



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:58 AM UTC

PDB ID : 6HWH / pdb_00006hwh
EMDB ID : EMD-0289
Title : Structure of a functional obligate respiratory supercomplex from *Mycobacterium smegmatis*
Authors : Wiseman, B.; Nitharwal, R.G.; Fedotovskaya, O.; Schafer, J.; Guo, H.; Kuang, Q.; Benlekhir, S.; Sjostrand, D.; Adelroth, P.; Rubinstein, J.L.; Brzezinski, P.; Hogbom, M.
Deposited on : 2018-10-12
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:

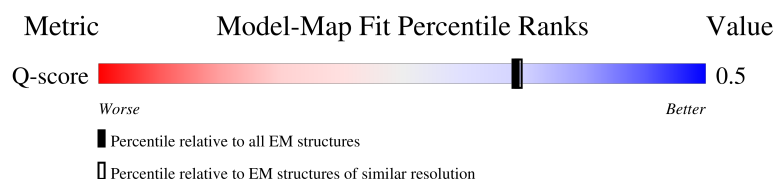
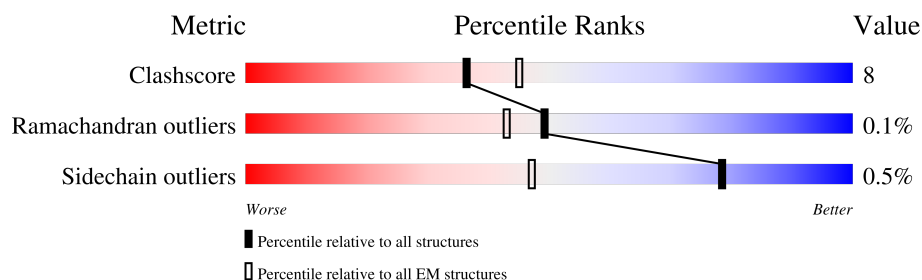
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	408	
1	B	408	
2	C	74	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	74	99% .
3	D	65	5% 100%
3	H	65	29% 100%
4	E	20	5% 100%
4	I	20	20% 100%
5	F	35	97% .
5	J	35	97% .
6	K	268	10% . 89%
6	M	268	9% . 89%
6	i	268	39% 46% 14% 40%
6	j	268	19% 54% 7% 40%
7	L	341	68% 14% 18%
7	P	341	69% 13% 18%
8	N	79	63% 5% 32%
8	R	79	65% . 32%
9	O	157	80% 10% 10%
9	T	157	82% 8% 10%
10	Q	583	76% 18% 6%
10	V	583	76% 18% . 6%
11	S	139	86% 14%
11	X	139	88% 12%
12	W	203	80% 10% 9%
12	Z	203	81% 9% 9%
13	Y	554	85% 12% .
13	b	554	83% 13% .

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
14	FES	B	501	-	-	X	-
18	HAS	Q	801	X	-	-	-
18	HAS	Q	802	X	-	-	-
18	HAS	V	801	X	-	-	-
18	HAS	V	802	X	-	-	-
19	HEC	V	804	-	-	X	-
19	HEC	j	301	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 40632 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 Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		
1	B	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		

- Molecule 2 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	74	Total	C	N	O	0	0
			370	222	74	74		
2	C	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 3 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	65	Total	C	N	O	0	0
			325	195	65	65		
3	D	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 4 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	20	Total	C	N	O	0	0
			100	60	20	20		
4	E	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 5 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	35	Total	C	N	O	0	0
			175	105	35	35		
5	F	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 6 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	30	Total	C	N	O	S	0	0
			211	139	35	33	4		
6	K	30	Total	C	N	O	S	0	0
			211	139	35	33	4		
6	i	162	Total	C	N	O		0	0
			648	324	162	162			
6	j	162	Total	C	N	O		0	0
			648	324	162	162			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	281	Total	C	N	O	S	0	0
			2236	1450	368	409	9		
7	L	281	Total	C	N	O	S	0	0
			2236	1450	368	409	9		

- Molecule 8 is a protein called MSMEG_4693.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	54	Total	C	N	O	S	0	0
			415	276	67	70	2		
8	N	54	Total	C	N	O	S	0	0
			415	276	67	70	2		

- Molecule 9 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	142	Total	C	N	O	S	0	0
			1019	644	173	200	2		
9	O	142	Total	C	N	O	S	0	0
			1019	644	173	200	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		
10	Q	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
11	S	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		
12	W	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

- Molecule 13 is a protein called Ubiquinol-cytochrome C reductase QcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		
13	Y	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		

There are 16 discrepancies between the modelled and reference sequences:

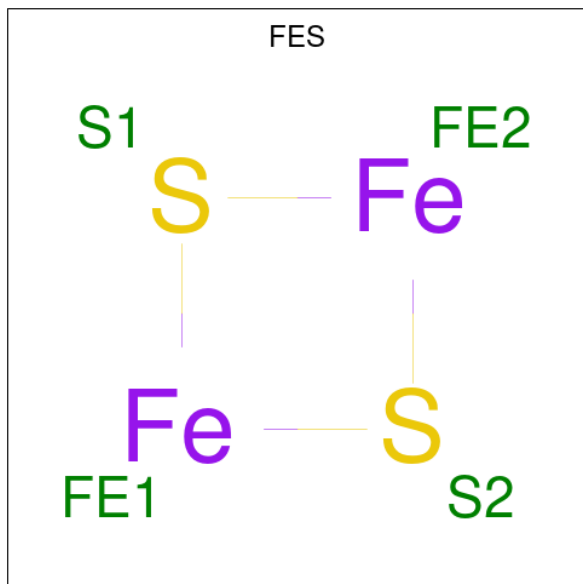
Chain	Residue	Modelled	Actual	Comment	Reference
b	547	ASP	-	expression tag	UNP I7FGS8
b	548	TYR	-	expression tag	UNP I7FGS8
b	549	LYS	-	expression tag	UNP I7FGS8
b	550	ASP	-	expression tag	UNP I7FGS8
b	551	ASP	-	expression tag	UNP I7FGS8
b	552	ASP	-	expression tag	UNP I7FGS8
b	553	ASP	-	expression tag	UNP I7FGS8
b	554	LYS	-	expression tag	UNP I7FGS8
Y	547	ASP	-	expression tag	UNP I7FGS8
Y	548	TYR	-	expression tag	UNP I7FGS8
Y	549	LYS	-	expression tag	UNP I7FGS8

Continued on next page...

Continued from previous page...

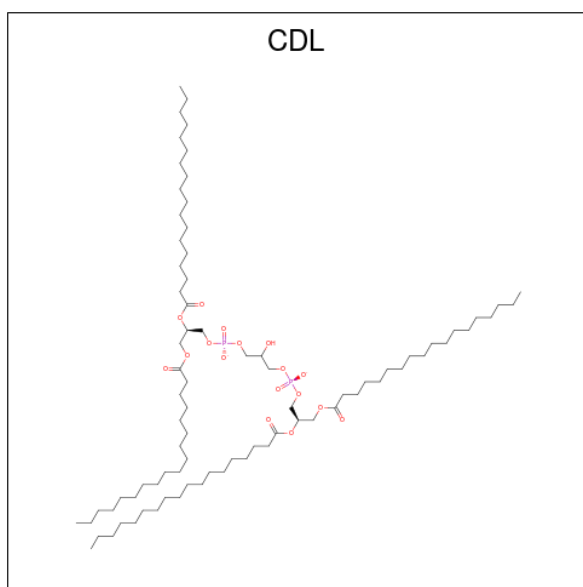
Chain	Residue	Modelled	Actual	Comment	Reference
Y	550	ASP	-	expression tag	UNP I7FGS8
Y	551	ASP	-	expression tag	UNP I7FGS8
Y	552	ASP	-	expression tag	UNP I7FGS8
Y	553	ASP	-	expression tag	UNP I7FGS8
Y	554	LYS	-	expression tag	UNP I7FGS8

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



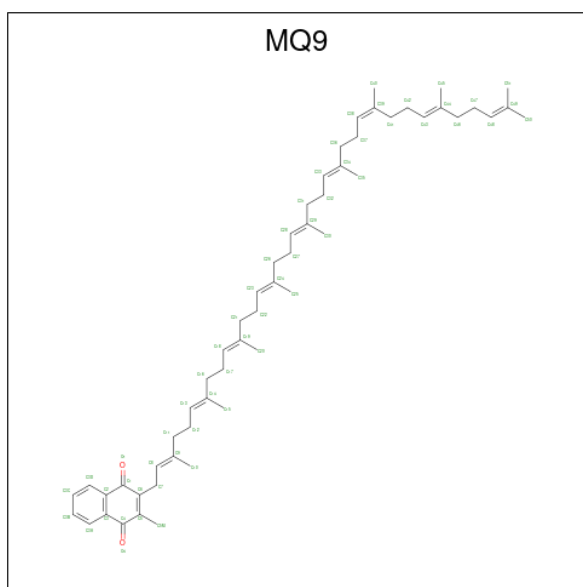
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	Fe	S	0
			4	2	2	
14	B	1	Total	Fe	S	0
			4	2	2	

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			100	81	17	2	
15	V	1	Total	C	O	P	0
			87	68	17	2	
15	b	1	Total	C	O	P	0
			92	73	17	2	
15	b	1	Total	C	O	P	0
			91	72	17	2	
15	K	1	Total	C	O	P	0
			100	81	17	2	
15	Q	1	Total	C	O	P	0
			87	68	17	2	
15	Y	1	Total	C	O	P	0
			91	72	17	2	
15	Y	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).

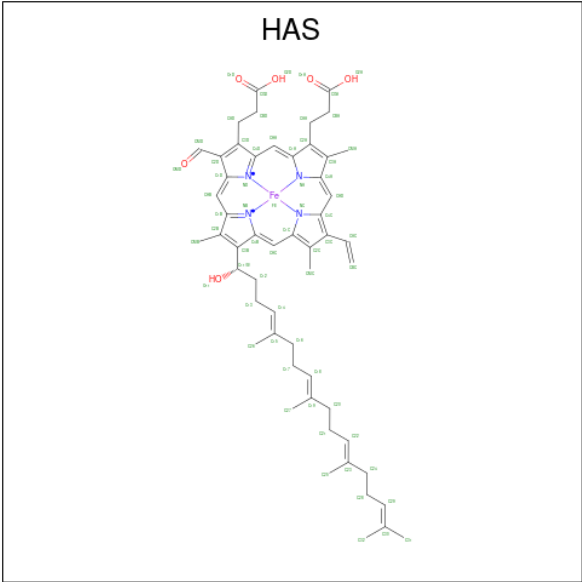


Mol	Chain	Residues	Atoms			AltConf
16	M	1	Total	C	O	0
			58	56	2	
16	b	1	Total	C	O	0
			58	56	2	
16	Y	1	Total	C	O	0
			58	56	2	
16	Y	1	Total	C	O	0
			58	56	2	

- Molecule 17 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

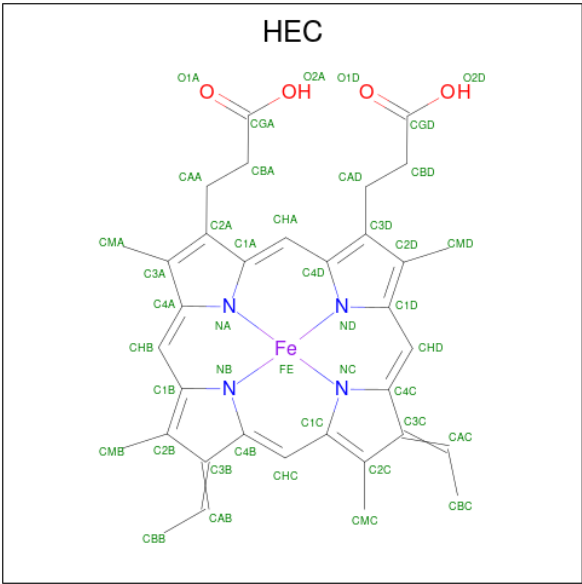
Mol	Chain	Residues	Atoms		AltConf
17	P	2	Total	Cu	0
			2	2	
17	V	1	Total	Cu	0
			1	1	
17	L	2	Total	Cu	0
			2	2	
17	Q	1	Total	Cu	0
			1	1	

- Molecule 18 is HEME-AS (CCD ID: HAS) (formula: C₅₄H₆₄FeN₄O₆).



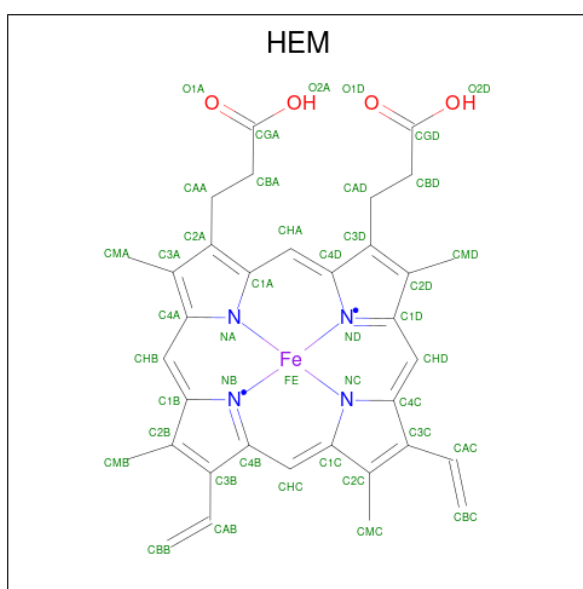
Mol	Chain	Residues	Atoms					AltConf
18	V	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	V	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	Q	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	Q	1	Total	C	Fe	N	O	0
			65	54	1	4	6	

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
19	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
19	i	1	Total 43	C 34	Fe 1	N 4	O 4	0
19	j	1	Total 43	C 34	Fe 1	N 4	O 4	0
19	j	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

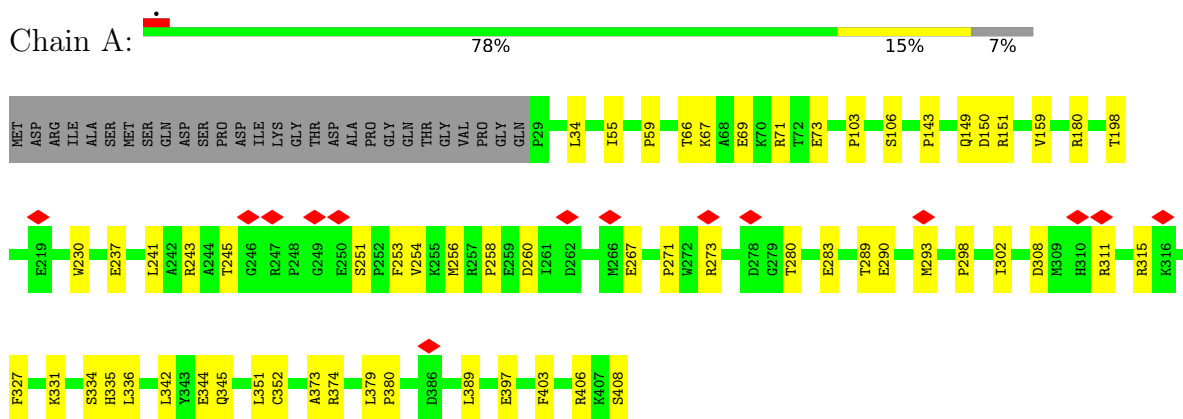


Mol	Chain	Residues	Atoms					AltConf
20	b	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	b	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	Y	1	Total 43	C 34	Fe 1	N 4	O 4	0
20	Y	1	Total 43	C 34	Fe 1	N 4	O 4	0

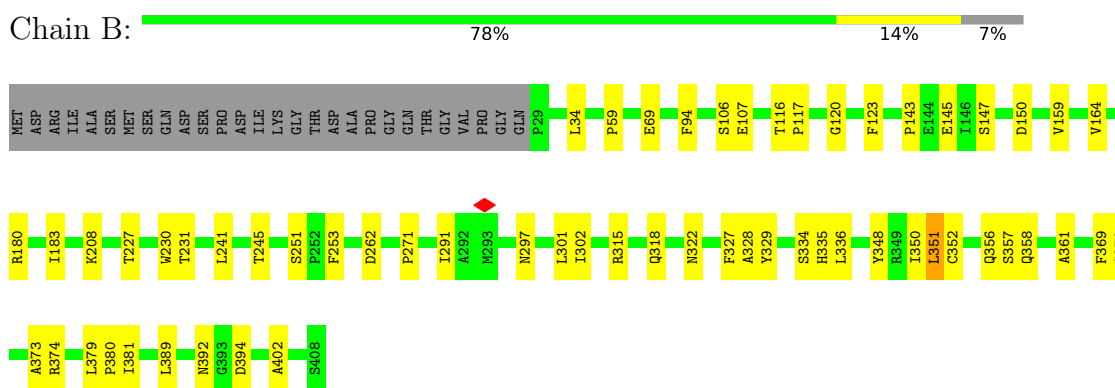
3 Residue-property plots

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.

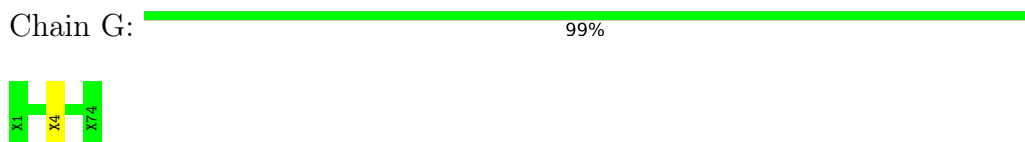
- Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit



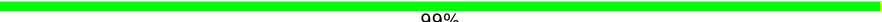
- Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 2: Co-purified unknown transmembrane helices built as polyALA



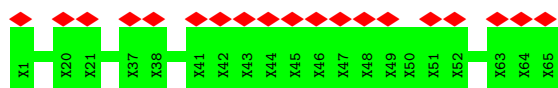
- Molecule 2: Co-purified unknown transmembrane helices built as polyALA

Chain C:  99%



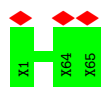
- Molecule 3: Co-purified unknown transmembrane helices built as polyALA

Chain H:  29% 100%



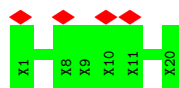
- Molecule 3: Co-purified unknown transmembrane helices built as polyALA

Chain D:  5% 100%



- Molecule 4: Co-purified unknown peptide built as polyALA

Chain I:  20% 100%



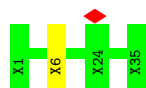
- Molecule 4: Co-purified unknown peptide built as polyALA

Chain E:  5% 100%



- Molecule 5: Co-purified unknown peptide built as polyALA

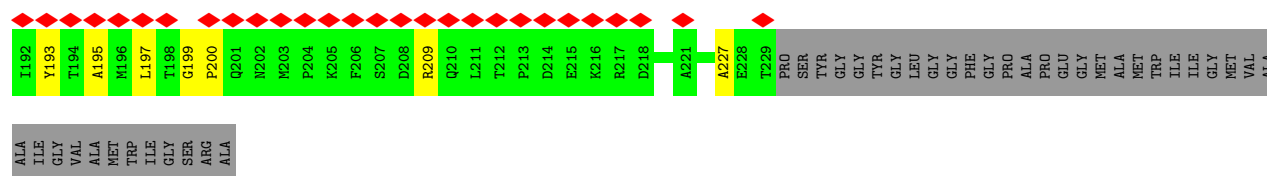
Chain J:  97%



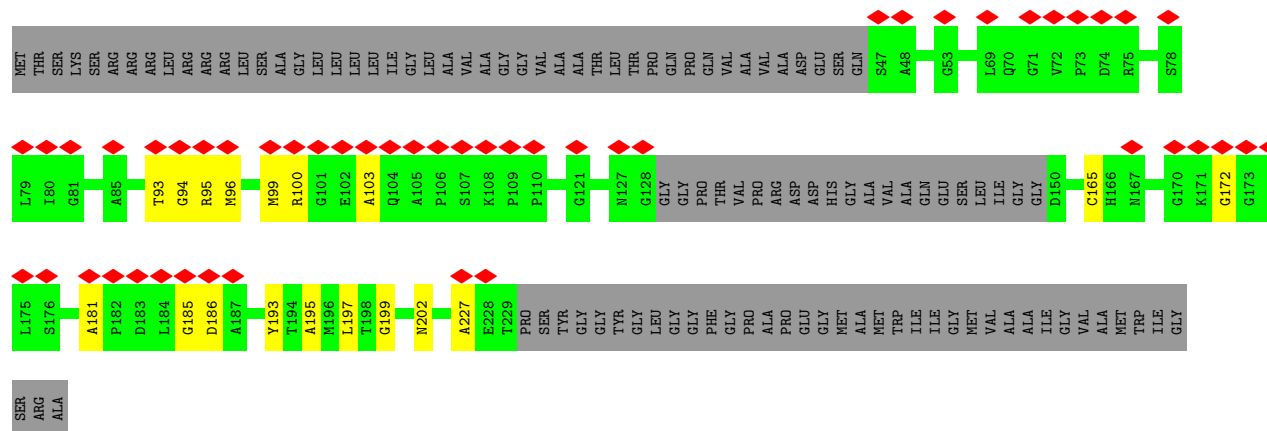
- Molecule 5: Co-purified unknown peptide built as polyALA

Chain F:  97%

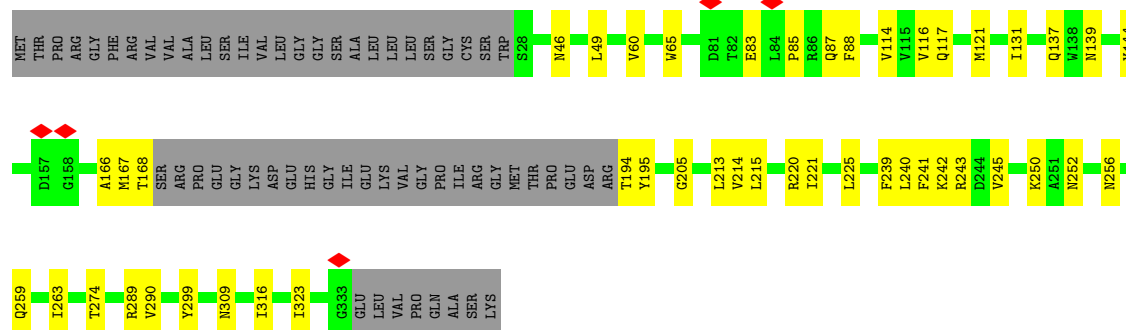




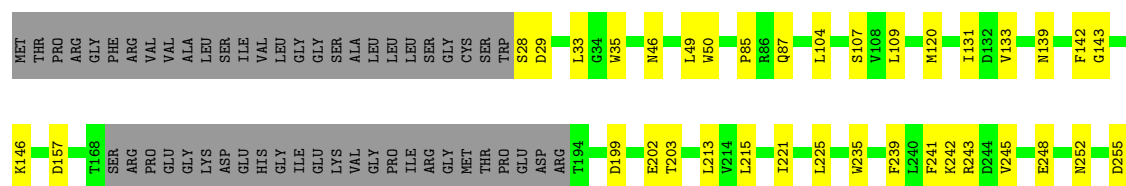
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit



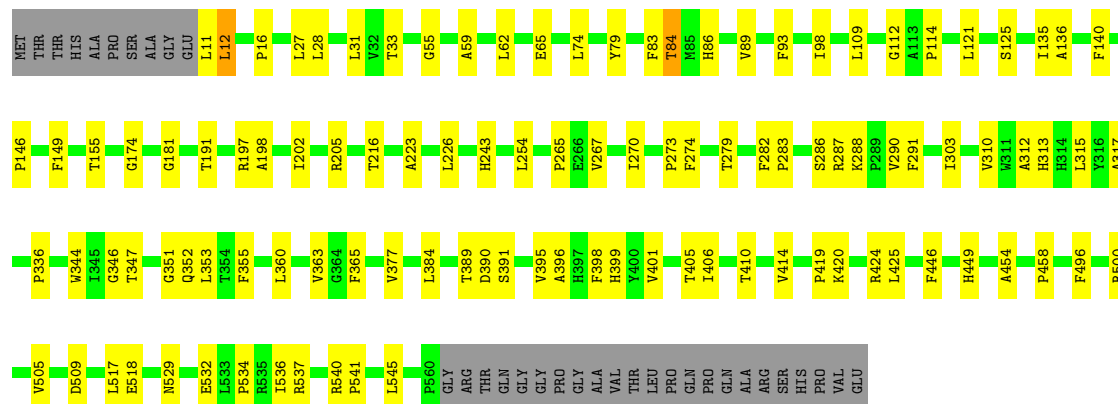
• Molecule 7: Cytochrome c oxidase subunit 2



• Molecule 7: Cytochrome c oxidase subunit 2



Chain Q:  76% 18% 6%



- Molecule 11: Cytochrome c oxidase polypeptide 4

Chain X:  88% 12%



- Molecule 11: Cytochrome c oxidase polypeptide 4

Chain S:  86% 14%



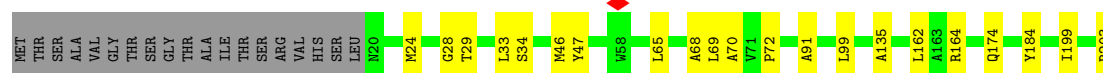
- Molecule 12: Cytochrome c oxidase subunit 3

Chain Z:  81% 9% 9%



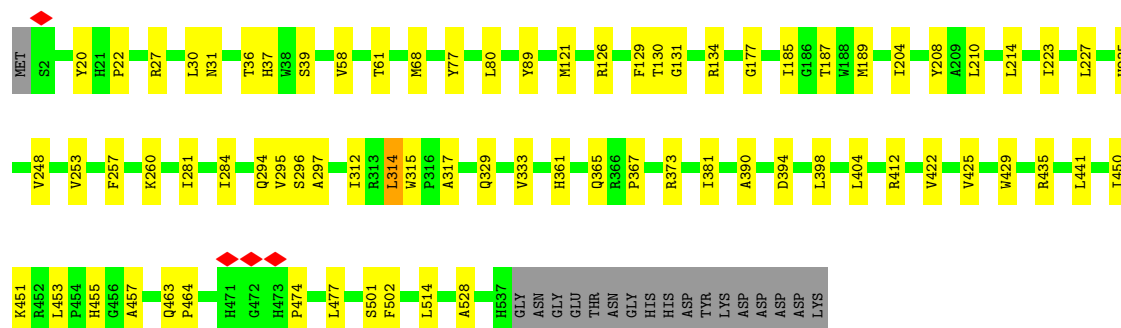
- Molecule 12: Cytochrome c oxidase subunit 3

Chain W:  80% 10% 9%



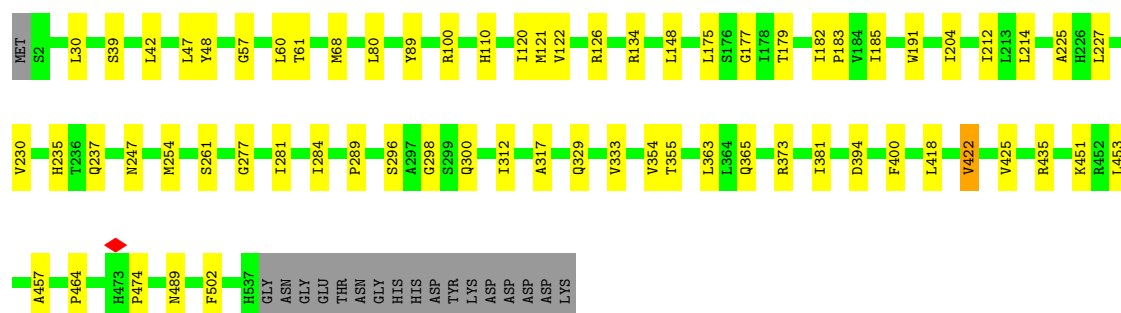
- Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain b:  83% 13% .



• Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain Y: 85% 12% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104198	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.884	Depositor
Minimum map value	-3.920	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.475	Depositor
Map size (Å)	402.8, 402.8, 402.8	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU, FES, HAS, MQ9, HEC, HEM, 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	0.28	0/3039	0.54	0/4120
1	B	0.34	0/3039	0.58	0/4120
6	K	0.38	0/217	0.53	0/293
6	M	0.35	0/217	0.51	0/293
6	i	1.19	2/646 (0.3%)	1.80	2/804 (0.2%)
6	j	1.10	2/646 (0.3%)	1.82	1/804 (0.1%)
7	L	0.37	0/2297	0.66	2/3126 (0.1%)
7	P	0.30	0/2297	0.59	2/3126 (0.1%)
8	N	0.28	0/430	0.56	0/591
8	R	0.23	0/430	0.51	0/591
9	O	0.31	0/1037	0.50	0/1416
9	T	0.26	0/1037	0.48	0/1416
10	Q	0.47	0/4515	0.69	3/6176 (0.0%)
10	V	0.42	0/4515	0.66	0/6176
11	S	0.39	0/1112	0.58	0/1524
11	X	0.33	0/1112	0.54	0/1524
12	W	0.38	0/1488	0.57	0/2032
12	Z	0.32	0/1488	0.53	0/2032
13	Y	0.42	0/4324	0.61	1/5897 (0.0%)
13	b	0.38	0/4324	0.61	3/5897 (0.1%)
All	All	0.43	4/38210 (0.0%)	0.68	14/51958 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	j	193	TYR	CA-C	-6.02	1.45	1.52
6	i	193	TYR	CA-C	-5.99	1.45	1.52
6	i	197	LEU	C-O	-5.23	1.18	1.24
6	j	197	LEU	C-O	-5.22	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	314	LEU	CA-C-N	-7.06	110.47	120.49
13	b	314	LEU	C-N-CA	-7.06	110.47	120.49
10	Q	420	LYS	N-CA-C	-6.03	107.16	114.75
6	i	227	ALA	N-CA-C	5.92	117.81	111.36
6	j	227	ALA	N-CA-C	5.89	117.78	111.36
10	Q	84	THR	CB-CA-C	5.82	119.97	110.95
13	Y	422	VAL	N-CA-C	-5.77	106.67	113.42
10	Q	155	THR	N-CA-C	5.47	121.90	109.81
13	b	31	ASN	N-CA-CB	5.18	118.44	110.46
6	i	76	GLY	N-CA-C	-5.14	108.70	115.22
7	L	316	ILE	CA-C-N	5.12	129.68	122.46
7	L	316	ILE	C-N-CA	5.12	129.68	122.46
7	P	316	ILE	CA-C-N	5.04	129.57	122.46
7	P	316	ILE	C-N-CA	5.04	129.57	122.46

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	A	2960	0	2963	64	0
1	B	2960	0	2965	47	0
2	C	370	0	80	1	0
2	G	370	0	80	1	0
3	D	325	0	67	0	0
3	H	325	0	67	0	0
4	E	100	0	23	0	0
4	I	100	0	23	0	0
5	F	175	0	38	1	0
5	J	175	0	41	1	0
6	K	211	0	212	2	0
6	M	211	0	212	5	0
6	i	648	0	182	105	0
6	j	648	0	185	33	0
7	L	2236	0	2189	30	0
7	P	2236	0	2189	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	415	0	424	4	0
8	R	415	0	424	3	0
9	O	1019	0	1030	11	0
9	T	1019	0	1030	11	0
10	Q	4354	0	4342	70	0
10	V	4354	0	4341	92	0
11	S	1077	0	1058	20	0
11	X	1077	0	1058	14	0
12	W	1441	0	1439	17	0
12	Z	1441	0	1439	13	0
13	Y	4190	0	4211	47	0
13	b	4190	0	4211	99	0
14	A	4	0	0	0	0
14	B	4	0	0	2	0
15	K	100	0	154	6	0
15	M	100	0	154	4	0
15	Q	87	0	118	3	0
15	V	87	0	118	2	0
15	Y	183	0	266	9	0
15	b	183	0	266	2	0
16	M	58	0	80	6	0
16	Y	116	0	160	10	0
16	b	58	0	80	2	0
17	L	2	0	0	0	0
17	P	2	0	0	0	0
17	Q	1	0	0	0	0
17	V	1	0	0	0	0
18	Q	130	0	124	6	0
18	V	130	0	124	6	0
19	V	43	0	32	21	0
19	i	43	0	32	18	0
19	j	86	0	63	34	0
20	Y	86	0	60	6	0
20	b	86	0	60	0	0
All	All	40632	0	38414	612	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 8.

