



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:51 PM UTC

PDB ID : 4I8V / pdb_00004i8v
Title : Human Cytochrome P450 1A1 in complex with alpha-naphthoflavone
Authors : Walsh, A.A.; Scott, E.E.
Deposited on : 2012-12-04
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

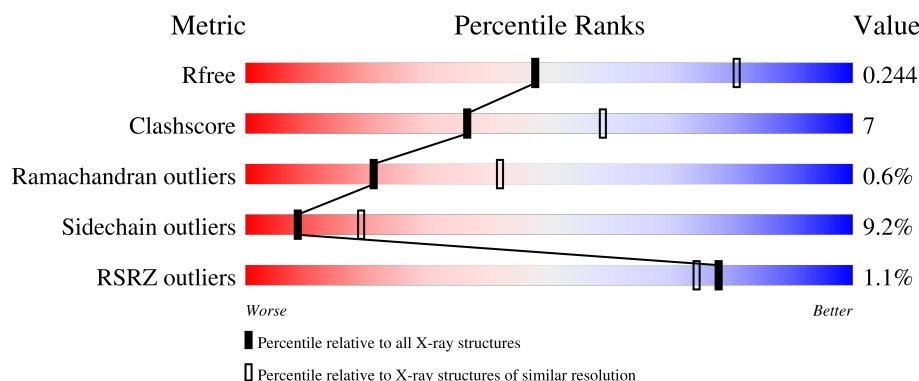
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

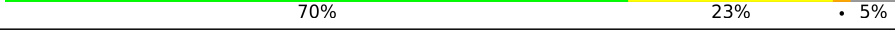
The reported resolution of this entry is 2.60 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	491	
1	B	491	
1	C	491	
1	D	491	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome P450 1A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3816	2442	664	689	21			
1	B	472	Total	C	N	O	S	0	0	0
			3776	2420	657	678	21			
1	C	468	Total	C	N	O	S	0	0	0
			3750	2404	652	673	21			
1	D	467	Total	C	N	O	S	0	0	0
			3741	2398	650	672	21			

There are 52 discrepancies between the modelled and reference sequences:

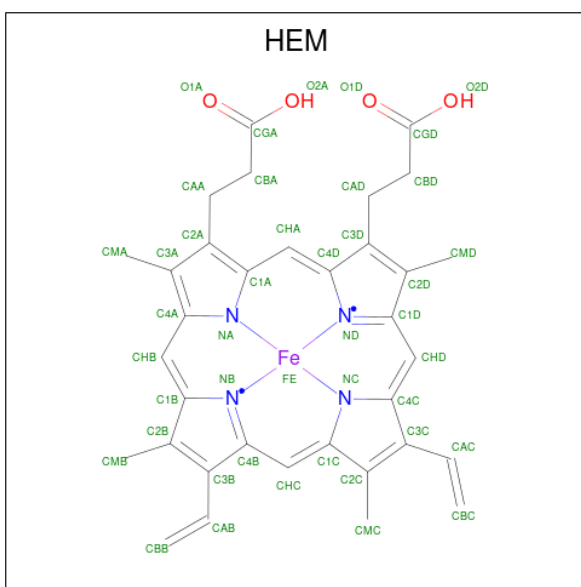
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP P04798
A	29	ALA	-	expression tag	UNP P04798
A	30	LYS	-	expression tag	UNP P04798
A	31	LYS	-	expression tag	UNP P04798
A	32	THR	-	expression tag	UNP P04798
A	33	SER	-	expression tag	UNP P04798
A	34	SER	-	expression tag	UNP P04798
A	513	HIS	-	expression tag	UNP P04798
A	514	HIS	-	expression tag	UNP P04798
A	515	HIS	-	expression tag	UNP P04798
A	516	HIS	-	expression tag	UNP P04798
A	517	HIS	-	expression tag	UNP P04798
A	518	HIS	-	expression tag	UNP P04798
B	28	MET	-	expression tag	UNP P04798
B	29	ALA	-	expression tag	UNP P04798
B	30	LYS	-	expression tag	UNP P04798
B	31	LYS	-	expression tag	UNP P04798
B	32	THR	-	expression tag	UNP P04798
B	33	SER	-	expression tag	UNP P04798
B	34	SER	-	expression tag	UNP P04798
B	513	HIS	-	expression tag	UNP P04798

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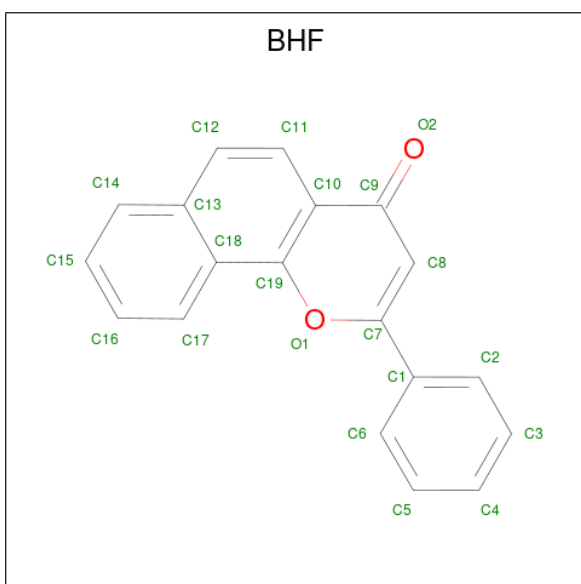
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	HIS	-	expression tag	UNP P04798
B	515	HIS	-	expression tag	UNP P04798
B	516	HIS	-	expression tag	UNP P04798
B	517	HIS	-	expression tag	UNP P04798
B	518	HIS	-	expression tag	UNP P04798
C	28	MET	-	expression tag	UNP P04798
C	29	ALA	-	expression tag	UNP P04798
C	30	LYS	-	expression tag	UNP P04798
C	31	LYS	-	expression tag	UNP P04798
C	32	THR	-	expression tag	UNP P04798
C	33	SER	-	expression tag	UNP P04798
C	34	SER	-	expression tag	UNP P04798
C	513	HIS	-	expression tag	UNP P04798
C	514	HIS	-	expression tag	UNP P04798
C	515	HIS	-	expression tag	UNP P04798
C	516	HIS	-	expression tag	UNP P04798
C	517	HIS	-	expression tag	UNP P04798
C	518	HIS	-	expression tag	UNP P04798
D	28	MET	-	expression tag	UNP P04798
D	29	ALA	-	expression tag	UNP P04798
D	30	LYS	-	expression tag	UNP P04798
D	31	LYS	-	expression tag	UNP P04798
D	32	THR	-	expression tag	UNP P04798
D	33	SER	-	expression tag	UNP P04798
D	34	SER	-	expression tag	UNP P04798
D	513	HIS	-	expression tag	UNP P04798
D	514	HIS	-	expression tag	UNP P04798
D	515	HIS	-	expression tag	UNP P04798
D	516	HIS	-	expression tag	UNP P04798
D	517	HIS	-	expression tag	UNP P04798
D	518	HIS	-	expression tag	UNP P04798

