73-C74
14	a	405	PEE	C32-C33-C34-C35
14	A	405	PEE	C34-C35-C36-C37
15	A	406	CDL	C75-C76-C77-C78
15	A	406	CDL	CA6-CA4-OA6-CA5
15	a	406	CDL	OB5-CB3-CB4-CB6
14	a	405	PEE	C2-C1-O3P-P
15	a	406	CDL	CB3-OB5-PB2-OB2
15	A	406	CDL	CB3-CB4-CB6-OB8
14	a	405	PEE	C38-C39-C40-C41
15	A	406	CDL	C53-C54-C55-C56
15	A	406	CDL	CA4-CA3-OA5-PA1
14	A	405	PEE	C36-C37-C38-C39
15	A	406	CDL	C55-C56-C57-C58
14	a	405	PEE	C13-C14-C15-C16
15	A	406	CDL	C15-C16-C17-C18
14	a	405	PEE	C35-C36-C37-C38
15	a	406	CDL	C54-C55-C56-C57
15	A	406	CDL	C73-C74-C75-C76
14	a	405	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
15	a	406	CDL	C13-C14-C15-C16
13	A	403	HEM	CAA-CBA-CGA-O2A
13	a	404	HEM	CAA-CBA-CGA-O2A
15	a	406	CDL	C32-C31-CA7-OA8
13	a	403	HEM	CAA-CBA-CGA-O2A
14	A	405	PEE	C24-C25-C26-C27
15	a	406	CDL	C53-C54-C55-C56
15	A	406	CDL	C11-C12-C13-C14
16	b	401	HEC	CAD-CBD-CGD-O1D
13	a	403	HEM	CAA-CBA-CGA-O1A
13	a	403	HEM	C4B-C3B-CAB-CBB
14	a	405	PEE	C18-C19-C20-C21
15	a	406	CDL	C51-C52-C53-C54
16	b	401	HEC	CAD-CBD-CGD-O2D
13	a	403	HEM	CAD-CBD-CGD-O1D
13	a	404	HEM	CAA-CBA-CGA-O1A
15	a	406	CDL	C12-C11-CA5-OA6
13	A	403	HEM	CAA-CBA-CGA-O1A
14	A	405	PEE	C22-C23-C24-C25
14	A	405	PEE	C20-C21-C22-C23
15	a	406	CDL	C32-C31-CA7-OA9
16	B	401	HEC	CAA-CBA-CGA-O2A
12	A	401	A1D6P	N2-C8-O1-C7
12	a	401	A1D6P	N2-C8-O1-C7
15	A	406	CDL	CA3-OA5-PA1-OA3
16	B	401	HEC	CAD-CBD-CGD-O2D
16	B	401	HEC	CAA-CBA-CGA-O1A
13	a	403	HEM	CAD-CBD-CGD-O2D
16	b	401	HEC	C3A-C2A-CAA-CBA
16	B	401	HEC	CAD-CBD-CGD-O1D
13	A	404	HEM	CAA-CBA-CGA-O1A
14	A	405	PEE	O3-C30-C31-C32
15	a	406	CDL	C12-C11-CA5-OA7

There are no ring outliers.

6 monomers are involved in 20 short contacts:

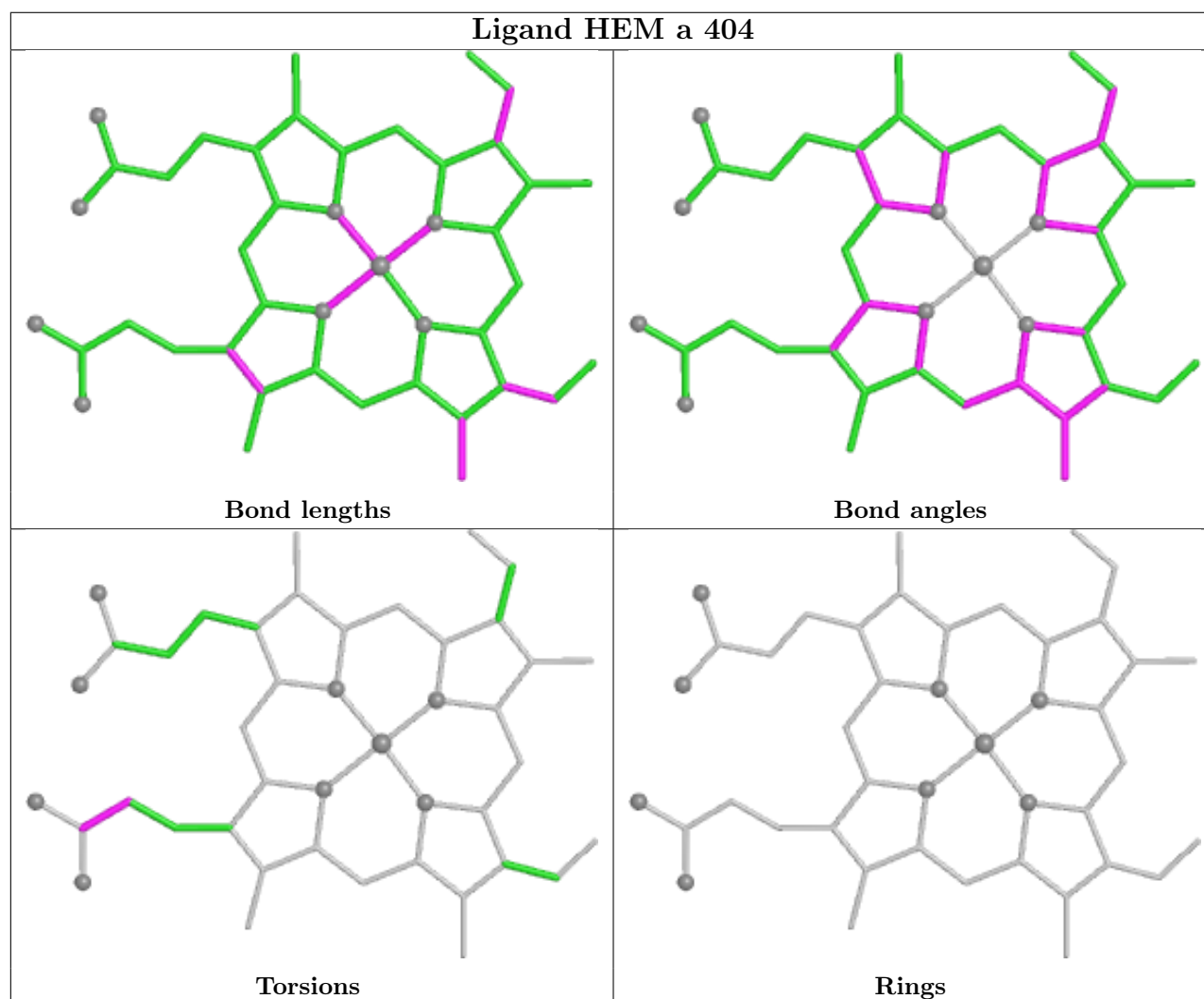
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	401	HEC	4	0
15	A	406	CDL	2	0
14	a	405	PEE	3	0
16	B	401	HEC	5	0

Continued on next page...

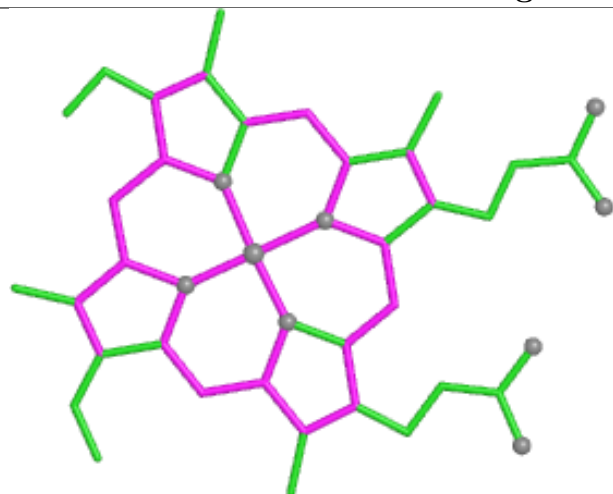
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a	406	CDL	2	0
14	A	405	PEE	4	0

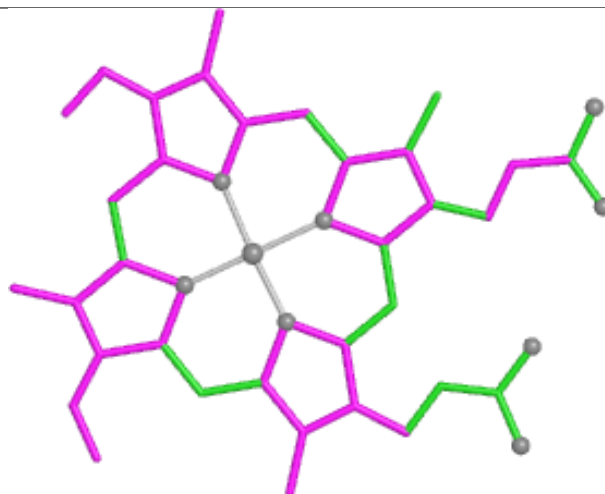
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