All (612) 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)
13:b:404:LEU:HD13	6:i:72:VAL:CA	1.19	1.55
10:V:161:MET:CG	19:V:804:HEC:HBC2	1.36	1.53
13:b:404:LEU:CD1	6:i:72:VAL:N	1.77	1.46
6:j:93:THR:CA	19:j:302:HEC:O2D	1.65	1.43
13:b:297:ALA:HB2	6:i:64:CYS:CA	1.51	1.39
13:b:404:LEU:HD12	6:i:71:GLY:C	1.42	1.39
6:j:96:MET:N	19:j:301:HEC:HMA2	1.34	1.38
7:P:166:ALA:HB1	6:i:152:ALA:C	1.47	1.38
6:j:96:MET:H	19:j:301:HEC:CMA	1.35	1.35
13:b:404:LEU:HD13	6:i:72:VAL:N	1.31	1.34
10:V:161:MET:CB	19:V:804:HEC:HBC2	1.58	1.31
13:b:297:ALA:CB	6:i:64:CYS:C	2.06	1.27
6:j:95:ARG:N	19:j:301:HEC:CMA	1.99	1.25
6:j:195:ALA:O	6:j:199:GLY:HA2	1.13	1.24
10:V:161:MET:CG	19:V:804:HEC:CBC	2.15	1.23
13:b:404:LEU:CD1	6:i:71:GLY:C	2.09	1.21
1:A:256:MET:HB2	6:i:109:PRO:N	1.56	1.20
6:i:159:ARG:O	6:i:163:ALA:CA	1.88	1.20
10:V:161:MET:HG2	19:V:804:HEC:CBC	1.73	1.19
13:b:404:LEU:CD1	6:i:72:VAL:CA	2.14	1.18
6:j:195:ALA:O	6:j:199:GLY:CA	1.92	1.17
10:V:161:MET:O	19:V:804:HEC:HBC1	1.46	1.16
6:j:96:MET:N	19:j:301:HEC:CMA	1.99	1.16
13:b:297:ALA:HB2	6:i:64:CYS:C	1.66	1.15
13:b:297:ALA:CB	6:i:64:CYS:CA	2.25	1.12
6:j:95:ARG:N	19:j:301:HEC:HMA1	1.58	1.11
6:j:95:ARG:CA	19:j:301:HEC:CMA	2.31	1.09
6:j:95:ARG:C	19:j:301:HEC:HMA2	1.75	1.08
13:b:295:VAL:HG13	6:i:63:SER:N	1.69	1.08
10:V:161:MET:C	19:V:804:HEC:HBC1	1.78	1.08
10:V:161:MET:HB2	19:V:804:HEC:HBC2	1.35	1.07
10:V:161:MET:CB	19:V:804:HEC:CBC	2.31	1.06
6:j:95:ARG:H	19:j:301:HEC:HMA1	1.05	1.06
13:b:295:VAL:HG13	6:i:63:SER:H	1.21	1.06
19:V:804:HEC:O2D	19:i:301:HEC:O1A	1.76	1.03
7:P:166:ALA:HB1	6:i:152:ALA:O	1.56	1.03
11:S:63:LEU:HD23	11:S:64:ASP:O	1.58	1.03
19:j:301:HEC:O1A	19:j:302:HEC:O2D	1.76	1.02
1:A:256:MET:CB	6:i:109:PRO:N	2.24	1.01
6:i:159:ARG:O	6:i:163:ALA:N	1.92	1.00
10:Q:62:LEU:HD21	18:Q:802:HAS:HBD2	1.42	1.00
10:V:161:MET:HG3	19:V:804:HEC:HBC2	1.40	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:95:ARG:CA	19:j:301:HEC:HMA2	1.91	1.00
10:V:161:MET:HB2	19:V:804:HEC:CBC	1.89	0.99
13:b:297:ALA:HB2	6:i:64:CYS:N	1.78	0.98
6:j:96:MET:H	19:j:301:HEC:C3A	1.75	0.98
1:A:342:LEU:HD13	19:i:301:HEC:HMB3	1.44	0.98
11:S:63:LEU:CD2	11:S:64:ASP:O	2.12	0.97
7:P:167:MET:HA	6:i:153:ARG:O	1.64	0.97
6:j:93:THR:N	19:j:302:HEC:O2D	1.98	0.95
6:j:103:ALA:H	6:j:186:ASP:CA	1.80	0.94
6:i:195:ALA:O	6:i:199:GLY:O	1.89	0.91
7:P:166:ALA:CB	6:i:152:ALA:C	2.40	0.90
6:j:94:GLY:HA3	19:j:301:HEC:HAA1	1.54	0.90
13:b:398:LEU:HD22	6:i:69:LEU:CA	2.04	0.88
13:b:297:ALA:HA	6:i:63:SER:O	1.74	0.88
13:b:297:ALA:N	6:i:62:VAL:O	2.07	0.87
6:i:96:MET:N	19:i:301:HEC:HMA1	1.89	0.87
13:b:295:VAL:HG13	6:i:63:SER:CA	2.06	0.84
7:P:137:GLN:HB3	6:i:164:SER:O	1.76	0.84
1:A:345:GLN:NE2	6:i:92:SER:O	2.10	0.84
6:j:95:ARG:N	19:j:301:HEC:HMA2	1.73	0.83
7:P:167:MET:CA	6:i:153:ARG:O	2.24	0.83
13:b:296:SER:HA	6:i:62:VAL:O	1.77	0.83
6:i:195:ALA:O	6:i:199:GLY:CA	2.26	0.83
1:A:256:MET:CG	6:i:109:PRO:N	2.42	0.82
7:P:137:GLN:HB2	6:i:164:SER:CA	2.11	0.81
13:b:297:ALA:HB3	6:i:64:CYS:C	2.05	0.80
1:A:256:MET:HA	6:i:108:LYS:N	1.98	0.78
1:A:342:LEU:CD1	19:i:301:HEC:HMB3	2.13	0.78
10:Q:84:THR:OG1	10:Q:149:PHE:O	2.01	0.75
10:Q:62:LEU:HD23	10:Q:62:LEU:O	1.88	0.74
6:j:94:GLY:HA3	19:j:301:HEC:CAA	2.17	0.73
13:b:404:LEU:HD12	6:i:71:GLY:O	1.86	0.72
1:A:351:LEU:HD23	1:A:352:CYS:N	2.04	0.72
7:P:166:ALA:HB1	6:i:153:ARG:N	2.04	0.72
6:j:202:ASN:CA	19:j:302:HEC:HMD1	2.20	0.71
1:A:243:ARG:HD3	6:i:109:PRO:CA	2.19	0.71
10:V:398:PHE:HA	10:V:401:VAL:HG12	1.73	0.71
7:P:166:ALA:CB	6:i:152:ALA:O	2.38	0.71
10:Q:62:LEU:CD1	10:Q:83:PHE:HB3	2.21	0.70
6:i:96:MET:N	19:i:301:HEC:CMA	2.53	0.70
6:j:95:ARG:C	19:j:301:HEC:CMA	2.47	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:S:63:LEU:HD23	11:S:63:LEU:C	2.17	0.70
10:Q:62:LEU:HD11	10:Q:83:PHE:HB3	1.74	0.70
10:V:32:VAL:HG21	13:b:429:TRP:CZ3	2.26	0.70
13:b:297:ALA:CB	6:i:64:CYS:O	2.41	0.69
13:b:394:ASP:HB2	6:i:71:GLY:HA3	1.74	0.69
6:i:195:ALA:O	6:i:199:GLY:C	2.36	0.69
10:Q:62:LEU:CD2	18:Q:802:HAS:HBD2	2.22	0.68
6:j:94:GLY:HA3	19:j:301:HEC:CBA	2.23	0.68
7:P:167:MET:HA	6:i:157:LEU:H	1.58	0.68
13:b:295:VAL:HG22	6:i:63:SER:CA	2.23	0.68
10:V:402:LEU:HD13	18:V:802:HAS:HAC	1.74	0.68
10:V:161:MET:HB2	19:V:804:HEC:CAC	2.24	0.68
7:P:167:MET:HA	6:i:157:LEU:N	2.09	0.68
6:i:96:MET:H	19:i:301:HEC:CMA	2.07	0.68
13:b:297:ALA:HB1	6:i:64:CYS:C	2.18	0.67
6:j:195:ALA:O	6:j:199:GLY:N	2.27	0.67
1:A:342:LEU:CD1	19:i:301:HEC:CMB	2.72	0.67
1:A:254:VAL:HG13	6:i:108:LYS:CA	2.25	0.67
11:S:63:LEU:HD23	11:S:64:ASP:N	2.09	0.67
1:A:351:LEU:HD23	1:A:351:LEU:C	2.20	0.67
13:b:394:ASP:CB	6:i:71:GLY:HA3	2.24	0.67
10:V:161:MET:C	19:V:804:HEC:CBC	2.64	0.67
13:b:297:ALA:CA	6:i:63:SER:O	2.44	0.66
6:j:96:MET:H	19:j:301:HEC:HMA2	0.95	0.66
7:P:263:ILE:HG21	7:P:290:VAL:HG11	1.76	0.66
13:b:297:ALA:HB2	6:i:63:SER:C	2.20	0.66
10:V:161:MET:O	19:V:804:HEC:CBC	2.35	0.65
7:P:83:GLU:HG2	7:P:85:PRO:HD3	1.77	0.65
10:V:32:VAL:HG21	13:b:429:TRP:CH2	2.32	0.65
10:Q:391:SER:HA	10:Q:458:PRO:HA	1.79	0.65
9:T:31:VAL:HG23	10:V:509:ASP:HB3	1.79	0.65
7:L:225:LEU:HB3	7:L:245:VAL:HG12	1.78	0.65
1:A:342:LEU:HD13	19:i:301:HEC:CMB	2.25	0.64
9:O:31:VAL:HG23	10:Q:509:ASP:HB3	1.79	0.64
13:b:296:SER:CA	6:i:62:VAL:O	2.46	0.64
1:A:345:GLN:NE2	6:i:94:GLY:O	2.24	0.64
1:B:335:HIS:NE2	13:Y:329:GLN:OE1	2.30	0.63
1:A:344:GLU:HA	6:i:95:ARG:O	1.99	0.62
6:j:95:ARG:CA	19:j:301:HEC:HMA3	2.29	0.62
7:P:121:MET:SD	7:P:243:ARG:NH2	2.72	0.62
10:V:391:SER:HA	10:V:458:PRO:HA	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:HA	1:A:293:MET:HB2	1.81	0.62
6:M:262:MET:HE2	6:M:267:ARG:HH11	1.64	0.61
1:B:334:SER:O	1:B:374:ARG:NH2	2.33	0.61
1:B:350:ILE:O	1:B:350:ILE:HG22	2.00	0.61
12:W:68:ALA:O	12:W:69:LEU:HB3	2.00	0.61
1:A:151:ARG:NH2	13:b:235:HIS:O	2.33	0.61
9:O:130:ALA:HB2	9:O:146:ALA:HB2	1.83	0.61
6:j:103:ALA:N	6:j:186:ASP:CA	2.59	0.61
11:X:48:LEU:HG	12:Z:34:SER:HB3	1.82	0.61
13:b:30:LEU:O	13:b:253:VAL:HB	1.99	0.61
10:V:197:ARG:NH2	11:X:4:GLU:OE2	2.33	0.61
13:b:294:GLN:CD	6:i:59:THR:CA	2.65	0.61
13:Y:365:GLN:OE1	13:Y:373:ARG:NH1	2.33	0.60
10:Q:197:ARG:NH2	11:S:4:GLU:OE2	2.34	0.60
7:L:263:ILE:HG21	7:L:290:VAL:HG11	1.82	0.60
13:b:404:LEU:HD12	6:i:71:GLY:CA	2.27	0.60
13:b:297:ALA:HB1	6:i:64:CYS:CA	2.27	0.60
10:V:109:LEU:HB3	10:V:518:GLU:HB3	1.84	0.60
1:B:351:LEU:C	1:B:351:LEU:HD13	2.26	0.60
7:P:242:LYS:NZ	10:V:387:HIS:O	2.35	0.60
6:j:202:ASN:CA	19:j:302:HEC:CMD	2.80	0.60
10:Q:398:PHE:HA	10:Q:401:VAL:HG12	1.83	0.59
7:P:139:ASN:ND2	7:P:205:GLY:O	2.35	0.59
6:i:96:MET:CA	19:i:301:HEC:HMA1	2.32	0.59
6:i:195:ALA:O	6:i:199:GLY:HA2	2.02	0.59
10:V:161:MET:HG2	19:V:804:HEC:HBC1	1.79	0.59
10:V:538:SER:HB3	10:V:555:ARG:HH12	1.68	0.59
7:L:87:GLN:NE2	10:Q:287:ARG:O	2.35	0.59
11:S:48:LEU:HG	12:W:34:SER:HB3	1.84	0.59
11:S:81:GLU:HA	13:Y:451:LYS:HA	1.85	0.58
15:M:301:CDL:HA22	11:X:137:GLU:HG2	1.86	0.58
13:b:210:LEU:HA	13:b:214:LEU:HB2	1.85	0.58
13:b:295:VAL:O	6:i:62:VAL:C	2.46	0.58
13:b:296:SER:HA	6:i:62:VAL:C	2.27	0.58
10:V:310:VAL:O	10:V:313:HIS:ND1	2.29	0.58
13:b:314:LEU:HD11	13:b:390:ALA:HB1	1.84	0.58
1:B:351:LEU:HD23	1:B:358:GLN:HG2	1.84	0.58
10:V:270:ILE:HG23	10:V:406:ILE:HD11	1.86	0.58
7:P:252:ASN:ND2	10:V:250:GLY:O	2.36	0.58
7:P:225:LEU:HB3	7:P:245:VAL:HG12	1.86	0.57
1:B:335:HIS:ND1	14:B:501:FES:S1	2.78	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HD13	1:B:352:CYS:N	2.19	0.57
1:A:336:LEU:HG	13:b:177:GLY:HA3	1.85	0.57
7:P:167:MET:CB	6:i:157:LEU:N	2.61	0.57
1:B:208:LYS:HB2	13:Y:191:TRP:HB3	1.86	0.57
12:W:69:LEU:HD12	12:W:69:LEU:O	2.04	0.57
10:Q:270:ILE:HG23	10:Q:406:ILE:HD11	1.86	0.57
11:S:42:LEU:HA	11:S:45:THR:HG22	1.86	0.57
13:Y:418:LEU:HD21	15:Y:604:CDL:H621	1.87	0.57
10:V:30:LYS:HG2	10:V:30:LYS:O	2.03	0.57
10:V:112:GLY:HA3	10:V:198:ALA:HB2	1.86	0.57
1:A:243:ARG:NH1	6:i:109:PRO:N	2.35	0.57
13:b:314:LEU:O	13:b:412:ARG:HD3	2.04	0.57
7:P:289:ARG:HH12	7:P:323:ILE:HG23	1.70	0.56
6:K:242:PRO:HG2	13:Y:300:GLN:HG3	1.87	0.56
9:T:25:SER:OG	10:V:532:GLU:OE2	2.24	0.56
10:V:279:THR:HG22	10:V:344:TRP:HE1	1.70	0.56
7:L:87:GLN:OE1	10:Q:540:ARG:NH2	2.35	0.56
1:A:373:ALA:HB2	13:b:317:ALA:HB1	1.88	0.56
6:i:96:MET:CA	19:i:301:HEC:CHB	2.82	0.56
7:L:248:GLU:O	7:L:252:ASN:ND2	2.38	0.56
1:A:241:LEU:HD12	1:A:389:LEU:HB3	1.87	0.56
1:B:241:LEU:HD12	1:B:389:LEU:HB3	1.86	0.56
9:O:25:SER:OG	10:Q:532:GLU:OE2	2.22	0.56
9:T:25:SER:H	10:V:532:GLU:HG2	1.71	0.56
10:Q:291:PHE:H	10:Q:347:THR:HB	1.71	0.56
13:Y:39:SER:HB3	13:Y:126:ARG:HG3	1.87	0.56
7:P:167:MET:CA	6:i:157:LEU:N	2.69	0.55
12:Z:131:ILE:HG23	12:Z:132:PRO:HD3	1.88	0.55
13:b:295:VAL:CG1	6:i:63:SER:CA	2.80	0.55
15:Y:603:CDL:H132	15:Y:603:CDL:H512	1.89	0.55
6:K:256:ALA:HB2	15:K:301:CDL:H432	1.89	0.55
1:A:256:MET:HG3	6:i:109:PRO:N	2.21	0.55
7:L:35:TRP:HZ3	7:L:46:ASN:HB3	1.72	0.55
13:Y:121:MET:HB3	16:Y:606:MQ9:H272	1.86	0.55
10:V:29:TYR:O	10:V:30:LYS:HB3	2.06	0.55
8:N:51:ALA:HB2	9:O:55:LEU:HB3	1.87	0.55
10:Q:283:PRO:HG2	10:Q:290:VAL:HG22	1.88	0.55
10:Q:312:ALA:HA	10:Q:315:LEU:HD13	1.89	0.55
15:V:805:CDL:H441	12:Z:149:LEU:HD22	1.88	0.55
10:Q:197:ARG:NH1	11:S:68:GLU:O	2.39	0.55
11:X:82:LEU:HB2	13:b:450:ILE:HB	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:PHE:O	13:Y:100:ARG:NH2	2.38	0.55
13:Y:134:ARG:NH1	13:Y:363:LEU:O	2.40	0.55
1:A:335:HIS:NE2	13:b:329:GLN:OE1	2.33	0.54
13:b:312:ILE:HG12	13:b:333:VAL:HG21	1.89	0.54
8:R:44:HIS:NE2	9:T:40:HIS:O	2.41	0.54
1:B:322:ASN:HD22	1:B:327:PHE:HE1	1.54	0.54
10:Q:496:PHE:O	10:Q:500:ARG:NH1	2.41	0.54
13:Y:212:ILE:HG23	20:Y:601:HEM:HAC	1.90	0.54
6:i:195:ALA:O	6:i:199:GLY:N	2.40	0.54
1:A:243:ARG:HH11	6:i:109:PRO:N	1.51	0.54
13:b:20:TYR:HB2	13:b:22:PRO:HD3	1.90	0.54
6:i:113:ASP:O	6:i:117:ILE:N	2.31	0.54
1:A:180:ARG:NH1	1:B:69:GLU:OE2	2.40	0.54
13:Y:464:PRO:HB3	13:Y:474:PRO:HB3	1.88	0.54
11:S:52:THR:HG1	12:W:34:SER:HG	1.54	0.54
1:B:59:PRO:HA	1:B:143:PRO:HB3	1.89	0.54
15:Q:804:CDL:OA3	12:W:164:ARG:NH2	2.41	0.53
1:A:345:GLN:HG2	6:i:96:MET:O	2.08	0.53
7:P:137:GLN:CB	6:i:164:SER:O	2.53	0.53
6:i:181:ALA:O	6:i:185:GLY:N	2.41	0.53
1:A:342:LEU:HD12	19:i:301:HEC:HMB1	1.89	0.53
13:Y:225:ALA:HB2	16:Y:605:MQ9:H451	1.91	0.53
1:B:120:GLY:HA3	13:Y:277:GLY:HA3	1.91	0.53
11:S:5:ALA:HB3	11:S:57:ARG:HH21	1.73	0.53
2:C:5:UNK:O	13:Y:435:ARG:NH1	2.42	0.53
10:Q:395:VAL:O	10:Q:399:HIS:ND1	2.32	0.53
15:b:603:CDL:H711	15:b:603:CDL:H512	1.91	0.53
10:Q:140:PHE:HA	10:Q:146:PRO:HD3	1.89	0.53
1:A:342:LEU:HD12	19:i:301:HEC:CMB	2.38	0.53
7:P:215:LEU:HD22	7:P:221:ILE:HG21	1.91	0.53
6:j:181:ALA:O	6:j:185:GLY:N	2.41	0.52
13:b:294:GLN:NE2	6:i:59:THR:CA	2.72	0.52
12:W:65:LEU:O	12:W:203:ARG:NH2	2.42	0.52
13:b:297:ALA:CB	6:i:65:HIS:N	2.68	0.52
1:B:357:SER:OG	14:B:501:FES:S1	2.68	0.52
10:Q:317:ALA:HB2	10:Q:389:THR:HG21	1.91	0.52
11:X:42:LEU:HA	11:X:45:THR:HG22	1.90	0.52
10:Q:33:THR:HG22	11:S:90:TRP:HB3	1.90	0.52
2:G:4:UNK:O	13:b:435:ARG:NH1	2.37	0.52
10:V:63:ARG:NH2	18:V:802:HAS:OMD	2.42	0.52
11:X:81:GLU:HA	13:b:451:LYS:HA	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:202:ILE:HG12	10:V:205:ARG:HG2	1.92	0.52
10:V:291:PHE:O	10:V:343:ASN:ND2	2.42	0.52
10:Q:279:THR:HG22	10:Q:344:TRP:HE1	1.74	0.52
13:b:365:GLN:HE21	13:b:373:ARG:HH12	1.58	0.52
10:V:534:PRO:HB3	10:V:545:LEU:HD22	1.91	0.52
1:A:403:PHE:HB2	13:b:187:THR:HG21	1.91	0.52
1:A:243:ARG:HD3	6:i:109:PRO:C	2.35	0.51
10:V:32:VAL:HG21	13:b:429:TRP:HZ3	1.74	0.51
12:W:162:LEU:HB3	13:Y:502:PHE:HZ	1.75	0.51
7:L:133:VAL:HG21	7:L:225:LEU:HD23	1.92	0.51
6:j:99:MET:O	6:j:100:ARG:C	2.53	0.51
1:B:145:GLU:OE1	1:B:147:SER:OG	2.28	0.51
8:N:35:THR:HG22	9:O:44:PRO:HD3	1.91	0.51
1:A:253:PHE:HE2	1:A:290:GLU:HG2	1.75	0.51
10:Q:65:GLU:HG3	10:Q:74:LEU:HD12	1.92	0.51
13:b:422:VAL:HA	13:b:425:VAL:HG12	1.91	0.51
8:N:44:HIS:NE2	9:O:40:HIS:O	2.43	0.51
7:P:168:THR:N	6:i:153:ARG:O	2.44	0.51
13:b:27:ARG:HB2	1:B:164:VAL:HG22	1.93	0.51
7:L:33:LEU:H	7:L:50:TRP:HE1	1.58	0.51
10:V:161:MET:HG3	19:V:804:HEC:CMC	2.41	0.51
9:O:100:SER:HB2	9:O:105:ALA:HB3	1.91	0.51
1:A:245:THR:HG1	1:A:251:SER:HG	1.54	0.51
10:V:355:PHE:HE1	10:V:363:VAL:HG21	1.76	0.50
12:Z:25:VAL:HG12	12:Z:180:VAL:HG11	1.93	0.50
7:L:131:ILE:HD13	7:L:213:LEU:HD11	1.92	0.50
13:Y:30:LEU:HG	13:Y:254:MET:HB2	1.93	0.50
13:Y:230:VAL:HG21	20:Y:602:HEM:HAD1	1.92	0.50
10:Q:223:ALA:HB2	10:Q:265:PRO:HB2	1.93	0.50
1:A:237:GLU:OE2	1:A:273:ARG:NH1	2.43	0.50
1:A:267:GLU:OE1	6:i:110:PRO:N	2.44	0.50
10:Q:114:PRO:O	10:Q:529:ASN:ND2	2.44	0.50
9:T:55:LEU:HD23	9:T:147:VAL:HG11	1.94	0.50
10:V:81:GLN:HB2	10:V:146:PRO:HG2	1.92	0.50
10:Q:216:THR:HG21	10:Q:273:PRO:HD3	1.93	0.50
1:A:280:THR:OG1	1:A:283:GLU:OE1	2.30	0.50
13:b:314:LEU:HD11	13:b:390:ALA:CB	2.41	0.50
7:L:143:GLY:HA2	7:L:202:GLU:HA	1.94	0.50
1:B:351:LEU:C	1:B:351:LEU:CD1	2.85	0.50
13:Y:296:SER:OG	13:Y:298:GLY:O	2.29	0.50
10:V:291:PHE:H	10:V:347:THR:HB	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:Q:310:VAL:O	10:Q:313:HIS:ND1	2.45	0.50
10:V:535:ARG:HH22	11:X:72:ASP:HB2	1.76	0.49
1:A:315:ARG:NH1	1:A:397:GLU:OE2	2.38	0.49
10:V:312:ALA:HA	10:V:315:LEU:HD13	1.93	0.49
10:V:536:ILE:HD13	10:V:541:PRO:HG3	1.94	0.49
13:b:464:PRO:HB3	13:b:474:PRO:HG3	1.93	0.49
12:Z:71:VAL:HA	12:Z:74:THR:HG22	1.95	0.49
10:Q:446:PHE:HA	10:Q:449:HIS:HD1	1.77	0.49
7:P:65:TRP:HZ2	10:V:371:LEU:HD11	1.77	0.49
1:B:245:THR:HG1	1:B:251:SER:HG	1.60	0.49
10:V:191:THR:HG22	12:Z:27:VAL:HG12	1.95	0.49
13:b:68:MET:HG2	13:b:204:ILE:HD12	1.94	0.49
7:L:28:SER:OG	7:L:29:ASP:N	2.46	0.49
15:Y:604:CDL:H512	15:Y:604:CDL:H711	1.94	0.49
10:V:52:PHE:HA	10:V:90:MET:HE1	1.94	0.49
10:V:125:SER:OG	10:V:181:GLY:O	2.26	0.49
10:Q:534:PRO:HB3	10:Q:545:LEU:HD22	1.93	0.49
15:K:301:CDL:H182	15:K:301:CDL:H412	1.93	0.49
13:Y:453:LEU:HB2	13:Y:457:ALA:HB3	1.94	0.49
10:V:27:LEU:O	10:V:31:LEU:HB2	2.13	0.49
10:V:120:ARG:NH2	11:X:128:LEU:O	2.45	0.49
10:V:216:THR:HG21	10:V:273:PRO:HD3	1.95	0.49
1:B:150:ASP:OD1	1:B:150:ASP:N	2.45	0.49
11:S:63:LEU:CD2	11:S:63:LEU:C	2.86	0.49
5:F:13:UNK:HA	11:S:84:PHE:HB2	1.93	0.49
7:L:274:THR:HB	10:Q:390:ASP:HB3	1.95	0.49
6:j:96:MET:N	19:j:301:HEC:HMA3	2.12	0.49
13:Y:47:LEU:HD11	13:Y:227:LEU:HD21	1.95	0.48
1:B:245:THR:OG1	1:B:251:SER:OG	2.28	0.48
10:Q:287:ARG:HD3	10:Q:352:GLN:HG2	1.94	0.48
10:Q:377:VAL:HG21	18:Q:801:HAS:H241	1.95	0.48
10:V:159:ASN:O	10:V:238:ARG:NH1	2.45	0.48
1:B:328:ALA:HB2	1:B:381:ILE:HD11	1.95	0.48
7:P:220:ARG:NH2	7:P:259:GLN:OE1	2.47	0.48
10:Q:136:ALA:HB2	10:Q:174:GLY:HA3	1.95	0.48
13:Y:148:LEU:HB2	20:Y:602:HEM:HBB1	1.95	0.48
13:Y:312:ILE:HG12	13:Y:333:VAL:HG21	1.94	0.48
10:V:254:LEU:HD21	12:Z:46:MET:HG2	1.95	0.48
10:V:424:ARG:NH1	10:V:500:ARG:O	2.46	0.48
13:b:129:PHE:HB3	13:b:367:PRO:HB3	1.96	0.48
7:L:239:PHE:O	7:L:241:PHE:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:O	1:A:374:ARG:NH2	2.46	0.48
1:A:59:PRO:HA	1:A:143:PRO:HB3	1.94	0.48
13:Y:126:ARG:HH22	20:Y:602:HEM:HBA1	1.78	0.48
15:Y:603:CDL:H251	15:Y:604:CDL:H272	1.96	0.48
7:P:60:VAL:HG11	18:V:801:HAS:H22	1.96	0.48
8:R:49:TRP:CG	10:V:16:PRO:HG3	2.49	0.48
1:B:379:LEU:HD12	1:B:380:PRO:HD2	1.95	0.48
6:M:245:GLU:HG2	13:b:281:ILE:HA	1.95	0.47
6:M:266:SER:OG	13:b:36:THR:O	2.32	0.47
15:K:301:CDL:H791	15:K:301:CDL:H762	1.63	0.47
15:Y:603:CDL:H712	15:Y:604:CDL:H712	1.96	0.47
1:A:351:LEU:C	1:A:351:LEU:CD2	2.86	0.47
1:A:260:ASP:OD1	6:i:105:ALA:O	2.31	0.47
16:M:302:MQ9:H272	13:b:121:MET:HB3	1.96	0.47
10:V:310:VAL:HG11	10:V:333:ILE:HD11	1.96	0.47
7:P:167:MET:O	7:P:194:THR:N	2.47	0.47
10:Q:55:GLY:O	10:Q:86:HIS:ND1	2.43	0.47
7:P:239:PHE:O	7:P:241:PHE:N	2.48	0.47
13:b:295:VAL:CG2	6:i:63:SER:CA	2.93	0.47
7:L:215:LEU:HD22	7:L:221:ILE:HD13	1.97	0.47
10:Q:536:ILE:HD13	10:Q:541:PRO:HG3	1.95	0.47
7:P:167:MET:HB3	7:P:194:THR:HG23	1.95	0.47
12:Z:36:GLU:OE1	12:Z:150:HIS:NE2	2.48	0.47
13:b:404:LEU:HD11	6:i:72:VAL:N	2.08	0.47
1:B:231:THR:HA	1:B:394:ASP:HB3	1.95	0.47
9:O:85:LEU:HD21	9:O:111:GLY:HA2	1.96	0.47
10:Q:135:ILE:HD11	11:S:100:SER:HB2	1.97	0.47
18:Q:801:HAS:H172	18:Q:801:HAS:H202	1.74	0.47
13:Y:89:TYR:OH	13:Y:284:ILE:O	2.29	0.47
13:Y:227:LEU:HA	13:Y:230:VAL:HG12	1.97	0.47
15:M:301:CDL:H572	11:X:123:THR:HG21	1.96	0.47
13:Y:57:GLY:O	13:Y:61:THR:OG1	2.25	0.47
1:B:348:TYR:HB3	1:B:361:ALA:HB3	1.97	0.47
7:L:199:ASP:OD1	7:L:199:ASP:N	2.45	0.47
10:Q:254:LEU:HD21	12:W:46:MET:HG2	1.97	0.47
10:V:270:ILE:HG22	18:V:801:HAS:HBC2	1.96	0.47
13:Y:68:MET:HG2	13:Y:204:ILE:HD12	1.96	0.47
6:j:96:MET:CA	19:j:301:HEC:CHB	2.93	0.47
1:A:256:MET:HB2	6:i:108:LYS:C	2.32	0.46
9:T:43:PHE:HZ	9:T:139:LEU:HD23	1.80	0.46
9:O:55:LEU:HD23	9:O:147:VAL:HG11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:114:VAL:HG12	9:O:117:ARG:HH11	1.80	0.46
1:A:243:ARG:HD3	6:i:110:PRO:N	2.30	0.46
16:b:605:MQ9:H303	16:b:605:MQ9:H322	1.61	0.46
10:Q:112:GLY:HA3	10:Q:198:ALA:HB2	1.98	0.46
13:Y:120:ILE:HG12	20:Y:602:HEM:HMC1	1.97	0.46
10:Q:424:ARG:NH1	10:Q:500:ARG:O	2.42	0.46
1:A:103:PRO:HG2	1:A:106:SER:HB2	1.96	0.46
1:A:256:MET:CA	6:i:108:LYS:N	2.75	0.46
10:V:535:ARG:NH1	10:V:536:ILE:O	2.48	0.46
13:b:294:GLN:HE22	6:i:59:THR:CA	2.28	0.46
16:Y:605:MQ9:H303	16:Y:605:MQ9:H351	1.97	0.46
10:V:382:PRO:HA	10:V:385:ASP:HB3	1.98	0.46
7:L:85:PRO:HG2	10:Q:351:GLY:HA2	1.98	0.46
19:i:301:HEC:HBC2	19:i:301:HEC:HMC3	1.98	0.46
1:A:379:LEU:HD12	1:A:380:PRO:HD2	1.98	0.46
1:B:357:SER:HA	1:B:370:GLY:HA3	1.98	0.46
7:P:250:LYS:HE2	7:P:256:ASN:HD22	1.80	0.46
9:T:38:SER:OG	10:V:504:PRO:O	2.30	0.46
11:S:2:HIS:HE1	11:S:6:ARG:HH21	1.63	0.46
6:i:96:MET:H	19:i:301:HEC:HMA3	1.78	0.46
13:b:39:SER:HB3	13:b:126:ARG:HG3	1.97	0.46
7:L:319:PRO:HA	7:L:320:PRO:HD3	1.79	0.46
19:i:301:HEC:HMB3	19:i:301:HEC:HBB2	1.98	0.46
7:P:194:THR:OG1	7:P:195:TYR:N	2.44	0.46
1:B:116:THR:HG23	1:B:117:PRO:HD3	1.97	0.46
1:A:256:MET:CG	6:i:109:PRO:CA	2.72	0.46
7:P:85:PRO:HG2	7:P:87:GLN:HG3	1.98	0.46
13:b:126:ARG:O	13:b:130:THR:OG1	2.30	0.46
1:A:308:ASP:HB3	1:A:311:ARG:HH21	1.81	0.45
19:V:804:HEC:HMC1	19:V:804:HEC:HBC3	1.98	0.45
13:b:315:TRP:HB2	13:b:329:GLN:HE21	1.80	0.45
1:B:230:TRP:CE2	1:B:271:PRO:HG3	2.51	0.45
19:j:302:HEC:HBB2	19:j:302:HEC:HMB3	1.98	0.45
10:Q:396:ALA:HB2	10:Q:449:HIS:HB2	1.98	0.45
15:M:301:CDL:H751	15:M:301:CDL:H781	1.69	0.45
7:L:109:LEU:HD12	18:Q:801:HAS:H321	1.99	0.45
15:Q:804:CDL:HB62	15:Q:804:CDL:H712	1.73	0.45
19:V:804:HEC:HMB1	19:V:804:HEC:HBB3	1.98	0.45
10:Q:288:LYS:NZ	10:Q:346:GLY:O	2.32	0.45
13:Y:237:GLN:NE2	13:Y:247:ASN:O	2.49	0.45
19:i:301:HEC:HMB3	19:i:301:HEC:CBB	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:302:MQ9:H353	16:M:302:MQ9:H371	1.78	0.45
9:T:24:SER:HB3	13:b:455:HIS:HB2	1.98	0.45
7:L:235:TRP:HB2	7:L:242:LYS:HG3	1.97	0.45
19:j:301:HEC:HBC2	19:j:301:HEC:HMC3	1.98	0.45
9:T:85:LEU:HD21	9:T:111:GLY:HA2	1.98	0.45
10:V:288:LYS:NZ	10:V:346:GLY:O	2.46	0.45
13:b:296:SER:C	6:i:62:VAL:O	2.58	0.45
13:b:297:ALA:HB1	6:i:64:CYS:O	2.12	0.45
1:B:373:ALA:HB2	13:Y:317:ALA:HB1	1.97	0.45
10:Q:109:LEU:HB3	10:Q:518:GLU:HB3	1.98	0.45
10:V:420:LYS:HG3	10:V:421:MET:HE2	1.99	0.45
9:O:122:ALA:O	9:O:126:GLY:N	2.49	0.45
19:j:302:HEC:HMC1	19:j:302:HEC:HBC3	1.98	0.45
13:b:58:VAL:HG13	13:Y:214:LEU:HD11	1.97	0.45
13:b:394:ASP:HB2	6:i:71:GLY:CA	2.43	0.45
7:L:35:TRP:CD1	10:Q:454:ALA:HB1	2.51	0.45
10:Q:11:LEU:HD13	10:Q:12:LEU:HB2	1.98	0.45
19:j:301:HEC:HBB2	19:j:301:HEC:HMB3	1.98	0.45
10:V:283:PRO:HB2	10:V:515:ASN:HD21	1.82	0.45
19:V:804:HEC:HMB1	19:V:804:HEC:CBB	2.47	0.45
13:b:297:ALA:HB2	6:i:65:HIS:N	2.22	0.45
7:L:142:PHE:HB2	7:L:203:THR:HB	1.98	0.45
10:Q:98:ILE:HG23	10:Q:274:PHE:HZ	1.82	0.45
19:i:301:HEC:HMC3	19:i:301:HEC:CBC	2.47	0.45
19:V:804:HEC:CBC	19:V:804:HEC:HMC1	2.47	0.44
13:b:398:LEU:CD2	6:i:69:LEU:CA	2.85	0.44
10:Q:365:PHE:HE1	10:Q:405:THR:HG22	1.81	0.44
10:V:259:PHE:O	10:V:263:GLY:N	2.50	0.44
12:Z:192:TRP:O	12:Z:196:PHE:N	2.47	0.44
19:j:301:HEC:HMC3	19:j:301:HEC:CBC	2.47	0.44
7:P:166:ALA:CB	6:i:153:ARG:N	2.66	0.44
13:Y:235:HIS:NE2	20:Y:602:HEM:O2D	2.46	0.44
12:Z:133:GLY:HA2	6:i:209:ARG:O	2.17	0.44
10:Q:355:PHE:HE1	10:Q:363:VAL:HG21	1.82	0.44
19:j:302:HEC:HMC1	19:j:302:HEC:CBC	2.47	0.44
10:V:11:LEU:HD13	10:V:12:LEU:HB2	1.99	0.44
10:V:98:ILE:HG23	10:V:274:PHE:HZ	1.82	0.44
10:V:446:PHE:HA	10:V:449:HIS:HD1	1.82	0.44
7:L:289:ARG:HH12	7:L:323:ILE:HG23	1.83	0.44
7:L:299:TYR:OH	7:L:309:ASN:OD1	2.33	0.44
15:Y:604:CDL:H351	16:Y:606:MQ9:H202	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:9:GLU:HA	11:X:12:THR:HG22	2.00	0.44
13:b:134:ARG:HE	13:b:361:HIS:CG	2.36	0.44
1:A:55:ILE:HG22	13:b:528:ALA:HB1	1.99	0.44
13:b:89:TYR:OH	13:b:284:ILE:O	2.29	0.44
13:Y:48:TYR:OH	13:Y:261:SER:OG	2.34	0.44
11:S:108:LEU:HD13	13:Y:400:PHE:HA	2.00	0.44
6:j:94:GLY:C	19:j:301:HEC:HMA2	2.38	0.44
19:j:301:HEC:HMB3	19:j:301:HEC:CBB	2.47	0.44
10:V:96:THR:HG22	10:V:269:ILE:HD11	1.99	0.44
13:b:77:TYR:HD2	13:b:80:LEU:HB2	1.83	0.44
10:Q:59:ALA:HB2	10:Q:86:HIS:CE1	2.52	0.44
19:j:302:HEC:HMB3	19:j:302:HEC:CBB	2.47	0.44
1:A:67:LYS:HG2	1:A:71:ARG:HH21	1.83	0.43
10:V:169:ASP:OD1	10:V:238:ARG:NE	2.40	0.43
1:B:230:TRP:NE1	1:B:297:ASN:O	2.47	0.43
10:Q:282:PHE:O	10:Q:286:SER:OG	2.34	0.43
15:V:805:CDL:OA4	12:Z:164:ARG:NH2	2.51	0.43
13:b:295:VAL:O	6:i:62:VAL:CA	2.66	0.43
1:A:230:TRP:CE2	1:A:271:PRO:HG3	2.54	0.43
7:P:46:ASN:ND2	7:P:240:LEU:O	2.50	0.43
13:b:314:LEU:O	13:b:412:ARG:CD	2.65	0.43
13:b:441:LEU:HD22	13:b:477:LEU:HB2	2.01	0.43
7:P:88:PHE:HA	10:V:558:SER:HA	2.00	0.43
7:P:215:LEU:HD13	7:P:221:ILE:HD13	2.00	0.43
9:T:88:VAL:HA	9:T:89:PRO:HD3	1.92	0.43
10:V:29:TYR:O	10:V:30:LYS:CB	2.66	0.43
13:b:453:LEU:HB2	13:b:457:ALA:HB3	2.00	0.43
10:Q:202:ILE:HG12	10:Q:205:ARG:HG2	2.01	0.43
16:Y:605:MQ9:H153	16:Y:605:MQ9:H171	1.71	0.43
10:V:372:GLY:HA3	10:V:401:VAL:HB	2.00	0.43
10:Q:121:LEU:HD11	15:Q:804:CDL:H712	2.01	0.43
10:Q:517:LEU:HG	10:Q:541:PRO:HG2	2.00	0.43
1:A:342:LEU:HD13	19:i:301:HEC:HBB2	2.00	0.43
10:V:33:THR:HG22	11:X:90:TRP:HB3	2.00	0.43
13:b:257:PHE:HA	13:b:260:LYS:HG2	2.00	0.43
7:L:300:ILE:O	7:L:304:ASN:N	2.43	0.43
7:P:131:ILE:HD13	7:P:213:LEU:HD11	2.01	0.43
16:b:605:MQ9:H272	16:b:605:MQ9:H253	1.69	0.43
15:K:301:CDL:H451	15:K:301:CDL:H611	1.76	0.43
10:Q:27:LEU:HG	10:Q:31:LEU:HD13	2.01	0.43
11:S:63:LEU:HD23	11:S:64:ASP:C	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:HG23	1:A:327:PHE:HB2	2.01	0.43
10:V:452:LEU:HD12	10:V:473:LEU:HB3	2.01	0.43
1:B:358:GLN:HB2	1:B:369:PHE:HB3	2.00	0.43
5:J:6:UNK:N	12:Z:21:ARG:O	2.52	0.43
7:P:242:LYS:HE3	7:P:274:THR:HG21	2.00	0.43
12:W:91:ALA:HB2	12:W:99:LEU:HD13	2.00	0.43
13:Y:110:HIS:HB3	13:Y:281:ILE:HG12	2.00	0.43
7:P:114:VAL:HA	7:P:117:GLN:HG2	2.01	0.42
13:b:398:LEU:HD22	6:i:69:LEU:N	2.34	0.42
1:B:336:LEU:HG	13:Y:177:GLY:HA3	2.01	0.42
10:V:378:ILE:HG23	10:V:384:LEU:HD23	2.00	0.42
10:V:394:VAL:HG12	10:V:398:PHE:HE2	1.85	0.42
1:B:315:ARG:HB3	1:B:318:GLN:HB2	1.99	0.42
13:Y:422:VAL:HA	13:Y:425:VAL:HG12	2.01	0.42
6:M:268:ALA:H	13:b:37:HIS:CD2	2.37	0.42
16:Y:605:MQ9:H253	16:Y:605:MQ9:H271	1.64	0.42
1:A:198:THR:HG22	1:B:123:PHE:HE1	1.85	0.42
7:L:146:LYS:HA	7:L:157:ASP:HA	2.02	0.42
10:Q:537:ARG:HE	11:S:72:ASP:HB2	1.84	0.42
10:V:59:ALA:HB2	10:V:86:HIS:CE1	2.53	0.42
1:B:351:LEU:HD23	1:B:358:GLN:CG	2.48	0.42
12:W:70:ALA:N	12:W:72:PRO:HD2	2.34	0.42
16:Y:606:MQ9:H71	16:Y:606:MQ9:H5M3	1.84	0.42
7:L:215:LEU:HD22	7:L:221:ILE:HG21	2.00	0.42
12:W:164:ARG:O	12:W:174:GLN:NE2	2.49	0.42
13:Y:42:LEU:HD13	13:Y:122:VAL:HG12	2.01	0.42
10:V:382:PRO:O	10:V:386:PHE:N	2.50	0.42
13:Y:422:VAL:HG13	15:Y:604:CDL:H771	2.02	0.42
16:M:302:MQ9:H221	16:M:302:MQ9:H262	1.83	0.42
7:P:144:TYR:OH	7:P:214:VAL:O	2.28	0.42
10:V:391:SER:OG	10:V:392:TYR:N	2.52	0.42
15:K:301:CDL:H832	11:S:119:ALA:HB2	2.01	0.42
1:A:34:LEU:HD11	1:B:159:VAL:HG12	2.02	0.42
6:M:247:MET:SD	16:M:302:MQ9:H3D	2.60	0.42
13:Y:80:LEU:HD11	13:Y:289:PRO:HD3	2.02	0.42
16:Y:606:MQ9:H203	16:Y:606:MQ9:H221	1.80	0.42
6:j:165:CYS:O	6:j:172:GLY:N	2.52	0.42
1:A:66:THR:HB	13:b:514:LEU:HD11	2.02	0.42
16:M:302:MQ9:H172	16:M:302:MQ9:H211	1.84	0.42
10:Q:62:LEU:HG	10:Q:79:TYR:CZ	2.54	0.42
12:W:47:TYR:CZ	12:W:199:ILE:HG22	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Y:182:ILE:HA	13:Y:183:PRO:HD3	1.92	0.42
10:V:197:ARG:HB2	11:X:68:GLU:HG2	2.02	0.41
10:V:161:MET:HG3	19:V:804:HEC:HMC2	2.01	0.41
12:Z:69:LEU:HD21	12:Z:119:TYR:HD2	1.85	0.41
15:K:301:CDL:H371	15:K:301:CDL:H142	2.01	0.41
6:j:94:GLY:CA	19:j:301:HEC:CBA	2.97	0.41
1:A:159:VAL:HG12	1:B:34:LEU:HD11	2.02	0.41
18:V:801:HAS:H251	18:V:801:HAS:H281	1.79	0.41
10:Q:89:VAL:HG22	10:Q:93:PHE:HD2	1.85	0.41
13:b:77:TYR:HE2	13:b:80:LEU:HD23	1.85	0.41
13:b:394:ASP:CA	6:i:71:GLY:HA3	2.51	0.41
7:L:243:ARG:HH12	7:L:255:ASP:HB3	1.85	0.41
10:Q:243:HIS:HB2	12:W:135:ALA:HA	2.02	0.41
16:M:302:MQ9:H18	15:b:603:CDL:H341	2.02	0.41
10:Q:410:THR:O	10:Q:414:VAL:N	2.49	0.41
1:A:73:GLU:HB2	1:B:183:ILE:HD11	2.02	0.41
15:M:301:CDL:H471	15:M:301:CDL:H861	2.03	0.41
7:P:49:LEU:HD22	7:P:116:VAL:HG21	2.03	0.41
13:b:398:LEU:CD2	6:i:69:LEU:N	2.84	0.41
10:V:31:LEU:O	10:V:34:THR:HG22	2.21	0.41
10:V:420:LYS:NZ	10:V:521:THR:O	2.54	0.41
18:Q:802:HAS:H171	18:Q:802:HAS:H261	1.74	0.41
12:W:29:THR:O	12:W:33:LEU:N	2.48	0.41
12:W:33:LEU:HD21	12:W:184:TYR:HD1	1.86	0.41
15:Y:604:CDL:H181	16:Y:606:MQ9:H18	2.03	0.41
1:A:150:ASP:OD1	1:A:150:ASP:N	2.51	0.41
7:P:167:MET:C	6:i:153:ARG:O	2.63	0.41
10:V:299:ALA:O	10:V:302:SER:OG	2.39	0.41
1:B:227:THR:HA	1:B:231:THR:HG21	2.02	0.41
1:B:374:ARG:CZ	1:B:402:ALA:HB2	2.51	0.41
1:B:380:PRO:HB2	1:B:392:ASN:HB2	2.02	0.41
7:L:49:LEU:HG	10:Q:384:LEU:HD11	2.02	0.41
8:N:49:TRP:CG	10:Q:16:PRO:HG3	2.55	0.41
10:Q:425:LEU:HG	10:Q:505:VAL:HG22	2.03	0.41
13:Y:175:LEU:O	13:Y:179:THR:OG1	2.39	0.41
13:Y:489:ASN:N	13:Y:489:ASN:OD1	2.54	0.41
13:b:501:SER:OG	13:b:502:PHE:N	2.53	0.41
7:L:46:ASN:ND2	7:L:120:MET:HE1	2.36	0.41
10:Q:62:LEU:HG	10:Q:79:TYR:CE1	2.55	0.41
10:Q:191:THR:HG21	12:W:28:GLY:HA2	2.03	0.41
1:A:406:ARG:NE	1:A:408:SER:OG	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:480:GLY:HA2	10:V:483:ILE:HD12	2.03	0.40
13:b:61:THR:OG1	13:b:208:TYR:OH	2.27	0.40
13:b:463:GLN:HA	13:b:464:PRO:HD3	1.87	0.40
1:B:356:GLN:NE2	13:Y:394:ASP:HB3	2.35	0.40
1:A:149:GLN:O	13:b:248:VAL:N	2.54	0.40
1:B:262:ASP:OD1	1:B:262:ASP:N	2.54	0.40
10:Q:125:SER:OG	10:Q:181:GLY:O	2.30	0.40
10:Q:419:PRO:HG3	10:Q:425:LEU:HD23	2.03	0.40
13:Y:354:VAL:HG23	13:Y:355:THR:HG23	2.04	0.40
1:A:69:GLU:OE2	1:B:180:ARG:NH1	2.45	0.40
7:P:87:GLN:HG2	10:V:288:LYS:HA	2.02	0.40
13:b:131:GLY:O	13:b:134:ARG:NH2	2.54	0.40
13:b:223:ILE:HG23	13:b:227:LEU:HD13	2.02	0.40
13:b:297:ALA:HB3	6:i:65:HIS:N	2.35	0.40
1:B:253:PHE:HZ	1:B:291:ILE:HD11	1.86	0.40
7:L:104:LEU:HA	7:L:107:SER:HB3	2.03	0.40
10:Q:274:PHE:CE1	10:Q:410:THR:HG22	2.57	0.40
1:A:258:PRO:HB3	1:A:389:LEU:HD21	2.03	0.40
1:A:345:GLN:CD	6:i:92:SER:O	2.64	0.40
10:V:71:LEU:HD12	10:V:463:ASP:HB2	2.03	0.40
10:V:135:ILE:HD11	11:X:100:SER:HB2	2.03	0.40
10:V:313:HIS:HD2	18:V:801:HAS:C2D	2.35	0.40
1:B:106:SER:OG	1:B:107:GLU:N	2.53	0.40
1:B:302:ILE:HD12	1:B:329:TYR:HD2	1.86	0.40
10:Q:303:ILE:HG13	10:Q:336:PRO:HB2	2.03	0.40
1:A:298:PRO:HB2	1:A:331:LYS:HD3	2.04	0.40
7:P:167:MET:HB3	6:i:157:LEU:N	2.32	0.40
7:P:299:TYR:OH	7:P:309:ASN:OD1	2.37	0.40
8:R:51:ALA:HB2	9:T:55:LEU:HB3	2.02	0.40
10:V:55:GLY:O	10:V:86:HIS:ND1	2.40	0.40
10:V:173:PHE:HB3	11:X:103:ALA:HB1	2.04	0.40
13:b:185:ILE:HD11	13:b:189:MET:HB2	2.02	0.40
12:W:24:MET:HE3	12:W:24:MET:HB2	1.93	0.40
13:Y:61:THR:HG23	13:Y:212:ILE:HD13	2.03	0.40
15:Y:603:CDL:H782	15:Y:604:CDL:H781	2.02	0.40
16:Y:605:MQ9:H303	16:Y:605:MQ9:H322	1.69	0.40
6:i:99:MET:O	6:i:111:HIS:CA	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
1	B	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
6	K	28/268 (10%)	27 (96%)	1 (4%)	0	100	100
6	M	28/268 (10%)	26 (93%)	2 (7%)	0	100	100
6	i	158/268 (59%)	143 (90%)	11 (7%)	4 (2%)	4	23
6	j	158/268 (59%)	145 (92%)	13 (8%)	0	100	100
7	L	277/341 (81%)	234 (84%)	43 (16%)	0	100	100
7	P	277/341 (81%)	236 (85%)	41 (15%)	0	100	100
8	N	52/79 (66%)	41 (79%)	11 (21%)	0	100	100
8	R	52/79 (66%)	44 (85%)	8 (15%)	0	100	100
9	O	140/157 (89%)	130 (93%)	10 (7%)	0	100	100
9	T	140/157 (89%)	129 (92%)	11 (8%)	0	100	100
10	Q	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
10	V	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
11	S	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
11	X	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
12	W	182/203 (90%)	166 (91%)	16 (9%)	0	100	100
12	Z	182/203 (90%)	169 (93%)	13 (7%)	0	100	100
13	Y	534/554 (96%)	489 (92%)	45 (8%)	0	100	100
13	b	534/554 (96%)	486 (91%)	48 (9%)	0	100	100
All	All	4868/6000 (81%)	4405 (90%)	459 (9%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	i	73	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	i	77	PRO
6	i	110	PRO
6	i	200	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	310/333 (93%)	310 (100%)	0	100	100
1	B	310/333 (93%)	308 (99%)	2 (1%)	78	81
6	K	18/197 (9%)	18 (100%)	0	100	100
6	M	18/197 (9%)	18 (100%)	0	100	100
7	L	239/288 (83%)	238 (100%)	1 (0%)	84	84
7	P	239/288 (83%)	239 (100%)	0	100	100
8	N	44/59 (75%)	44 (100%)	0	100	100
8	R	44/59 (75%)	44 (100%)	0	100	100
9	O	105/114 (92%)	105 (100%)	0	100	100
9	T	105/114 (92%)	105 (100%)	0	100	100
10	Q	456/481 (95%)	450 (99%)	6 (1%)	61	74
10	V	456/481 (95%)	450 (99%)	6 (1%)	61	74
11	S	106/106 (100%)	106 (100%)	0	100	100
11	X	106/106 (100%)	106 (100%)	0	100	100
12	W	146/161 (91%)	146 (100%)	0	100	100
12	Z	146/161 (91%)	146 (100%)	0	100	100
13	Y	431/446 (97%)	428 (99%)	3 (1%)	76	80
13	b	431/446 (97%)	430 (100%)	1 (0%)	87	88
All	All	3710/4370 (85%)	3691 (100%)	19 (0%)	78	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	V	12	LEU
10	V	226	LEU
10	V	267	VAL
10	V	269	ILE
10	V	360	LEU
10	V	392	TYR
13	b	381	ILE
1	B	301	LEU
1	B	351	LEU
7	L	139	ASN
10	Q	12	LEU
10	Q	28	LEU
10	Q	226	LEU
10	Q	267	VAL
10	Q	353	LEU
10	Q	360	LEU
13	Y	60	LEU
13	Y	185	ILE
13	Y	381	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
7	P	145	GLN
7	P	256	ASN
8	R	7	HIS
9	T	40	HIS
10	V	528	HIS
11	X	88	HIS
12	Z	53	GLN
12	Z	117	GLN
13	b	110	HIS
13	b	401	HIS
13	b	443	HIS
13	b	519	HIS
1	B	102	GLN
1	B	356	GLN
1	B	378	GLN
7	L	139	ASN
7	L	252	ASN
8	N	7	HIS
10	Q	343	ASN
11	S	88	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	Y	70	HIS
13	Y	247	ASN
13	Y	405	ASN
13	Y	434	GLN
13	Y	443	HIS
13	Y	537	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	HEM	b	602	13	50,50,50	1.68	11 (22%)	67,82,82	2.04	18 (26%)
19	HEC	i	301	-	46,50,50	2.61	23 (50%)	58,82,82	2.08	21 (36%)
20	HEM	b	601	13	50,50,50	1.63	12 (24%)	67,82,82	2.21	22 (32%)
19	HEC	j	302	-	46,50,50	2.61	23 (50%)	58,82,82	2.07	21 (36%)
16	MQ9	Y	606	-	59,59,59	1.27	7 (11%)	73,75,75	1.44	14 (19%)
14	FES	B	501	1	0,4,4	-	-	-	-	-
14	FES	A	501	1	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	HAS	V	801	10	72,72,72	1.12	5 (6%)	87,109,109	1.26	13 (14%)
20	HEM	Y	601	13	50,50,50	1.65	11 (22%)	67,82,82	1.81	17 (25%)
20	HEM	Y	602	13	50,50,50	1.66	10 (20%)	67,82,82	1.92	19 (28%)
18	HAS	Q	801	10	72,72,72	1.12	7 (9%)	87,109,109	1.23	8 (9%)
15	CDL	b	604	-	90,90,99	1.25	9 (10%)	96,102,111	0.98	4 (4%)
18	HAS	V	802	10	72,72,72	1.14	6 (8%)	87,109,109	1.17	8 (9%)
15	CDL	M	301	-	99,99,99	1.23	8 (8%)	105,111,111	0.99	4 (3%)
19	HEC	j	301	-	46,50,50	2.61	23 (50%)	58,82,82	2.08	21 (36%)
15	CDL	b	603	-	91,91,99	1.21	7 (7%)	97,103,111	1.09	5 (5%)
16	MQ9	Y	605	-	59,59,59	0.92	1 (1%)	73,75,75	1.48	13 (17%)
19	HEC	V	804	-	46,50,50	2.62	23 (50%)	58,82,82	2.08	21 (36%)
15	CDL	V	805	-	86,86,99	1.27	9 (10%)	92,98,111	1.02	4 (4%)
15	CDL	K	301	-	99,99,99	1.22	8 (8%)	105,111,111	0.99	5 (4%)
16	MQ9	b	605	-	59,59,59	0.94	2 (3%)	73,75,75	1.54	16 (21%)
15	CDL	Q	804	-	86,86,99	1.26	8 (9%)	92,98,111	1.07	4 (4%)
15	CDL	Y	604	-	91,91,99	1.21	7 (7%)	97,103,111	1.05	5 (5%)
16	MQ9	M	302	-	59,59,59	1.04	4 (6%)	73,75,75	1.38	12 (16%)
18	HAS	Q	802	10	72,72,72	1.18	7 (9%)	87,109,109	1.16	7 (8%)
15	CDL	Y	603	-	90,90,99	1.23	8 (8%)	96,102,111	1.04	5 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	HEM	b	602	13	-	8/14/54/54	-
19	HEC	i	301	-	-	3/14/54/54	-
20	HEM	b	601	13	-	12/14/54/54	-
19	HEC	j	302	-	-	3/14/54/54	-
16	MQ9	Y	606	-	-	9/53/73/73	0/2/2/2
14	FES	B	501	1	-	-	0/1/1/1
18	HAS	V	801	10	1/1/8/18	11/42/82/82	-
20	HEM	Y	601	13	-	7/14/54/54	-
20	HEM	Y	602	13	-	6/14/54/54	-
14	FES	A	501	1	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	HAS	Q	801	10	1/1/8/18	6/42/82/82	-
15	CDL	b	604	-	-	54/101/101/110	-
18	HAS	V	802	10	1/1/8/18	10/42/82/82	-
15	CDL	M	301	-	-	56/110/110/110	-
19	HEC	j	301	-	-	3/14/54/54	-
15	CDL	b	603	-	-	44/102/102/110	-
16	MQ9	Y	605	-	-	16/53/73/73	0/2/2/2
19	HEC	V	804	-	-	3/14/54/54	-
15	CDL	V	805	-	-	44/97/97/110	-
15	CDL	K	301	-	-	56/110/110/110	-
16	MQ9	b	605	-	-	16/53/73/73	0/2/2/2
15	CDL	Q	804	-	-	46/97/97/110	-
15	CDL	Y	604	-	-	61/102/102/110	-
16	MQ9	M	302	-	-	8/53/73/73	0/2/2/2
18	HAS	Q	802	10	1/1/8/18	10/42/82/82	-
15	CDL	Y	603	-	-	56/101/101/110	-