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



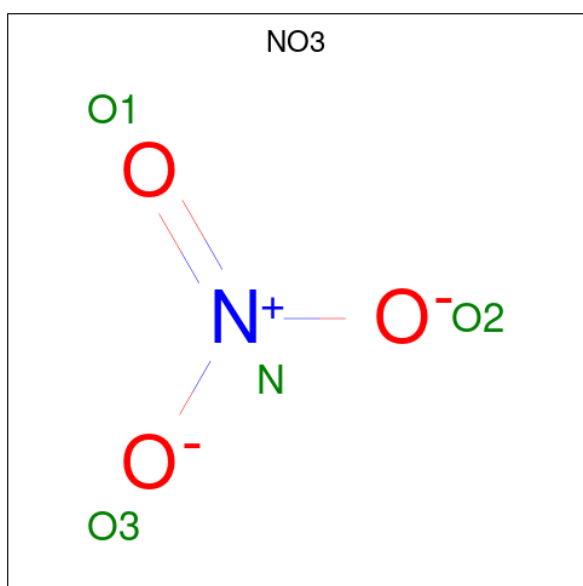
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 2-PHENYL-4H-BENZO[H]CHROMEN-4-ONE (CCD ID: BHF) (formula: $C_{19}H_{12}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	19	2		
3	B	1	Total	C	O	0	0
			21	19	2		
3	C	1	Total	C	O	0	0
			21	19	2		
3	D	1	Total	C	O	0	0
			21	19	2		

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	76	Total	O	0	0
			76	76		
5	C	10	Total	O	0	0
			10	10		

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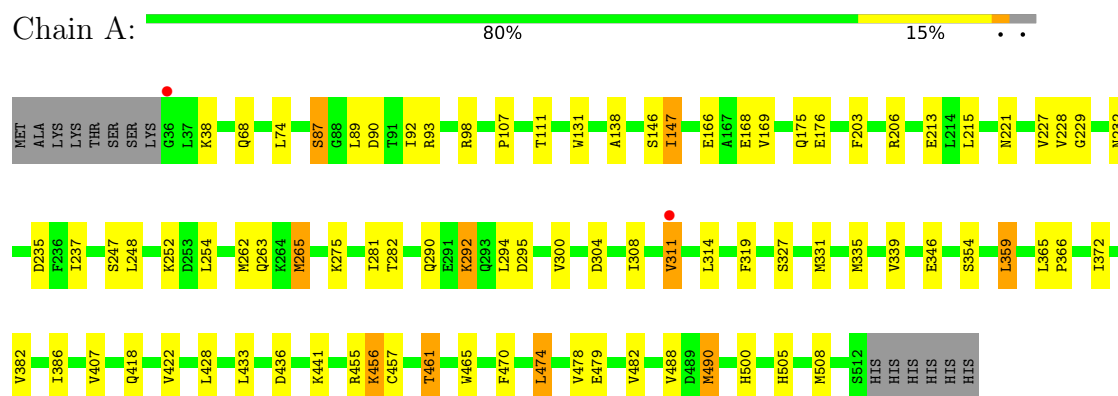
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	8	Total	O	0	0
			8	8		

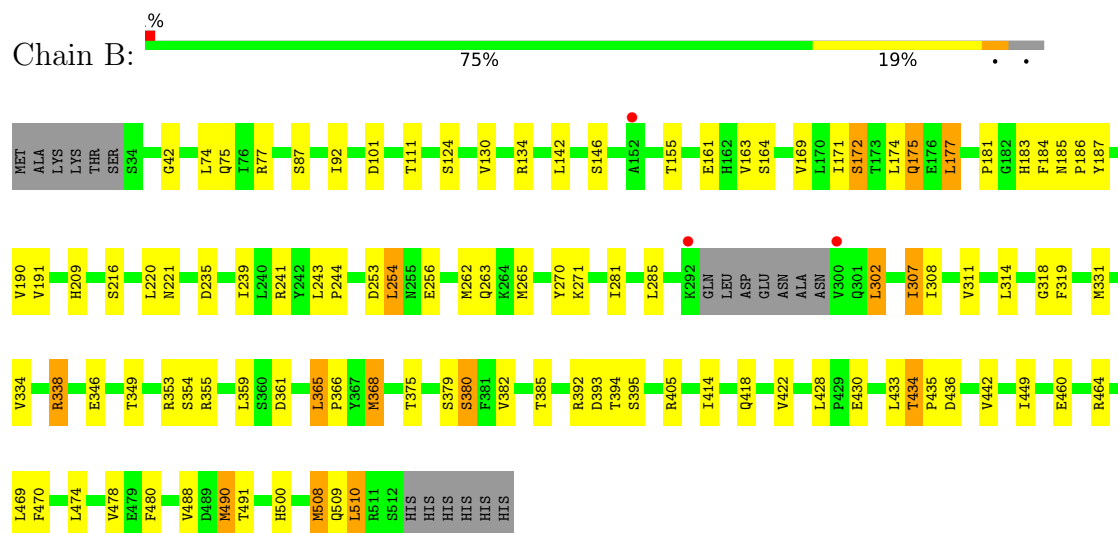
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

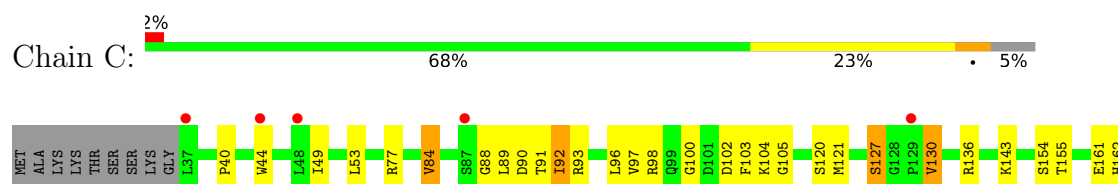
• Molecule 1: Cytochrome P450 1A1

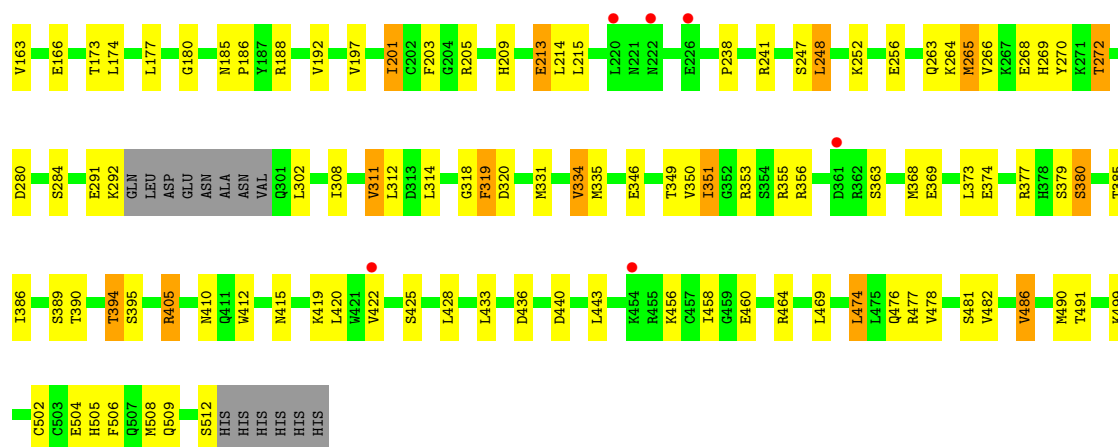


• Molecule 1: Cytochrome P450 1A1

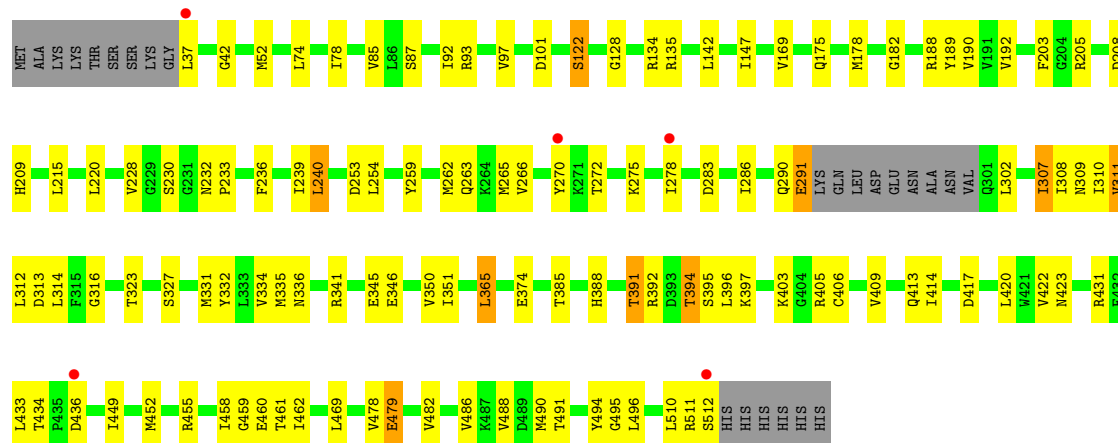


• Molecule 1: Cytochrome P450 1A1





• Molecule 1: Cytochrome P450 1A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.00Å 195.49Å 235.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.24 – 2.60 38.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.24-2.60) 99.9 (38.24-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7	Depositor
R, R_{free}	0.188 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	4687 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15532	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NO3, BHF