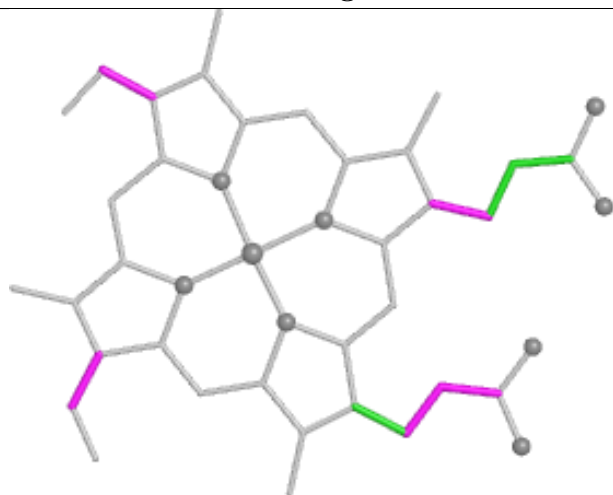
Ligand HEC b 401



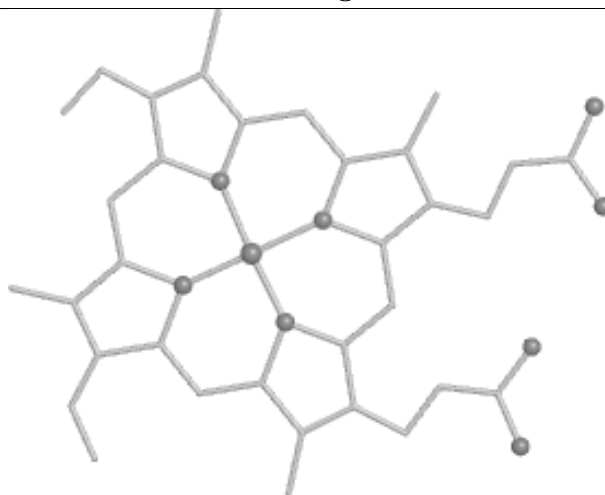
Bond lengths



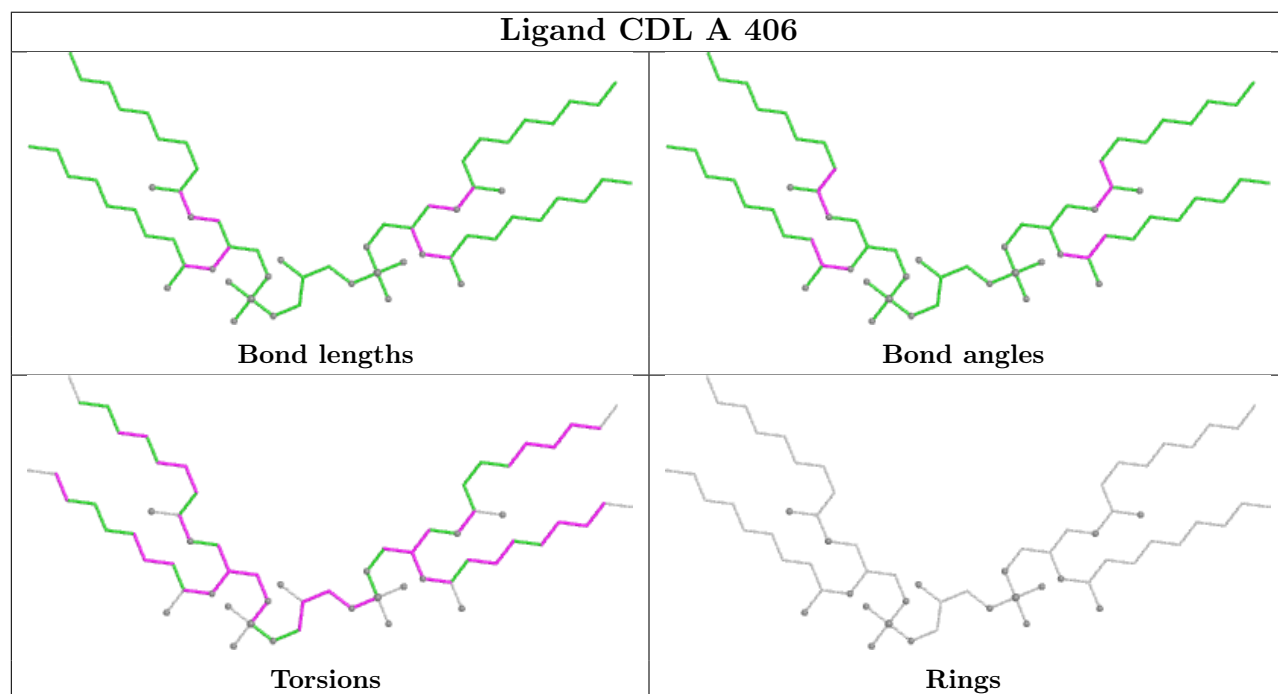
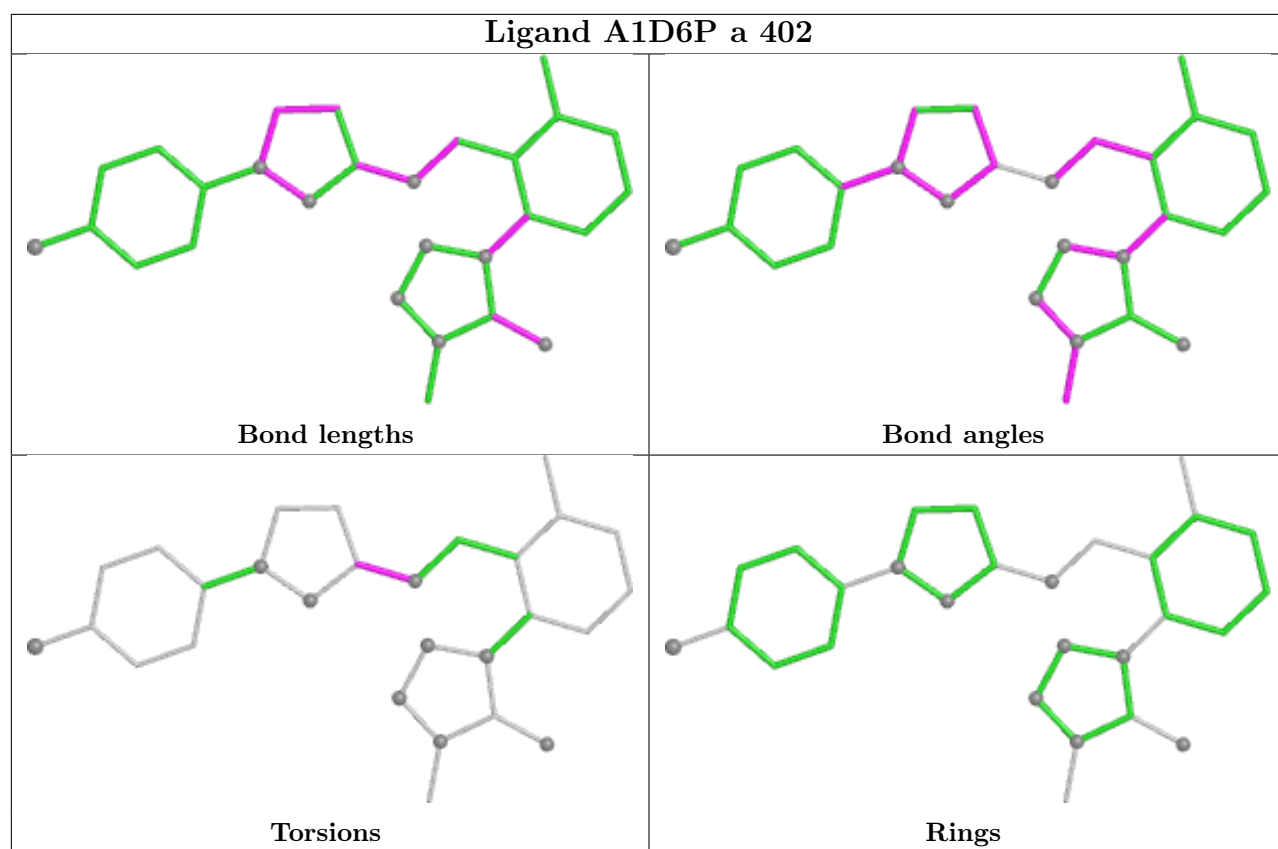
Bond angles

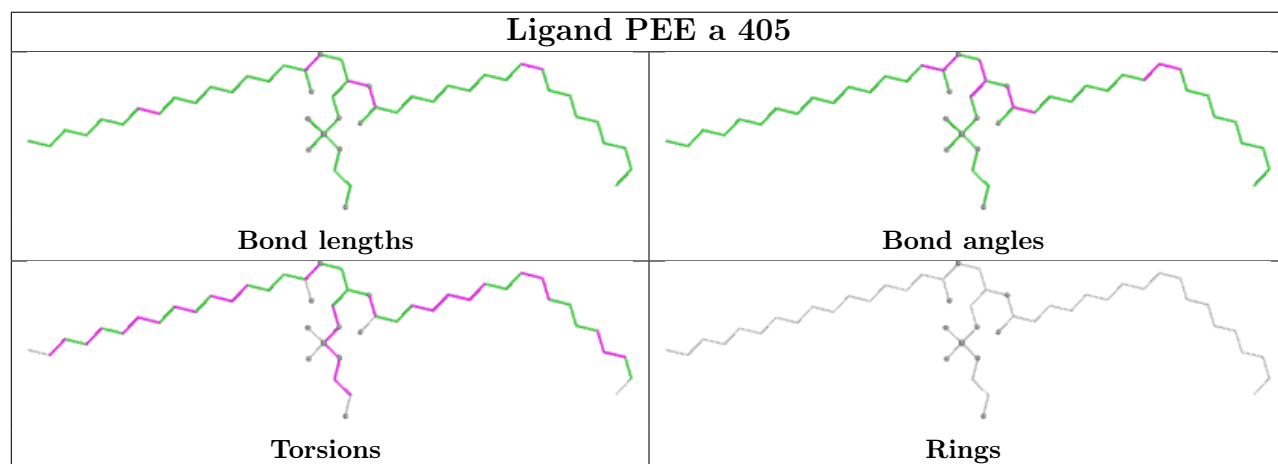
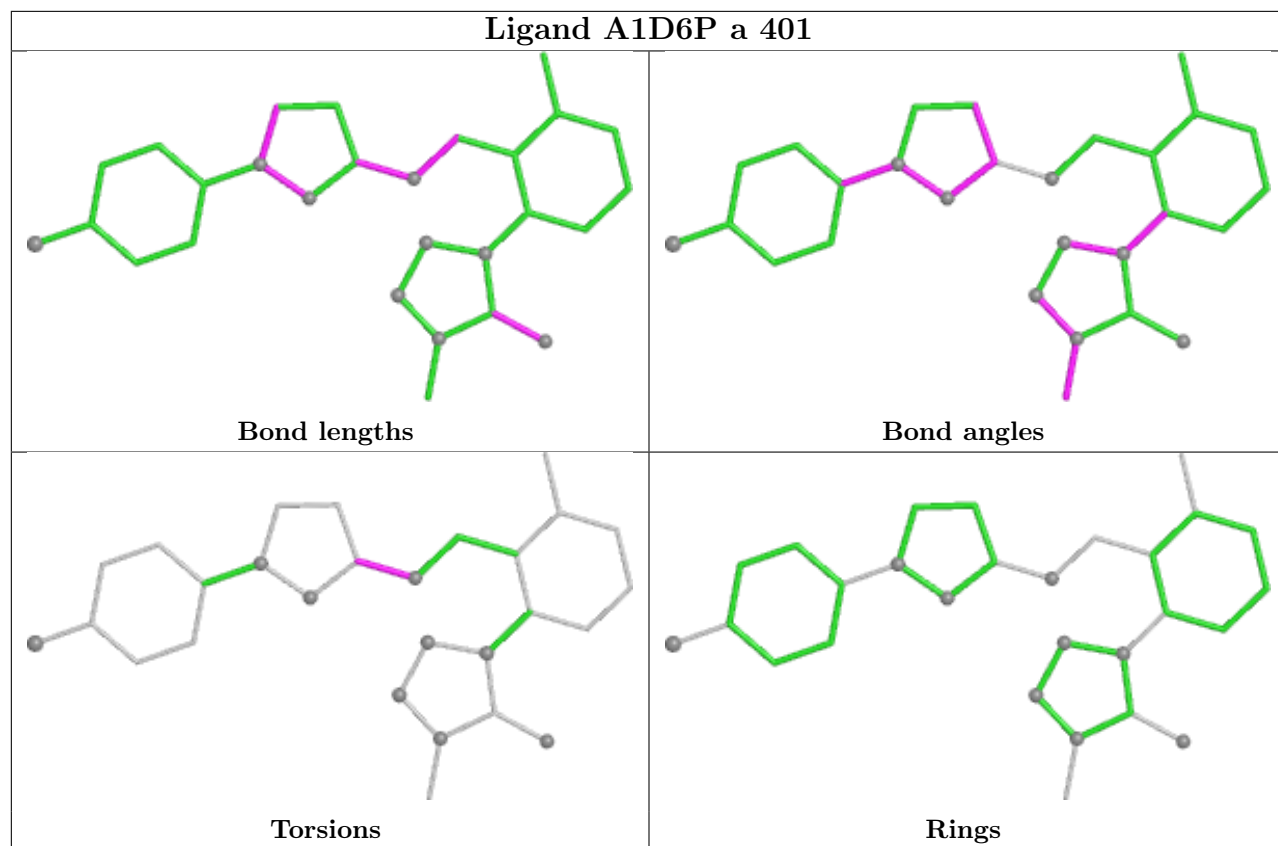