All (239) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	j	301	HEC	C2A-C3A	5.02	1.47	1.36
19	V	804	HEC	C2A-C3A	5.01	1.47	1.36
19	i	301	HEC	C2A-C3A	5.01	1.47	1.36
19	j	302	HEC	CHB-C4A	5.00	1.48	1.38
19	j	302	HEC	C2A-C3A	4.97	1.47	1.36
19	j	301	HEC	CHC-C4B	4.97	1.48	1.38
19	V	804	HEC	CHB-C4A	4.97	1.48	1.38
19	j	302	HEC	CHA-C1A	4.95	1.48	1.38
19	V	804	HEC	CHD-C4C	4.95	1.48	1.38
19	j	302	HEC	CHD-C4C	4.95	1.48	1.38
19	i	301	HEC	CHB-C4A	4.95	1.48	1.38
19	j	301	HEC	CHB-C4A	4.95	1.48	1.38
19	V	804	HEC	CHA-C1A	4.94	1.48	1.38
19	i	301	HEC	CHC-C4B	4.94	1.48	1.38
20	Y	601	HEM	FE-ND	4.92	2.10	1.94
19	V	804	HEC	CHC-C4B	4.92	1.48	1.38
19	i	301	HEC	CHA-C1A	4.92	1.48	1.38
19	j	302	HEC	CHC-C4B	4.92	1.48	1.38
19	j	301	HEC	CHA-C1A	4.92	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	i	301	HEC	CHD-C4C	4.87	1.47	1.38
19	j	301	HEC	CHD-C4C	4.83	1.47	1.38
20	b	602	HEM	FE-ND	4.72	2.09	1.94
20	Y	602	HEM	FE-ND	4.71	2.09	1.94
20	b	602	HEM	CBB-CAB	4.41	1.51	1.30
20	b	601	HEM	FE-ND	4.32	2.08	1.94
19	V	804	HEC	CAB-C3B	4.26	1.48	1.35
19	i	301	HEC	CAB-C3B	4.25	1.48	1.35
19	j	301	HEC	CAB-C3B	4.25	1.48	1.35
19	j	302	HEC	CAB-C3B	4.25	1.48	1.35
19	V	804	HEC	CAC-C3C	4.24	1.48	1.35
19	j	302	HEC	CAC-C3C	4.24	1.48	1.35
20	Y	601	HEM	CBB-CAB	4.20	1.50	1.30
19	i	301	HEC	CAC-C3C	4.20	1.48	1.35
20	Y	602	HEM	CBB-CAB	4.20	1.50	1.30
19	j	301	HEC	CAC-C3C	4.18	1.48	1.35
20	b	601	HEM	CBB-CAB	4.01	1.49	1.30
19	V	804	HEC	CHC-C1C	3.89	1.48	1.39
19	i	301	HEC	CHB-C1B	3.89	1.48	1.39
19	V	804	HEC	CHA-C4D	3.89	1.48	1.39
19	j	302	HEC	CHA-C4D	3.89	1.48	1.39
19	j	302	HEC	CHC-C1C	3.89	1.48	1.39
19	j	301	HEC	CHD-C1D	3.88	1.48	1.39
19	j	301	HEC	CHC-C1C	3.88	1.48	1.39
19	j	302	HEC	CHB-C1B	3.87	1.48	1.39
19	i	301	HEC	CHC-C1C	3.87	1.48	1.39
19	i	301	HEC	CHD-C1D	3.87	1.48	1.39
19	V	804	HEC	CHB-C1B	3.86	1.48	1.39
19	i	301	HEC	CHA-C4D	3.86	1.48	1.39
19	j	301	HEC	CHB-C1B	3.86	1.48	1.39
19	j	301	HEC	CHA-C4D	3.85	1.48	1.39
19	V	804	HEC	CHD-C1D	3.82	1.48	1.39
19	j	302	HEC	CHD-C1D	3.79	1.47	1.39
20	b	602	HEM	FE-NA	3.70	2.07	1.95
15	K	301	CDL	OA8-CA7	3.68	1.44	1.33
16	Y	606	MQ9	C25-C24	-3.63	1.41	1.50
15	b	604	CDL	OA6-CA4	-3.56	1.38	1.46
15	Y	604	CDL	OA8-CA7	3.52	1.43	1.33
15	b	604	CDL	OA8-CA7	3.50	1.43	1.33
15	Y	603	CDL	OA8-CA7	3.50	1.43	1.33
15	Y	603	CDL	OA6-CA4	-3.49	1.38	1.46
15	M	301	CDL	OA8-CA7	3.49	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	301	CDL	OA6-CA4	-3.46	1.38	1.46
15	b	603	CDL	OA8-CA7	3.44	1.43	1.33
20	b	601	HEM	C4D-ND	-3.42	1.34	1.40
20	Y	601	HEM	FE-NA	3.41	2.06	1.95
18	V	801	HAS	CAC-C3C	-3.39	1.38	1.47
15	Q	804	CDL	OA8-CA7	3.36	1.43	1.33
15	b	603	CDL	OA6-CA4	-3.33	1.38	1.46
19	j	301	HEC	C3D-C2D	3.33	1.47	1.38
15	V	805	CDL	OA8-CA7	3.33	1.43	1.33
19	i	301	HEC	C3D-C2D	3.32	1.47	1.38
20	b	602	HEM	FE-NC	3.32	2.06	1.95
15	K	301	CDL	OB8-CB7	3.32	1.43	1.33
20	b	601	HEM	FE-NA	3.30	2.06	1.95
15	Q	804	CDL	OA6-CA4	-3.30	1.38	1.46
19	V	804	HEC	C3D-C2D	3.29	1.47	1.38
15	Q	804	CDL	OB8-CB7	3.27	1.42	1.33
19	j	302	HEC	C3D-C2D	3.27	1.47	1.38
20	Y	602	HEM	C4D-ND	-3.26	1.34	1.40
15	V	805	CDL	OA6-CA4	-3.25	1.39	1.46
15	Y	604	CDL	OB6-CB5	3.25	1.43	1.34
20	b	601	HEM	FE-NC	3.23	2.05	1.95
20	b	602	HEM	C4D-ND	-3.22	1.34	1.40
15	Q	804	CDL	OB6-CB5	3.21	1.43	1.34
15	V	805	CDL	OB8-CB7	3.20	1.42	1.33
20	Y	602	HEM	FE-NC	3.20	2.05	1.95
15	Y	604	CDL	OA6-CA4	-3.20	1.39	1.46
18	Q	801	HAS	CAC-C3C	-3.18	1.38	1.47
15	b	604	CDL	OB6-CB5	3.17	1.43	1.34
18	V	802	HAS	C14-C15	3.17	1.40	1.33
20	Y	602	HEM	FE-NA	3.17	2.05	1.95
15	V	805	CDL	OB6-CB5	3.16	1.43	1.34
18	Q	802	HAS	CAC-C3C	-3.16	1.39	1.47
15	b	603	CDL	OB8-CB7	3.16	1.42	1.33
15	M	301	CDL	OA6-CA4	-3.15	1.39	1.46
16	Y	606	MQ9	C46-C44	-3.14	1.44	1.51
15	b	603	CDL	OB6-CB5	3.14	1.43	1.34
18	Q	802	HAS	C22-C23	3.14	1.40	1.33
15	b	604	CDL	OB8-CB7	3.13	1.42	1.33
15	M	301	CDL	OB8-CB7	3.13	1.42	1.33
15	M	301	CDL	OB6-CB5	3.12	1.43	1.34
18	V	802	HAS	C22-C23	3.12	1.40	1.33
20	Y	601	HEM	FE-NC	3.10	2.05	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	601	HEM	C4D-ND	-3.10	1.34	1.40
20	b	602	HEM	C1B-NB	-3.09	1.34	1.40
15	Y	603	CDL	OB8-CB7	3.07	1.42	1.33
16	Y	606	MQ9	C11-C9	-3.06	1.45	1.51
18	V	801	HAS	C14-C15	3.06	1.40	1.33
15	K	301	CDL	OB6-CB5	3.00	1.42	1.34
18	Q	801	HAS	C14-C15	3.00	1.40	1.33
20	Y	602	HEM	C1A-NA	-2.96	1.34	1.39
15	Y	603	CDL	OB6-CB5	2.96	1.42	1.34
15	Y	603	CDL	OB6-CB4	-2.95	1.39	1.46
20	Y	601	HEM	C1A-NA	-2.93	1.34	1.39
20	Y	601	HEM	C1C-NC	-2.92	1.34	1.39
15	Y	604	CDL	OB8-CB7	2.91	1.41	1.33
18	Q	801	HAS	C18-C19	2.89	1.39	1.33
15	K	301	CDL	OB6-CB4	-2.86	1.39	1.46
20	b	601	HEM	C4B-NB	-2.86	1.33	1.38
18	Q	802	HAS	C14-C15	2.85	1.39	1.33
18	Q	801	HAS	C22-C23	2.83	1.39	1.33
18	V	801	HAS	C18-C19	2.80	1.39	1.33
18	V	801	HAS	C22-C23	2.77	1.39	1.33
18	V	802	HAS	C18-C19	2.77	1.39	1.33
20	Y	602	HEM	C1C-NC	-2.76	1.34	1.39
18	Q	802	HAS	C18-C19	2.74	1.39	1.33
15	Q	804	CDL	OB6-CB4	-2.74	1.40	1.46
18	V	802	HAS	CAC-C3C	-2.72	1.40	1.47
20	b	601	HEM	C1C-NC	-2.72	1.34	1.39
15	M	301	CDL	OB6-CB4	-2.71	1.40	1.46
15	V	805	CDL	OB6-CB4	-2.71	1.40	1.46
15	b	604	CDL	OB6-CB4	-2.71	1.40	1.46
20	Y	602	HEM	C4B-NB	-2.70	1.33	1.38
19	j	301	HEC	C1B-C2B	2.69	1.49	1.43
19	i	301	HEC	C1B-C2B	2.68	1.49	1.43
19	V	804	HEC	C1B-C2B	2.67	1.49	1.43
19	V	804	HEC	C1C-C2C	2.66	1.49	1.43
15	b	603	CDL	OB6-CB4	-2.66	1.40	1.46
19	j	302	HEC	C1B-C2B	2.65	1.49	1.43
19	j	302	HEC	C1C-C2C	2.65	1.49	1.43
19	i	301	HEC	C1C-C2C	2.65	1.49	1.43
20	Y	601	HEM	C1B-NB	-2.64	1.35	1.40
18	V	802	HAS	C29-C30	2.63	1.40	1.32
19	j	301	HEC	C1C-C2C	2.63	1.49	1.43
18	Q	802	HAS	C29-C30	2.61	1.40	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	801	HAS	C29-C30	2.60	1.40	1.32
20	b	601	HEM	C1B-NB	-2.60	1.35	1.40
16	b	605	MQ9	C7-C6	2.56	1.56	1.51
15	Y	604	CDL	OB6-CB4	-2.52	1.40	1.46
19	V	804	HEC	C1D-C2D	2.51	1.49	1.43
19	i	301	HEC	C1D-C2D	2.51	1.49	1.43
18	Q	801	HAS	C29-C30	2.51	1.40	1.32
19	j	302	HEC	C1D-C2D	2.51	1.49	1.43
19	j	301	HEC	C1D-C2D	2.49	1.49	1.43
20	b	602	HEM	C1A-NA	-2.48	1.34	1.39
20	b	602	HEM	C1C-NC	-2.47	1.35	1.39
16	M	302	MQ9	C16-C14	-2.45	1.46	1.51
16	Y	605	MQ9	C36-C34	-2.41	1.46	1.51
20	b	602	HEM	C4B-NB	-2.39	1.34	1.38
20	Y	602	HEM	C1B-NB	-2.36	1.36	1.40
15	M	301	CDL	OA6-CA5	2.36	1.40	1.34
20	b	601	HEM	C1A-NA	-2.36	1.35	1.39
16	Y	606	MQ9	C22-C23	-2.33	1.43	1.50
15	Q	804	CDL	OA6-CA5	2.32	1.40	1.34
15	V	805	CDL	OA6-CA5	2.31	1.40	1.34
19	j	301	HEC	C4D-C3D	2.29	1.49	1.44
16	M	302	MQ9	C21-C19	-2.29	1.46	1.51
20	b	602	HEM	C4A-NA	-2.26	1.35	1.39
19	i	301	HEC	C4D-C3D	2.26	1.49	1.44
18	Q	802	HAS	O2D-CGD	-2.25	1.23	1.30
19	j	302	HEC	C4D-C3D	2.22	1.49	1.44
19	V	804	HEC	C4D-C3D	2.21	1.49	1.44
19	j	302	HEC	C1A-C2A	2.20	1.49	1.45
20	Y	601	HEM	C4B-NB	-2.19	1.34	1.38
20	Y	602	HEM	O2A-CGA	-2.19	1.23	1.30
16	M	302	MQ9	C25-C24	-2.19	1.45	1.50
15	Q	804	CDL	PA1-OA5	2.18	1.67	1.59
15	b	604	CDL	PA1-OA5	2.18	1.67	1.59
19	i	301	HEC	C1D-ND	-2.17	1.35	1.39
19	j	301	HEC	C1D-ND	-2.17	1.35	1.39
15	M	301	CDL	PA1-OA5	2.17	1.67	1.59
16	M	302	MQ9	C41-C39	-2.17	1.46	1.51
19	V	804	HEC	C1A-C2A	2.17	1.49	1.45
19	j	301	HEC	C4A-NA	-2.17	1.35	1.39
19	i	301	HEC	C1A-C2A	2.16	1.49	1.45
18	V	802	HAS	CBC-CAC	2.16	1.40	1.30
16	Y	606	MQ9	C30-C29	-2.16	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	i	301	HEC	C4A-NA	-2.16	1.35	1.39
15	V	805	CDL	C51-CB5	2.16	1.57	1.50
19	V	804	HEC	C4A-NA	-2.15	1.35	1.39
19	j	302	HEC	C4D-ND	-2.15	1.35	1.39
18	Q	802	HAS	CBC-CAC	2.15	1.40	1.30
19	j	302	HEC	C1A-NA	-2.15	1.35	1.39
19	V	804	HEC	C1A-NA	-2.15	1.35	1.39
19	V	804	HEC	C4C-NC	-2.14	1.35	1.39
19	j	302	HEC	C1D-ND	-2.14	1.35	1.39
15	M	301	CDL	C51-CB5	2.14	1.56	1.50
15	V	805	CDL	PA1-OA5	2.14	1.67	1.59
19	V	804	HEC	C4D-ND	-2.14	1.35	1.39
15	Q	804	CDL	C51-CB5	2.14	1.56	1.50
18	Q	801	HAS	O2D-CGD	-2.14	1.23	1.30
19	j	302	HEC	C4A-NA	-2.14	1.35	1.39
19	j	301	HEC	C1A-C2A	2.13	1.48	1.45
19	V	804	HEC	C1D-ND	-2.13	1.35	1.39
15	Y	603	CDL	PA1-OA5	2.13	1.67	1.59
15	b	603	CDL	OA6-CA5	2.13	1.40	1.34
19	i	301	HEC	C1A-NA	-2.12	1.35	1.39
15	K	301	CDL	OA6-CA5	2.12	1.40	1.34
16	Y	606	MQ9	C15-C14	-2.12	1.45	1.50
19	i	301	HEC	C4D-ND	-2.12	1.35	1.39
15	Y	603	CDL	PA1-OA2	2.12	1.67	1.59
15	V	805	CDL	PA1-OA2	2.11	1.67	1.59
19	j	301	HEC	C4B-NB	-2.11	1.35	1.39
19	i	301	HEC	C4C-NC	-2.11	1.35	1.39
15	K	301	CDL	PA1-OA5	2.11	1.67	1.59
15	Y	604	CDL	PA1-OA2	2.11	1.67	1.59
19	j	302	HEC	C4C-NC	-2.10	1.35	1.39
19	j	302	HEC	C4B-NB	-2.10	1.35	1.39
19	V	804	HEC	C4B-NB	-2.10	1.35	1.39
20	b	601	HEM	O2A-CGA	-2.09	1.23	1.30
19	j	301	HEC	C1A-NA	-2.09	1.35	1.39
20	Y	601	HEM	C4A-NA	-2.09	1.35	1.39
15	K	301	CDL	PA1-OA2	2.09	1.67	1.59
19	i	301	HEC	C4B-NB	-2.09	1.35	1.39
20	b	601	HEM	C4A-NA	-2.09	1.35	1.39
15	b	604	CDL	C51-CB5	2.08	1.56	1.50
19	j	301	HEC	C4D-ND	-2.08	1.35	1.39
20	b	602	HEM	O2A-CGA	-2.08	1.23	1.30
15	b	604	CDL	OA6-CA5	2.07	1.40	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	604	CDL	OA6-CA5	2.07	1.40	1.34
15	Y	603	CDL	OA6-CA5	2.07	1.40	1.34
19	j	301	HEC	C4C-NC	-2.06	1.35	1.39
18	Q	801	HAS	CBC-CAC	2.05	1.40	1.30
15	b	603	CDL	PA1-OA5	2.03	1.67	1.59
16	Y	606	MQ9	C36-C34	-2.03	1.47	1.51
15	b	604	CDL	PA1-OA2	2.02	1.67	1.59
20	b	601	HEM	C3B-C4B	-2.00	1.41	1.44
16	b	605	MQ9	C30-C29	-2.00	1.45	1.50
20	Y	601	HEM	O2A-CGA	-2.00	1.24	1.30