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	1.14	3/3911 (0.1%)	1.15	11/5300 (0.2%)
1	B	1.04	1/3870 (0.0%)	1.09	8/5241 (0.2%)
1	C	0.76	0/3844	0.99	9/5207 (0.2%)
1	D	0.80	0/3835	0.99	8/5196 (0.2%)
All	All	0.95	4/15460 (0.0%)	1.06	36/20944 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	42	GLY	C-O	-6.49	1.15	1.24
1	A	107	PRO	N-CA	-5.52	1.40	1.47
1	A	68	GLN	C-O	-5.49	1.17	1.24
1	A	407	VAL	C-O	-5.10	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ILE	N-CA-C	-7.15	101.10	108.96
1	A	229	GLY	N-CA-C	7.14	119.72	111.36
1	A	275	LYS	N-CA-C	6.76	119.51	111.33
1	C	386	ILE	N-CA-C	-6.51	101.80	108.96
1	D	350	VAL	N-CA-C	6.31	116.48	110.42
1	A	295	ASP	N-CA-C	-6.26	100.09	110.17
1	A	232	ASN	CA-C-N	6.18	126.36	119.32
1	A	232	ASN	C-N-CA	6.18	126.36	119.32
1	D	42	GLY	CA-C-N	6.03	126.00	120.21
1	D	42	GLY	C-N-CA	6.03	126.00	120.21
1	B	491	THR	CA-C-N	-6.01	113.78	119.85
1	B	491	THR	C-N-CA	-6.01	113.78	119.85
1	D	327	SER	N-CA-C	-5.99	104.38	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	GLY	CA-C-N	5.88	125.75	119.28
1	D	128	GLY	C-N-CA	5.88	125.75	119.28
1	C	385	THR	N-CA-C	-5.80	102.85	110.33
1	C	491	THR	CA-C-N	-5.75	114.34	120.03
1	C	491	THR	C-N-CA	-5.75	114.34	120.03
1	B	385	THR	N-CA-C	-5.71	102.97	110.33
1	B	124	SER	CA-C-N	5.62	125.71	119.87
1	B	124	SER	C-N-CA	5.62	125.71	119.87
1	B	368	MET	N-CA-C	-5.57	105.13	111.14
1	C	89	LEU	N-CA-C	5.56	117.14	111.14
1	D	169	VAL	CB-CA-C	-5.49	104.94	111.97
1	B	375	THR	N-CA-C	-5.36	104.86	111.40
1	C	40	PRO	CA-C-N	5.24	125.70	120.14
1	C	40	PRO	C-N-CA	5.24	125.70	120.14
1	A	237	ILE	CB-CA-C	-5.21	106.13	111.08
1	A	138	ALA	N-CA-C	-5.21	105.68	111.36
1	A	422	VAL	CA-C-N	-5.19	116.46	123.46
1	A	422	VAL	C-N-CA	-5.19	116.46	123.46
1	A	372	ILE	N-CA-C	-5.17	105.80	110.82
1	C	394	THR	N-CA-C	5.17	115.18	107.88
1	D	434	THR	N-CA-C	-5.05	102.83	110.50
1	B	169	VAL	CB-CA-C	-5.01	105.47	112.04
1	C	40	PRO	N-CA-C	5.01	115.94	110.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3816	0	3809	33	0
1	B	3776	0	3780	56	0
1	C	3750	0	3750	65	0
1	D	3741	0	3737	56	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	3	0
2	D	43	0	30	5	0
3	A	21	0	12	0	0
3	B	21	0	12	0	0
3	C	21	0	12	0	0
3	D	21	0	12	1	0
4	A	8	0	0	0	0
4	B	4	0	0	0	0
5	A	87	0	0	3	0
5	B	76	0	0	5	0
5	C	10	0	0	1	0
5	D	8	0	0	0	0
All	All	15532	0	15244	221	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 7.