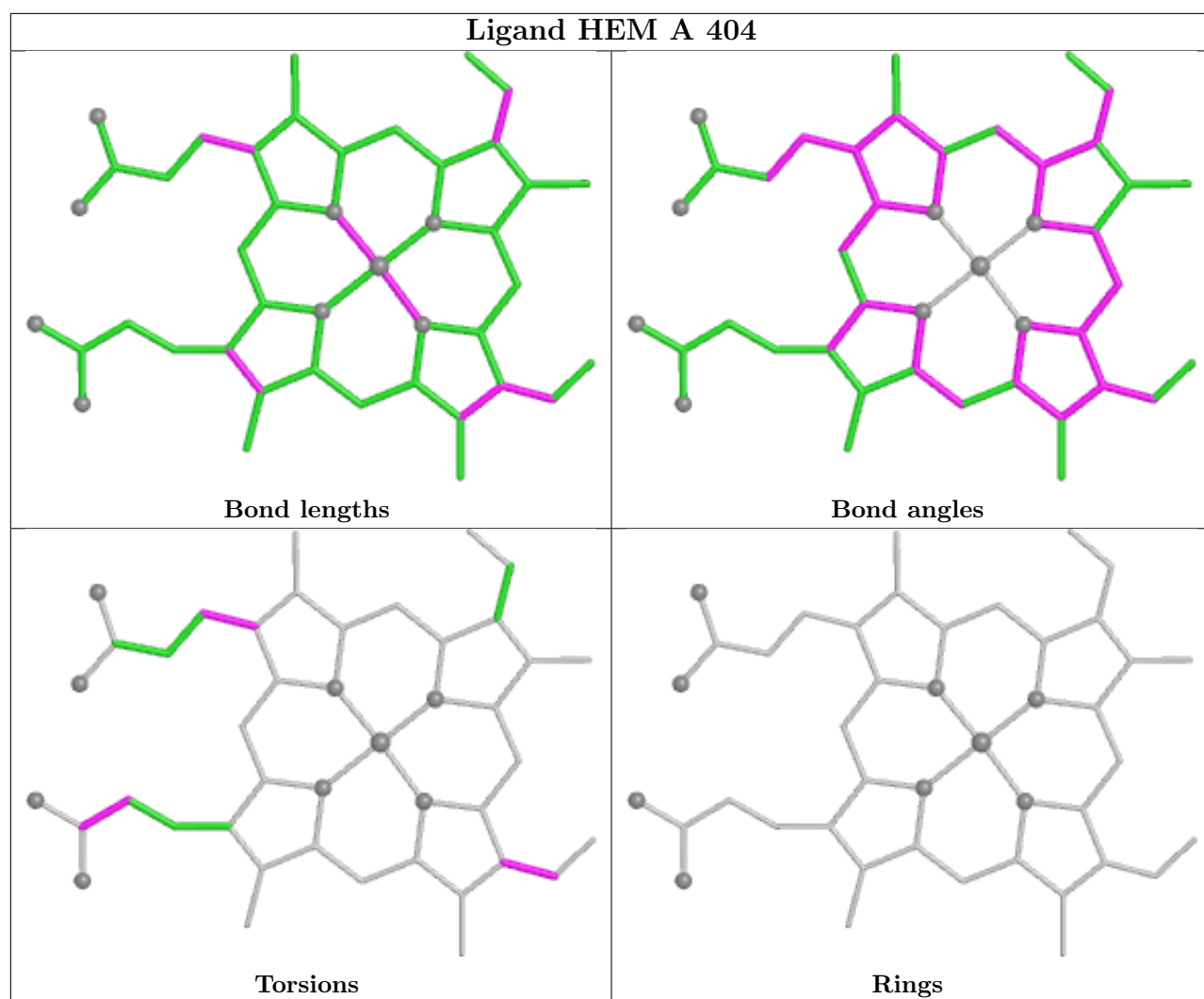
Torsions

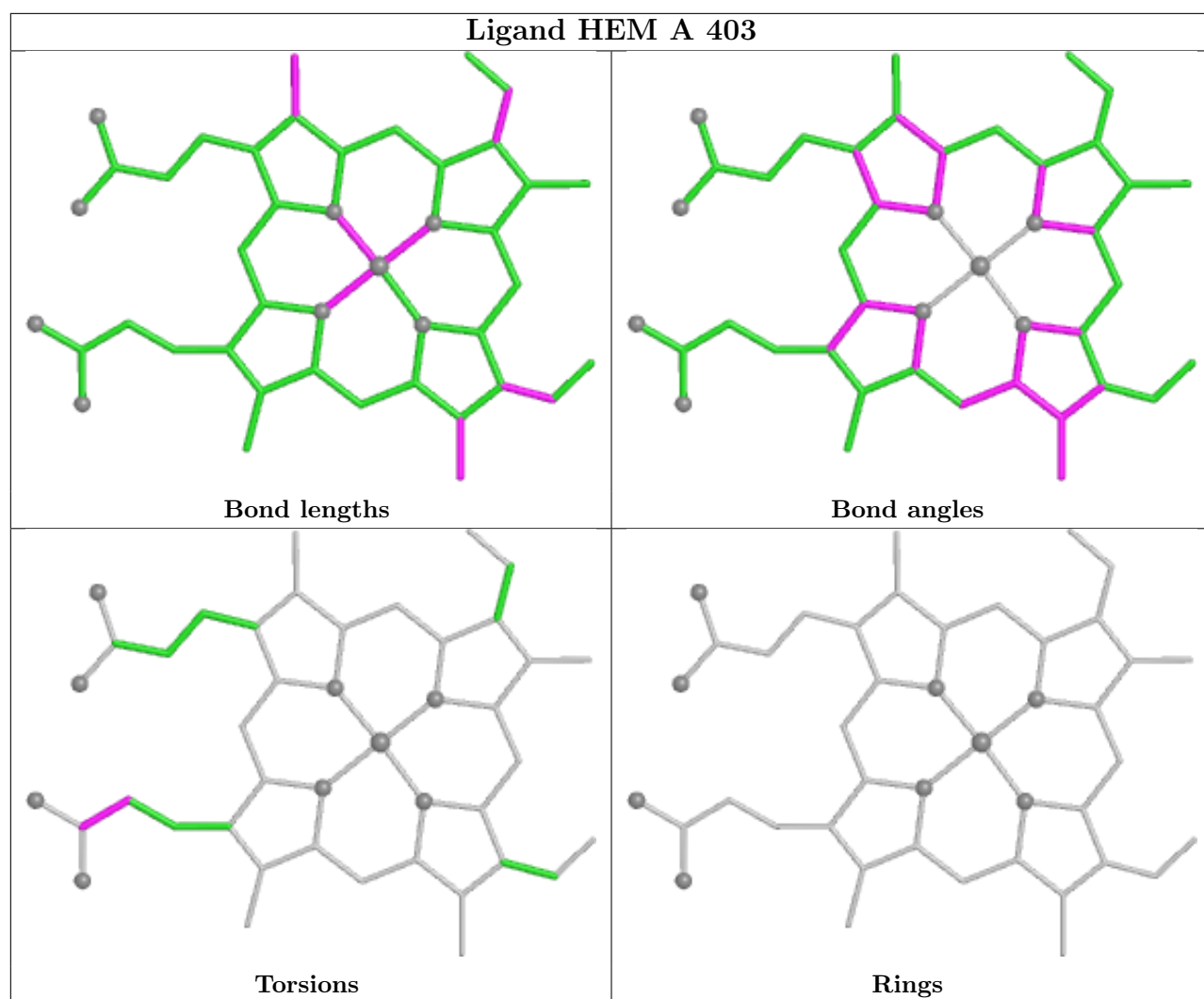


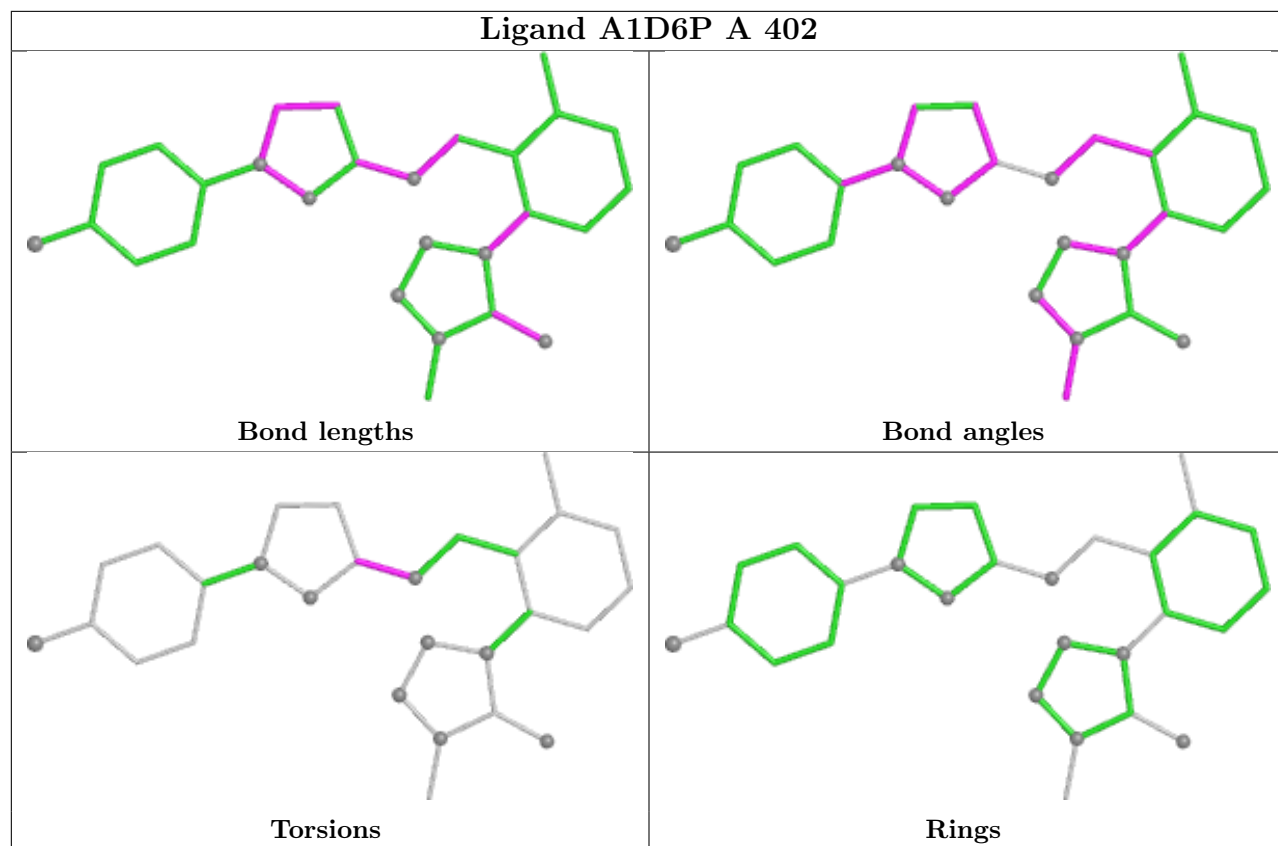