All (287) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	602	HEM	CBA-CAA-C2A	5.35	127.33	112.53
20	b	601	HEM	CHC-C4B-NB	5.24	130.06	124.42
19	j	302	HEC	C2A-C1A-NA	5.09	115.23	110.32
19	V	804	HEC	C2A-C1A-NA	5.08	115.22	110.32
19	j	301	HEC	C2A-C1A-NA	5.02	115.16	110.32
19	i	301	HEC	C2A-C1A-NA	5.01	115.16	110.32
20	b	601	HEM	C1B-NB-C4B	5.01	111.14	105.21
20	Y	601	HEM	C1B-NB-C4B	4.89	111.00	105.21
20	Y	602	HEM	C1B-NB-C4B	4.85	110.94	105.21
20	b	601	HEM	C4D-ND-C1D	4.75	110.84	105.21
20	b	601	HEM	CBA-CAA-C2A	4.70	125.52	112.53
20	b	601	HEM	CAA-C2A-C1A	4.68	134.09	124.94
15	b	603	CDL	OB6-CB5-C51	4.65	121.55	111.48
15	Y	604	CDL	OB6-CB5-C51	4.64	121.53	111.48
20	b	602	HEM	CHB-C1B-NB	4.63	130.09	124.37
20	Y	602	HEM	CHC-C4B-NB	4.59	129.36	124.42
20	b	602	HEM	C1B-NB-C4B	4.56	110.61	105.21
19	i	301	HEC	C3D-C4D-ND	4.55	115.20	110.15
19	V	804	HEC	C3D-C4D-ND	4.55	115.20	110.15
19	j	301	HEC	C3D-C4D-ND	4.52	115.16	110.15
19	j	302	HEC	C3D-C4D-ND	4.50	115.15	110.15
15	M	301	CDL	OA6-CA5-C11	4.28	120.74	111.48
15	Q	804	CDL	OB6-CB5-C51	4.27	120.71	111.48
15	V	805	CDL	OB6-CB5-C51	4.26	120.70	111.48
15	Y	603	CDL	OB6-CB5-C51	4.24	120.65	111.48
20	b	602	HEM	C4D-ND-C1D	4.18	110.15	105.21
15	b	603	CDL	OA6-CA5-C11	4.17	120.51	111.48
20	b	601	HEM	CHD-C1D-ND	4.11	128.84	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	804	CDL	OA6-CA5-C11	4.05	120.25	111.48
20	b	602	HEM	CHC-C1C-NC	4.05	128.86	124.45
20	Y	601	HEM	CHB-C1B-NB	4.04	129.36	124.37
15	K	301	CDL	OB6-CB5-C51	4.00	120.12	111.48
20	Y	601	HEM	CHD-C4C-NC	3.98	128.78	124.45
18	V	802	HAS	CAD-CBD-CGD	-3.97	103.14	113.67
15	b	604	CDL	OB6-CB5-C51	3.94	120.01	111.48
15	V	805	CDL	OA6-CA5-C11	3.93	119.99	111.48
20	b	602	HEM	CAA-C2A-C1A	3.93	132.62	124.94
20	b	602	HEM	CMB-C2B-C1B	-3.91	118.92	125.03
18	Q	802	HAS	CAD-CBD-CGD	-3.91	103.31	113.67
15	Y	604	CDL	OA6-CA5-C11	3.85	119.80	111.48
20	Y	602	HEM	CHD-C4C-NC	3.82	128.61	124.45
20	Y	602	HEM	CHD-C1D-ND	3.79	128.50	124.42
16	b	605	MQ9	C25-C24-C26	3.77	121.77	115.23
15	K	301	CDL	OA6-CA5-C11	3.77	119.63	111.48
20	b	602	HEM	CHC-C4B-NB	3.76	128.47	124.42
19	j	301	HEC	CBB-CAB-C3B	-3.75	119.94	127.43
20	Y	602	HEM	C4D-ND-C1D	3.75	109.64	105.21
19	i	301	HEC	CBC-CAC-C3C	-3.74	119.95	127.43
19	i	301	HEC	CBB-CAB-C3B	-3.74	119.95	127.43
19	j	301	HEC	CBC-CAC-C3C	-3.74	119.96	127.43
19	j	302	HEC	CBB-CAB-C3B	-3.73	119.98	127.43
19	V	804	HEC	CBB-CAB-C3B	-3.72	120.00	127.43
15	Y	603	CDL	OA6-CA5-C11	3.72	119.53	111.48
19	V	804	HEC	CBC-CAC-C3C	-3.72	120.01	127.43
19	j	302	HEC	CBC-CAC-C3C	-3.71	120.01	127.43
20	Y	601	HEM	CHC-C1C-NC	3.71	128.50	124.45
16	Y	606	MQ9	C25-C24-C23	-3.70	114.13	123.63
15	M	301	CDL	OB6-CB5-C51	3.69	119.47	111.48
20	b	601	HEM	CAA-C2A-C3A	-3.65	118.88	127.07
16	b	605	MQ9	C30-C29-C31	3.64	121.54	115.23
16	M	302	MQ9	C7-C8-C9	-3.62	120.59	126.83
16	b	605	MQ9	C7-C6-C5	-3.58	118.76	124.89
20	b	601	HEM	CBB-CAB-C3B	-3.57	109.70	127.53
20	Y	601	HEM	C4D-ND-C1D	3.56	109.43	105.21
19	V	804	HEC	C1D-C2D-C3D	-3.55	102.75	106.82
15	b	604	CDL	OA6-CA5-C11	3.54	119.13	111.48
19	i	301	HEC	C1D-C2D-C3D	-3.53	102.77	106.82
19	j	302	HEC	C1D-C2D-C3D	-3.53	102.78	106.82
19	j	301	HEC	C1D-C2D-C3D	-3.51	102.79	106.82
20	b	601	HEM	CHA-C4D-ND	3.50	128.70	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	301	HEC	C2C-C1C-NC	3.50	115.76	110.14
19	j	302	HEC	C2C-C1C-NC	3.50	115.75	110.14
19	V	804	HEC	C2C-C1C-NC	3.50	115.75	110.14
19	i	301	HEC	C2C-C1C-NC	3.49	115.74	110.14
16	b	605	MQ9	C7-C8-C9	-3.49	120.83	126.83
19	V	804	HEC	C2B-C1B-NB	3.48	115.73	110.14
19	j	302	HEC	C2B-C1B-NB	3.48	115.73	110.14
19	i	301	HEC	C2B-C1B-NB	3.48	115.72	110.14
16	Y	605	MQ9	C15-C14-C16	3.47	121.24	115.23
20	b	601	HEM	C2A-C1A-NA	-3.46	106.31	110.15
19	j	301	HEC	C2B-C1B-NB	3.46	115.69	110.14
20	b	601	HEM	CHD-C4C-NC	3.41	128.17	124.45
20	Y	601	HEM	CHA-C4D-ND	3.39	128.56	124.37
20	Y	602	HEM	CAA-CBA-CGA	-3.34	104.80	113.67
16	Y	606	MQ9	C7-C8-C9	-3.33	121.09	126.83
15	Q	804	CDL	OB8-CB7-C71	3.30	121.88	111.83
20	Y	601	HEM	CHD-C1D-ND	3.29	127.97	124.42
20	b	602	HEM	CHA-C4D-ND	3.29	128.43	124.37
20	b	601	HEM	C4A-NA-C1A	3.26	111.14	105.82
19	V	804	HEC	C1A-C2A-C3A	-3.26	102.81	107.11
19	j	302	HEC	C1A-C2A-C3A	-3.26	102.81	107.11
16	Y	605	MQ9	C30-C29-C31	3.25	120.88	115.23
19	i	301	HEC	C1A-C2A-C3A	-3.25	102.83	107.11
19	j	301	HEC	C1A-C2A-C3A	-3.24	102.84	107.11
20	Y	602	HEM	CHA-C4D-ND	3.24	128.37	124.37
20	b	601	HEM	CHC-C1C-NC	3.23	127.97	124.45
19	j	301	HEC	C2D-C1D-ND	3.23	115.31	110.14
20	Y	601	HEM	C3B-C4B-NB	-3.21	107.16	109.47
19	i	301	HEC	C2D-C1D-ND	3.21	115.29	110.14
20	b	602	HEM	CHD-C4C-NC	3.20	127.94	124.45
19	V	804	HEC	C2D-C1D-ND	3.19	115.26	110.14
19	j	302	HEC	C2D-C1D-ND	3.17	115.22	110.14
20	Y	602	HEM	CHB-C1B-NB	3.16	128.28	124.37
15	M	301	CDL	OB8-CB7-C71	3.13	121.39	111.83
20	Y	602	HEM	CHC-C1C-NC	3.13	127.86	124.45
18	Q	801	HAS	CMB-C2B-C3B	-3.11	124.27	130.28
18	Q	802	HAS	CMC-C2C-C1C	-3.10	120.69	125.42
16	Y	605	MQ9	C7-C8-C9	-3.09	121.50	126.83
18	Q	801	HAS	CAD-CBD-CGD	-3.09	105.47	113.67
15	K	301	CDL	OA8-CA7-C31	3.06	121.17	111.83
20	Y	602	HEM	C4A-NA-C1A	3.04	110.78	105.82
19	j	301	HEC	C3A-C4A-NA	3.03	115.25	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	302	HEC	C3A-C4A-NA	3.03	115.24	109.64
20	Y	601	HEM	C4C-C3C-C2C	3.02	109.44	106.81
19	i	301	HEC	C3A-C4A-NA	3.02	115.22	109.64
16	Y	605	MQ9	C40-C39-C41	3.01	120.46	115.23
19	V	804	HEC	C3A-C4A-NA	3.01	115.20	109.64
15	b	603	CDL	OB8-CB7-C71	2.98	120.92	111.83
20	b	601	HEM	CAA-CBA-CGA	-2.97	105.78	113.67
20	b	601	HEM	CHB-C4A-NA	2.97	129.24	123.86
15	Y	603	CDL	OB8-CB7-C71	2.96	120.86	111.83
16	Y	605	MQ9	C25-C24-C26	2.95	120.34	115.23
15	b	603	CDL	OA8-CA7-C31	2.92	120.74	111.83
18	V	802	HAS	CAD-C3D-C4D	2.92	129.78	124.70
18	V	801	HAS	CMB-C2B-C3B	-2.89	124.68	130.28
20	Y	602	HEM	CHA-C1A-NA	2.89	129.11	123.86
15	b	604	CDL	OB8-CB7-C71	2.87	120.58	111.83
15	V	805	CDL	OB8-CB7-C71	2.86	120.54	111.83
15	Y	604	CDL	OA8-CA7-C31	2.85	120.52	111.83
16	Y	605	MQ9	C27-C28-C29	-2.84	121.11	127.62
16	b	605	MQ9	C7-C6-C1	2.84	121.57	118.58
19	j	301	HEC	C4A-C3A-C2A	-2.84	102.77	106.97
19	V	804	HEC	C4A-C3A-C2A	-2.83	102.77	106.97
19	j	302	HEC	C4A-C3A-C2A	-2.83	102.78	106.97
19	i	301	HEC	C4A-C3A-C2A	-2.82	102.78	106.97
18	V	801	HAS	C13-C14-C15	-2.82	121.17	127.62
15	Y	604	CDL	OB8-CB7-C71	2.80	120.36	111.83
20	b	601	HEM	C4C-CHD-C1D	-2.79	120.09	126.02
20	Y	602	HEM	CBB-CAB-C3B	-2.78	113.64	127.53
20	b	602	HEM	CHD-C1D-ND	2.78	127.41	124.42
18	V	801	HAS	C17-C18-C19	-2.76	121.32	127.62
16	Y	605	MQ9	C7-C6-C5	-2.75	120.18	124.89
16	M	302	MQ9	C25-C24-C26	2.75	120.00	115.23
20	b	601	HEM	C3B-C4B-NB	-2.74	107.50	109.47
20	Y	602	HEM	C4C-NC-C1C	2.74	110.30	105.82
15	M	301	CDL	OA8-CA7-C31	2.74	120.18	111.83
19	j	301	HEC	CMC-C2C-C1C	2.73	129.58	125.42
16	M	302	MQ9	C25-C24-C23	-2.73	116.62	123.63
20	Y	601	HEM	C4C-NC-C1C	2.73	110.27	105.82
20	Y	602	HEM	C2A-C1A-NA	-2.72	107.13	110.15
19	i	301	HEC	CMC-C2C-C1C	2.72	129.56	125.42
19	V	804	HEC	CMC-C2C-C1C	2.70	129.54	125.42
16	Y	606	MQ9	C25-C24-C26	2.70	119.91	115.23
19	j	302	HEC	CMC-C2C-C1C	2.68	129.51	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	b	604	CDL	OA8-CA7-C31	2.68	120.01	111.83
18	Q	801	HAS	C3C-C4C-NC	2.68	112.05	109.80
15	K	301	CDL	OB8-CB7-C71	2.67	119.98	111.83
15	Y	603	CDL	OA8-CA7-C31	2.66	119.96	111.83
20	b	601	HEM	C2B-C1B-NB	-2.66	106.78	109.84
16	Y	606	MQ9	C47-C46-C44	-2.66	104.37	113.19
18	V	801	HAS	C17-C16-C15	-2.66	104.39	113.19
19	j	302	HEC	CMB-C2B-C1B	2.66	129.46	125.42
20	b	602	HEM	C2D-C1D-ND	-2.65	106.84	109.90
19	V	804	HEC	CMB-C2B-C1B	2.65	129.45	125.42
19	j	301	HEC	C4D-C3D-C2D	-2.64	102.78	106.87
19	i	301	HEC	C4D-C3D-C2D	-2.63	102.80	106.87
16	M	302	MQ9	C12-C13-C14	-2.63	121.60	127.62
19	j	301	HEC	CMB-C2B-C1B	2.61	129.40	125.42
20	b	601	HEM	C3D-C4D-ND	-2.61	107.31	110.17
20	b	602	HEM	C4C-NC-C1C	2.61	110.07	105.82
19	i	301	HEC	CMB-C2B-C1B	2.60	129.38	125.42
20	Y	601	HEM	CHA-C1A-NA	2.60	128.57	123.86
16	b	605	MQ9	C25-C24-C23	-2.59	116.97	123.63
19	V	804	HEC	C4D-C3D-C2D	-2.59	102.86	106.87
19	j	302	HEC	C4D-C3D-C2D	-2.58	102.87	106.87
18	V	801	HAS	C21-C22-C23	-2.58	121.71	127.62
16	b	605	MQ9	C27-C28-C29	-2.56	121.76	127.62
15	Q	804	CDL	OA8-CA7-C31	2.54	119.58	111.83
20	b	602	HEM	CAA-C2A-C3A	-2.54	121.38	127.07
18	Q	801	HAS	C21-C22-C23	-2.54	121.82	127.62
15	Y	603	CDL	CA4-OA6-CA5	-2.52	111.76	117.80
18	Q	801	HAS	C17-C18-C19	-2.51	121.88	127.62
18	V	801	HAS	C12-C13-C14	2.50	118.74	112.16
20	b	601	HEM	C4C-NC-C1C	2.49	109.88	105.82
16	M	302	MQ9	C35-C34-C36	2.48	119.54	115.23
19	j	302	HEC	CHA-C1A-C2A	-2.48	120.95	124.86
20	Y	602	HEM	C3B-C4B-NB	-2.48	107.69	109.47
20	b	601	HEM	CHB-C1B-NB	2.48	127.43	124.37
19	V	804	HEC	CHA-C1A-C2A	-2.46	120.97	124.86
16	Y	606	MQ9	C7-C6-C5	-2.45	120.70	124.89
20	b	602	HEM	C4C-C3C-C2C	2.44	108.93	106.81
20	Y	601	HEM	C4A-NA-C1A	2.43	109.78	105.82
18	V	802	HAS	C3C-C4C-NC	2.43	111.84	109.80
19	i	301	HEC	CHA-C1A-C2A	-2.42	121.04	124.86
18	V	802	HAS	C21-C22-C23	-2.41	122.10	127.62
19	j	301	HEC	CHA-C1A-C2A	-2.40	121.08	124.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	601	HEM	C2D-C1D-ND	-2.39	107.14	109.90
16	Y	606	MQ9	C15-C14-C16	2.39	119.38	115.23
16	b	605	MQ9	C30-C29-C28	-2.39	117.50	123.63
18	V	802	HAS	C12-C11-C3B	-2.38	108.40	112.12
15	V	805	CDL	OA8-CA7-C31	2.38	119.10	111.83
20	Y	602	HEM	C4C-CHD-C1D	-2.38	120.96	126.02
16	M	302	MQ9	C37-C38-C39	-2.37	122.19	127.62
18	Q	802	HAS	CMC-C2C-C3C	2.37	132.12	126.55
20	Y	601	HEM	CHC-C4B-NB	2.37	126.97	124.42
16	b	605	MQ9	O1-C1-C2	-2.36	117.80	121.57
16	b	605	MQ9	C40-C39-C41	2.35	119.31	115.23
20	Y	602	HEM	CHB-C4A-NA	2.35	128.12	123.86
16	Y	606	MQ9	C20-C19-C21	2.34	119.29	115.23
18	Q	802	HAS	C17-C18-C19	-2.34	122.28	127.62
18	Q	801	HAS	C13-C14-C15	-2.34	122.28	127.62
19	V	804	HEC	CHB-C1B-C2B	-2.32	120.69	127.43
19	j	302	HEC	CHB-C1B-C2B	-2.32	120.69	127.43
19	i	301	HEC	CHB-C1B-C2B	-2.31	120.71	127.43
19	j	301	HEC	CHB-C1B-C2B	-2.31	120.73	127.43
16	b	605	MQ9	C32-C33-C34	-2.31	122.35	127.62
20	Y	601	HEM	C2D-C1D-ND	-2.30	107.24	109.90
16	b	605	MQ9	C12-C13-C14	-2.29	122.38	127.62
16	M	302	MQ9	C7-C6-C5	-2.29	120.96	124.89
16	Y	606	MQ9	C51-C49-C50	2.29	119.86	114.59
19	j	301	HEC	CHC-C1C-C2C	-2.29	120.78	127.43
20	Y	601	HEM	C4C-CHD-C1D	-2.29	121.16	126.02
19	i	301	HEC	CHC-C1C-C2C	-2.29	120.79	127.43
20	b	602	HEM	C4A-NA-C1A	2.28	109.54	105.82
19	V	804	HEC	CHC-C1C-C2C	-2.27	120.83	127.43
18	Q	801	HAS	CMB-C2B-C1B	2.27	128.57	125.03
19	j	302	HEC	CHC-C1C-C2C	-2.26	120.87	127.43
16	Y	605	MQ9	C10-C9-C11	2.25	119.14	115.23
16	M	302	MQ9	C42-C43-C44	-2.25	122.47	127.62
20	Y	602	HEM	C4C-C3C-C2C	2.24	108.76	106.81
16	Y	605	MQ9	C45-C44-C46	2.24	119.12	115.23
19	j	301	HEC	CMA-C3A-C4A	2.24	128.67	124.73
20	Y	601	HEM	C2B-C1B-NB	-2.23	107.27	109.84
18	V	801	HAS	CMA-C3A-C4A	2.23	128.66	124.73
18	V	801	HAS	CAA-CBA-CGA	-2.23	107.75	113.67
19	V	804	HEC	CMA-C3A-C4A	2.22	128.65	124.73
19	j	302	HEC	CHD-C1D-C2D	-2.22	120.97	127.43
19	V	804	HEC	CHD-C1D-C2D	-2.22	120.97	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	i	301	HEC	CMA-C3A-C4A	2.22	128.64	124.73
19	i	301	HEC	CHD-C1D-C2D	-2.22	120.99	127.43
19	j	301	HEC	CHD-C1D-C2D	-2.21	121.02	127.43
19	j	302	HEC	CMA-C3A-C4A	2.20	128.60	124.73
18	Q	801	HAS	CBA-CAA-C2A	2.20	118.61	112.53
18	V	801	HAS	CMC-C2C-C3C	2.19	131.70	126.55
19	j	301	HEC	CHB-C4A-C3A	-2.17	120.97	125.49
19	i	301	HEC	CHB-C4A-C3A	-2.17	120.98	125.49
16	Y	606	MQ9	C45-C44-C46	2.16	118.98	115.23
20	b	602	HEM	CMB-C2B-C3B	2.16	133.66	128.43
19	V	804	HEC	CHB-C4A-C3A	-2.15	121.01	125.49
19	j	302	HEC	CHB-C4A-C3A	-2.15	121.02	125.49
20	b	602	HEM	CAA-CBA-CGA	-2.15	107.96	113.67
16	Y	606	MQ9	C12-C11-C9	-2.15	106.08	113.19
16	Y	605	MQ9	C32-C33-C34	-2.14	122.72	127.62
16	b	605	MQ9	C42-C43-C44	-2.14	122.74	127.62
16	Y	605	MQ9	C51-C49-C50	2.13	119.50	114.59
18	V	801	HAS	C25-C23-C24	2.13	118.93	115.23
16	b	605	MQ9	C51-C49-C50	2.13	119.48	114.59
16	Y	606	MQ9	C26-C24-C23	2.12	125.93	121.17
16	M	302	MQ9	C51-C49-C50	2.11	119.44	114.59
16	Y	605	MQ9	C30-C29-C28	-2.10	118.22	123.63
19	j	302	HEC	CMD-C2D-C1D	2.10	128.62	125.42
20	Y	602	HEM	C2B-C1B-NB	-2.10	107.42	109.84
15	K	301	CDL	OB4-PB2-OB3	-2.10	102.68	112.44
18	V	801	HAS	CMB-C2B-C1B	2.10	128.31	125.03
16	b	605	MQ9	C45-C44-C46	2.10	118.87	115.23
19	V	804	HEC	CMD-C2D-C1D	2.10	128.61	125.42
15	Y	604	CDL	CA4-OA6-CA5	-2.09	112.79	117.80
16	M	302	MQ9	C32-C33-C34	-2.09	122.83	127.62
18	V	802	HAS	C17-C18-C19	-2.09	122.85	127.62
18	Q	802	HAS	C26-C15-C16	2.08	118.83	115.23
18	Q	802	HAS	O11-C11-C3B	2.07	115.06	111.26
16	Y	606	MQ9	C12-C13-C14	-2.07	122.88	127.62
16	Y	606	MQ9	C15-C14-C13	-2.07	118.32	123.63
16	M	302	MQ9	C45-C44-C46	2.06	118.81	115.23
18	V	801	HAS	CMC-C2C-C1C	-2.06	122.28	125.42
16	b	605	MQ9	C5M-C5-C6	-2.06	121.07	124.45
19	i	301	HEC	CMD-C2D-C1D	2.05	128.55	125.42
19	j	301	HEC	CMD-C2D-C1D	2.05	128.55	125.42
15	b	603	CDL	OB4-PB2-OB3	-2.05	102.92	112.44
20	Y	601	HEM	CBC-CAC-C3C	-2.04	117.32	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	605	MQ9	C25-C24-C23	-2.04	118.39	123.63
18	V	802	HAS	C25-C23-C24	2.04	118.76	115.23
18	V	802	HAS	C2B-C1B-NB	2.04	112.26	109.90
18	V	801	HAS	CAD-CBD-CGD	-2.03	108.29	113.67
16	Y	606	MQ9	C27-C28-C29	-2.02	122.99	127.62
18	Q	802	HAS	CHC-C4B-NB	-2.00	121.89	124.37
16	M	302	MQ9	C17-C16-C14	-2.00	106.54	113.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	V	801	HAS	NA
18	V	802	HAS	NA
18	Q	801	HAS	NA
18	Q	802	HAS	NA