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:O	1:B:181:PRO:HD2	1.71	0.89
1:A:308:ILE:O	1:A:311:VAL:HG22	1.79	0.83
2:A:601:HEM:HMB1	2:A:601:HEM:HBB2	1.67	0.76
1:C:105:GLY:HA2	1:C:127:SER:OG	1.87	0.75
1:D:346:GLU:HG2	1:D:365:LEU:HD12	1.70	0.74
1:D:92:ILE:HD12	1:D:414:ILE:HD11	1.70	0.72
1:C:331:MET:HB3	1:C:490:MET:HE1	1.70	0.72
1:D:302:LEU:HD12	1:D:302:LEU:O	1.90	0.72
1:C:460:GLU:O	1:C:464:ARG:HG3	1.91	0.71
2:D:600:HEM:HBB2	2:D:600:HEM:HMB2	1.72	0.71
1:B:361:ASP:O	1:B:365:LEU:HD22	1.92	0.69
1:C:205:ARG:NH2	1:C:268:GLU:OE1	2.25	0.69
1:D:52:MET:HE1	1:D:233:PRO:HB3	1.72	0.69
1:B:480:PHE:CE2	1:B:508:MET:HE3	2.27	0.68
1:B:474:LEU:O	1:B:478:VAL:HG22	1.94	0.68
1:A:308:ILE:O	1:A:311:VAL:CG2	2.43	0.67
2:A:601:HEM:HBC2	2:A:601:HEM:HMC2	1.76	0.66
1:C:203:PHE:CD1	1:C:265:MET:HG2	2.33	0.64
1:C:320:ASP:OD2	1:C:499:LYS:NZ	2.31	0.64
1:D:93:ARG:O	1:D:97:VAL:HG22	1.99	0.61
1:D:302:LEU:HD13	1:D:307:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:THR:O	1:C:177:LEU:HD12	2.01	0.60
1:C:331:MET:HB3	1:C:490:MET:CE	2.32	0.59
1:B:338:ARG:NH2	1:B:430:GLU:OE2	2.35	0.59
1:B:478:VAL:HG21	1:B:508:MET:HE2	1.84	0.59
1:D:351:ILE:HD11	1:D:365:LEU:HD21	1.84	0.58
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.85	0.58
1:C:477:ARG:HB3	1:C:478:VAL:HG13	1.85	0.58
1:B:142:LEU:O	1:B:146:SER:CB	2.52	0.58
1:C:374:GLU:OE1	1:C:374:GLU:HA	2.02	0.58
1:B:174:LEU:HD22	1:B:184:PHE:CE1	2.38	0.58
1:B:92:ILE:HD12	1:B:414:ILE:HD11	1.86	0.57
1:B:331:MET:HE3	1:B:490:MET:CE	2.34	0.57
1:A:474:LEU:O	1:A:478:VAL:HG22	2.04	0.57
2:C:600:HEM:HBB2	2:C:600:HEM:HMB2	1.86	0.57
1:C:374:GLU:OE2	1:C:377:ARG:NH2	2.37	0.57
2:D:600:HEM:HBB2	2:D:600:HEM:CMB	2.34	0.56
1:A:461:THR:HG23	5:A:771:HOH:O	2.06	0.56
1:B:430:GLU:N	1:B:430:GLU:OE1	2.38	0.56
1:D:335:MET:HG3	1:D:490:MET:HE2	1.88	0.56
1:A:455:ARG:NH2	5:A:703:HOH:O	2.21	0.55
1:B:349:THR:HG22	1:B:349:THR:O	2.03	0.55
1:D:332:TYR:O	1:D:336:ASN:HB2	2.05	0.55
1:D:422:VAL:O	1:D:431:ARG:NH2	2.40	0.55
1:A:90:ASP:OD1	1:A:98:ARG:NH2	2.40	0.55
1:D:479:GLU:HG2	1:D:511:ARG:HG2	1.89	0.55
1:B:392:ARG:O	1:B:393:ASP:C	2.48	0.55
1:D:374:GLU:HA	1:D:374:GLU:OE1	2.07	0.55
1:B:285:LEU:CD1	1:B:311:VAL:CG1	2.86	0.54
1:A:74:LEU:C	1:A:74:LEU:HD12	2.32	0.54
1:A:335:MET:HE3	1:A:488:VAL:HG11	1.90	0.53
1:C:84:VAL:HG23	1:C:405:ARG:HG2	1.89	0.53
1:A:455:ARG:O	2:A:601:HEM:HBA2	2.08	0.53
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.38	0.53
1:C:350:VAL:HG12	1:C:351:ILE:HD12	1.90	0.53
1:B:285:LEU:HD12	1:B:311:VAL:CG1	2.38	0.53
1:B:394:THR:OG1	1:B:395:SER:N	2.41	0.53
1:C:84:VAL:HG23	1:C:405:ARG:CG	2.39	0.53
1:C:103:PHE:CD1	1:C:390:THR:HG22	2.44	0.53
2:D:600:HEM:CMC	2:D:600:HEM:HBC2	2.39	0.53
1:C:379:SER:O	1:C:380:SER:C	2.51	0.52
2:D:600:HEM:HBC2	2:D:600:HEM:HMC2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ASP:C	1:C:440:ASP:OD1	2.53	0.52
1:D:239:ILE:CG2	1:D:240:LEU:N	2.73	0.52
1:C:509:GLN:OE1	1:C:509:GLN:HA	2.09	0.52
1:C:269:HIS:NE2	1:C:280:ASP:OD2	2.42	0.51
1:A:111:THR:HG23	1:A:235:ASP:OD1	2.11	0.51
1:B:142:LEU:O	1:B:146:SER:HB2	2.11	0.51
1:B:382:VAL:HG11	2:B:601:HEM:HMA2	1.93	0.51
1:D:278:ILE:HG23	1:D:283:ASP:HB3	1.92	0.51
1:C:335:MET:HE2	1:C:335:MET:HA	1.94	0.50
1:B:134:ARG:NH1	5:B:729:HOH:O	2.36	0.50
1:D:308:ILE:O	1:D:311:VAL:HG22	2.11	0.50
1:C:486:VAL:HG11	1:C:505:HIS:CG	2.46	0.50
1:D:175:GLN:HE21	1:D:510:LEU:HD11	1.75	0.50
1:D:142:LEU:HD22	1:D:462:ILE:CD1	2.41	0.50
1:B:490:MET:HE2	1:B:490:MET:HA	1.93	0.49
1:A:327:SER:OG	1:A:500:HIS:NE2	2.42	0.49
1:A:93:ARG:HD3	5:A:781:HOH:O	2.12	0.49
1:B:142:LEU:O	1:B:146:SER:HB3	2.12	0.49
1:B:346:GLU:OE2	1:B:366:PRO:HD2	2.13	0.49
1:A:131:TRP:CZ2	1:A:455:ARG:HD3	2.47	0.49
1:B:509:GLN:HA	1:B:509:GLN:OE1	2.12	0.49
1:C:490:MET:HE3	1:C:490:MET:HA	1.93	0.49
1:D:335:MET:HA	1:D:335:MET:HE2	1.94	0.49
1:D:101:ASP:O	1:D:391:THR:OG1	2.29	0.49
1:D:266:VAL:HG21	1:D:308:ILE:HG21	1.94	0.49
1:C:308:ILE:O	1:C:311:VAL:HG22	2.13	0.49
1:D:396:LEU:O	1:D:397:LYS:C	2.56	0.49
1:C:197:VAL:O	1:C:201:ILE:HD12	2.13	0.48
1:C:120:SER:O	1:C:121:MET:C	2.56	0.48
1:D:511:ARG:O	1:D:512:SER:C	2.57	0.48
1:A:203:PHE:CD1	1:A:265:MET:HG2	2.48	0.48
1:C:163:VAL:HG11	1:C:469:LEU:HB3	1.96	0.48
1:D:331:MET:HE3	1:D:490:MET:SD	2.53	0.48
1:C:49:ILE:CD1	1:C:53:LEU:HD13	2.43	0.48
2:C:600:HEM:HBC2	2:C:600:HEM:HMC2	1.96	0.48
1:B:187:TYR:O	1:B:191:VAL:HG12	2.14	0.48
1:D:392:ARG:HA	1:D:403:LYS:HD2	1.95	0.47
1:C:346:GLU:O	1:C:349:THR:HG22	2.14	0.47
1:A:331:MET:HB3	1:A:490:MET:HE1	1.96	0.47
1:B:221:ASN:N	5:B:750:HOH:O	2.28	0.47
1:A:359:LEU:HD11	1:A:465:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:MET:HE3	1:B:308:ILE:HG22	1.97	0.47
1:C:93:ARG:O	1:C:97:VAL:HG22	2.15	0.47
1:D:93:ARG:O	1:D:97:VAL:CG2	2.63	0.47
1:D:388:HIS:HE1	1:D:455:ARG:HB2	1.80	0.47
1:C:188:ARG:CZ	1:C:215:LEU:HD21	2.44	0.47
1:C:103:PHE:CE1	1:C:390:THR:HG22	2.50	0.47
1:D:190:VAL:HG12	1:D:323:THR:HG23	1.97	0.47
1:C:270:TYR:C	1:C:272:THR:H	2.23	0.47
1:D:309:ASN:OD1	1:D:309:ASN:C	2.59	0.47
1:B:302:LEU:HD22	1:B:307:ILE:HG13	1.96	0.46
1:A:456:LYS:O	1:A:457:CYS:C	2.58	0.46
1:B:331:MET:HE3	1:B:490:MET:HE2	1.95	0.46
1:D:308:ILE:C	1:D:310:ILE:H	2.23	0.46
1:B:355:ARG:NH1	1:D:436:ASP:CG	2.74	0.46