Rings

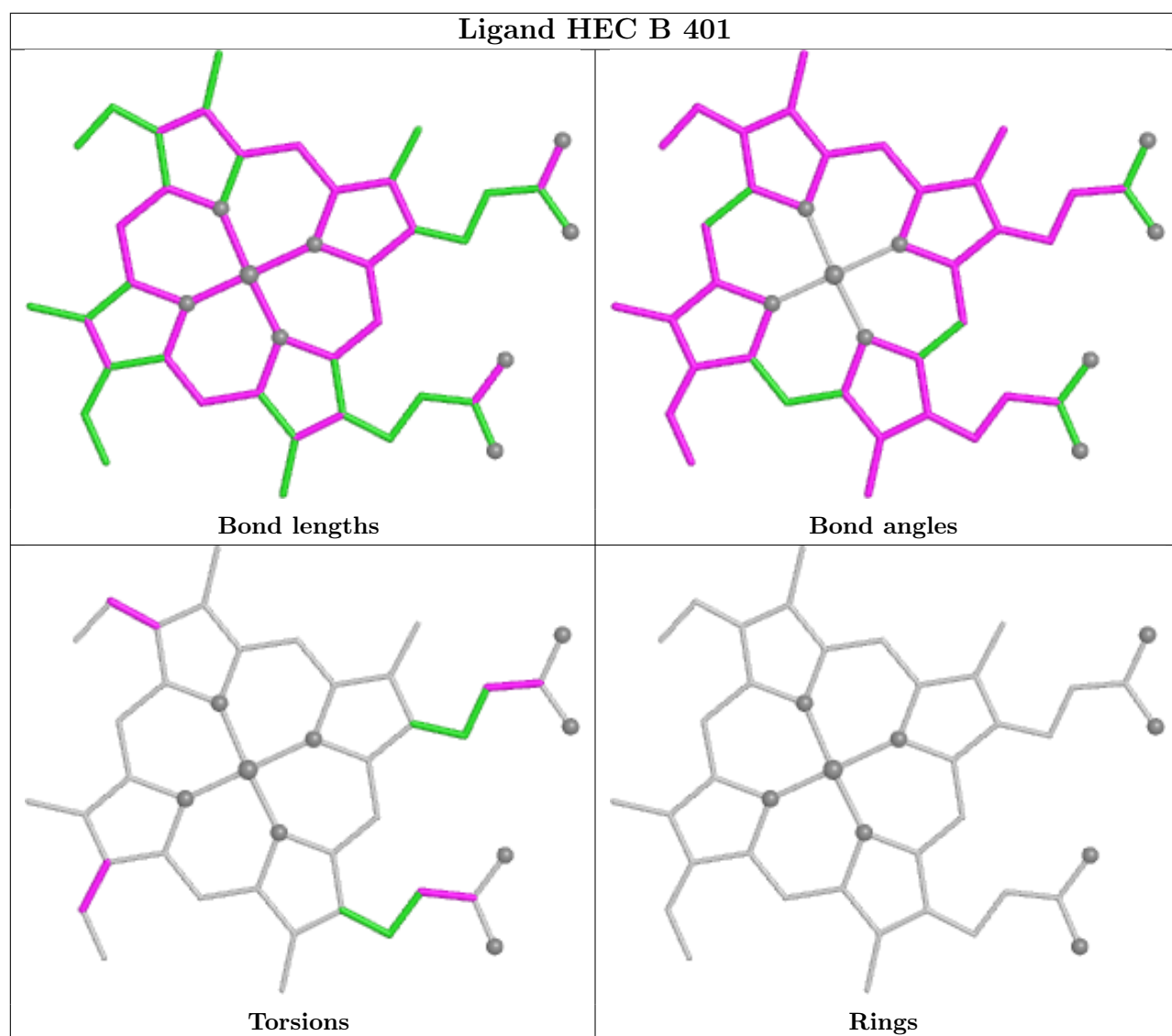


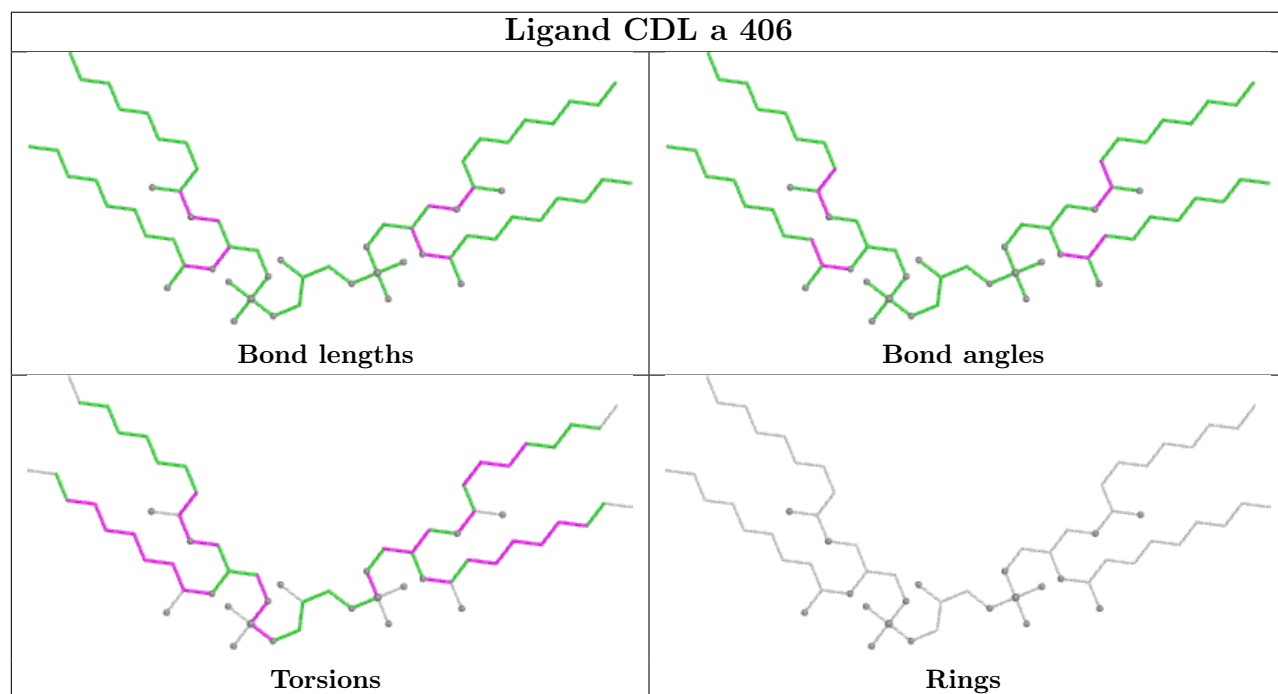
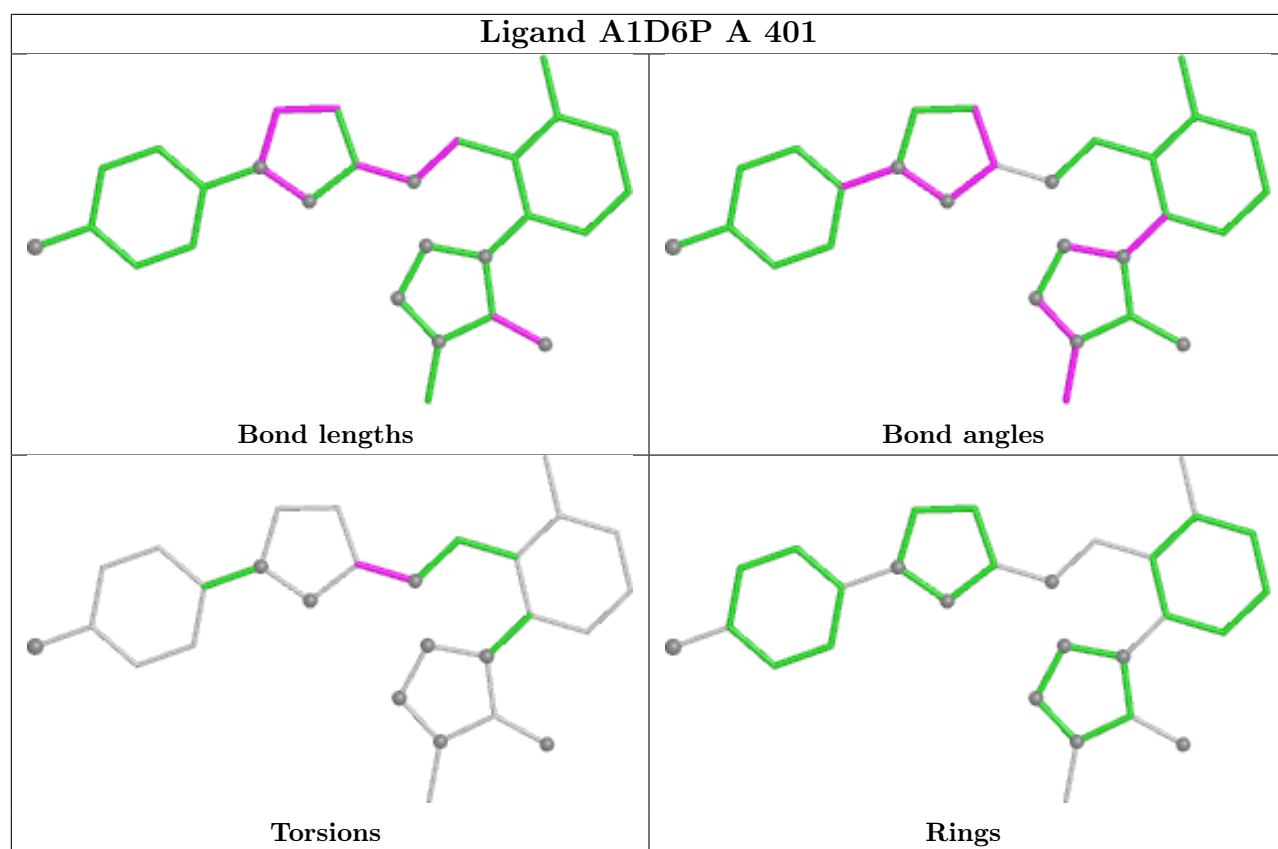