All (548) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	M	301	CDL	CA2-OA2-PA1-OA3
15	M	301	CDL	CA2-OA2-PA1-OA4
15	M	301	CDL	CA2-OA2-PA1-OA5
15	M	301	CDL	CA3-OA5-PA1-OA3
15	V	805	CDL	CA2-OA2-PA1-OA3
15	V	805	CDL	CA2-OA2-PA1-OA5
15	V	805	CDL	CB2-OB2-PB2-OB3
15	b	603	CDL	O1-C1-CA2-OA2
15	b	603	CDL	CB3-OB5-PB2-OB2
15	b	603	CDL	OB7-CB5-OB6-CB4
15	b	604	CDL	CA3-OA5-PA1-OA3
15	b	604	CDL	CA3-OA5-PA1-OA4
15	b	604	CDL	OA6-CA4-CA6-OA8
15	K	301	CDL	CA2-OA2-PA1-OA3
15	K	301	CDL	CA2-OA2-PA1-OA4
15	K	301	CDL	CA2-OA2-PA1-OA5
15	K	301	CDL	CA3-OA5-PA1-OA3
15	K	301	CDL	CA3-OA5-PA1-OA4
15	K	301	CDL	OA7-CA5-OA6-CA4
15	K	301	CDL	C11-CA5-OA6-CA4
15	K	301	CDL	OA9-CA7-OA8-CA6
15	K	301	CDL	C31-CA7-OA8-CA6
15	K	301	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	K	301	CDL	CB3-OB5-PB2-OB2
15	K	301	CDL	CB3-OB5-PB2-OB3
15	K	301	CDL	CB3-OB5-PB2-OB4
15	Q	804	CDL	CA3-OA5-PA1-OA3
15	Q	804	CDL	CB2-OB2-PB2-OB4
15	Q	804	CDL	CB3-OB5-PB2-OB2
15	Q	804	CDL	OB9-CB7-OB8-CB6
15	Q	804	CDL	C71-CB7-OB8-CB6
15	Y	603	CDL	CA2-OA2-PA1-OA3
15	Y	603	CDL	CA2-OA2-PA1-OA4
15	Y	603	CDL	CA3-OA5-PA1-OA2
15	Y	603	CDL	C11-CA5-OA6-CA4
15	Y	603	CDL	CB3-OB5-PB2-OB2
15	Y	603	CDL	CB3-OB5-PB2-OB3
15	Y	603	CDL	CB3-OB5-PB2-OB4
15	Y	604	CDL	O1-C1-CA2-OA2
15	Y	604	CDL	CA2-OA2-PA1-OA3
15	Y	604	CDL	CA2-OA2-PA1-OA4
15	Y	604	CDL	CA2-OA2-PA1-OA5
15	Y	604	CDL	CA3-OA5-PA1-OA2
15	Y	604	CDL	CA3-OA5-PA1-OA3
15	Y	604	CDL	C11-CA5-OA6-CA4
15	Y	604	CDL	CB2-OB2-PB2-OB3
15	Y	604	CDL	CB2-OB2-PB2-OB5
15	Y	604	CDL	CB3-OB5-PB2-OB3
15	Y	604	CDL	CB3-OB5-PB2-OB4
15	Y	604	CDL	OB7-CB5-OB6-CB4
15	Y	604	CDL	C51-CB5-OB6-CB4
16	Y	605	MQ9	C29-C31-C32-C33
18	V	801	HAS	C1D-C2D-CMD-OMD
18	V	801	HAS	C3D-C2D-CMD-OMD
18	V	801	HAS	C23-C24-C28-C29
18	V	802	HAS	C1D-C2D-CMD-OMD
18	V	802	HAS	C3D-C2D-CMD-OMD
18	Q	802	HAS	C3D-C2D-CMD-OMD
18	Q	802	HAS	C3B-C11-C12-C13
18	Q	802	HAS	O11-C11-C12-C13
18	Q	802	HAS	C26-C15-C16-C17
20	b	601	HEM	C2B-C3B-CAB-CBB
20	b	601	HEM	C4B-C3B-CAB-CBB
20	b	601	HEM	C2C-C3C-CAC-CBC
20	b	602	HEM	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	Y	601	HEM	C2C-C3C-CAC-CBC
20	Y	601	HEM	C4C-C3C-CAC-CBC
20	Y	602	HEM	C2C-C3C-CAC-CBC
15	b	603	CDL	OB9-CB7-OB8-CB6
15	b	604	CDL	OA9-CA7-OA8-CA6
15	Y	603	CDL	OA7-CA5-OA6-CA4
15	Y	604	CDL	OA7-CA5-OA6-CA4
15	b	604	CDL	C31-CA7-OA8-CA6
15	b	603	CDL	C51-CB5-OB6-CB4
15	Y	604	CDL	OB9-CB7-OB8-CB6
16	b	605	MQ9	C25-C24-C26-C27
16	Y	605	MQ9	C15-C14-C16-C17
16	Y	605	MQ9	C25-C24-C26-C27
16	Y	605	MQ9	C30-C29-C31-C32
16	Y	605	MQ9	C40-C39-C41-C42
18	V	801	HAS	C25-C23-C24-C28
18	V	802	HAS	C25-C23-C24-C28
16	b	605	MQ9	C23-C24-C26-C27
16	Y	605	MQ9	C13-C14-C16-C17
16	Y	605	MQ9	C23-C24-C26-C27
16	Y	605	MQ9	C28-C29-C31-C32
16	Y	605	MQ9	C38-C39-C41-C42
18	V	802	HAS	C22-C23-C24-C28
18	Q	802	HAS	C14-C15-C16-C17
15	b	603	CDL	C71-CB7-OB8-CB6
15	Y	604	CDL	C71-CB7-OB8-CB6
15	M	301	CDL	O1-C1-CA2-OA2
15	Y	603	CDL	O1-C1-CB2-OB2
15	Y	604	CDL	O1-C1-CB2-OB2
18	V	801	HAS	C22-C23-C24-C28
16	M	302	MQ9	C24-C26-C27-C28
16	M	302	MQ9	C44-C46-C47-C48
16	b	605	MQ9	C9-C11-C12-C13
16	b	605	MQ9	C39-C41-C42-C43
16	b	605	MQ9	C44-C46-C47-C48
16	Y	605	MQ9	C9-C11-C12-C13
16	Y	605	MQ9	C19-C21-C22-C23
16	Y	605	MQ9	C34-C36-C37-C38
16	Y	606	MQ9	C9-C11-C12-C13
16	Y	606	MQ9	C19-C21-C22-C23
18	V	802	HAS	C19-C20-C21-C22
18	Q	801	HAS	C23-C24-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	Q	802	HAS	C23-C24-C28-C29
20	b	601	HEM	C1A-C2A-CAA-CBA
20	b	602	HEM	C1A-C2A-CAA-CBA
20	b	602	HEM	C2A-CAA-CBA-CGA
15	M	301	CDL	CB2-C1-CA2-OA2
15	Y	603	CDL	CA2-C1-CB2-OB2
15	K	301	CDL	C71-CB7-OB8-CB6
15	Q	804	CDL	C31-CA7-OA8-CA6
15	M	301	CDL	C75-C76-C77-C78
16	b	605	MQ9	C30-C29-C31-C32
16	b	605	MQ9	C28-C29-C31-C32
15	Y	603	CDL	O1-C1-CA2-OA2
15	Q	804	CDL	OA9-CA7-OA8-CA6
15	V	805	CDL	CA5-C11-C12-C13
20	b	601	HEM	C3A-C2A-CAA-CBA
20	b	602	HEM	C3A-C2A-CAA-CBA
15	M	301	CDL	C11-CA5-OA6-CA4
15	Y	604	CDL	CB5-C51-C52-C53
15	K	301	CDL	C56-C57-C58-C59
15	Y	603	CDL	CA5-C11-C12-C13
16	M	302	MQ9	C19-C21-C22-C23
16	b	605	MQ9	C14-C16-C17-C18
16	b	605	MQ9	C34-C36-C37-C38
16	Y	605	MQ9	C44-C46-C47-C48
18	Q	801	HAS	C15-C16-C17-C18
15	K	301	CDL	C76-C77-C78-C79
15	Q	804	CDL	CA7-C31-C32-C33
15	Y	604	CDL	CA7-C31-C32-C33
15	K	301	CDL	OB9-CB7-OB8-CB6
20	b	601	HEM	C3D-CAD-CBD-CGD
15	V	805	CDL	CB7-C71-C72-C73
15	b	604	CDL	O1-C1-CB2-OB2
15	b	603	CDL	CA5-C11-C12-C13
15	Q	804	CDL	CA5-C11-C12-C13
15	V	805	CDL	C71-CB7-OB8-CB6
15	M	301	CDL	OA7-CA5-OA6-CA4
15	b	604	CDL	CA2-C1-CB2-OB2
15	Y	603	CDL	CB2-C1-CA2-OA2
15	Y	604	CDL	CB2-C1-CA2-OA2
15	Y	604	CDL	CA2-C1-CB2-OB2
15	M	301	CDL	C21-C22-C23-C24
15	b	604	CDL	C11-CA5-OA6-CA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b	604	CDL	OA7-CA5-OA6-CA4
16	b	605	MQ9	C29-C31-C32-C33
20	b	601	HEM	C2A-CAA-CBA-CGA
15	V	805	CDL	OB9-CB7-OB8-CB6
15	Y	603	CDL	C51-CB5-OB6-CB4
15	M	301	CDL	C77-C78-C79-C80
15	b	604	CDL	C51-C52-C53-C54
15	Y	604	CDL	C59-C60-C61-C62
15	b	604	CDL	C13-C14-C15-C16
15	b	604	CDL	C54-C55-C56-C57
15	K	301	CDL	C32-C33-C34-C35
15	Q	804	CDL	C12-C13-C14-C15
15	Q	804	CDL	C57-C58-C59-C60
15	M	301	CDL	C39-C40-C41-C42
15	b	604	CDL	C19-C20-C21-C22
15	Y	603	CDL	OB7-CB5-OB6-CB4
15	b	604	CDL	C37-C38-C39-C40
15	Y	603	CDL	C13-C14-C15-C16
15	K	301	CDL	C16-C17-C18-C19
15	Y	604	CDL	C35-C36-C37-C38
15	b	603	CDL	C14-C15-C16-C17
15	b	603	CDL	C11-CA5-OA6-CA4
15	b	603	CDL	C38-C39-C40-C41
15	b	604	CDL	C72-C73-C74-C75
15	Y	604	CDL	C23-C24-C25-C26
15	Y	604	CDL	C75-C76-C77-C78
15	V	805	CDL	C39-C40-C41-C42
15	b	603	CDL	C51-C52-C53-C54
15	b	603	CDL	C12-C13-C14-C15
15	K	301	CDL	C21-C22-C23-C24
15	b	603	CDL	C17-C18-C19-C20
15	b	604	CDL	C74-C75-C76-C77
15	b	603	CDL	CB2-C1-CA2-OA2
15	V	805	CDL	C31-CA7-OA8-CA6
15	M	301	CDL	C13-C14-C15-C16
15	V	805	CDL	C13-C14-C15-C16
15	K	301	CDL	C12-C13-C14-C15
15	Y	604	CDL	C54-C55-C56-C57
15	M	301	CDL	C60-C61-C62-C63
15	b	604	CDL	C60-C61-C62-C63
15	M	301	CDL	C38-C39-C40-C41
15	Y	604	CDL	C83-C84-C85-C86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	K	301	CDL	C42-C43-C44-C45
15	Y	603	CDL	C53-C54-C55-C56
15	Y	604	CDL	C56-C57-C58-C59
15	b	603	CDL	C54-C55-C56-C57
15	Y	604	CDL	C32-C33-C34-C35
15	b	604	CDL	C51-CB5-OB6-CB4
15	b	604	CDL	C71-CB7-OB8-CB6
15	b	603	CDL	C76-C77-C78-C79
15	b	604	CDL	C12-C13-C14-C15
15	K	301	CDL	C58-C59-C60-C61
20	Y	601	HEM	C3D-CAD-CBD-CGD
15	M	301	CDL	C15-C16-C17-C18
15	b	603	CDL	C35-C36-C37-C38
15	Y	604	CDL	C52-C53-C54-C55
15	M	301	CDL	C17-C18-C19-C20
15	V	805	CDL	C35-C36-C37-C38
15	b	603	CDL	C19-C20-C21-C22
15	b	603	CDL	OA7-CA5-OA6-CA4
15	b	604	CDL	C23-C24-C25-C26
15	K	301	CDL	C52-C53-C54-C55
15	K	301	CDL	C23-C24-C25-C26
15	M	301	CDL	C62-C63-C64-C65
15	b	603	CDL	C83-C84-C85-C86
15	M	301	CDL	C23-C24-C25-C26
15	b	603	CDL	C15-C16-C17-C18
15	Q	804	CDL	C39-C40-C41-C42
15	Y	603	CDL	C60-C61-C62-C63
15	Y	603	CDL	C75-C76-C77-C78
15	b	604	CDL	C15-C16-C17-C18
15	b	604	CDL	C17-C18-C19-C20
15	K	301	CDL	C75-C76-C77-C78
15	Y	604	CDL	C12-C13-C14-C15
15	Y	604	CDL	C15-C16-C17-C18
15	Y	603	CDL	C72-C73-C74-C75
15	Y	603	CDL	C71-CB7-OB8-CB6
15	Y	603	CDL	C41-C42-C43-C44
15	K	301	CDL	C17-C18-C19-C20
15	Q	804	CDL	C14-C15-C16-C17
15	Y	604	CDL	C19-C20-C21-C22
15	Y	604	CDL	C37-C38-C39-C40
20	Y	601	HEM	C2B-C3B-CAB-CBB
20	Y	602	HEM	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b	604	CDL	C20-C21-C22-C23
15	b	603	CDL	C34-C35-C36-C37
15	Y	603	CDL	C37-C38-C39-C40
15	V	805	CDL	OA9-CA7-OA8-CA6
15	K	301	CDL	C51-CB5-OB6-CB4
20	b	601	HEM	C4C-C3C-CAC-CBC
20	b	602	HEM	C4C-C3C-CAC-CBC
15	b	604	CDL	C32-C33-C34-C35
15	b	603	CDL	C32-C33-C34-C35
15	Y	604	CDL	C60-C61-C62-C63
15	M	301	CDL	C42-C43-C44-C45
15	b	604	CDL	C58-C59-C60-C61
15	Y	603	CDL	C56-C57-C58-C59
15	K	301	CDL	C38-C39-C40-C41
15	Y	603	CDL	C58-C59-C60-C61
15	K	301	CDL	C15-C16-C17-C18
15	Y	604	CDL	C51-C52-C53-C54
15	K	301	CDL	C54-C55-C56-C57
15	Y	604	CDL	C71-C72-C73-C74
15	Y	603	CDL	C11-C12-C13-C14
15	b	604	CDL	OB9-CB7-OB8-CB6
15	V	805	CDL	C11-C12-C13-C14
15	V	805	CDL	C61-C62-C63-C64
15	V	805	CDL	OB5-CB3-CB4-CB6
15	Y	603	CDL	C17-C18-C19-C20
15	Y	604	CDL	C13-C14-C15-C16
15	Y	604	CDL	C38-C39-C40-C41
15	Y	603	CDL	OB9-CB7-OB8-CB6
15	M	301	CDL	C24-C25-C26-C27
15	K	301	CDL	CA7-C31-C32-C33
15	K	301	CDL	C19-C20-C21-C22
15	M	301	CDL	C31-CA7-OA8-CA6
15	b	604	CDL	C57-C58-C59-C60
15	Y	604	CDL	C74-C75-C76-C77
15	b	604	CDL	OB7-CB5-OB6-CB4
15	M	301	CDL	CA3-CA4-CA6-OA8
15	b	604	CDL	CA3-CA4-CA6-OA8
15	V	805	CDL	C79-C80-C81-C82
15	V	805	CDL	C53-C54-C55-C56
15	V	805	CDL	C80-C81-C82-C83
15	Y	604	CDL	C58-C59-C60-C61
15	M	301	CDL	C51-C52-C53-C54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	Y	603	CDL	C15-C16-C17-C18
15	M	301	CDL	C52-C53-C54-C55
15	b	604	CDL	C55-C56-C57-C58
15	Y	604	CDL	C20-C21-C22-C23
15	M	301	CDL	C41-C42-C43-C44
15	b	604	CDL	C41-C42-C43-C44
15	b	603	CDL	C31-C32-C33-C34
15	Y	604	CDL	C21-C22-C23-C24
15	Q	804	CDL	C11-CA5-OA6-CA4
15	Y	603	CDL	C36-C37-C38-C39
15	M	301	CDL	C37-C38-C39-C40
15	V	805	CDL	C57-C58-C59-C60
15	Q	804	CDL	C79-C80-C81-C82
15	M	301	CDL	C53-C54-C55-C56
15	M	301	CDL	C57-C58-C59-C60
15	b	603	CDL	C72-C73-C74-C75
15	K	301	CDL	C72-C73-C74-C75
15	Q	804	CDL	OA6-CA4-CA6-OA8
15	V	805	CDL	C51-C52-C53-C54
15	K	301	CDL	C34-C35-C36-C37
15	b	603	CDL	C52-C53-C54-C55
15	Y	604	CDL	CB7-C71-C72-C73
15	M	301	CDL	C40-C41-C42-C43
15	b	603	CDL	C55-C56-C57-C58
15	V	805	CDL	C56-C57-C58-C59
15	M	301	CDL	OA9-CA7-OA8-CA6
15	Y	604	CDL	CA5-C11-C12-C13
15	M	301	CDL	C76-C77-C78-C79
15	M	301	CDL	C12-C13-C14-C15
15	b	603	CDL	C20-C21-C22-C23
15	b	604	CDL	C56-C57-C58-C59
15	Y	603	CDL	C35-C36-C37-C38
15	b	604	CDL	OB5-CB3-CB4-CB6
15	b	603	CDL	C23-C24-C25-C26
15	Y	603	CDL	C23-C24-C25-C26
15	V	805	CDL	C75-C76-C77-C78
15	b	604	CDL	C36-C37-C38-C39
15	M	301	CDL	CB3-CB4-CB6-OB8
15	K	301	CDL	CB3-CB4-CB6-OB8
15	Y	603	CDL	CB3-CB4-CB6-OB8
15	Q	804	CDL	C17-C18-C19-C20
15	b	604	CDL	C42-C43-C44-C45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b	604	CDL	C61-C62-C63-C64
15	Y	603	CDL	C76-C77-C78-C79
15	b	603	CDL	OB5-CB3-CB4-OB6
15	b	604	CDL	OB5-CB3-CB4-OB6
15	Q	804	CDL	OB5-CB3-CB4-OB6
15	b	604	CDL	C1-CA2-OA2-PA1
15	Y	603	CDL	C40-C41-C42-C43
15	Q	804	CDL	C62-C63-C64-C65
15	K	301	CDL	C11-C12-C13-C14
15	M	301	CDL	CA5-C11-C12-C13
15	M	301	CDL	OA6-CA4-CA6-OA8
15	b	603	CDL	OA6-CA4-CA6-OA8
15	Q	804	CDL	C32-C33-C34-C35
15	K	301	CDL	OB7-CB5-OB6-CB4
15	K	301	CDL	C39-C40-C41-C42
15	b	603	CDL	C16-C17-C18-C19
15	M	301	CDL	C55-C56-C57-C58
15	Q	804	CDL	C55-C56-C57-C58
15	K	301	CDL	C80-C81-C82-C83
15	Y	603	CDL	C73-C74-C75-C76
16	Y	606	MQ9	C24-C26-C27-C28
15	Q	804	CDL	C40-C41-C42-C43
15	Q	804	CDL	C81-C82-C83-C84
15	Q	804	CDL	C41-C42-C43-C44
15	Q	804	CDL	OB5-CB3-CB4-CB6
15	Y	603	CDL	C39-C40-C41-C42
15	V	805	CDL	C76-C77-C78-C79
15	Q	804	CDL	OA7-CA5-OA6-CA4
15	V	805	CDL	C15-C16-C17-C18
15	Y	603	CDL	OB5-CB3-CB4-OB6
15	b	603	CDL	CA3-CA4-CA6-OA8
15	Y	604	CDL	CA3-CA4-CA6-OA8
20	Y	602	HEM	C4B-C3B-CAB-CBB
20	Y	602	HEM	C4C-C3C-CAC-CBC
15	b	604	CDL	C34-C35-C36-C37
16	b	605	MQ9	C1-C6-C7-C8
15	K	301	CDL	OB6-CB4-CB6-OB8
15	Y	603	CDL	OB6-CB4-CB6-OB8
15	Y	604	CDL	OA6-CA4-CA6-OA8
15	Y	604	CDL	OB6-CB4-CB6-OB8
15	M	301	CDL	C31-C32-C33-C34
15	b	603	CDL	C57-C58-C59-C60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	V	805	CDL	C37-C38-C39-C40
15	Y	603	CDL	C19-C20-C21-C22
15	Y	604	CDL	C82-C83-C84-C85
15	Q	804	CDL	C53-C54-C55-C56
15	Y	603	CDL	C61-C62-C63-C64
16	M	302	MQ9	C45-C44-C46-C47
19	V	804	HEC	C3D-CAD-CBD-CGD
19	i	301	HEC	C3D-CAD-CBD-CGD
19	j	301	HEC	C3D-CAD-CBD-CGD
19	j	302	HEC	C3D-CAD-CBD-CGD
15	V	805	CDL	C32-C31-CA7-OA8
15	M	301	CDL	C56-C57-C58-C59
15	V	805	CDL	C33-C34-C35-C36
15	b	604	CDL	C64-C65-C66-C67
16	M	302	MQ9	C12-C11-C9-C10
15	M	301	CDL	OB5-CB3-CB4-CB6
15	Y	603	CDL	OB5-CB3-CB4-CB6
15	Q	804	CDL	C80-C81-C82-C83
15	b	603	CDL	C82-C83-C84-C85
15	Y	604	CDL	C57-C58-C59-C60
15	Q	804	CDL	C78-C79-C80-C81
15	Y	603	CDL	C18-C19-C20-C21
15	Y	603	CDL	C74-C75-C76-C77
15	M	301	CDL	OB5-CB3-CB4-OB6
15	V	805	CDL	OB5-CB3-CB4-OB6
15	K	301	CDL	C63-C64-C65-C66
18	Q	801	HAS	C1D-C2D-CMD-OMD
18	Q	802	HAS	C1D-C2D-CMD-OMD
15	Y	604	CDL	C80-C81-C82-C83
15	M	301	CDL	OB6-CB4-CB6-OB8
15	Y	603	CDL	C24-C25-C26-C27
15	Q	804	CDL	CA3-CA4-CA6-OA8
16	M	302	MQ9	C43-C44-C46-C47
15	V	805	CDL	C60-C61-C62-C63
15	K	301	CDL	C20-C21-C22-C23
15	M	301	CDL	CB2-OB2-PB2-OB3
15	V	805	CDL	CA2-OA2-PA1-OA4
15	V	805	CDL	CB3-OB5-PB2-OB3
15	b	603	CDL	CB3-OB5-PB2-OB3
15	b	604	CDL	CA2-OA2-PA1-OA3
15	b	604	CDL	CA3-OA5-PA1-OA2
15	b	604	CDL	CB3-OB5-PB2-OB2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	b	604	CDL	CB3-OB5-PB2-OB3
15	b	604	CDL	CB3-OB5-PB2-OB4
15	K	301	CDL	CA3-OA5-PA1-OA2
15	K	301	CDL	CB2-OB2-PB2-OB4
15	Q	804	CDL	CB2-OB2-PB2-OB5
15	Q	804	CDL	CB3-OB5-PB2-OB4
15	Y	603	CDL	CA2-OA2-PA1-OA5
15	Y	603	CDL	CA3-OA5-PA1-OA3
15	Y	603	CDL	CA3-OA5-PA1-OA4
15	Y	604	CDL	CB3-OB5-PB2-OB2
15	b	603	CDL	C18-C19-C20-C21
15	V	805	CDL	C71-C72-C73-C74
15	Q	804	CDL	C31-C32-C33-C34
15	b	604	CDL	C33-C34-C35-C36
15	Y	603	CDL	C59-C60-C61-C62
15	M	301	CDL	C32-C31-CA7-OA8
15	Q	804	CDL	OA5-CA3-CA4-OA6
15	K	301	CDL	C53-C54-C55-C56
15	V	805	CDL	C34-C35-C36-C37
15	Y	603	CDL	C12-C13-C14-C15
15	b	604	CDL	C11-C12-C13-C14
18	Q	801	HAS	O11-C11-C12-C13
15	V	805	CDL	C17-C18-C19-C20
15	V	805	CDL	C36-C37-C38-C39
15	Q	804	CDL	C52-C51-CB5-OB6
15	b	604	CDL	C14-C15-C16-C17
15	Q	804	CDL	C15-C16-C17-C18
15	M	301	CDL	C72-C71-CB7-OB8
15	Y	604	CDL	CB3-CB4-CB6-OB8
16	Y	605	MQ9	C24-C26-C27-C28
15	Q	804	CDL	C77-C78-C79-C80
15	M	301	CDL	C44-C45-C46-C47
16	b	605	MQ9	C5-C6-C7-C8
15	Y	603	CDL	C63-C64-C65-C66
15	Y	603	CDL	C55-C56-C57-C58
20	Y	601	HEM	C4B-C3B-CAB-CBB
15	b	604	CDL	C39-C40-C41-C42
15	Y	604	CDL	C76-C77-C78-C79
15	Y	604	CDL	C24-C25-C26-C27
15	b	604	CDL	C31-C32-C33-C34
20	b	601	HEM	CAD-CBD-CGD-O1D
16	M	302	MQ9	C12-C11-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	K	301	CDL	C74-C75-C76-C77
15	V	805	CDL	C40-C41-C42-C43
15	Y	604	CDL	C22-C23-C24-C25
15	b	603	CDL	CB3-CB4-OB6-CB5
15	b	603	CDL	CB6-CB4-OB6-CB5
15	Y	604	CDL	CB3-CB4-OB6-CB5
15	Y	604	CDL	CB6-CB4-OB6-CB5
15	Q	804	CDL	C38-C39-C40-C41
16	Y	606	MQ9	C20-C19-C21-C22
15	Y	603	CDL	C52-C53-C54-C55
18	Q	801	HAS	CAD-CBD-CGD-O2D
20	Y	602	HEM	CAD-CBD-CGD-O2D
15	K	301	CDL	O1-C1-CB2-OB2
15	M	301	CDL	C71-CB7-OB8-CB6
15	b	604	CDL	C52-C53-C54-C55
15	b	603	CDL	C21-C22-C23-C24
16	Y	605	MQ9	C35-C34-C36-C37
16	Y	606	MQ9	C12-C11-C9-C10
20	Y	602	HEM	CAD-CBD-CGD-O1D
18	V	802	HAS	CAD-CBD-CGD-O2D
18	Q	802	HAS	CAD-CBD-CGD-O1D
20	b	601	HEM	CAD-CBD-CGD-O2D
15	K	301	CDL	C35-C36-C37-C38
15	Q	804	CDL	C51-C52-C53-C54
15	b	604	CDL	C21-C22-C23-C24
18	V	802	HAS	C27-C19-C20-C21
16	Y	606	MQ9	C12-C11-C9-C8
20	b	602	HEM	CAD-CBD-CGD-O1D
15	K	301	CDL	C78-C79-C80-C81
15	Y	604	CDL	C84-C85-C86-C87
15	M	301	CDL	OB9-CB7-OB8-CB6
15	Q	804	CDL	C54-C55-C56-C57
18	V	802	HAS	CAD-CBD-CGD-O1D
18	Q	802	HAS	CAD-CBD-CGD-O2D
18	V	801	HAS	CAA-CBA-CGA-O2A
15	Y	603	CDL	C16-C17-C18-C19
18	Q	801	HAS	CAD-CBD-CGD-O1D
20	b	602	HEM	CAD-CBD-CGD-O2D
15	Y	603	CDL	C21-C22-C23-C24
16	b	605	MQ9	C40-C39-C41-C42
18	V	801	HAS	C27-C19-C20-C21
15	b	604	CDL	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	Y	601	HEM	CAA-CBA-CGA-O2A
19	j	302	HEC	CAD-CBD-CGD-O2D
15	V	805	CDL	C41-C42-C43-C44
19	V	804	HEC	CAD-CBD-CGD-O2D
19	j	301	HEC	CAD-CBD-CGD-O2D
15	V	805	CDL	C31-C32-C33-C34
18	V	801	HAS	C11-C12-C13-C14
19	i	301	HEC	CAD-CBD-CGD-O2D
15	b	603	CDL	OB5-CB3-CB4-CB6
15	Q	804	CDL	OA5-CA3-CA4-CA6
18	V	801	HAS	CAD-CBD-CGD-O2D
15	M	301	CDL	C34-C35-C36-C37
18	V	802	HAS	C18-C19-C20-C21
15	Q	804	CDL	C35-C36-C37-C38
18	V	801	HAS	CAD-CBD-CGD-O1D
15	K	301	CDL	C83-C84-C85-C86
18	V	801	HAS	CAA-CBA-CGA-O1A
19	V	804	HEC	CAD-CBD-CGD-O1D
19	j	302	HEC	CAD-CBD-CGD-O1D
19	i	301	HEC	CAD-CBD-CGD-O1D
19	j	301	HEC	CAD-CBD-CGD-O1D
20	Y	601	HEM	CAA-CBA-CGA-O1A
15	K	301	CDL	CA2-C1-CB2-OB2
15	V	805	CDL	C32-C33-C34-C35
20	b	601	HEM	CAA-CBA-CGA-O2A
15	Y	604	CDL	C61-C62-C63-C64
15	K	301	CDL	C59-C60-C61-C62
15	Q	804	CDL	C42-C43-C44-C45
16	M	302	MQ9	C39-C41-C42-C43
16	b	605	MQ9	C24-C26-C27-C28
16	Y	605	MQ9	C14-C16-C17-C18
15	K	301	CDL	C40-C41-C42-C43
15	M	301	CDL	C18-C19-C20-C21
16	Y	606	MQ9	C18-C19-C21-C22
15	M	301	CDL	C59-C60-C61-C62
15	M	301	CDL	C52-C51-CB5-OB6
15	Q	804	CDL	C72-C71-CB7-OB8
15	b	603	CDL	CB3-CB4-CB6-OB8
16	Y	606	MQ9	C45-C44-C46-C47
20	b	601	HEM	CAA-CBA-CGA-O1A
15	Y	603	CDL	C71-C72-C73-C74
16	b	605	MQ9	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	M	301	CDL	C19-C20-C21-C22
15	K	301	CDL	C77-C78-C79-C80
16	Y	606	MQ9	C34-C36-C37-C38
15	b	603	CDL	CB5-C51-C52-C53
15	K	301	CDL	C33-C34-C35-C36
15	V	805	CDL	C14-C15-C16-C17
16	b	605	MQ9	C38-C39-C41-C42
15	M	301	CDL	C81-C82-C83-C84
15	b	603	CDL	OB6-CB4-CB6-OB8
15	Q	804	CDL	C72-C71-CB7-OB9
15	V	805	CDL	C32-C31-CA7-OA9
18	V	802	HAS	C16-C17-C18-C19
15	V	805	CDL	C1-CA2-OA2-PA1
15	V	805	CDL	C72-C71-CB7-OB8
20	b	602	HEM	C2B-C3B-CAB-CBB
15	M	301	CDL	C73-C74-C75-C76
18	Q	802	HAS	O11-C11-C3B-C4B
15	Q	804	CDL	C36-C37-C38-C39
15	V	805	CDL	C52-C51-CB5-OB6
15	Y	604	CDL	C32-C31-CA7-OA8
15	M	301	CDL	C52-C51-CB5-OB7

There are no ring outliers.