1:D:417:ASP:CB	1:D:420:LEU:HD12	2.46	0.46
1:D:74:LEU:C	1:D:74:LEU:HD12	2.40	0.46
1:B:478:VAL:CB	1:B:508:MET:HE2	2.45	0.46
1:B:478:VAL:CG2	1:B:508:MET:HE2	2.45	0.46
1:C:319:PHE:CD1	1:C:319:PHE:C	2.93	0.46
1:C:419:LYS:HE2	1:C:420:LEU:HD12	1.98	0.46
1:D:134:ARG:O	1:D:135:ARG:C	2.59	0.46
1:B:285:LEU:CD1	1:B:311:VAL:HG13	2.46	0.45
1:B:111:THR:HG23	1:B:235:ASP:OD1	2.16	0.45
1:A:87:SER:HA	1:A:92:ILE:HD11	1.98	0.45
1:C:394:THR:OG1	1:C:395:SER:N	2.49	0.45
1:A:265:MET:HE2	1:A:265:MET:HA	1.99	0.45
1:B:216:SER:O	1:B:220:LEU:HB3	2.15	0.45
1:C:335:MET:HG3	1:C:490:MET:SD	2.57	0.45
1:C:263:GLN:O	1:C:264:LYS:C	2.60	0.45
1:D:290:GLN:O	1:D:291:GLU:OE2	2.34	0.45
1:A:248:LEU:O	1:A:252:LYS:HG3	2.17	0.45
1:A:346:GLU:OE2	1:A:366:PRO:HD2	2.17	0.45
1:A:456:LYS:HB3	1:A:456:LYS:HE2	1.49	0.45
1:A:479:GLU:O	1:A:508:MET:HA	2.17	0.45
1:C:248:LEU:O	1:C:252:LYS:HG3	2.17	0.44
1:D:205:ARG:CZ	1:D:265:MET:HE1	2.46	0.44
1:A:168:GLU:O	1:A:169:VAL:C	2.60	0.44
1:B:460:GLU:OE1	1:B:464:ARG:NH1	2.50	0.44
1:C:96:LEU:O	1:C:100:GLY:HA2	2.17	0.44
1:C:88:GLY:O	1:C:92:ILE:HB	2.16	0.44
1:B:349:THR:O	1:B:349:THR:CG2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:SER:O	1:D:494:TYR:OH	2.30	0.44
1:D:259:TYR:CZ	1:D:262:MET:HE1	2.53	0.44
1:A:262:MET:CE	1:A:263:GLN:HG3	2.48	0.44
1:A:292:LYS:HE2	1:A:304:ASP:OD1	2.17	0.44
1:B:74:LEU:HD12	1:B:74:LEU:C	2.43	0.44
1:B:75:GLN:HG2	5:B:712:HOH:O	2.18	0.44
1:B:353:ARG:O	1:B:355:ARG:N	2.50	0.44
2:A:601:HEM:HBB2	2:A:601:HEM:CMB	2.40	0.44
1:B:478:VAL:HG21	1:B:508:MET:CE	2.47	0.44
1:A:175:GLN:O	1:A:176:GLU:C	2.59	0.43
1:D:331:MET:HE1	1:D:488:VAL:HG13	1.99	0.43
1:B:175:GLN:OE1	1:B:510:LEU:HD23	2.19	0.43
1:D:178:MET:O	1:D:182:GLY:HA2	2.18	0.43
1:D:495:GLY:O	1:D:496:LEU:C	2.57	0.43
1:C:104:LYS:O	1:C:127:SER:OG	2.35	0.43
1:C:380:SER:HB2	1:C:412:TRP:CD1	2.54	0.43
1:C:102:ASP:O	1:C:390:THR:HA	2.19	0.43
1:D:394:THR:OG1	1:D:395:SER:N	2.52	0.43
1:B:186:PRO:O	1:B:190:VAL:HG23	2.18	0.43
1:A:470:PHE:O	1:A:474:LEU:HB2	2.19	0.43
1:B:318:GLY:HA2	2:B:601:HEM:HMC2	2.01	0.43
1:C:213:GLU:CG	1:C:214:LEU:N	2.81	0.43
1:D:240:LEU:HD13	1:D:240:LEU:HA	1.89	0.43
1:D:459:GLY:O	1:D:460:GLU:C	2.62	0.43
1:A:382:VAL:HG11	2:A:601:HEM:HMA2	2.00	0.43
1:B:338:ARG:HB3	5:B:745:HOH:O	2.18	0.43
1:C:186:PRO:HG2	1:C:506:PHE:CD2	2.54	0.43
1:B:77:ARG:NE	5:B:701:HOH:O	2.25	0.43
1:C:192:VAL:HG11	1:C:209:HIS:HA	2.02	0.42
1:D:422:VAL:O	1:D:423:ASN:HB2	2.19	0.42
1:B:243:LEU:HB3	1:B:244:PRO:HD2	2.01	0.42
1:B:488:VAL:O	1:B:488:VAL:HG23	2.18	0.42
1:C:410:ASN:OD1	1:C:410:ASN:C	2.62	0.42
1:D:122:SER:OG	1:D:313:ASP:OD1	2.23	0.42
1:A:166:GLU:OE2	1:A:206:ARG:NE	2.42	0.42
1:C:353:ARG:NH1	1:C:512:SER:O	2.52	0.42
1:C:508:MET:HA	5:C:708:HOH:O	2.20	0.42
1:A:482:VAL:HG23	1:A:505:HIS:O	2.18	0.42
1:C:84:VAL:CG2	1:C:405:ARG:HG2	2.50	0.42
1:C:460:GLU:OE1	1:C:464:ARG:NH1	2.52	0.42
1:D:78:ILE:HG22	1:D:236:PHE:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:GLN:C	1:D:413:GLN:OE1	2.63	0.42
1:C:97:VAL:HG23	1:C:98:ARG:N	2.34	0.42
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.48	0.42
1:B:379:SER:O	1:B:380:SER:C	2.63	0.42
1:B:270:TYR:O	1:B:271:LYS:C	2.63	0.42
1:C:130:VAL:HG12	1:C:302:LEU:CD1	2.50	0.42
1:C:162:HIS:O	1:C:166:GLU:HG2	2.20	0.42
1:C:186:PRO:CG	1:C:506:PHE:CD2	3.03	0.42
1:C:312:LEU:HD12	1:C:312:LEU:HA	1.93	0.42
1:D:203:PHE:HB3	1:D:265:MET:HE2	2.01	0.41
1:C:334:VAL:HG21	1:C:506:PHE:CE1	2.55	0.41
1:A:146:SER:OG	1:A:147:ILE:N	2.54	0.41
1:B:163:VAL:HG11	1:B:469:LEU:HB3	2.01	0.41
1:B:171:ILE:O	1:B:172:SER:C	2.63	0.41
1:C:185:ASN:C	1:C:185:ASN:OD1	2.62	0.41
1:D:188:ARG:HG2	1:D:189:TYR:CZ	2.55	0.41
1:D:331:MET:HE1	1:D:488:VAL:CG1	2.51	0.41
1:B:253:ASP:O	1:B:254:LEU:C	2.62	0.41
1:D:455:ARG:NH1	2:D:600:HEM:O2D	2.54	0.41
1:C:238:PRO:HA	1:C:241:ARG:NH1	2.36	0.41
1:C:350:VAL:HG12	1:C:351:ILE:CD1	2.51	0.41
1:B:331:MET:HB3	1:B:490:MET:HE1	2.03	0.41
1:B:469:LEU:O	1:B:470:PHE:C	2.62	0.41
1:C:318:GLY:HA2	2:C:600:HEM:HMC2	2.03	0.41
1:C:355:ARG:HG2	1:C:356:ARG:O	2.21	0.41
1:D:192:VAL:HB	1:D:209:HIS:CD2	2.56	0.41
1:A:281:ILE:O	1:A:282:THR:C	2.63	0.40
1:C:369:GLU:O	1:C:373:LEU:HG	2.21	0.40
1:D:232:ASN:HA	1:D:233:PRO:HD3	1.92	0.40
1:B:434:THR:HG23	1:B:435:PRO:HD2	2.02	0.40
1:C:474:LEU:O	1:C:478:VAL:HG22	2.21	0.40
1:D:178:MET:HA	1:D:182:GLY:HA2	2.03	0.40
1:B:331:MET:HE2	1:B:500:HIS:ND1	2.37	0.40
1:C:377:ARG:HD3	1:C:415:ASN:O	2.21	0.40
1:D:312:LEU:HD23	3:D:601:BHF:H15	2.02	0.40
1:D:385:THR:OG1	1:D:409:VAL:HB	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	475/491 (97%)	453 (95%)	22 (5%)	0	100	100
1	B	468/491 (95%)	447 (96%)	16 (3%)	5 (1%)	11	25
1	C	464/491 (94%)	426 (92%)	34 (7%)	4 (1%)	14	30
1	D	463/491 (94%)	426 (92%)	35 (8%)	2 (0%)	30	51
All	All	1870/1964 (95%)	1752 (94%)	107 (6%)	11 (1%)	21	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	SER
1	B	209	HIS
1	C	180	GLY
1	C	291	GLU
1	D	275	LYS
1	C	363	SER
1	C	380	SER
1	B	380	SER
1	D	316	GLY
1	B	449	ILE
1	B	422	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	426/439 (97%)	394 (92%)	32 (8%)	12	28
1	B	422/439 (96%)	385 (91%)	37 (9%)	9	21
1	C	419/439 (95%)	372 (89%)	47 (11%)	6	12
1	D	418/439 (95%)	379 (91%)	39 (9%)	8	18
All	All	1685/1756 (96%)	1530 (91%)	155 (9%)	8	19