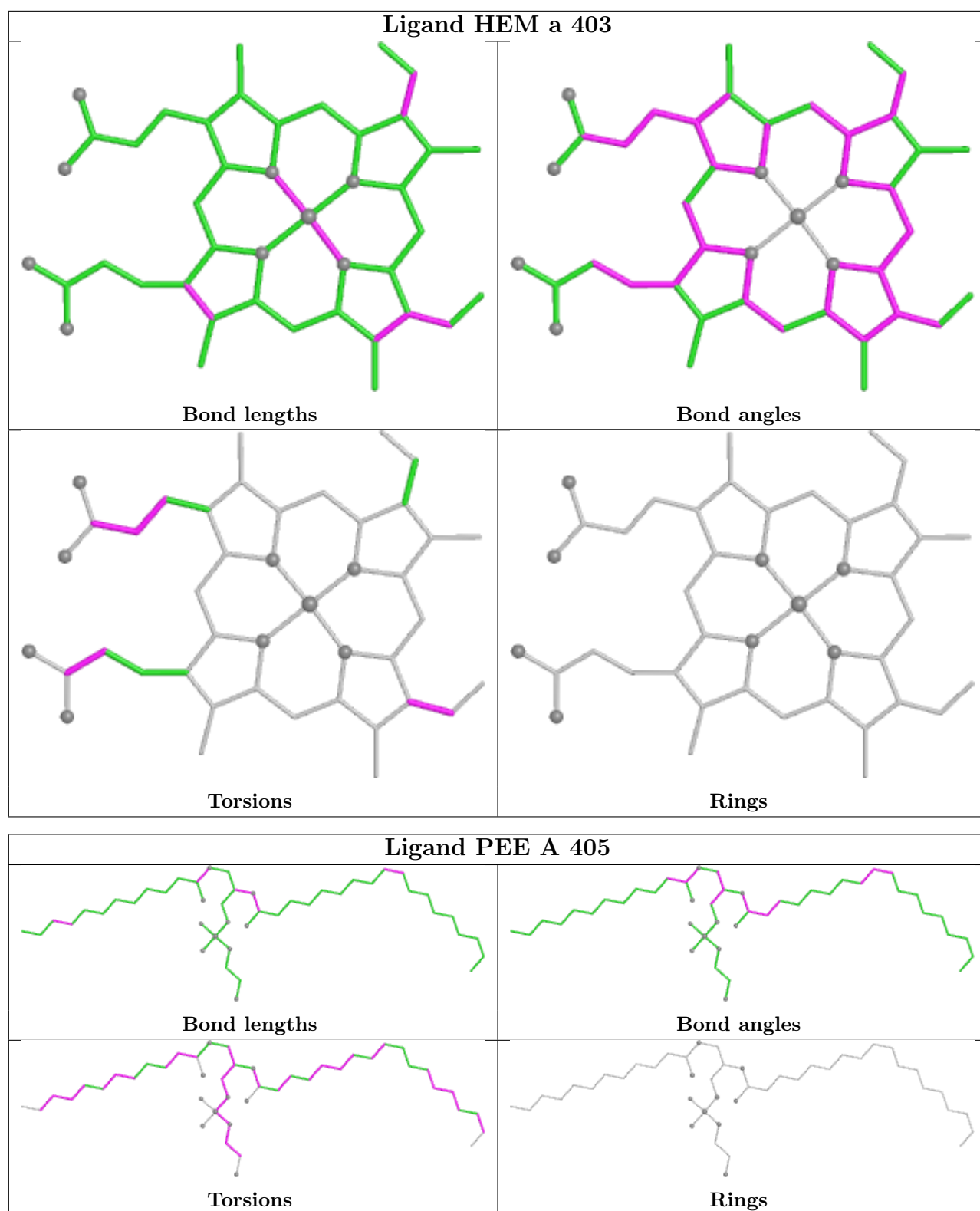












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

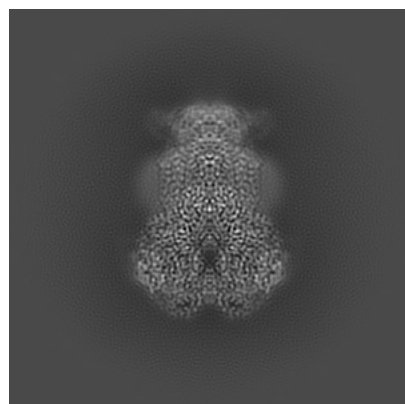
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60320. These allow visual inspection of the internal detail of the map and identification of artifacts.

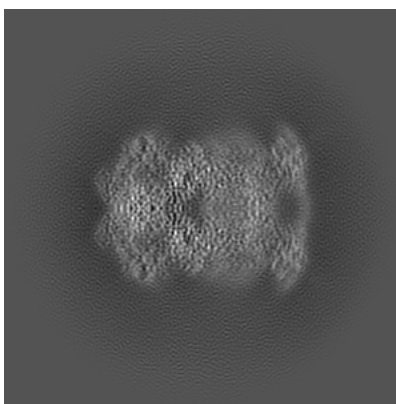
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

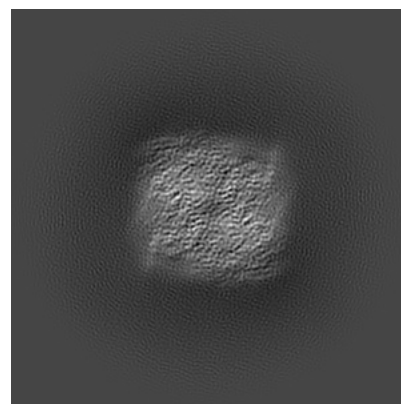
6.1.1 Primary map



X

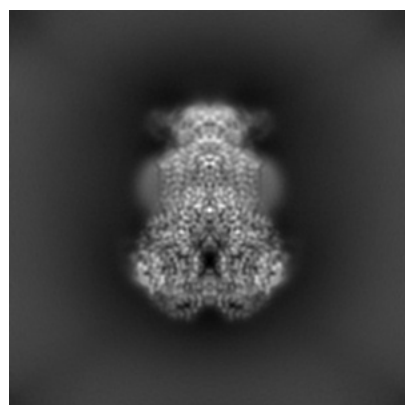


Y

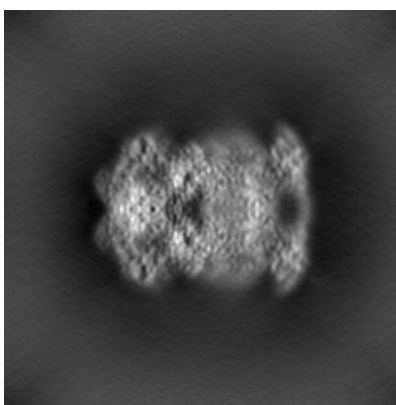


Z

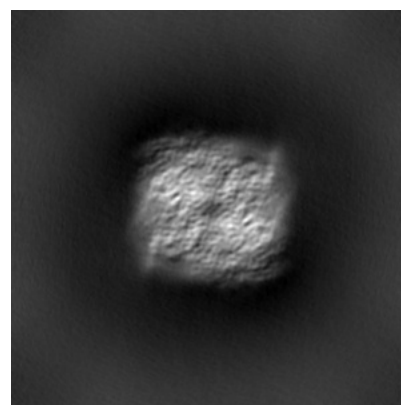
6.1.2 Raw map



X



Y

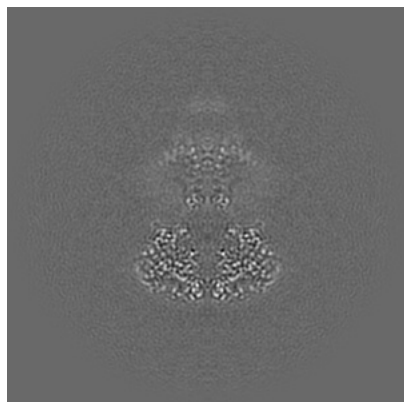


Z

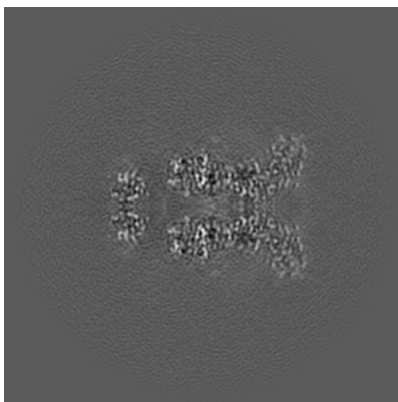
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

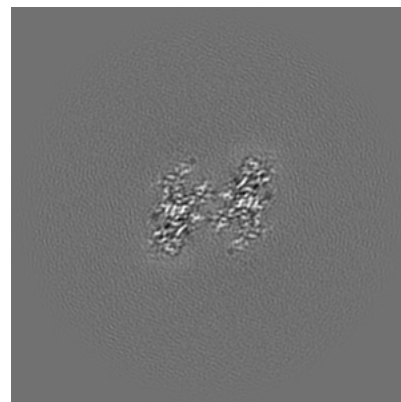
6.2.1 Primary map



X Index: 150

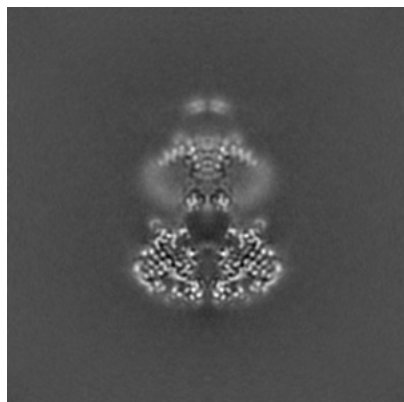


Y Index: 150

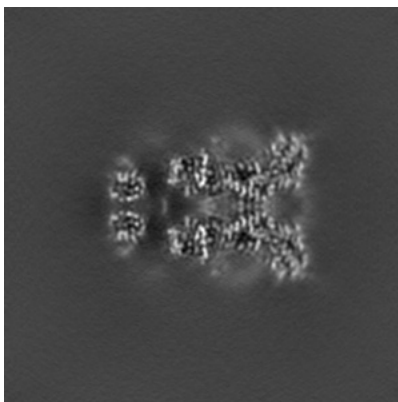


Z Index: 150

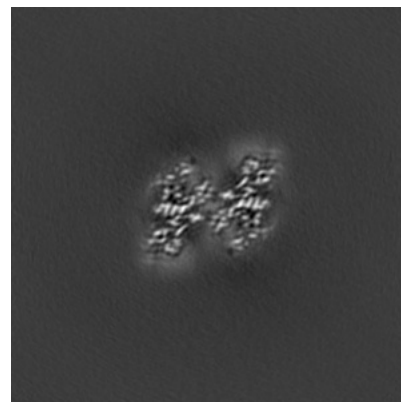
6.2.2 Raw map



X Index: 150



Y Index: 150

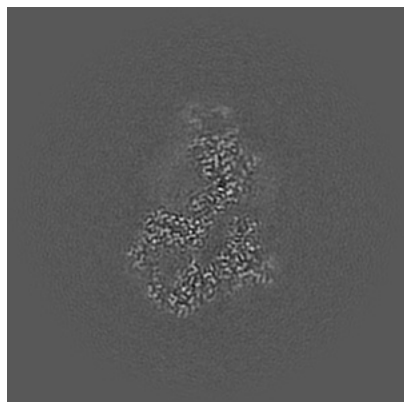


Z Index: 150

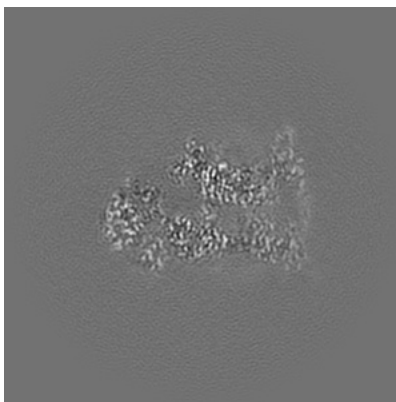
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