22 monomers are involved in 133 short contacts:

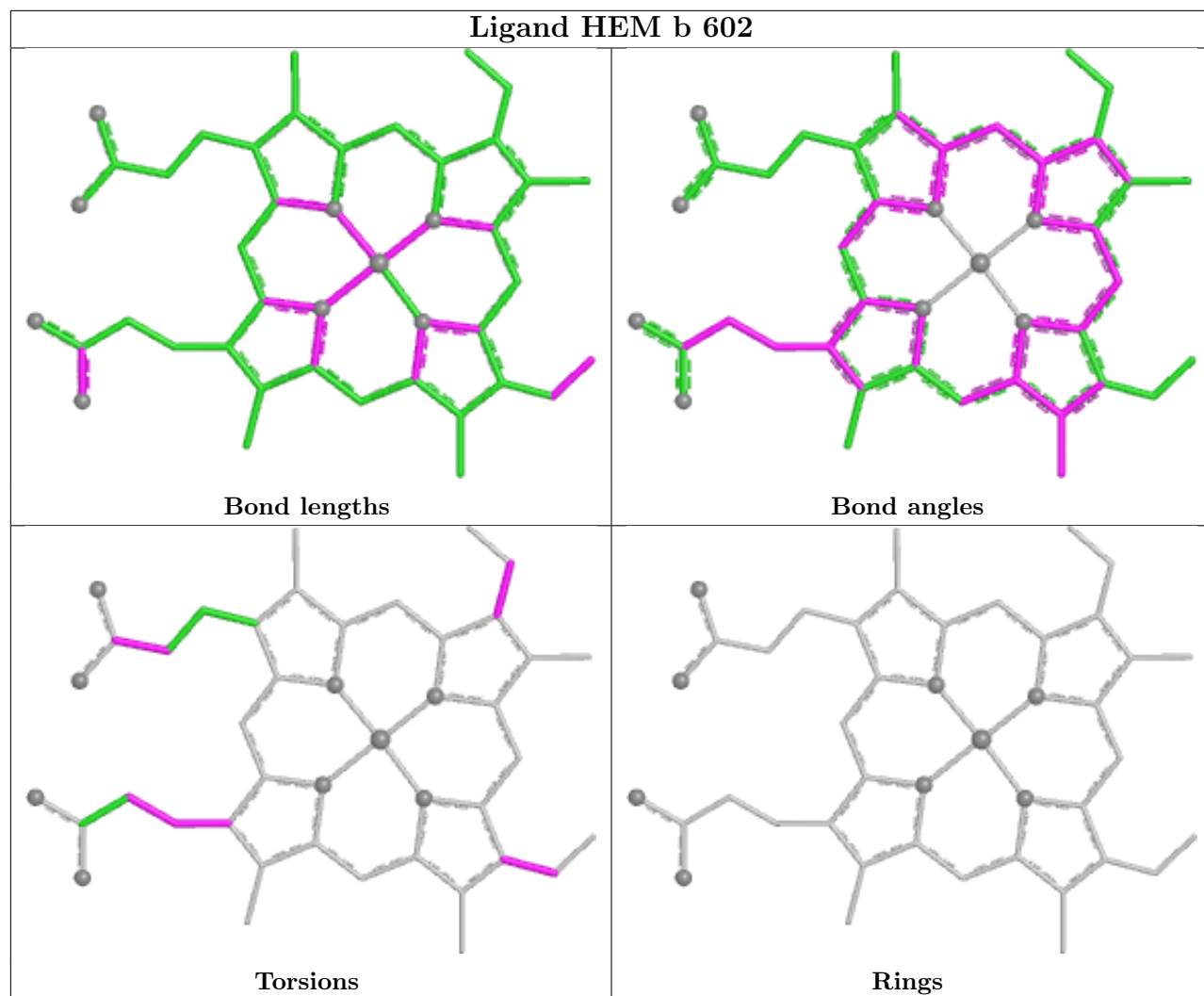
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	i	301	HEC	18	0
19	j	302	HEC	9	0
16	Y	606	MQ9	5	0
14	B	501	FES	2	0
18	V	801	HAS	4	0
20	Y	601	HEM	1	0
20	Y	602	HEM	5	0
18	Q	801	HAS	3	0
18	V	802	HAS	2	0
15	M	301	CDL	4	0
19	j	301	HEC	26	0
15	b	603	CDL	2	0
16	Y	605	MQ9	5	0
19	V	804	HEC	21	0
15	V	805	CDL	2	0
15	K	301	CDL	6	0

Continued on next page...

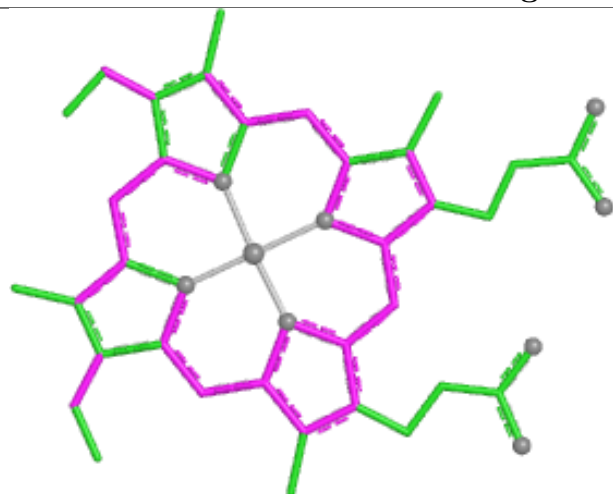
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	605	MQ9	2	0
15	Q	804	CDL	3	0
15	Y	604	CDL	8	0
16	M	302	MQ9	6	0
18	Q	802	HAS	3	0
15	Y	603	CDL	4	0

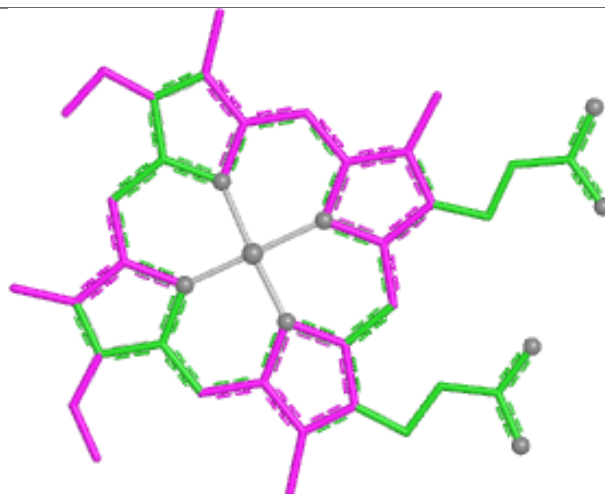
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



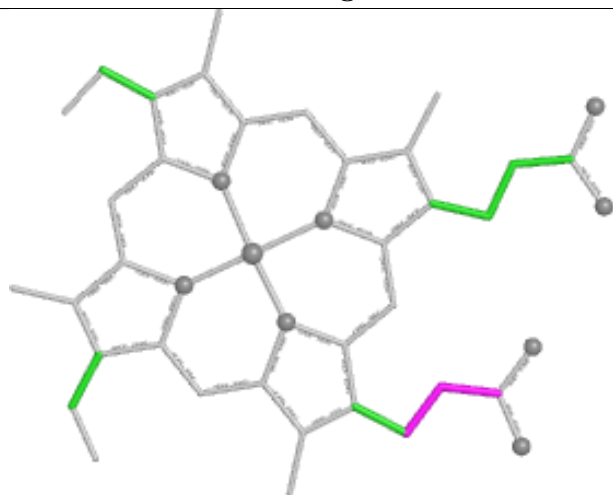
Ligand HEC i 301



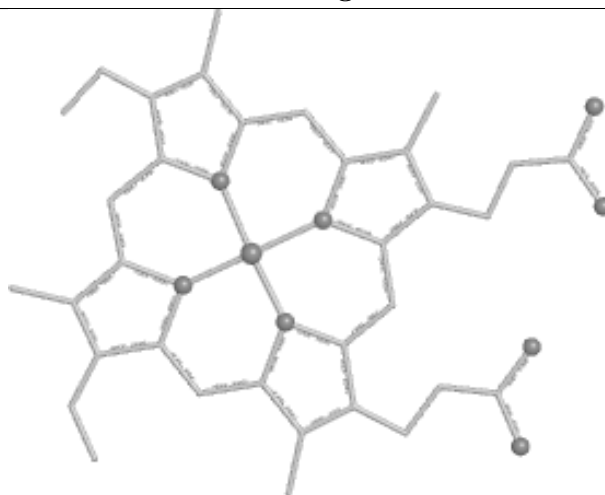
Bond lengths



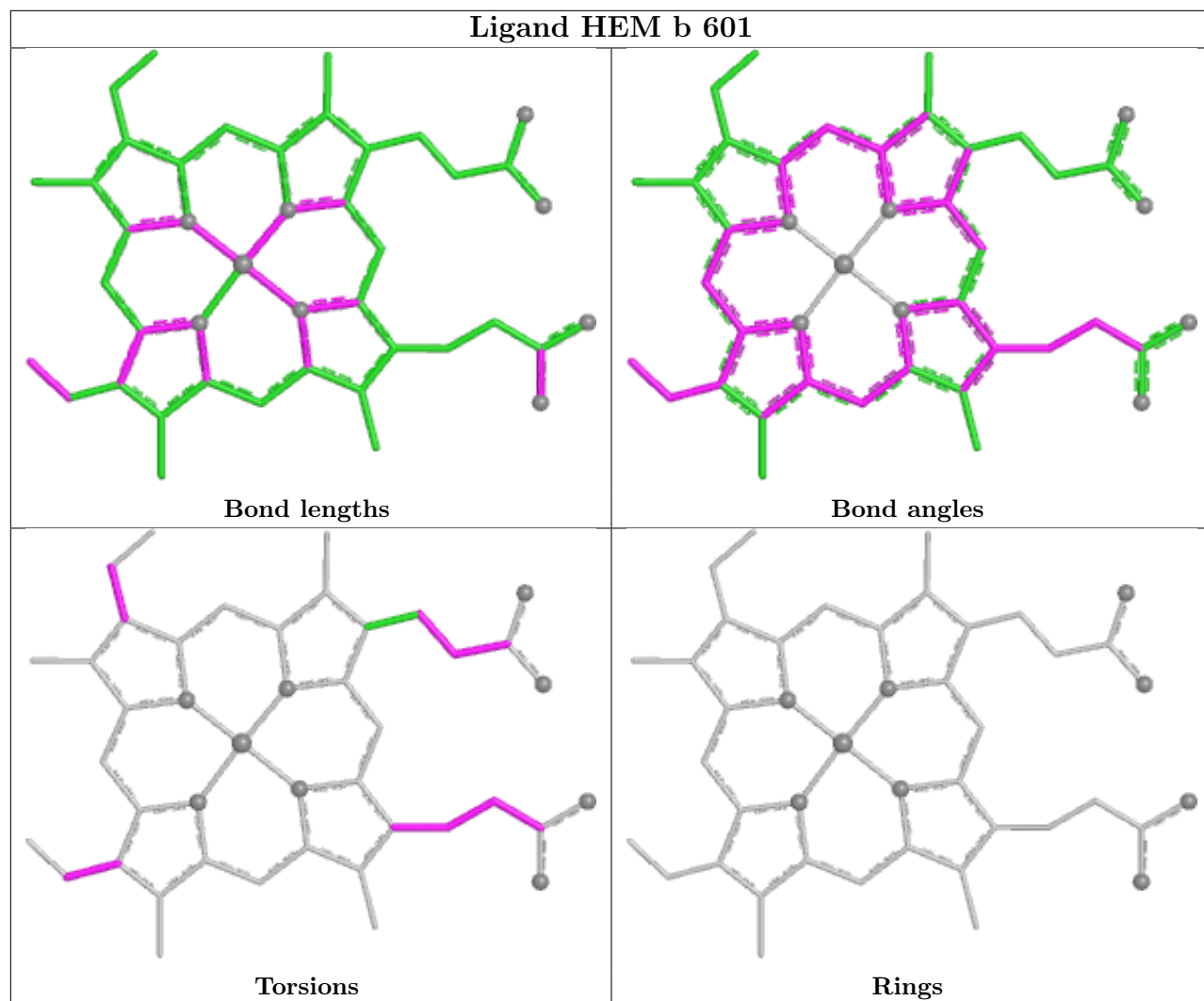
Bond angles



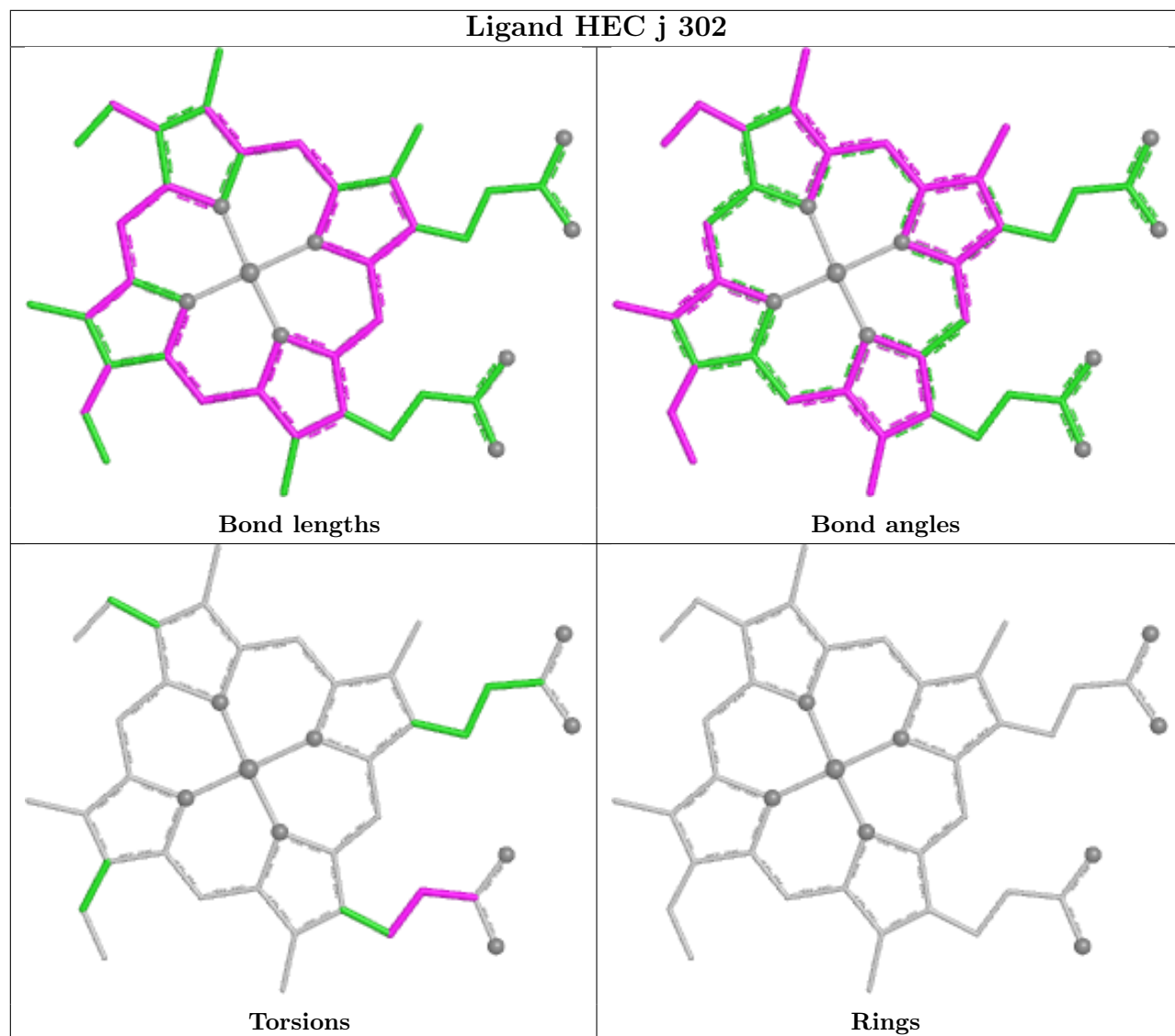
Torsions



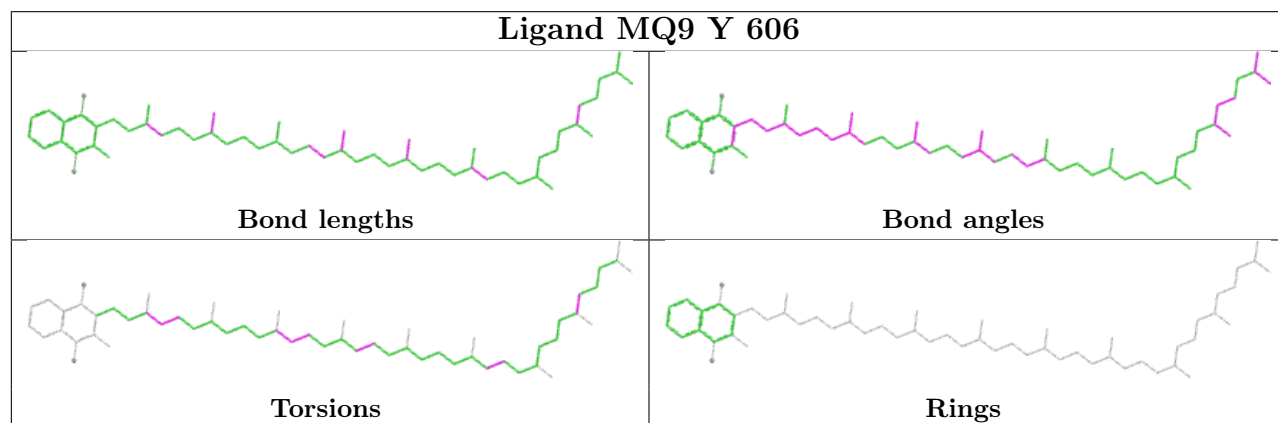
Rings



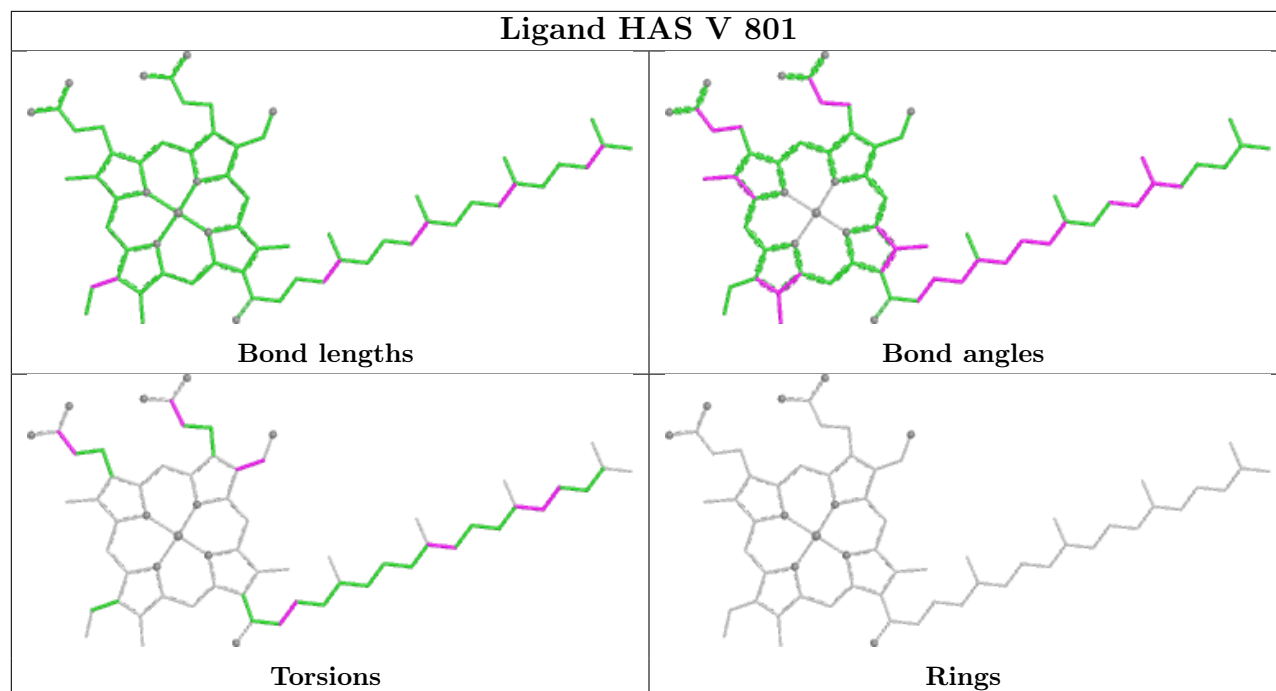
Ligand HEC j 302



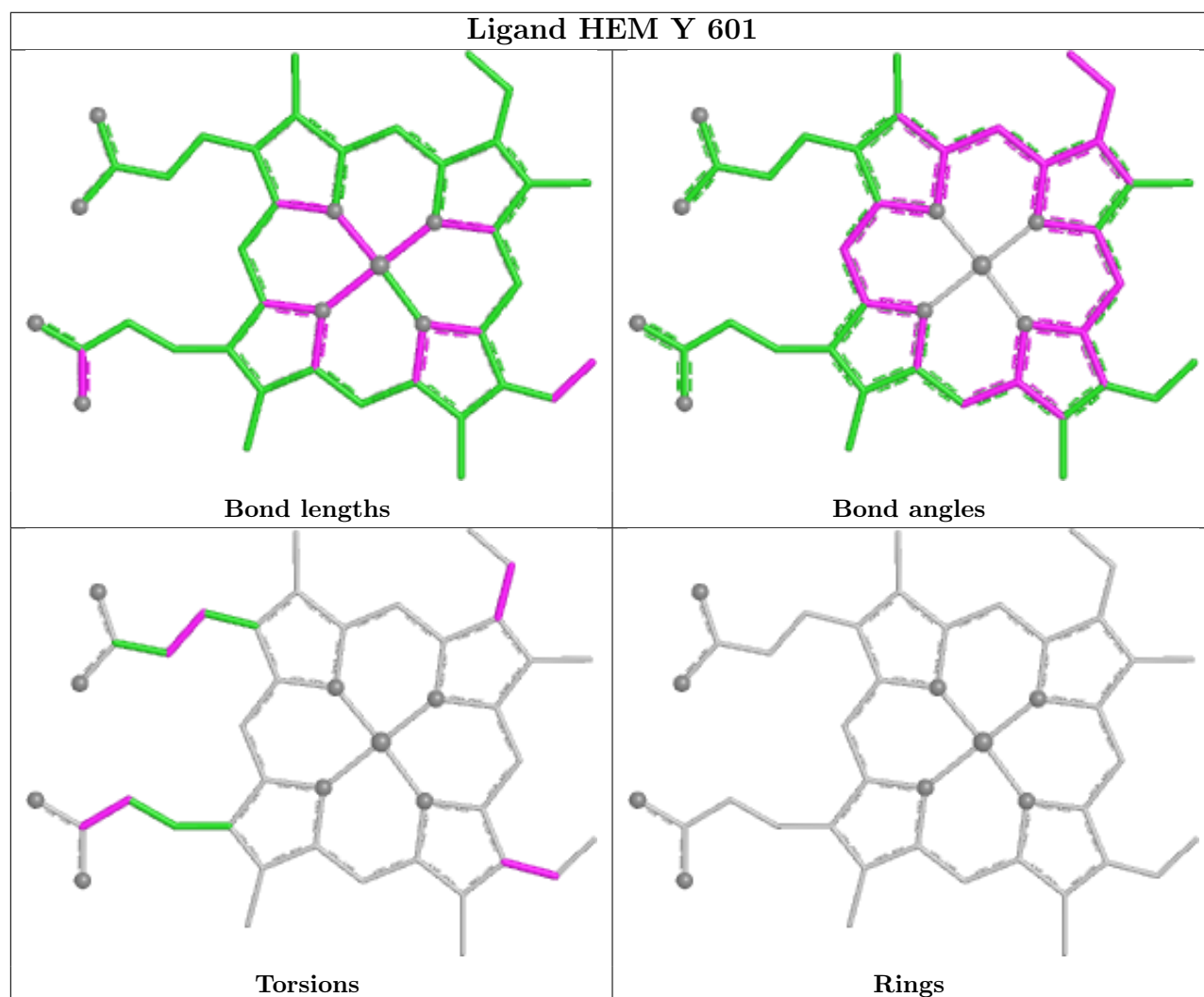
Ligand MQ9 Y 606

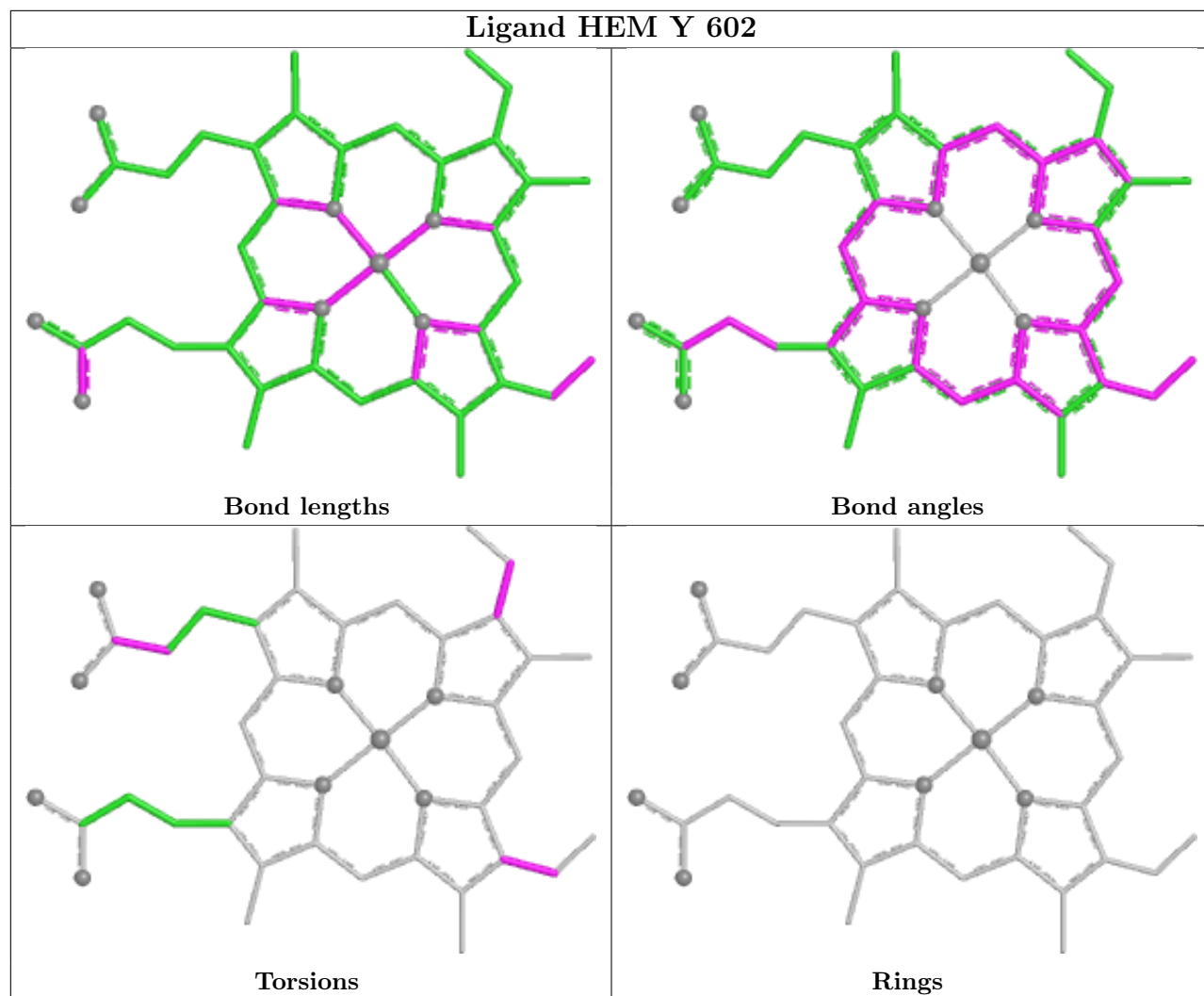


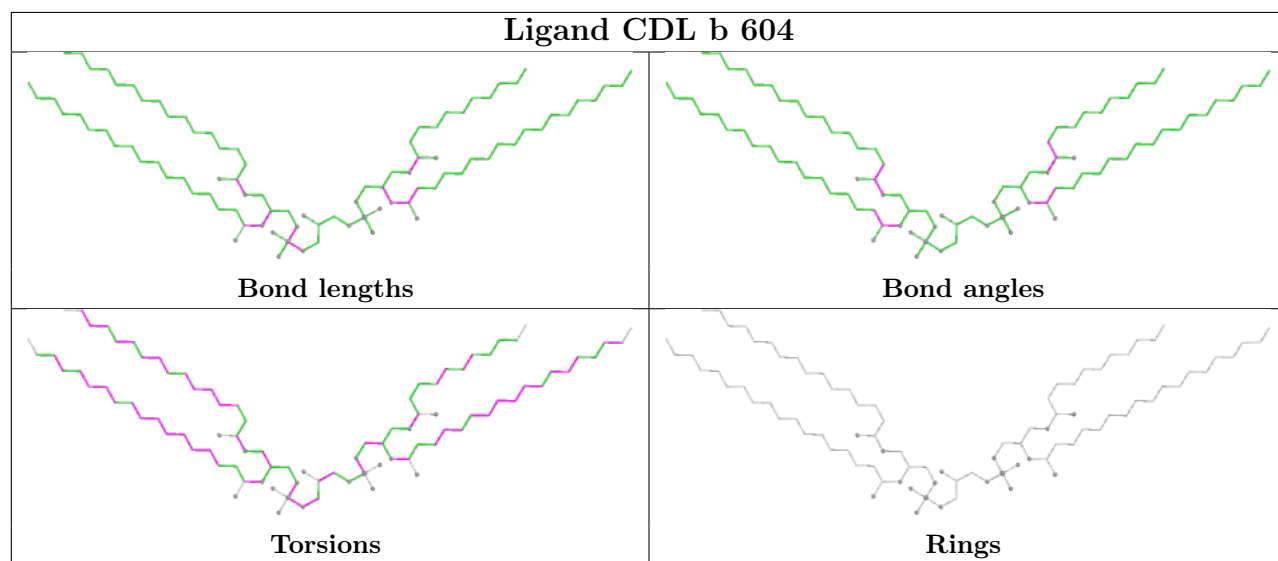
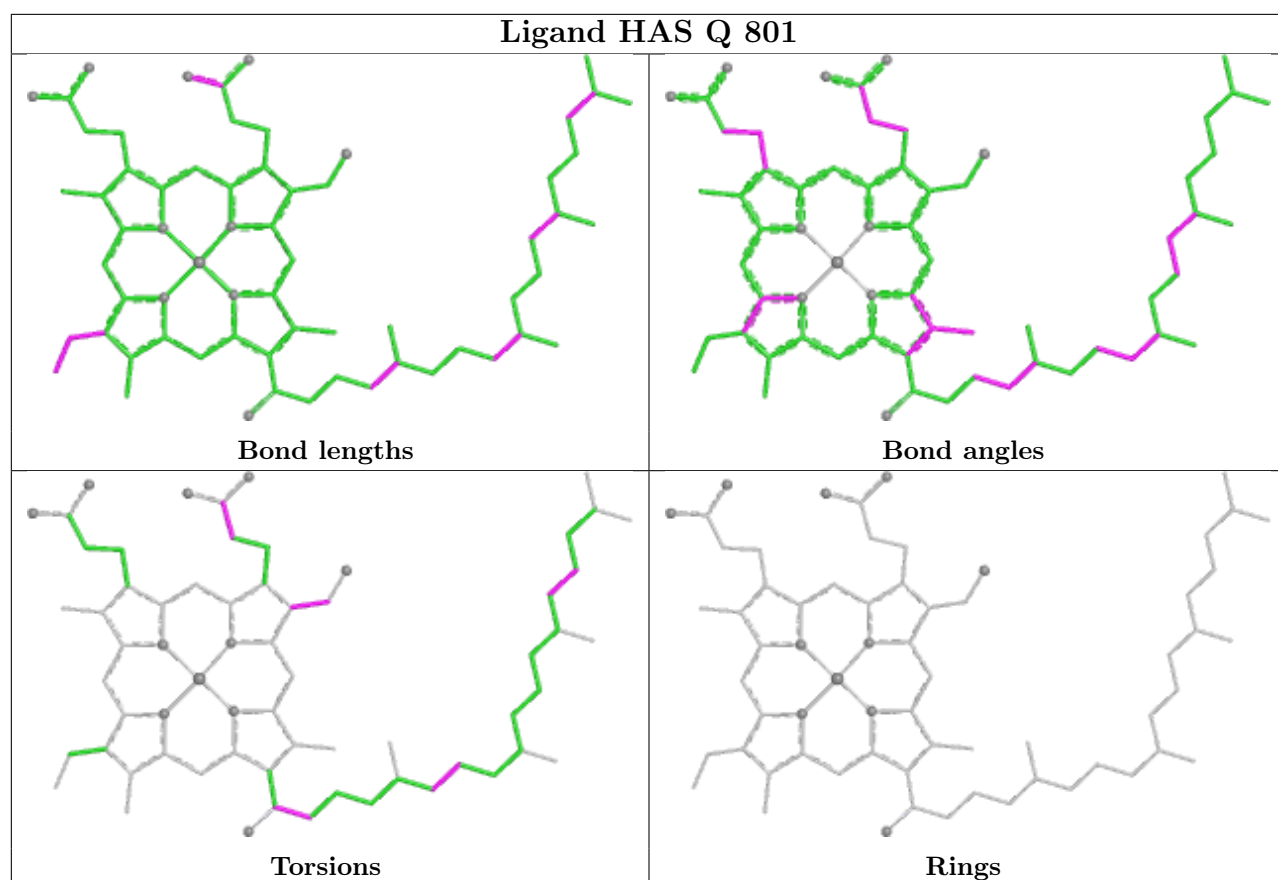
Ligand HAS V 801