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	87	SER
1	A	89	LEU
1	A	147	ILE
1	A	213	GLU
1	A	215	LEU
1	A	221	ASN
1	A	227	VAL
1	A	228	VAL
1	A	247	SER
1	A	254	LEU
1	A	265	MET
1	A	290	GLN
1	A	292	LYS
1	A	294	LEU
1	A	300	VAL
1	A	311	VAL
1	A	314	LEU
1	A	319	PHE
1	A	339	VAL
1	A	354	SER
1	A	359	LEU
1	A	365	LEU
1	A	418	GLN
1	A	428	LEU
1	A	433	LEU
1	A	436	ASP
1	A	441	LYS
1	A	456	LYS
1	A	461	THR
1	A	474	LEU
1	A	490	MET
1	B	87	SER

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Mol	Chain	Res	Type
1	B	101	ASP
1	B	130	VAL
1	B	155	THR
1	B	161	GLU
1	B	164	SER
1	B	172	SER
1	B	175	GLN
1	B	177	LEU
1	B	183	HIS
1	B	185	ASN
1	B	239	ILE
1	B	241	ARG
1	B	254	LEU
1	B	256	GLU
1	B	263	GLN
1	B	265	MET
1	B	281	ILE
1	B	302	LEU
1	B	307	ILE
1	B	314	LEU
1	B	319	PHE
1	B	334	VAL
1	B	338	ARG
1	B	359	LEU
1	B	365	LEU
1	B	368	MET
1	B	405	ARG
1	B	418	GLN
1	B	428	LEU
1	B	433	LEU
1	B	434	THR
1	B	436	ASP
1	B	442	VAL
1	B	490	MET
1	B	508	MET
1	B	510	LEU
1	C	44	TRP
1	C	77	ARG
1	C	84	VAL
1	C	90	ASP
1	C	91	THR
1	C	92	ILE

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Mol	Chain	Res	Type
1	C	127	SER
1	C	130	VAL
1	C	136	ARG
1	C	143	LYS
1	C	154	SER
1	C	155	THR
1	C	161	GLU
1	C	174	LEU
1	C	201	ILE
1	C	213	GLU
1	C	247	SER
1	C	248	LEU
1	C	256	GLU
1	C	265	MET
1	C	266	VAL
1	C	272	THR
1	C	284	SER
1	C	292	LYS
1	C	311	VAL
1	C	314	LEU
1	C	319	PHE
1	C	334	VAL
1	C	351	ILE
1	C	368	MET
1	C	389	SER
1	C	405	ARG
1	C	422	VAL
1	C	425	SER
1	C	428	LEU
1	C	433	LEU
1	C	436	ASP
1	C	443	LEU
1	C	456	LYS
1	C	458	ILE
1	C	474	LEU
1	C	476	GLN
1	C	481	SER
1	C	482	VAL
1	C	486	VAL
1	C	502	CYS
1	C	504	GLU
1	D	37	LEU

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Mol	Chain	Res	Type
1	D	85	VAL
1	D	87	SER
1	D	122	SER
1	D	147	ILE
1	D	208	ASP
1	D	215	LEU
1	D	220	LEU
1	D	228	VAL
1	D	240	LEU
1	D	253	ASP
1	D	254	LEU
1	D	263	GLN
1	D	270	TYR
1	D	272	THR
1	D	286	ILE
1	D	291	GLU
1	D	307	ILE
1	D	311	VAL
1	D	314	LEU
1	D	334	VAL
1	D	341	ARG
1	D	345	GLU
1	D	365	LEU
1	D	391	THR
1	D	394	THR
1	D	405	ARG
1	D	406	CYS
1	D	433	LEU
1	D	449	ILE
1	D	452	MET
1	D	458	ILE
1	D	461	THR
1	D	469	LEU
1	D	478	VAL
1	D	479	GLU
1	D	482	VAL
1	D	486	VAL
1	D	491	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	B	139	GLN
1	B	210	ASN
1	B	211	HIS
1	B	277	HIS
1	B	288	HIS
1	C	69	GLN
1	C	209	HIS
1	C	245	ASN
1	C	344	GLN
1	D	249	ASN
1	D	288	HIS
1	D	507	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BHF	C	601	-	24,24,24	1.64	3 (12%)	34,34,34	1.28	5 (14%)
4	NO3	B	603	-	1,3,3	0.90	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BHF	B	602	-	24,24,24	1.66	4 (16%)	34,34,34	2.00	11 (32%)
3	BHF	A	602	-	24,24,24	1.51	4 (16%)	34,34,34	2.22	14 (41%)
2	HEM	D	600	1	50,50,50	1.97	16 (32%)	67,82,82	1.57	10 (14%)
2	HEM	A	601	1	50,50,50	1.71	12 (24%)	67,82,82	1.80	19 (28%)
3	BHF	D	601	-	24,24,24	1.61	2 (8%)	34,34,34	1.66	6 (17%)
4	NO3	A	604	-	1,3,3	1.15	0	0,3,3	-	-
2	HEM	C	600	1	50,50,50	1.68	13 (26%)	67,82,82	2.02	11 (16%)
4	NO3	A	603	-	1,3,3	0.17	0	0,3,3	-	-
2	HEM	B	601	1	50,50,50	1.77	13 (26%)	67,82,82	1.71	15 (22%)