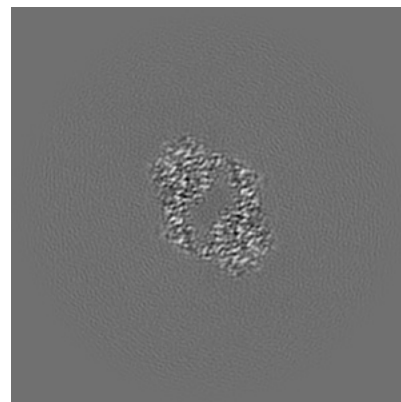
6.3.1 Primary map



X Index: 163

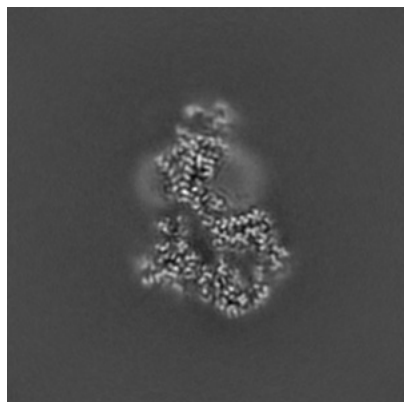


Y Index: 158

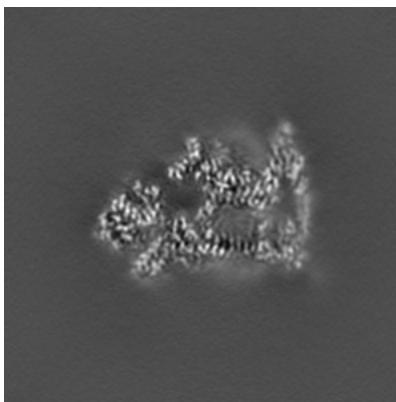


Z Index: 130

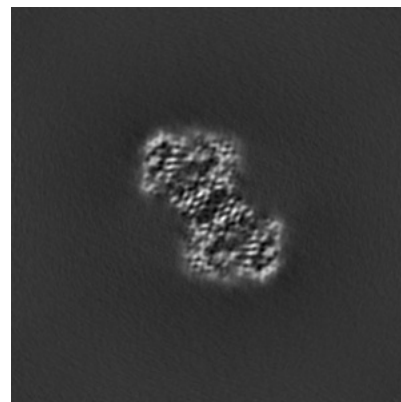
6.3.2 Raw map



X Index: 137



Y Index: 161

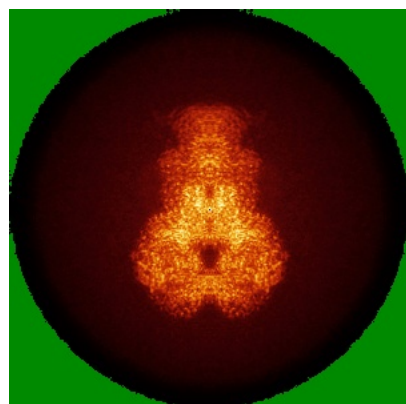


Z Index: 97

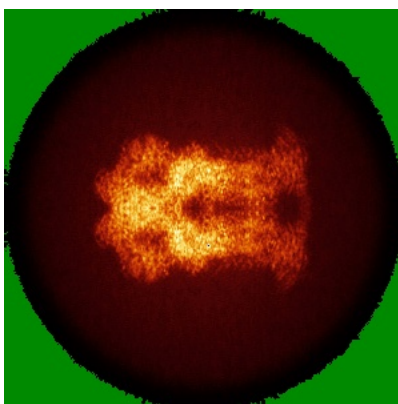
The images above show the largest variance slices of the map in three orthogonal directions.

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

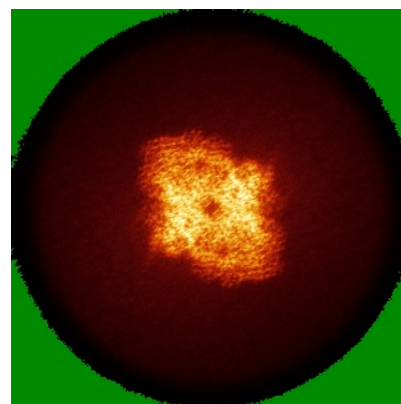
6.4.1 Primary map



X

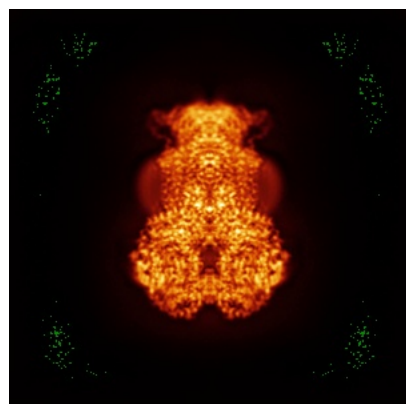


Y

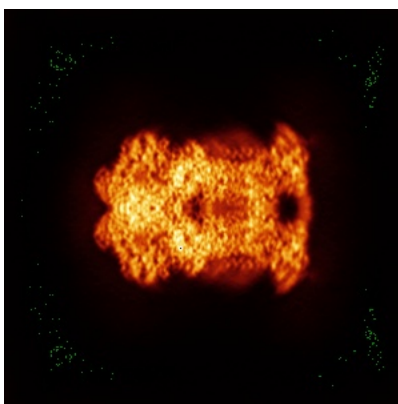


Z

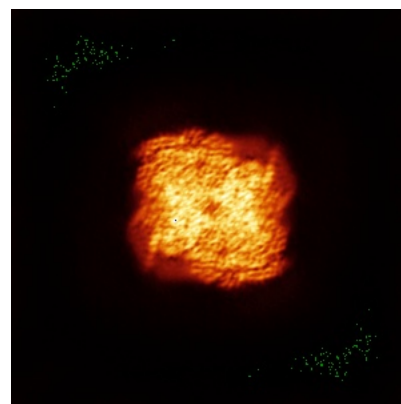
6.4.2 Raw map



X



Y



Z

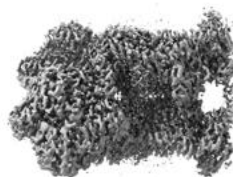
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



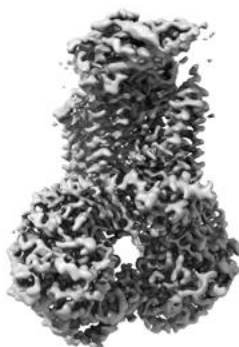
Y



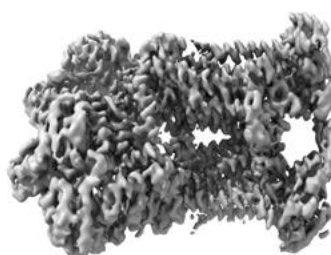
Z

The images above show the 3D surface view of the map at the recommended contour level 0.798. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

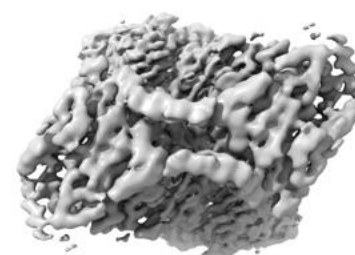
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

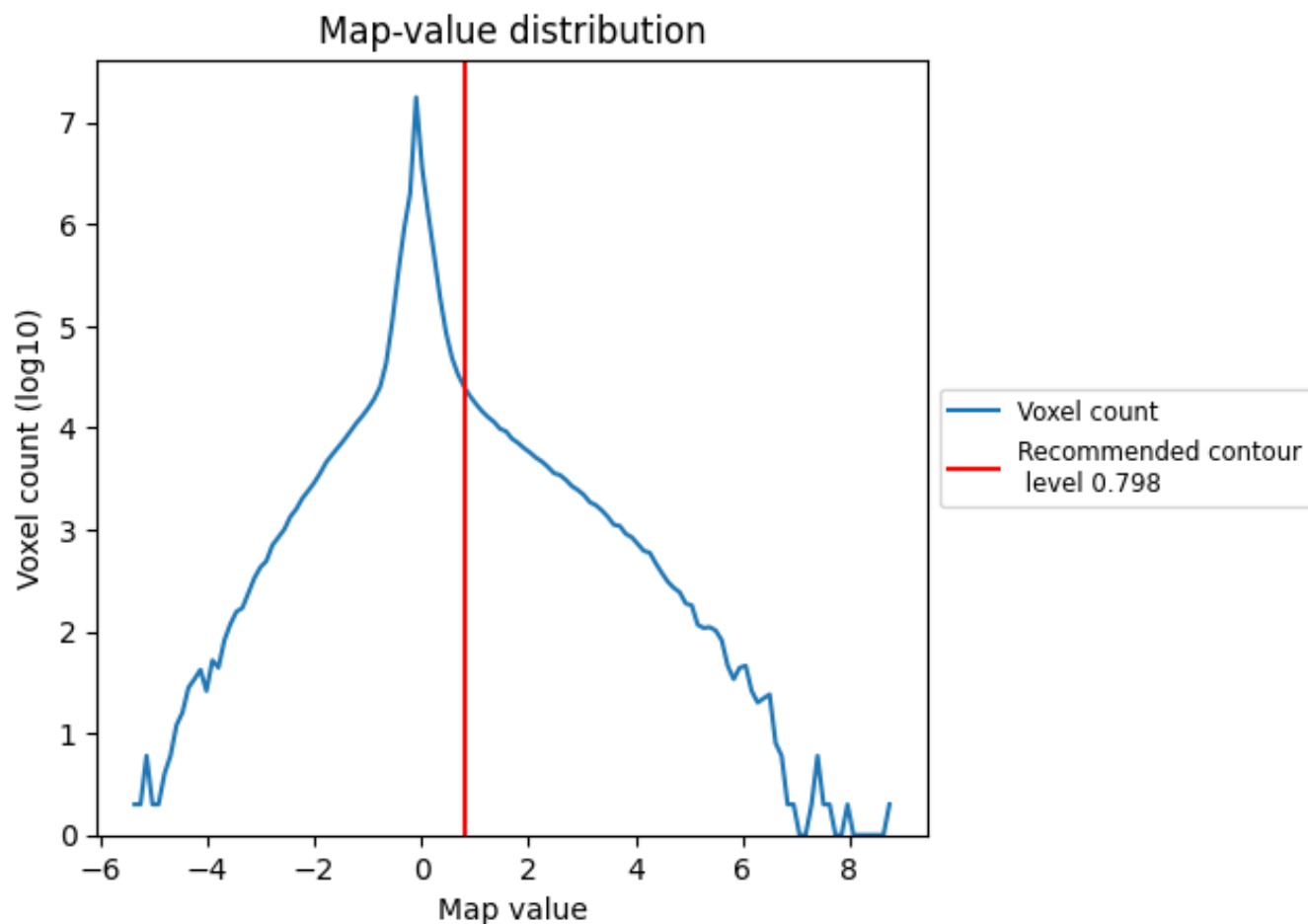
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