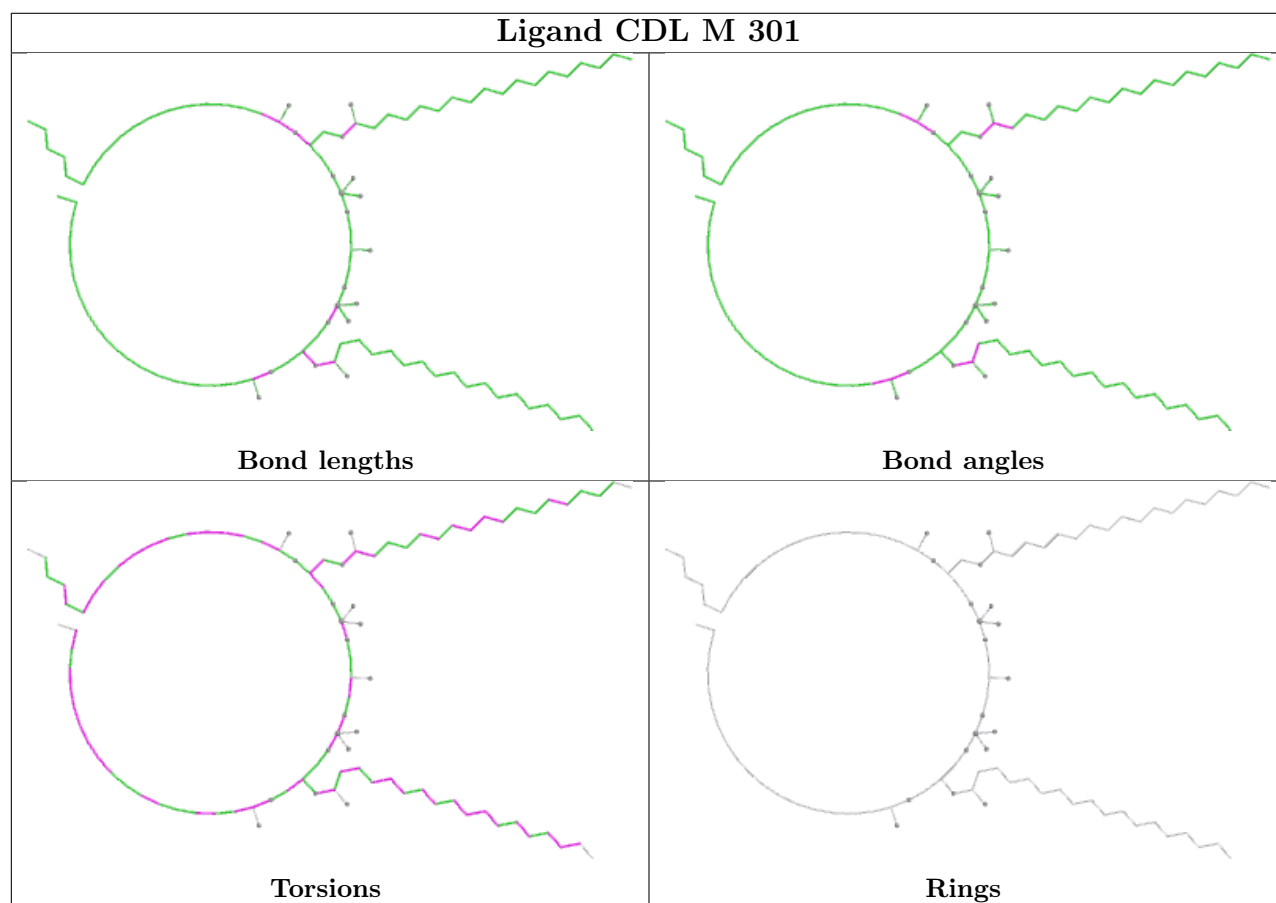
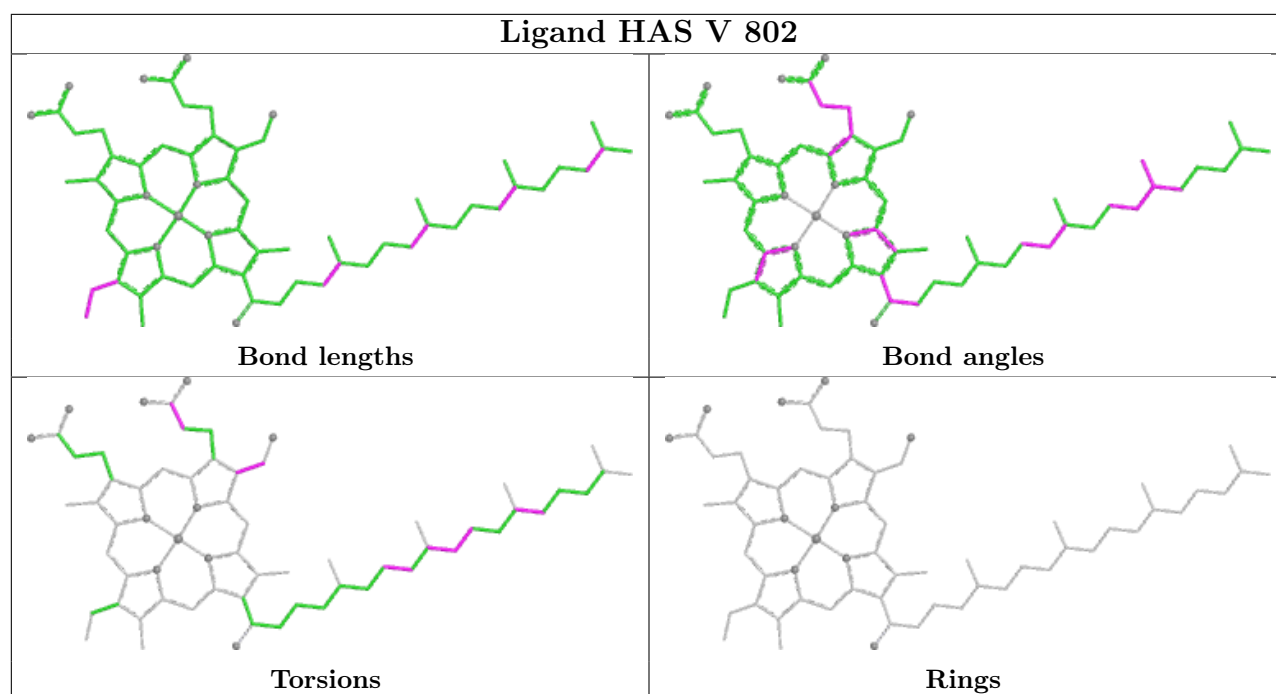


Ligand HEM Y 601

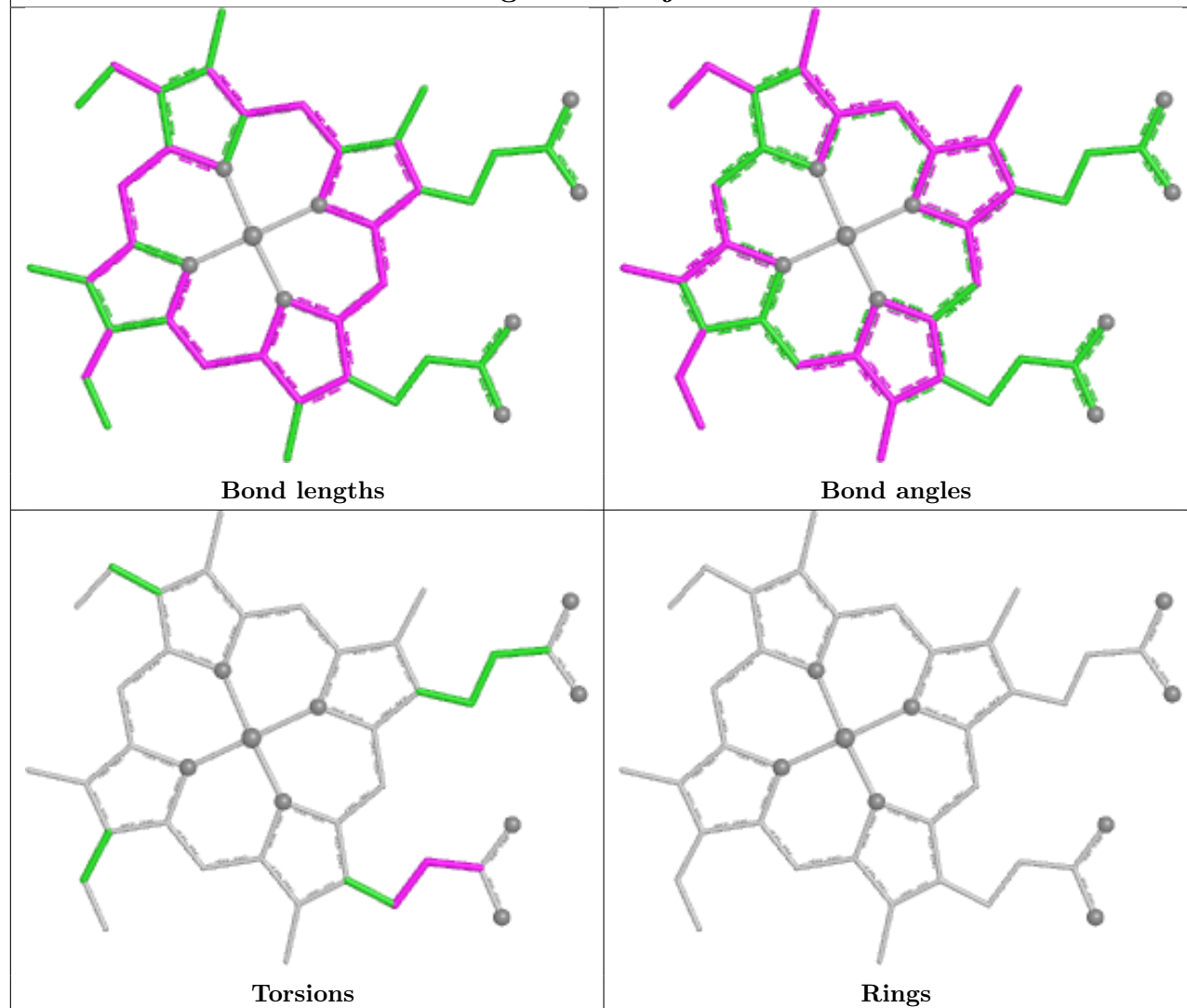




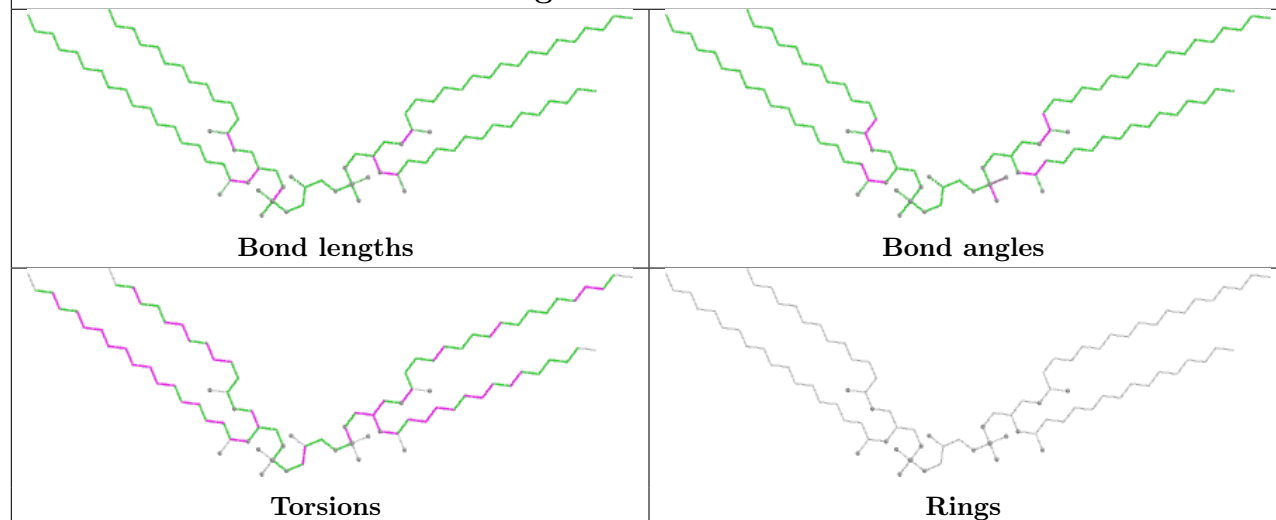


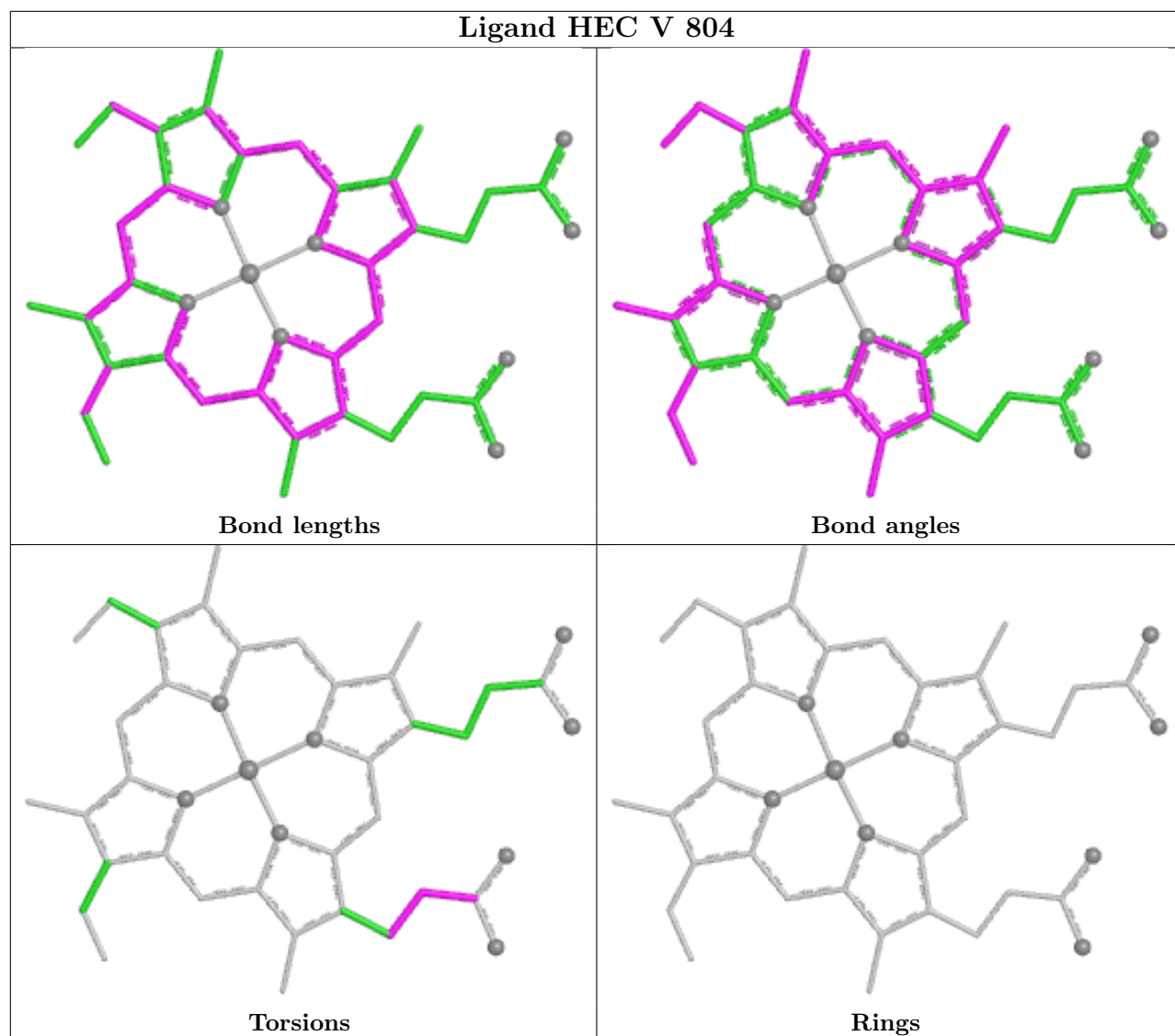
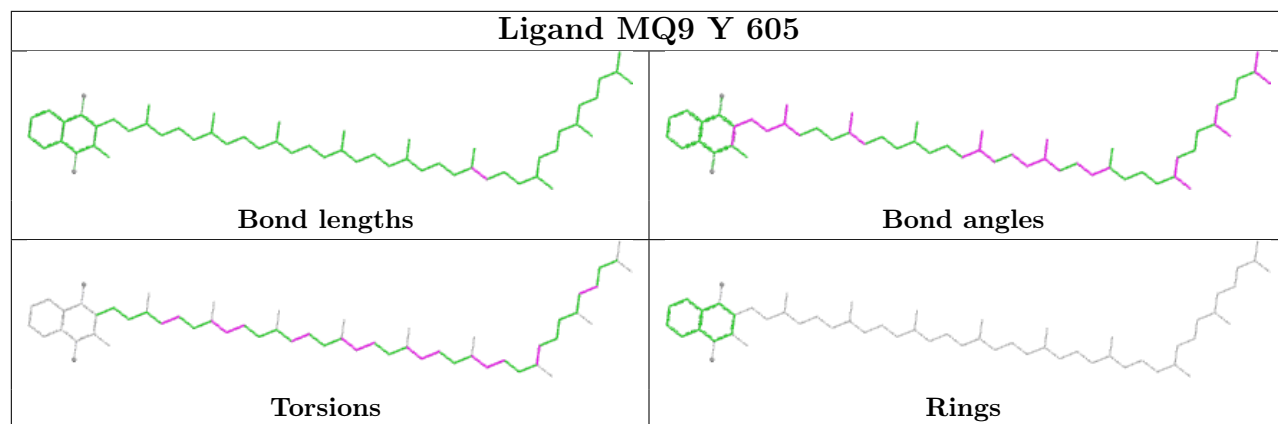


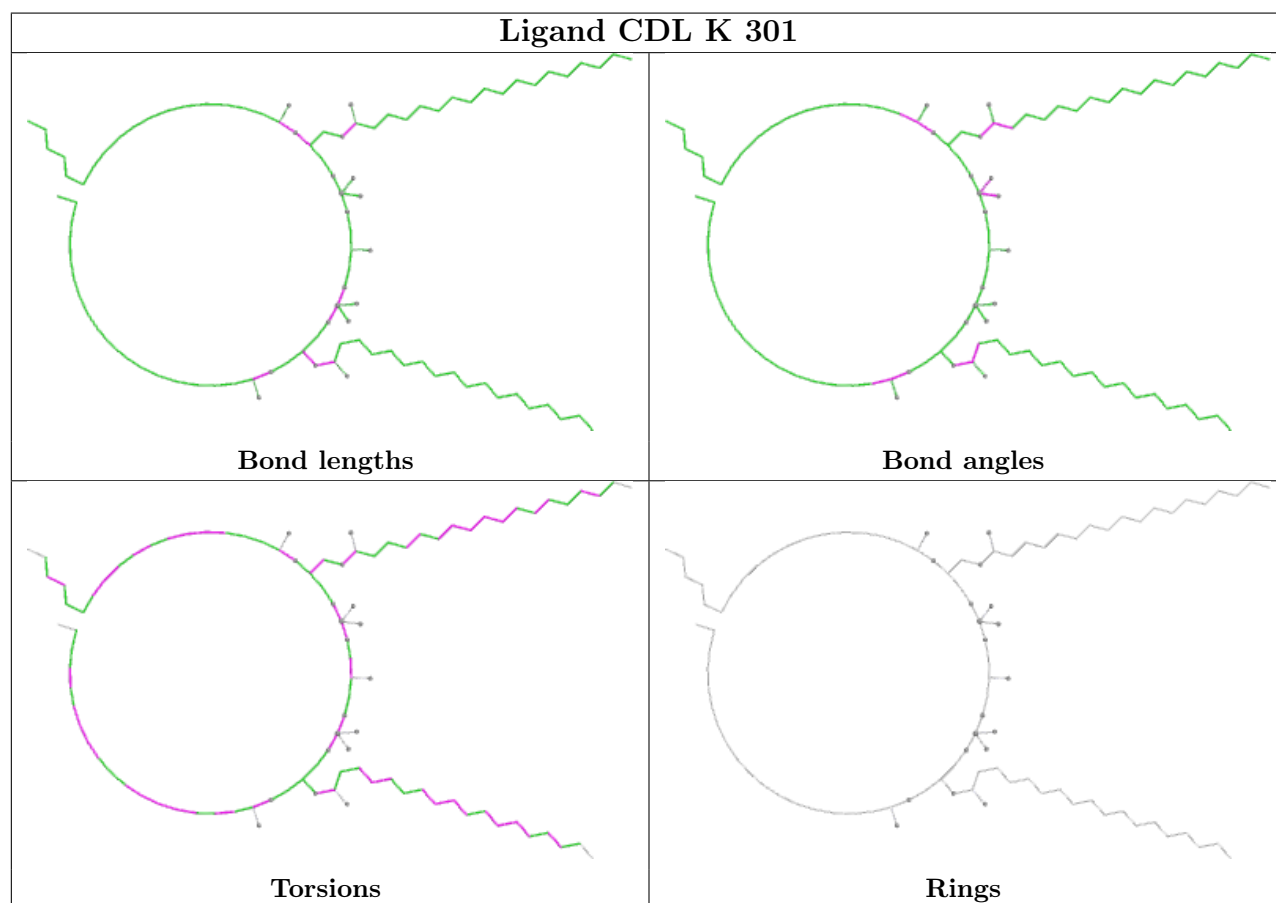
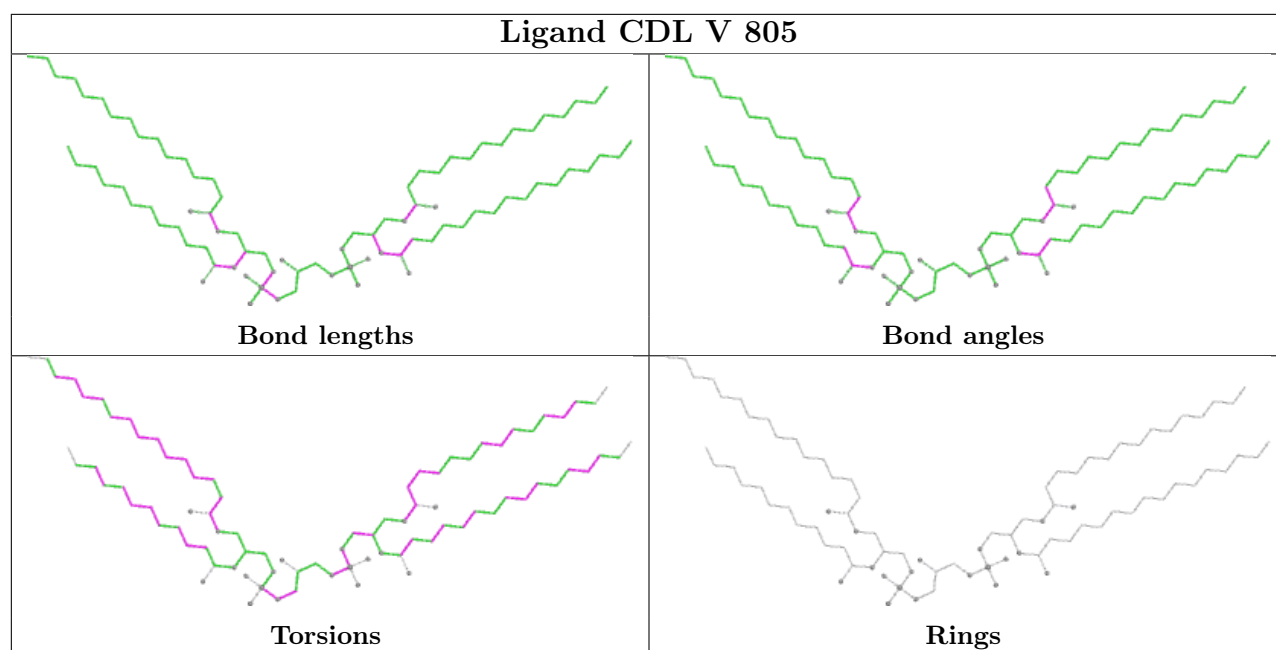
Ligand HEC j 301

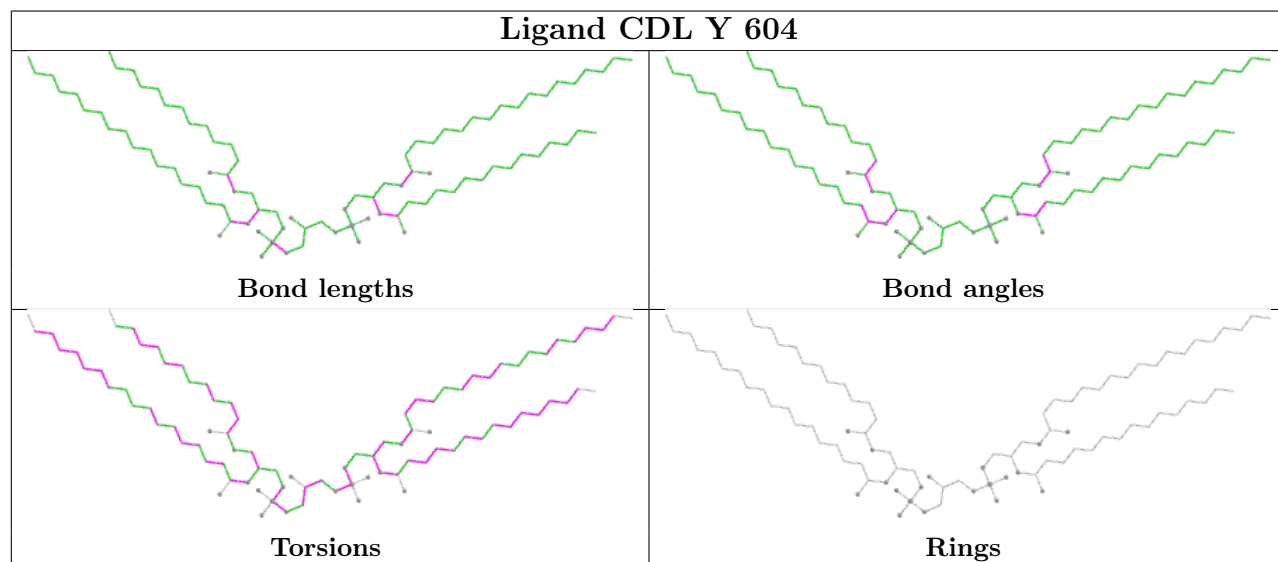
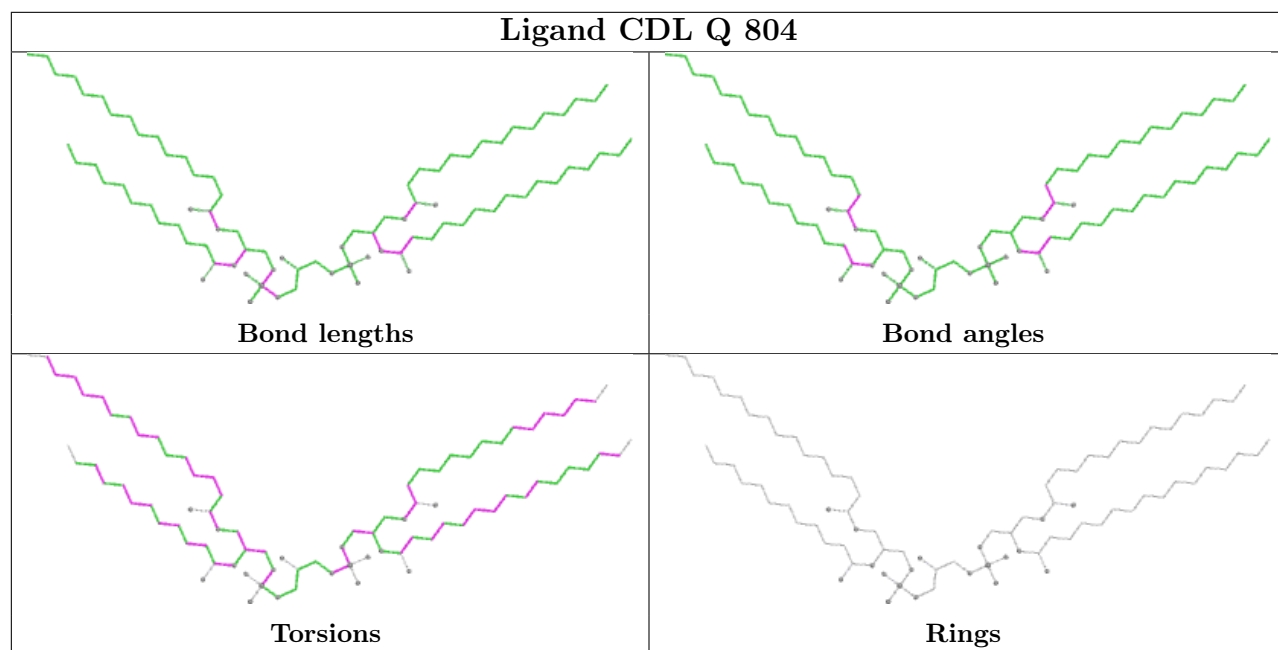
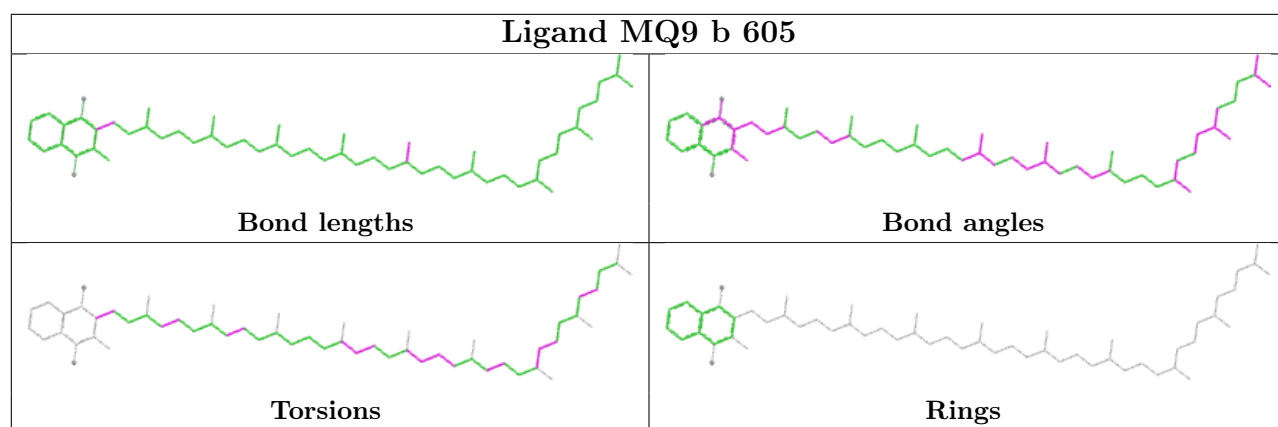


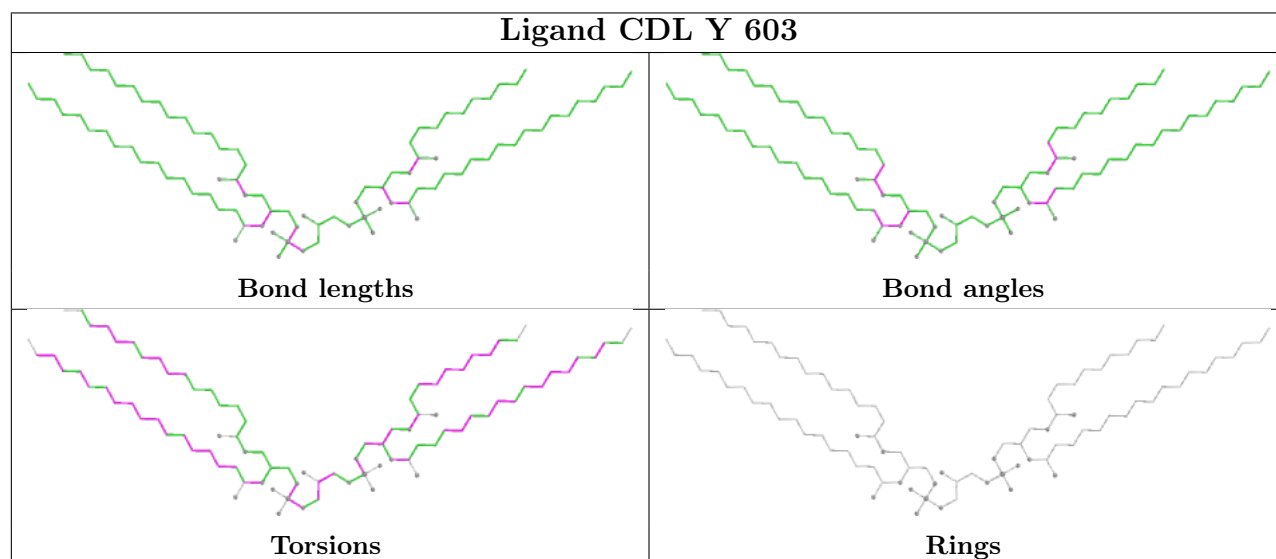
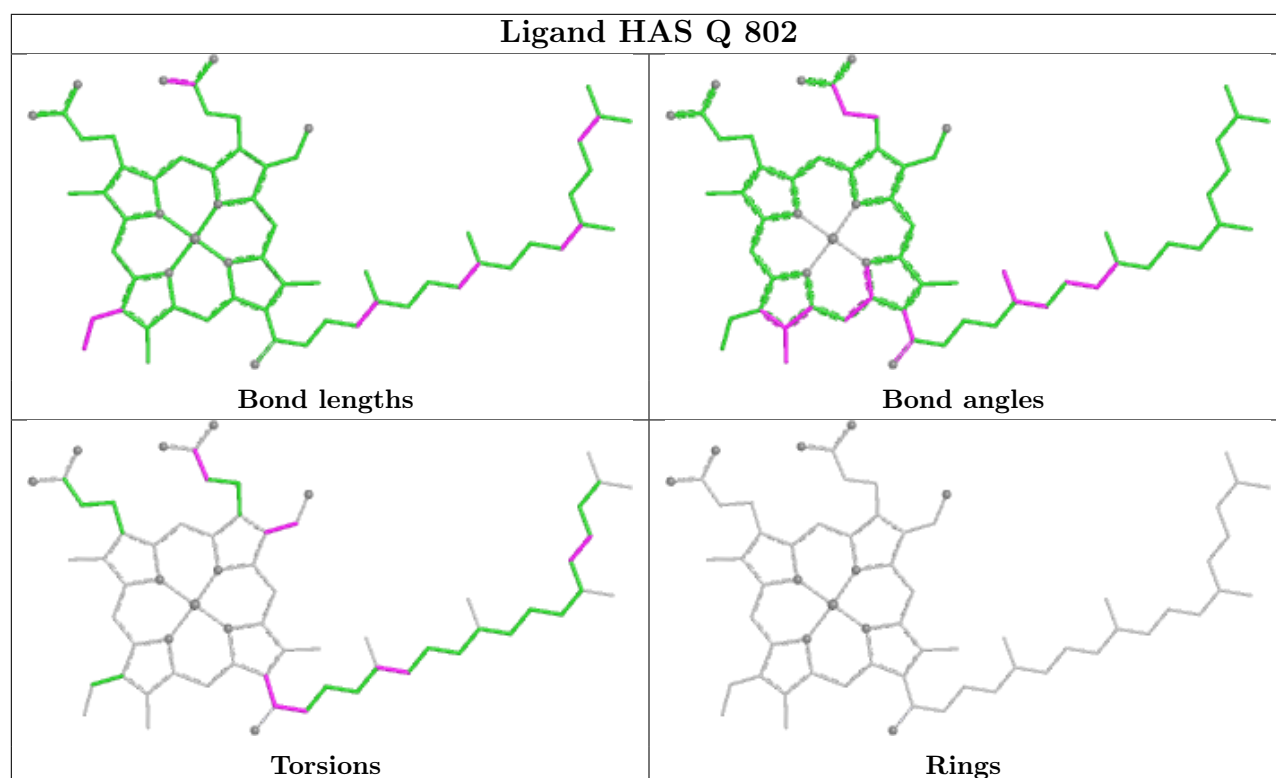
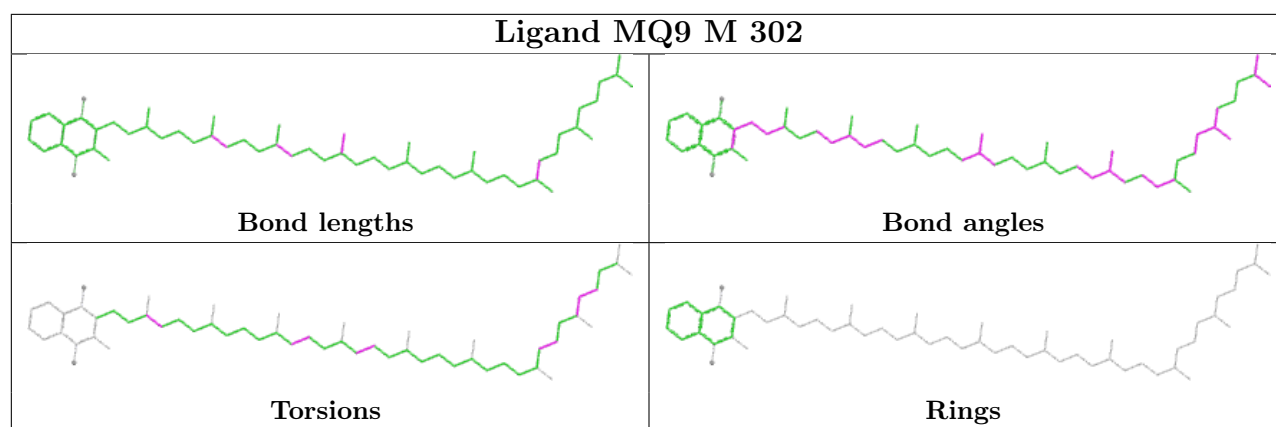
Ligand CDL b 603











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.