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
3	BHF	C	601	-	-	0/4/4/4	0/4/4/4
3	BHF	B	602	-	-	0/4/4/4	0/4/4/4
3	BHF	A	602	-	-	0/4/4/4	0/4/4/4
2	HEM	D	600	1	-	2/14/54/54	-
2	HEM	A	601	1	-	2/14/54/54	-
3	BHF	D	601	-	-	0/4/4/4	0/4/4/4
2	HEM	C	600	1	-	3/14/54/54	-
2	HEM	B	601	1	-	2/14/54/54	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	BHF	C10-C19	4.98	1.49	1.39
2	C	600	HEM	FE-NC	4.89	2.11	1.95
2	A	601	HEM	C4B-NB	-4.88	1.29	1.38
3	C	601	BHF	C10-C19	4.87	1.49	1.39
2	D	600	HEM	C1B-NB	-4.70	1.32	1.40
2	B	601	HEM	C1B-NB	-4.67	1.32	1.40
3	D	601	BHF	C10-C19	4.45	1.48	1.39
2	A	601	HEM	C1B-NB	-4.09	1.33	1.40
2	A	601	HEM	FE-NC	4.00	2.08	1.95
2	D	600	HEM	FE-NB	3.90	2.06	1.94
2	C	600	HEM	C1B-NB	-3.88	1.33	1.40
2	B	601	HEM	FE-NC	3.81	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	HEM	FE-NB	3.80	2.06	1.94
3	A	602	BHF	C10-C19	3.69	1.47	1.39
2	D	600	HEM	C4B-NB	-3.63	1.31	1.38
2	D	600	HEM	C1D-ND	-3.61	1.31	1.38
2	B	601	HEM	C4B-NB	-3.58	1.31	1.38
2	B	601	HEM	C1C-C2C	-3.55	1.38	1.45
2	D	600	HEM	C1C-C2C	-3.53	1.38	1.45
2	A	601	HEM	C4D-ND	-3.42	1.34	1.40
2	D	600	HEM	C4C-NC	-3.39	1.33	1.39
2	D	600	HEM	C4D-ND	-3.38	1.34	1.40
3	D	601	BHF	C18-C13	3.38	1.49	1.43
2	D	600	HEM	C4A-NA	-3.30	1.33	1.39
2	D	600	HEM	C3C-C4C	-3.21	1.40	1.46
2	C	600	HEM	FE-ND	-3.06	1.85	1.94
2	D	600	HEM	FE-NC	3.05	2.05	1.95
3	A	602	BHF	C8-C7	3.00	1.45	1.37
3	C	601	BHF	C18-C13	2.97	1.48	1.43
3	B	602	BHF	O1-C19	-2.96	1.34	1.38
2	C	600	HEM	C4D-ND	-2.92	1.35	1.40
2	B	601	HEM	FE-NB	2.92	2.03	1.94
2	A	601	HEM	C4A-NA	-2.90	1.34	1.39
2	D	600	HEM	C1C-NC	-2.82	1.34	1.39
2	B	601	HEM	C4D-ND	-2.74	1.35	1.40
2	C	600	HEM	C4C-NC	-2.68	1.34	1.39
2	C	600	HEM	CHD-C4C	-2.65	1.33	1.38
3	B	602	BHF	C8-C7	2.63	1.44	1.37
2	A	601	HEM	C1C-NC	-2.57	1.34	1.39
2	A	601	HEM	FE-NB	2.56	2.02	1.94
2	B	601	HEM	C1C-NC	-2.53	1.34	1.39
2	D	600	HEM	FE-ND	-2.53	1.87	1.94
2	A	601	HEM	C1C-C2C	-2.52	1.40	1.45
2	B	601	HEM	C4A-NA	-2.47	1.35	1.39
2	C	600	HEM	C1D-ND	-2.45	1.34	1.38
2	B	601	HEM	C2A-C3A	-2.43	1.32	1.38
2	A	601	HEM	O1D-CGD	2.38	1.29	1.22
3	A	602	BHF	C12-C11	2.37	1.41	1.36
2	C	600	HEM	C3C-C4C	-2.33	1.42	1.46
2	D	600	HEM	C3B-C4B	2.32	1.49	1.44
3	B	602	BHF	C12-C11	2.29	1.41	1.36
2	D	600	HEM	CHD-C4C	-2.27	1.33	1.38
2	C	600	HEM	C3B-C4B	2.26	1.49	1.44
2	C	600	HEM	C4D-C3D	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C4C-NC	-2.25	1.35	1.39
3	A	602	BHF	C18-C13	2.25	1.47	1.43
2	C	600	HEM	C1C-C2C	-2.23	1.40	1.45
2	D	600	HEM	C3D-C2D	-2.13	1.32	1.36
2	A	601	HEM	CHB-C4A	-2.10	1.34	1.39
2	B	601	HEM	O1D-CGD	2.09	1.28	1.22
2	A	601	HEM	C4C-NC	-2.08	1.35	1.39
2	B	601	HEM	FE-ND	-2.08	1.88	1.94
2	D	600	HEM	C1A-C2A	-2.06	1.40	1.44
2	C	600	HEM	C4B-NB	-2.06	1.34	1.38
2	A	601	HEM	C3C-C4C	-2.03	1.42	1.46
2	B	601	HEM	C1A-NA	-2.02	1.35	1.39
3	C	601	BHF	C8-C7	2.01	1.42	1.37

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	HEM	CHD-C1D-ND	8.08	133.11	124.42
2	C	600	HEM	CHC-C4B-NB	6.37	131.28	124.42
2	C	600	HEM	CHD-C1D-C2D	-6.00	115.56	125.03
3	A	602	BHF	C17-C18-C13	5.61	125.17	117.92
3	B	602	BHF	C17-C18-C13	5.16	124.59	117.92
2	A	601	HEM	CHC-C4B-NB	4.90	129.69	124.42
2	A	601	HEM	C1B-NB-C4B	4.88	110.98	105.21
2	B	601	HEM	CHC-C4B-NB	4.82	129.61	124.42
2	D	600	HEM	CHD-C1D-ND	4.81	129.60	124.42
3	D	601	BHF	C19-C10-C9	-4.77	115.57	119.55
2	C	600	HEM	C1B-NB-C4B	4.59	110.65	105.21
3	B	602	BHF	C19-C10-C9	-4.33	115.94	119.55
3	A	602	BHF	O1-C19-C10	4.16	125.36	121.63
2	D	600	HEM	C1B-NB-C4B	4.14	110.11	105.21
2	A	601	HEM	C3B-C4B-NB	-4.09	106.53	109.47
2	B	601	HEM	CHD-C1D-ND	3.96	128.69	124.42
2	D	600	HEM	CHC-C4B-NB	3.92	128.65	124.42
3	A	602	BHF	C19-C10-C9	-3.89	116.31	119.55
2	B	601	HEM	C1B-NB-C4B	3.85	109.77	105.21
2	C	600	HEM	C3B-C4B-NB	-3.83	106.72	109.47
3	D	601	BHF	C17-C18-C13	3.80	122.84	117.92
2	A	601	HEM	CHB-C1B-NB	3.75	129.01	124.37
2	A	601	HEM	CHD-C1D-ND	3.63	128.33	124.42
2	D	600	HEM	CHA-C4D-ND	3.58	128.79	124.37
2	B	601	HEM	CHA-C4D-ND	3.57	128.78	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	BHF	C14-C13-C18	-3.54	114.56	119.12
2	C	600	HEM	CAD-C3D-C4D	3.51	130.81	124.70
2	A	601	HEM	CHD-C1D-C2D	-3.47	119.55	125.03
2	B	601	HEM	CAD-C3D-C4D	3.46	130.72	124.70
3	A	602	BHF	C16-C17-C18	-3.43	116.28	120.91
2	D	600	HEM	CHD-C1D-C2D	-3.34	119.75	125.03
3	A	602	BHF	O2-C9-C10	-3.34	116.67	121.38
2	B	601	HEM	CHA-C4D-C3D	-3.31	119.13	125.23
2	A	601	HEM	O2A-CGA-CBA	3.25	124.28	114.00
3	A	602	BHF	C14-C13-C18	-3.25	114.93	119.12
3	A	602	BHF	C2-C1-C7	-3.22	115.65	120.77
2	A	601	HEM	CHA-C4D-ND	3.12	128.22	124.37
3	C	601	BHF	C19-C10-C9	-3.11	116.96	119.55
2	D	600	HEM	CHA-C4D-C3D	-3.07	119.56	125.23
3	B	602	BHF	C2-C1-C7	-3.03	115.95	120.77
3	C	601	BHF	C17-C18-C13	3.02	121.83	117.92
3	A	602	BHF	C6-C1-C2	2.94	122.31	118.57
2	A	601	HEM	CMD-C2D-C1D	2.87	129.52	125.03
2	B	601	HEM	C1A-CHA-C4D	-2.84	119.57	126.25
3	D	601	BHF	O1-C19-C18	2.75	119.15	114.77
2	B	601	HEM	CHD-C1D-C2D	-2.70	120.77	125.03
3	D	601	BHF	C11-C10-C19	2.67	121.61	118.42
3	D	601	BHF	C16-C17-C18	-2.66	117.32	120.91
2	D	600	HEM	C1A-CHA-C4D	-2.65	120.02	126.25
2	D	600	HEM	C3B-C4B-NB	-2.64	107.57	109.47
2	C	600	HEM	CHA-C4D-ND	2.63	127.62	124.37
2	B	601	HEM	C3B-C4B-NB	-2.58	107.61	109.47
3	B	602	BHF	O1-C19-C10	2.57	123.93	121.63
3	B	602	BHF	C6-C1-C2	2.56	121.82	118.57
2	A	601	HEM	CHA-C4D-C3D	-2.54	120.55	125.23
2	A	601	HEM	CHD-C4C-NC	2.49	127.16	124.45
2	B	601	HEM	O2A-CGA-CBA	2.47	121.79	114.00
2	C	600	HEM	O2D-CGD-O1D	-2.43	117.09	123.33
3	B	602	BHF	O1-C7-C1	-2.42	108.52	111.89
2	B	601	HEM	O2A-CGA-O1A	-2.40	117.16	123.33
3	A	602	BHF	C17-C18-C19	-2.40	117.72	122.07
3	A	602	BHF	O2-C9-C8	2.38	125.69	121.88
3	C	601	BHF	O1-C19-C18	2.38	118.57	114.77
3	B	602	BHF	C11-C10-C9	2.38	124.45	120.73
2	B	601	HEM	CMD-C2D-C1D	2.34	128.69	125.03
3	A	602	BHF	C11-C10-C19	2.33	121.20	118.42
2	B	601	HEM	C4C-NC-C1C	2.30	109.58	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	BHF	O2-C9-C10	-2.26	118.20	121.38
2	D	600	HEM	CAD-C3D-C4D	2.24	128.60	124.70
2	A	601	HEM	CAD-C3D-C4D	2.23	128.59	124.70
2	C	600	HEM	C4C-CHD-C1D	-2.22	121.29	126.02
2	C	600	HEM	CHB-C4A-NA	2.21	127.88	123.86
2	B	601	HEM	CAA-C2A-C1A	2.18	129.19	124.94
3	B	602	BHF	C16-C15-C14	2.15	123.28	120.40
2	A	601	HEM	CHB-C1B-C2B	-2.15	120.84	126.95
3	A	602	BHF	C12-C13-C18	2.13	121.87	119.12
3	C	601	BHF	C2-C1-C7	-2.12	117.40	120.77
2	A	601	HEM	C3B-C2B-C1B	-2.12	104.82	106.41
2	B	601	HEM	CAD-C3D-C2D	-2.10	123.94	127.87
2	A	601	HEM	CAA-C2A-C1A	2.06	128.97	124.94
2	D	600	HEM	O2D-CGD-CBD	2.06	120.51	114.00
2	A	601	HEM	O1A-CGA-CBA	-2.06	116.57	123.09
3	C	601	BHF	C11-C10-C19	2.06	120.88	118.42
3	A	602	BHF	O1-C7-C1	-2.05	109.03	111.89
2	C	600	HEM	CHB-C1B-NB	2.04	126.89	124.37
3	B	602	BHF	C19-C18-C13	-2.04	114.88	118.68
2	A	601	HEM	C4C-NC-C1C	2.02	109.11	105.82
3	B	602	BHF	C5-C4-C3	2.02	122.63	119.87
2	A	601	HEM	C1A-CHA-C4D	-2.02	121.50	126.25
2	A	601	HEM	CBA-CAA-C2A	2.01	118.10	112.53
3	A	602	BHF	C5-C4-C3	2.01	122.62	119.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