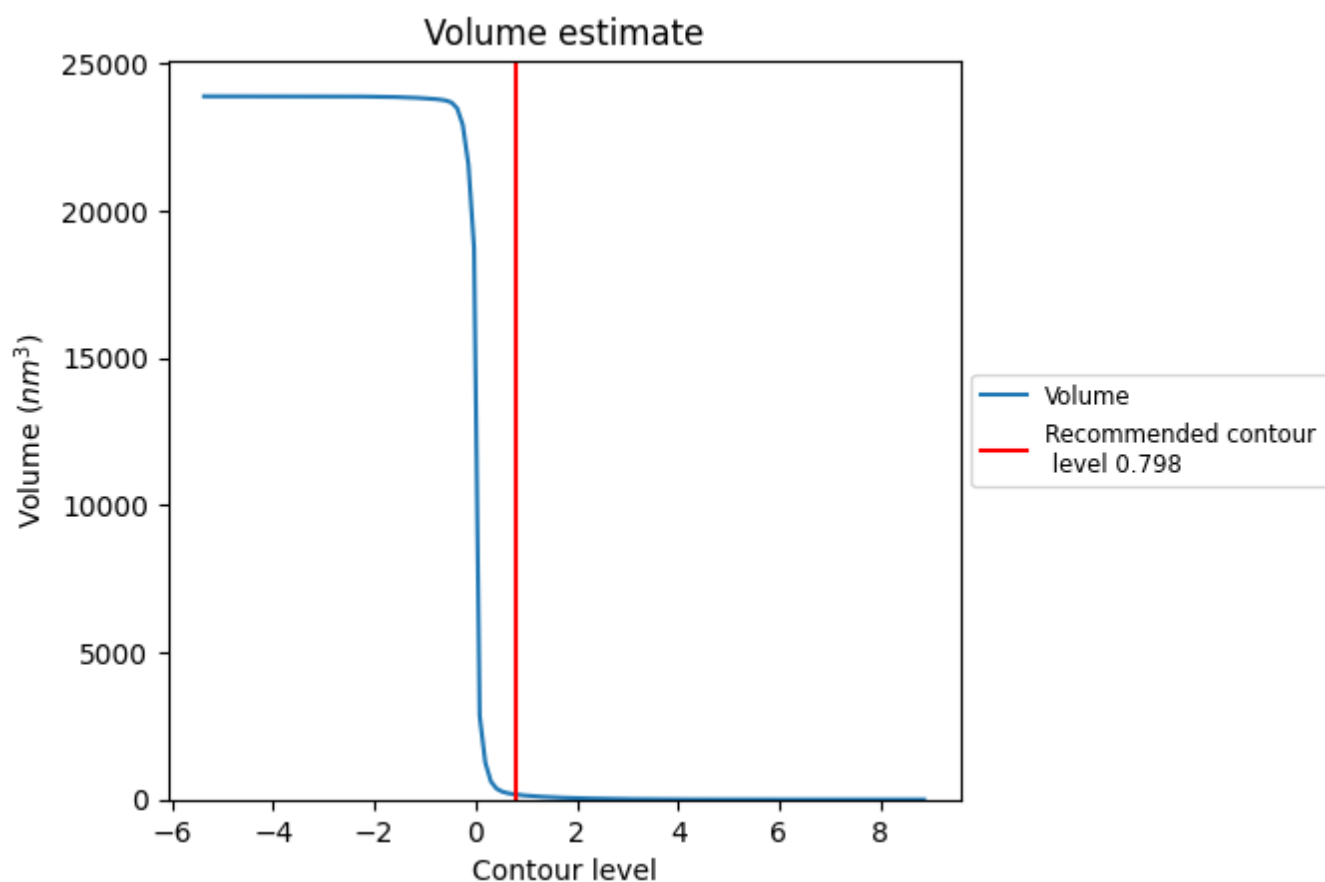
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

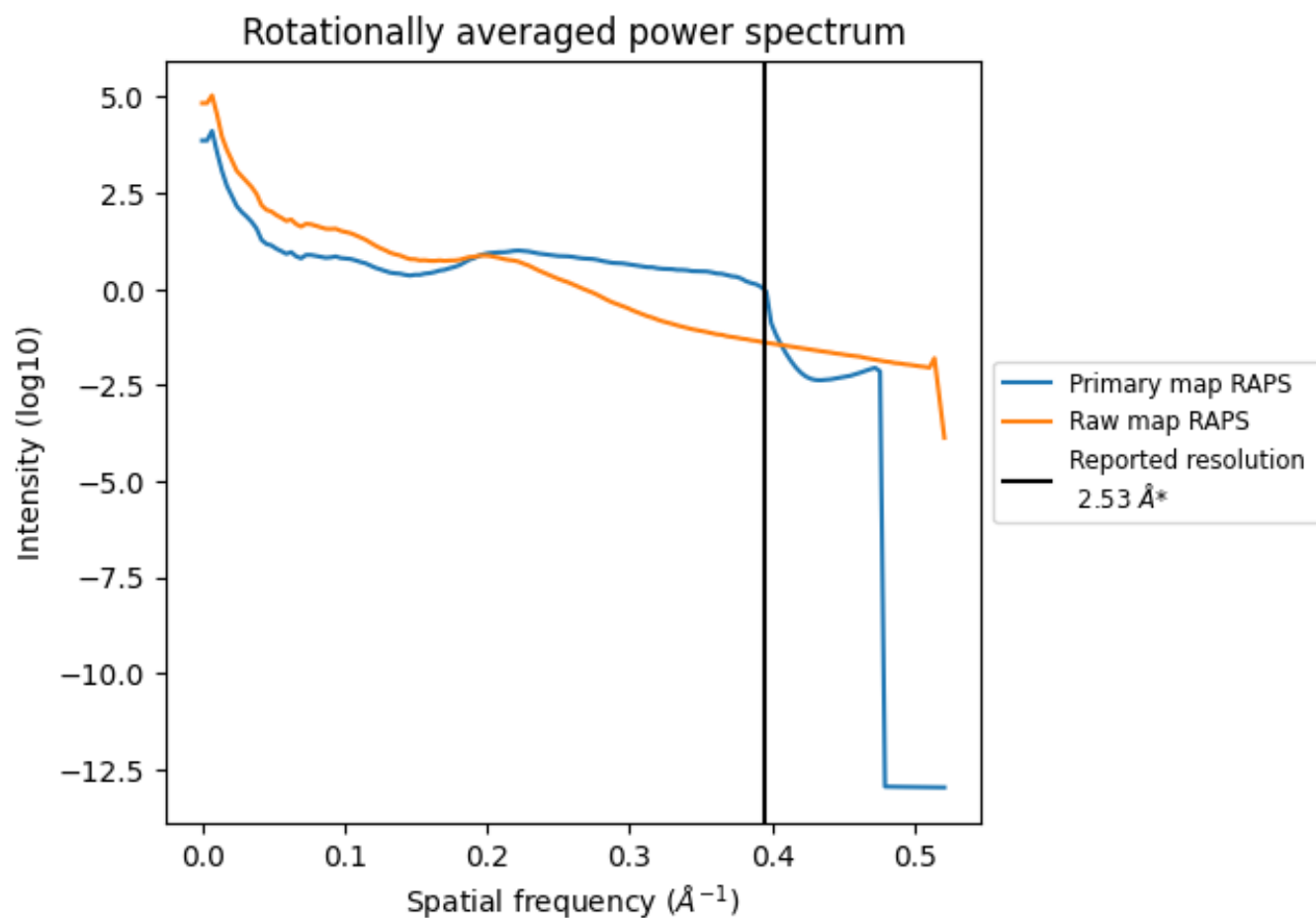
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 172 nm³; this corresponds to an approximate mass of 155 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 ⓘ

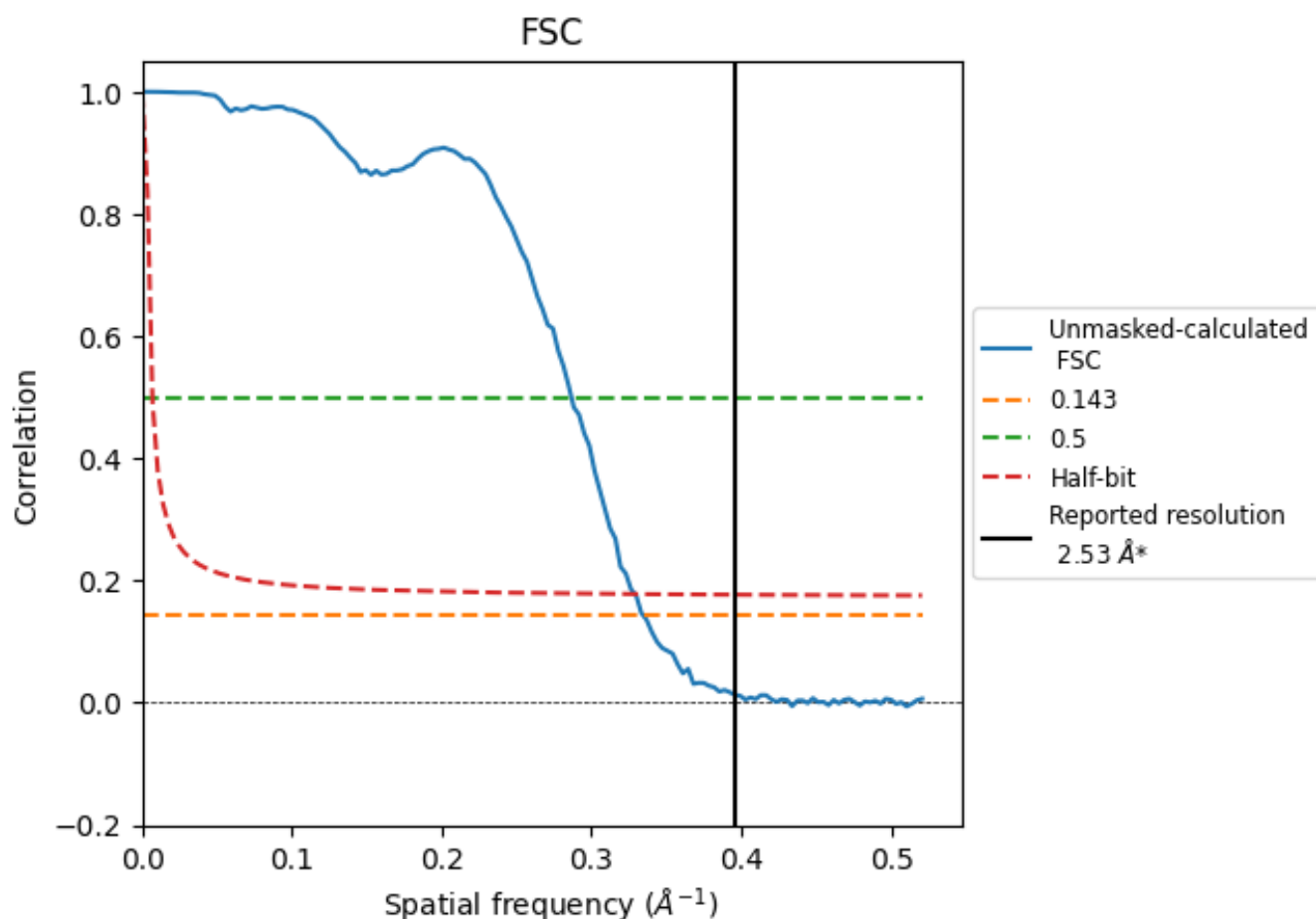


*Reported resolution corresponds to spatial frequency of 0.395 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.395 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