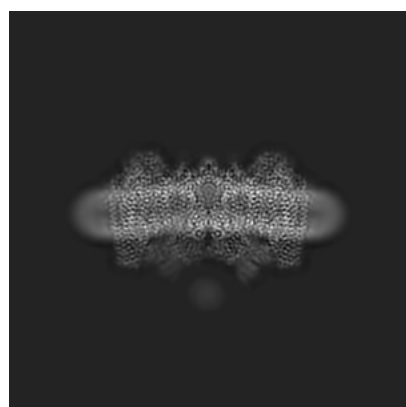
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0289. These allow visual inspection of the internal detail of the map and identification of artifacts.

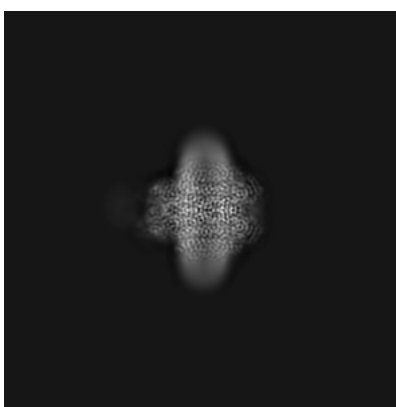
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

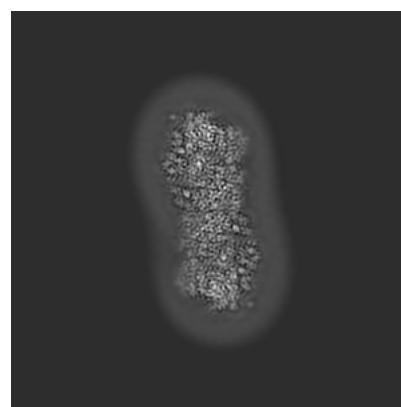
6.1.1 Primary map



X



Y

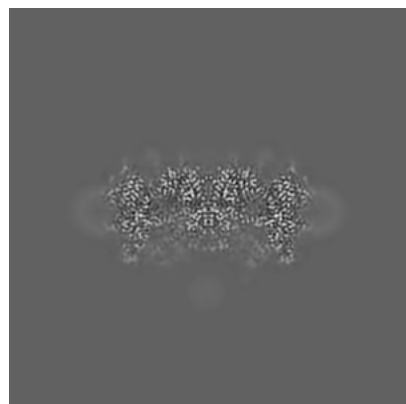


Z

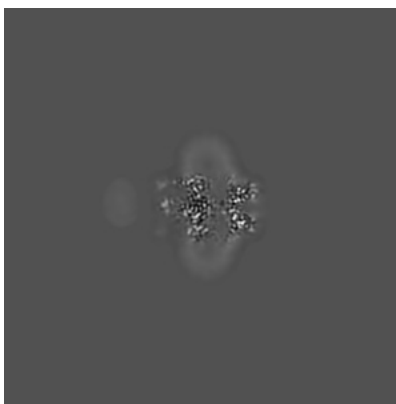
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

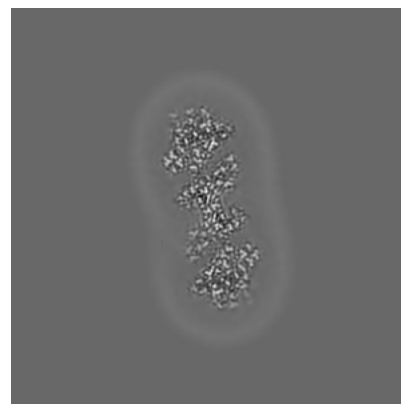
6.2.1 Primary map



X Index: 190



Y Index: 190

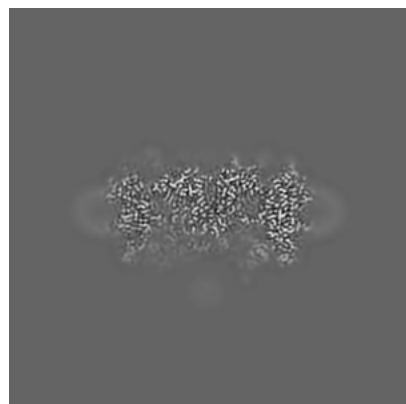


Z Index: 190

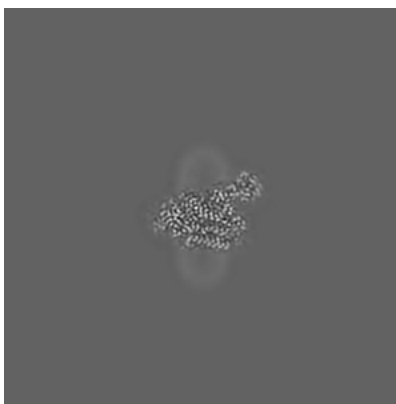
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

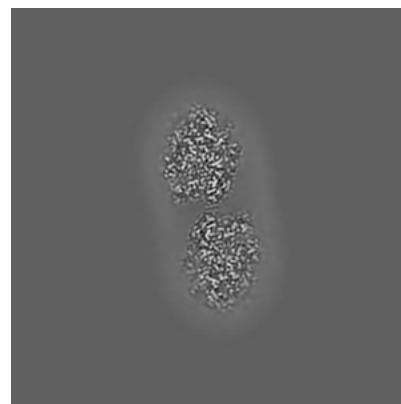
6.3.1 Primary map



X Index: 188



Y Index: 253

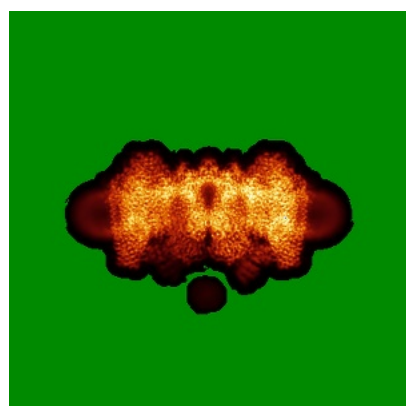


Z Index: 207

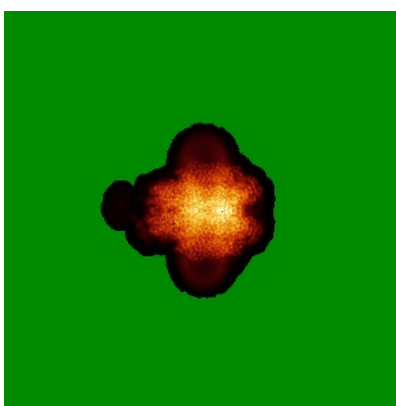
The images above show the largest variance slices of the map in three orthogonal directions.

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

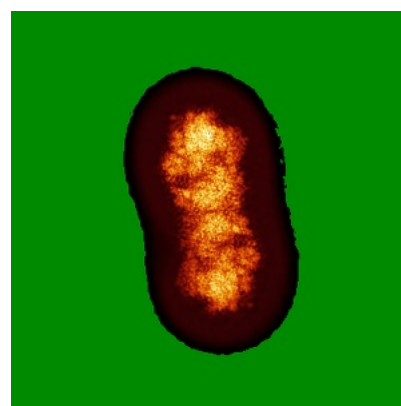
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

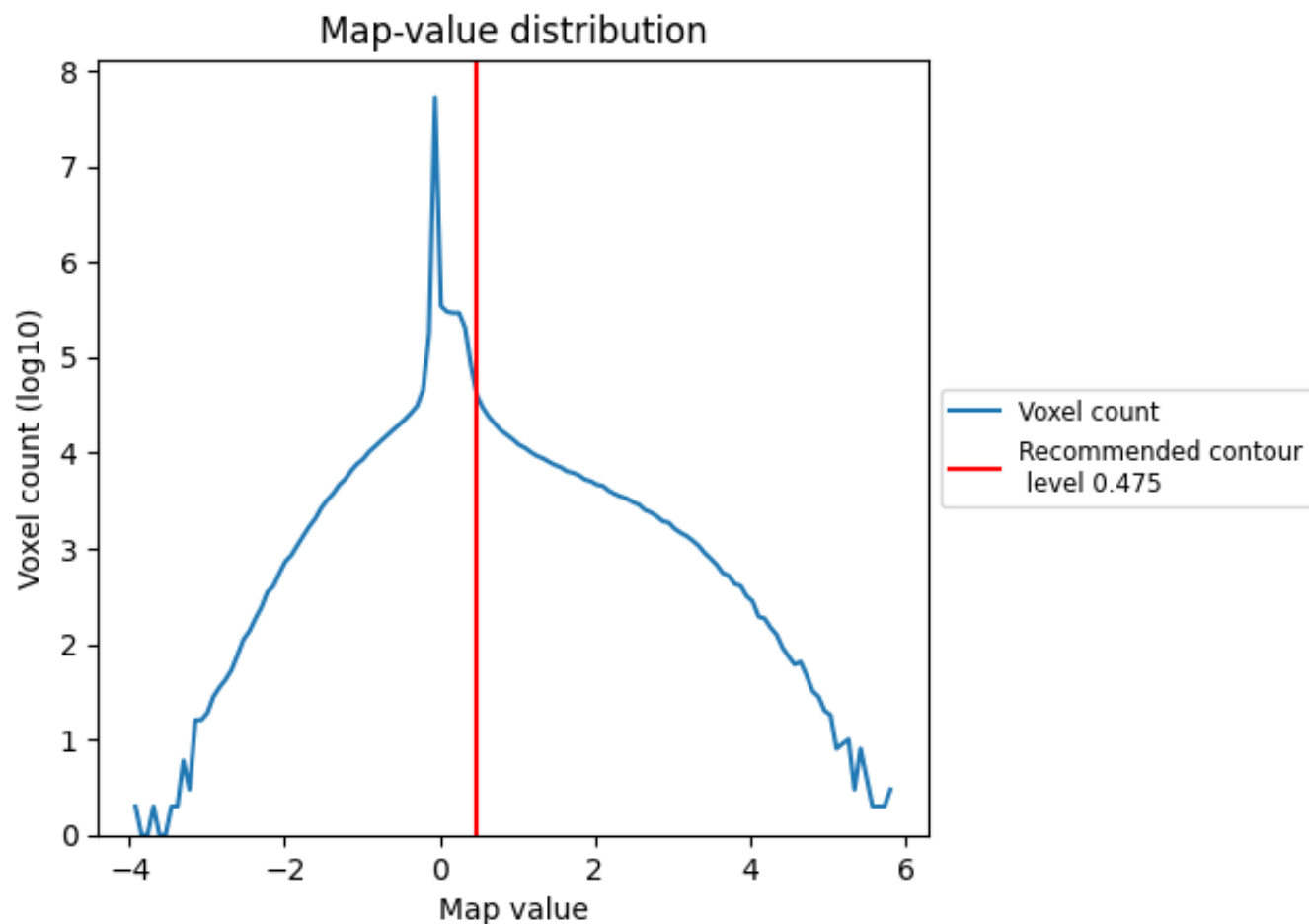
6.6 Mask visualisation

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

7 Map analysis [i](#)

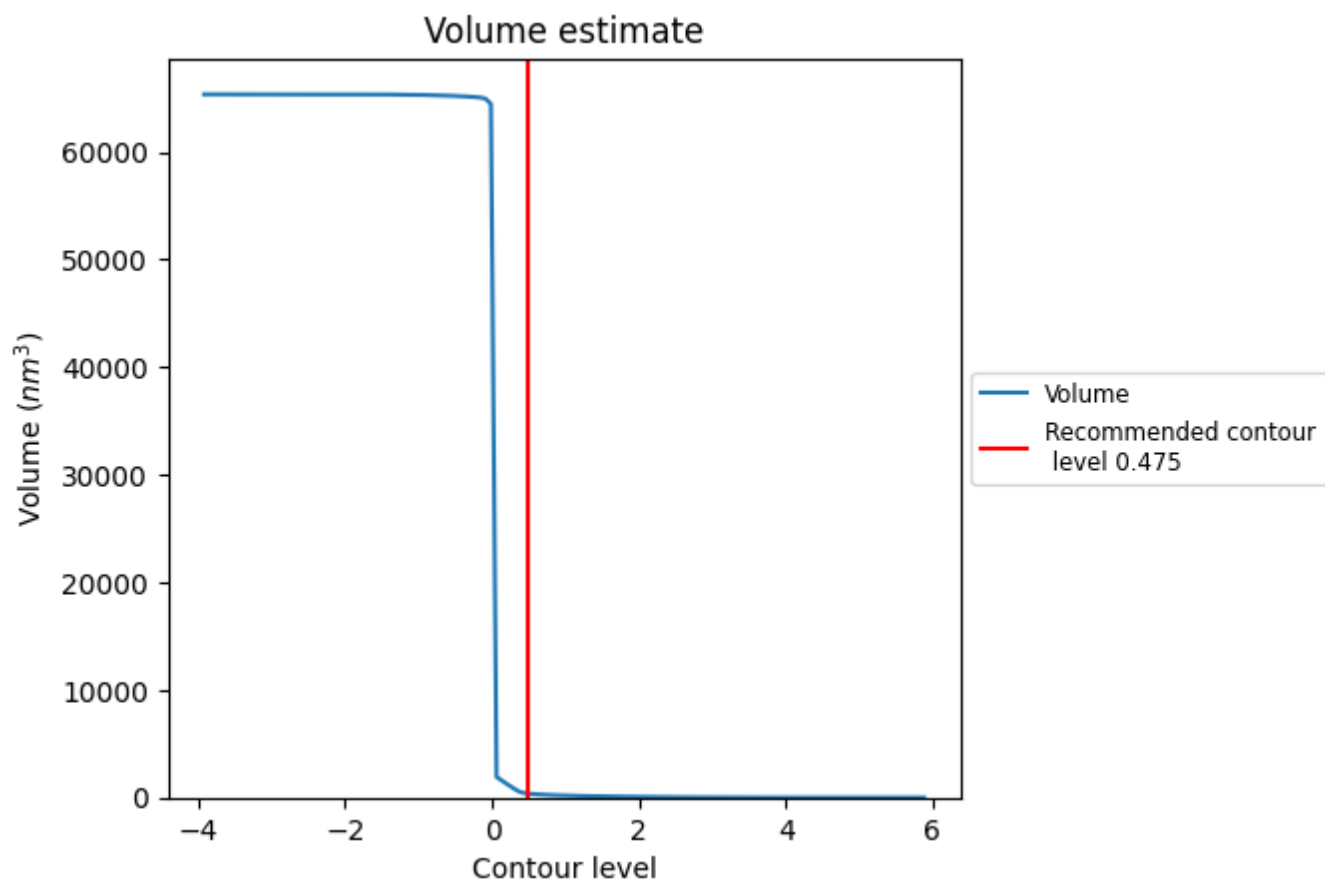
This section contains the results of statistical analysis of the map.

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.

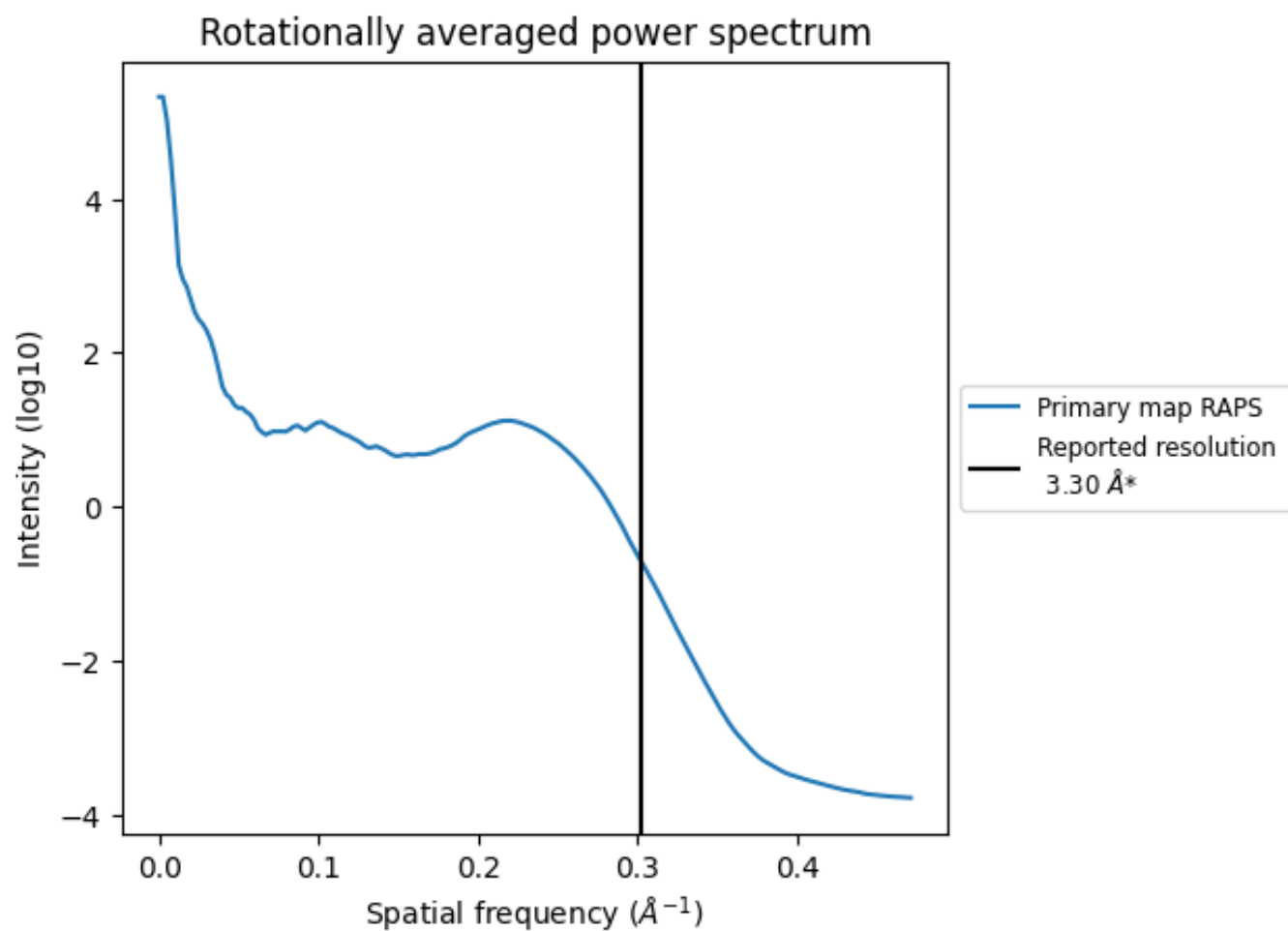
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

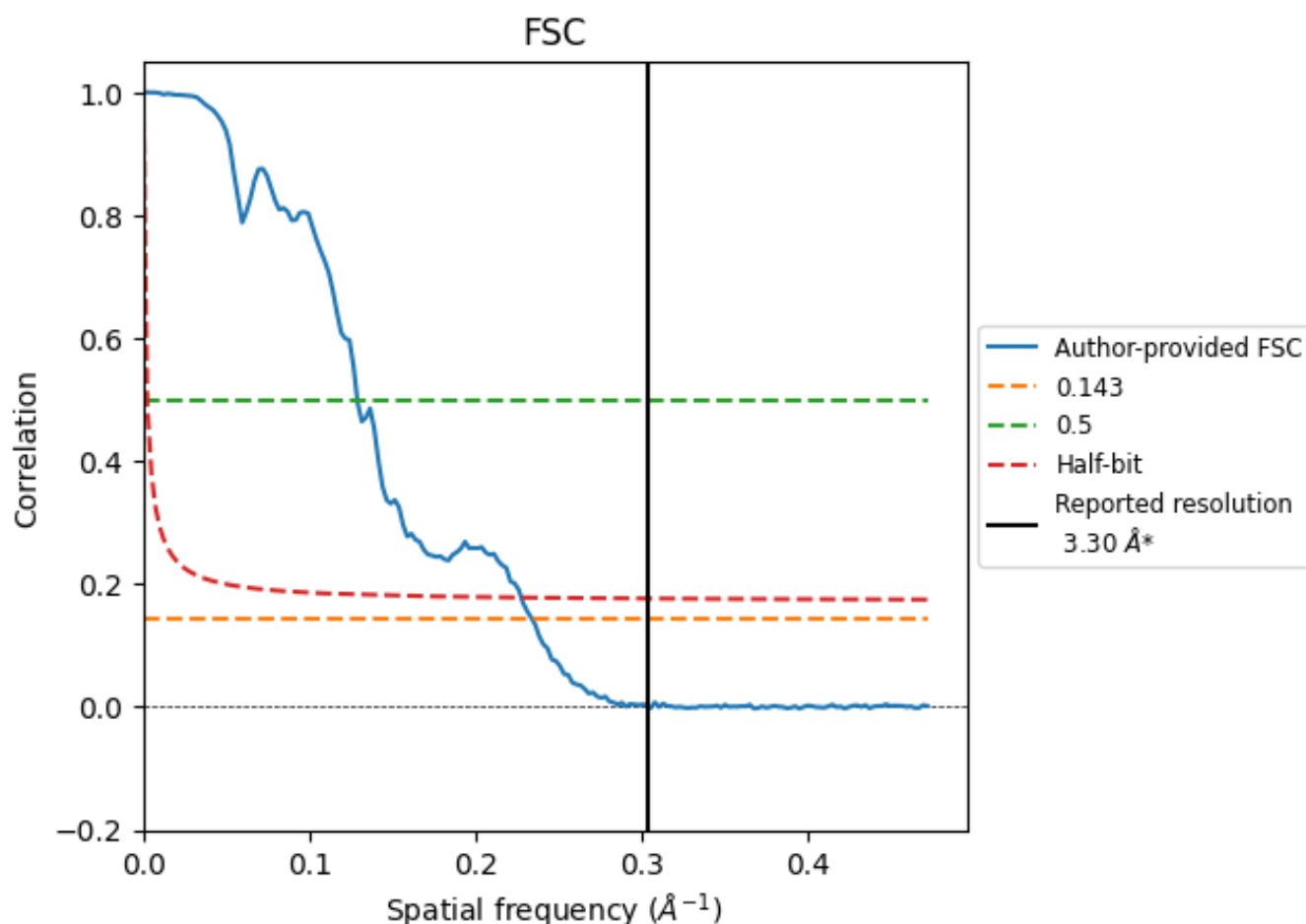


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 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	4.28	7.76	4.40
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.28 differs from the reported value 3.3 by more than 10 %

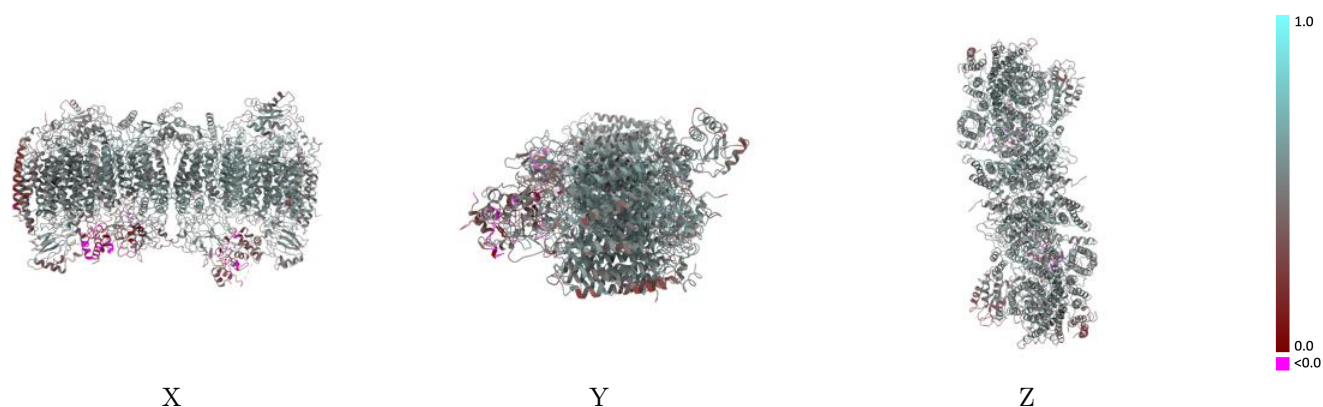
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0289 and PDB model 6HWH. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

This section was not generated.

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

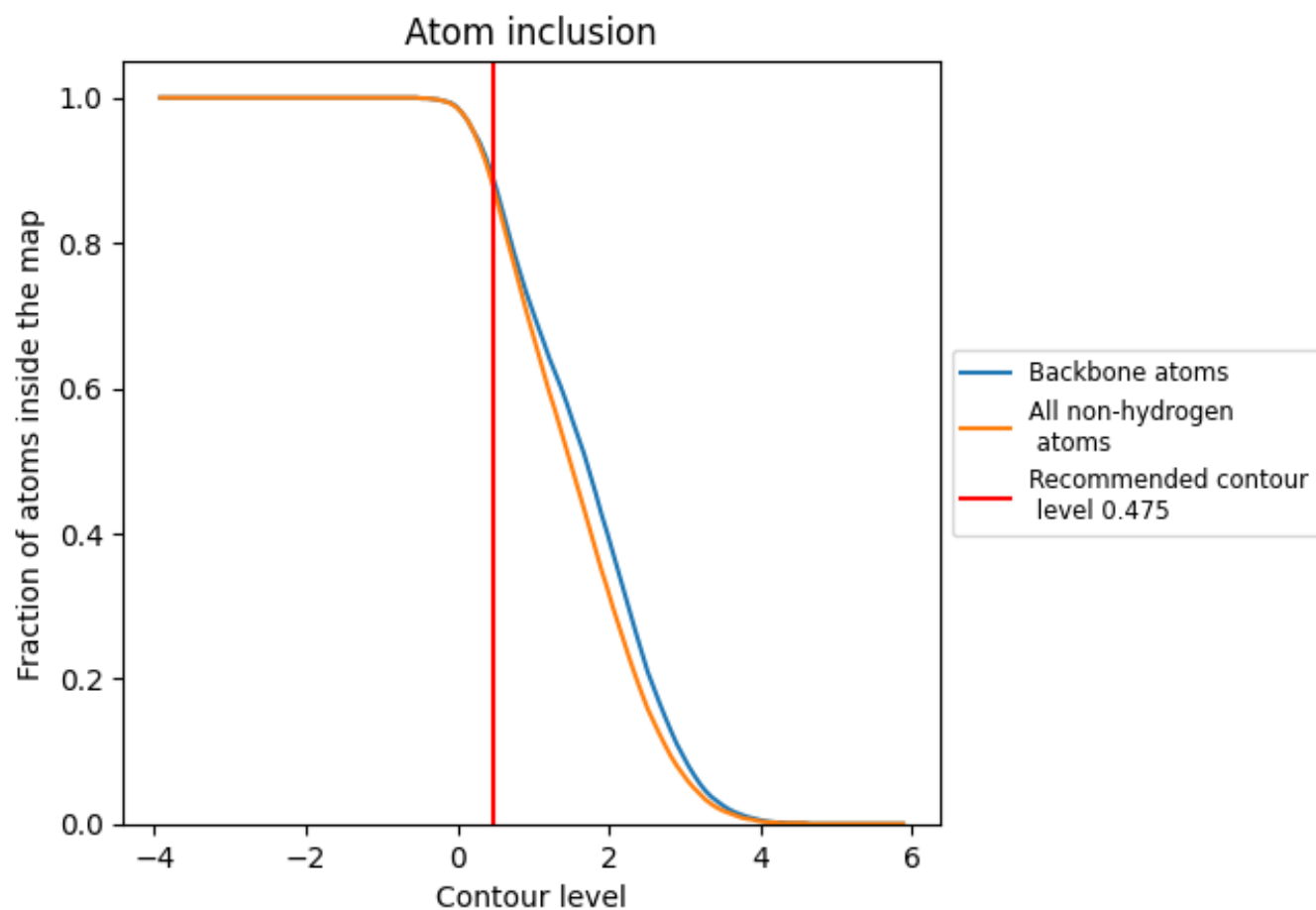


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.475) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.5000
A	 0.8140	 0.4750
B	 0.9000	 0.5080
C	 0.9680	 0.5510
D	 0.8090	 0.4240
E	 0.8500	 0.4370
F	 0.9890	 0.5580
G	 0.9080	 0.5140
H	 0.6190	 0.3030
I	 0.7400	 0.4140
J	 0.8460	 0.5110
K	 0.9220	 0.5650
L	 0.8880	 0.4920
M	 0.8790	 0.5450
N	 0.9120	 0.4960
O	 0.8870	 0.4840
P	 0.8400	 0.4560
Q	 0.9280	 0.5460
R	 0.8540	 0.4620
S	 0.9190	 0.5350
T	 0.8600	 0.4450
V	 0.9070	 0.5230
W	 0.8990	 0.5170
X	 0.8990	 0.5190
Y	 0.9240	 0.5450
Z	 0.8830	 0.5040
b	 0.9030	 0.5310
i	 0.2900	 0.1410
j	 0.6290	 0.1900