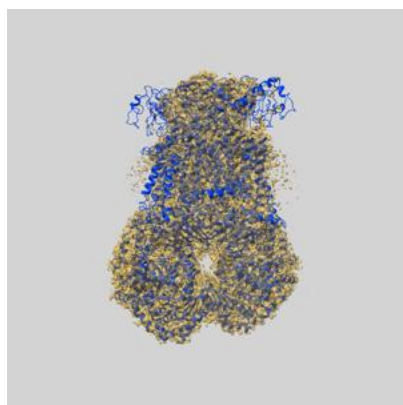
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.49	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.53 by more than 10 %

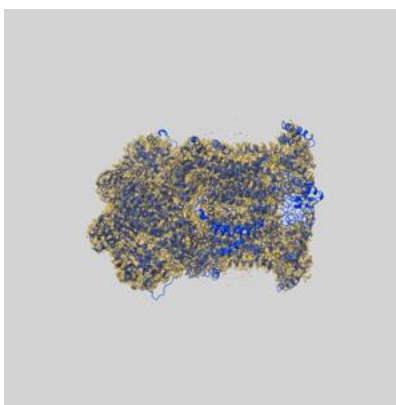
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60320 and PDB model 8ZOW. Per-residue inclusion information can be found in section [3](#) on page [10](#).

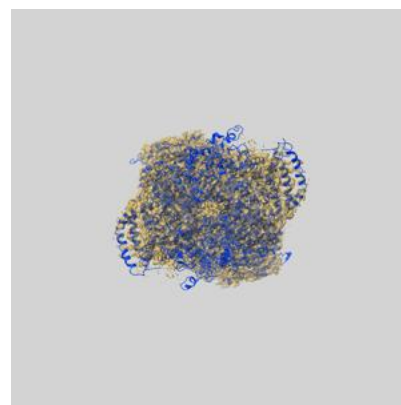
9.1 Map-model overlay [i](#)



X



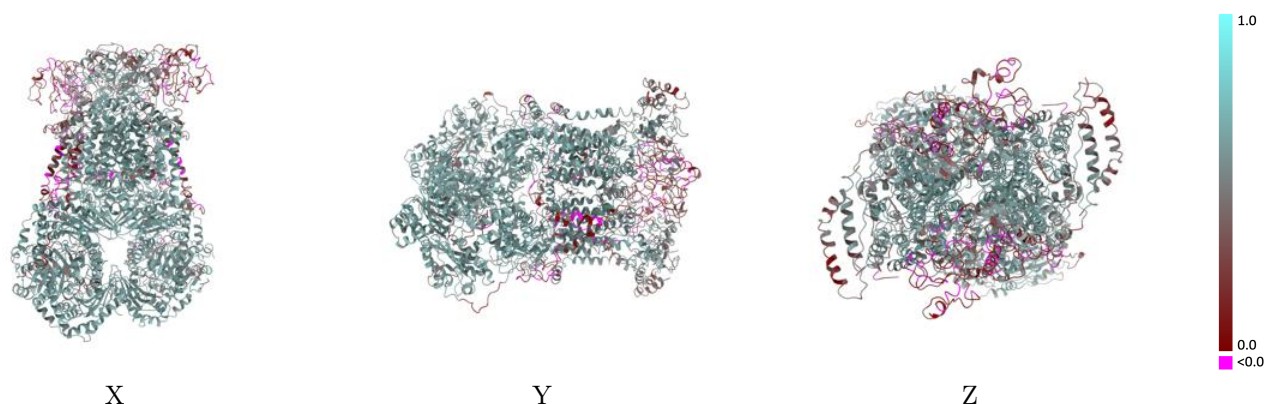
Y



Z

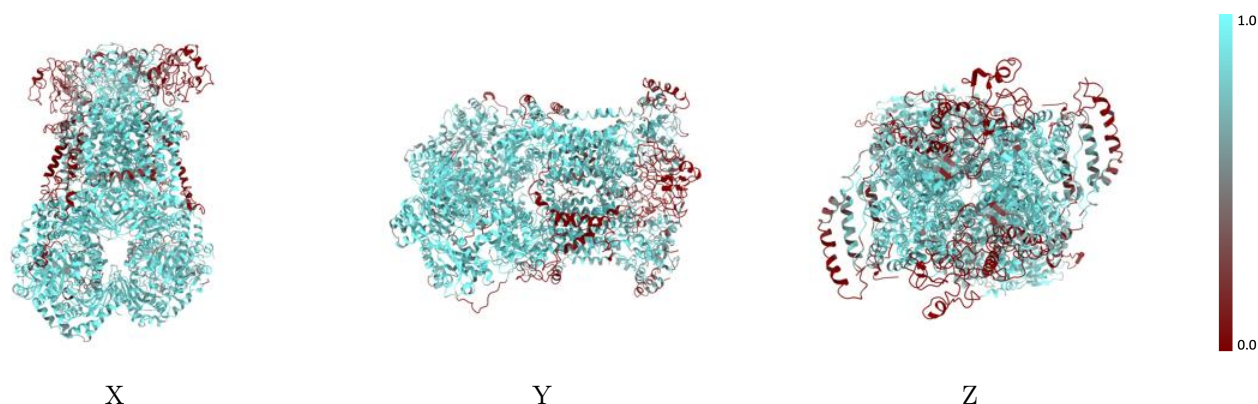
The images above show the 3D surface view of the map at the recommended contour level 0.798 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



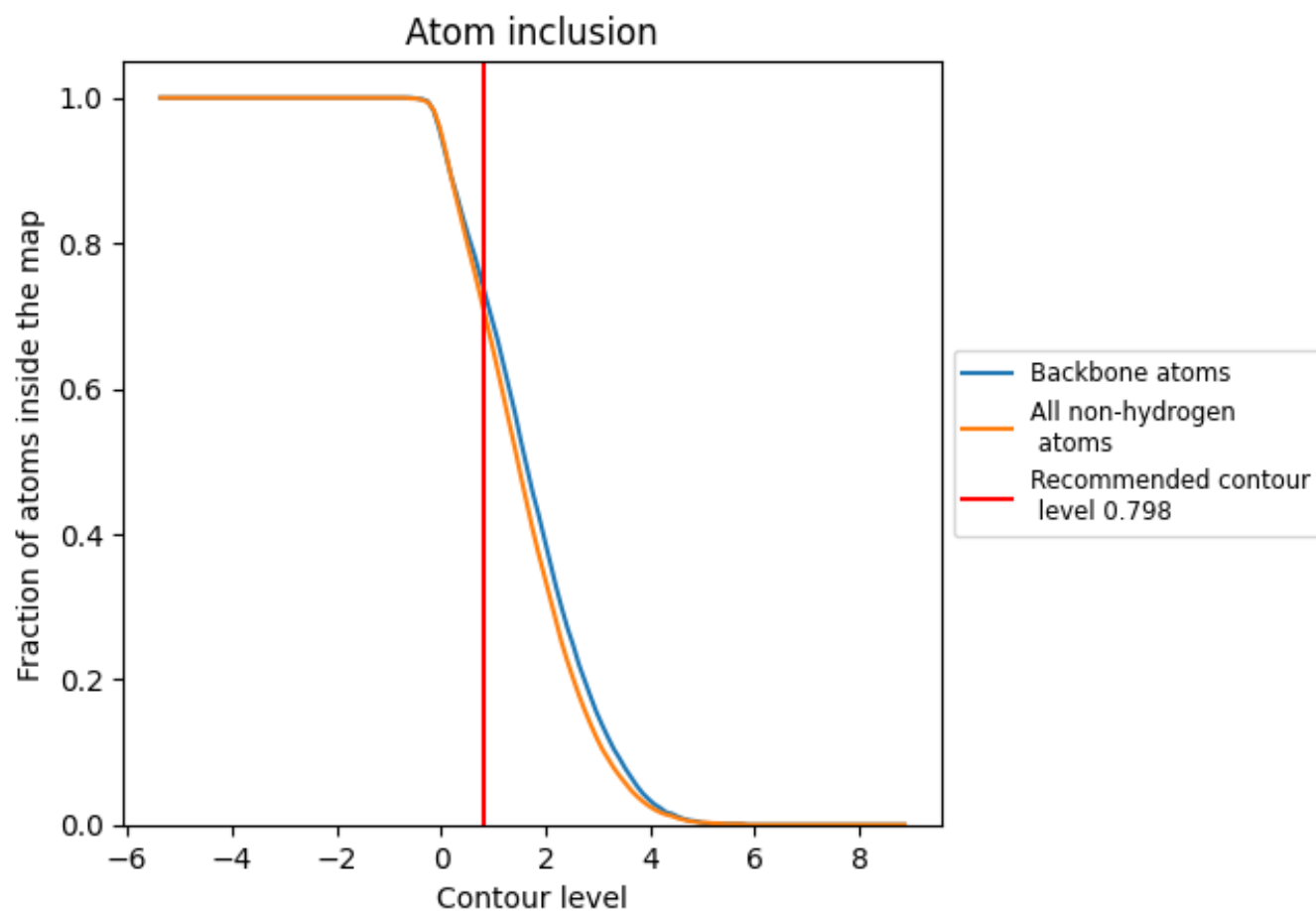
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.798).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 71% 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 (0.798) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7130	 0.5150
A	 0.8860	 0.5960
B	 0.7420	 0.5260
C	 0.0430	 0.1950
D	 0.8730	 0.5880
E	 0.8970	 0.6100
F	 0.3680	 0.4050
G	 0.8720	 0.5920
H	 0.6290	 0.5160
I	 0.2610	 0.2550
J	 0.0000	 0.1600
K	 0.3930	 0.2910
a	 0.8860	 0.5960
b	 0.7450	 0.5280
c	 0.0580	 0.1690
d	 0.8780	 0.5940
e	 0.8910	 0.6070
f	 0.3660	 0.4100
g	 0.8620	 0.5960
h	 0.5720	 0.4890
i	 0.2590	 0.2290
j	 0.0050	 0.1600
k	 0.4470	 0.3970