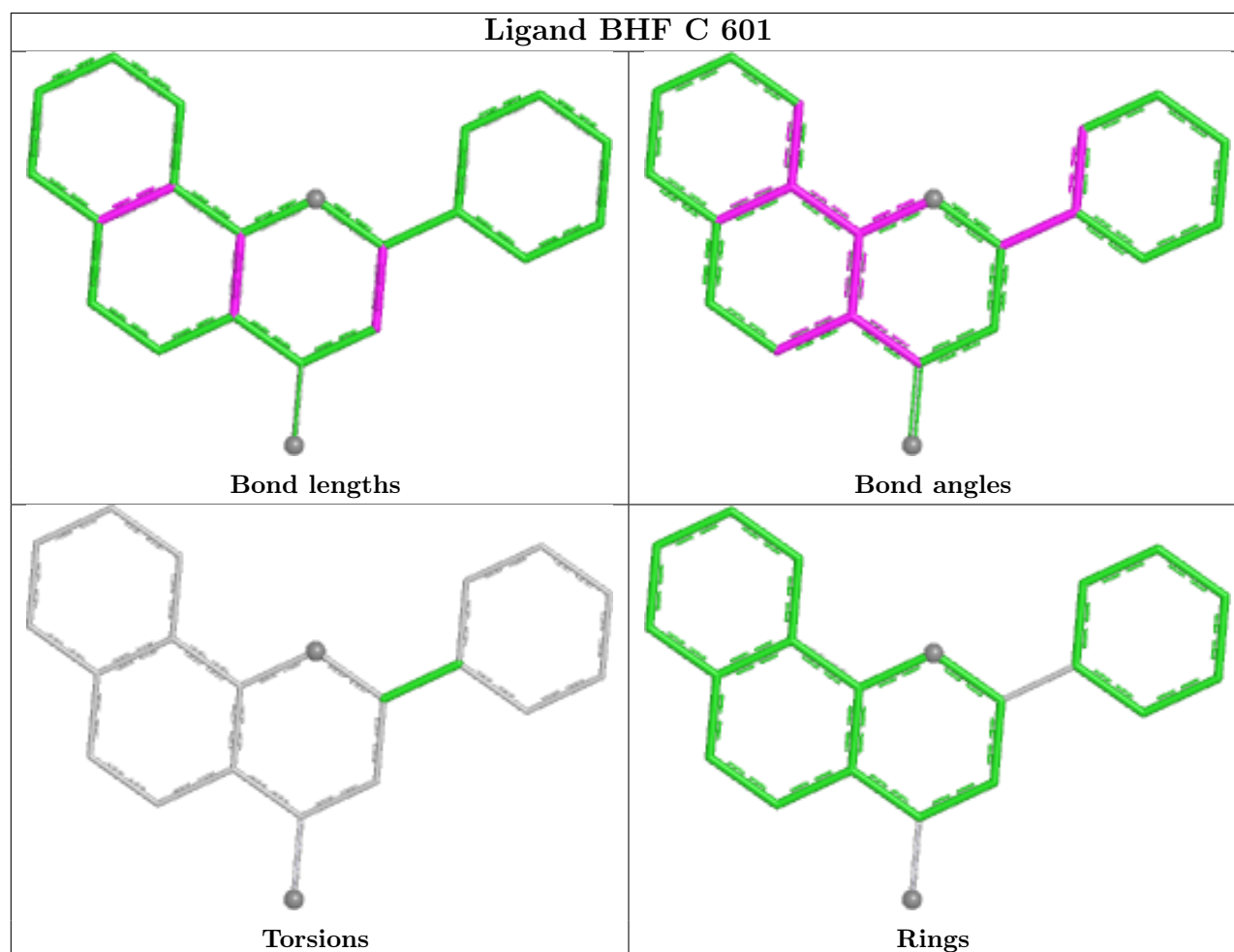
Mol	Chain	Res	Type	Atoms
2	C	600	HEM	C2D-C3D-CAD-CBD
2	C	600	HEM	C4D-C3D-CAD-CBD
2	C	600	HEM	C3D-CAD-CBD-CGD
2	D	600	HEM	CAA-CBA-CGA-O1A
2	B	601	HEM	CAA-CBA-CGA-O2A
2	B	601	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O1A

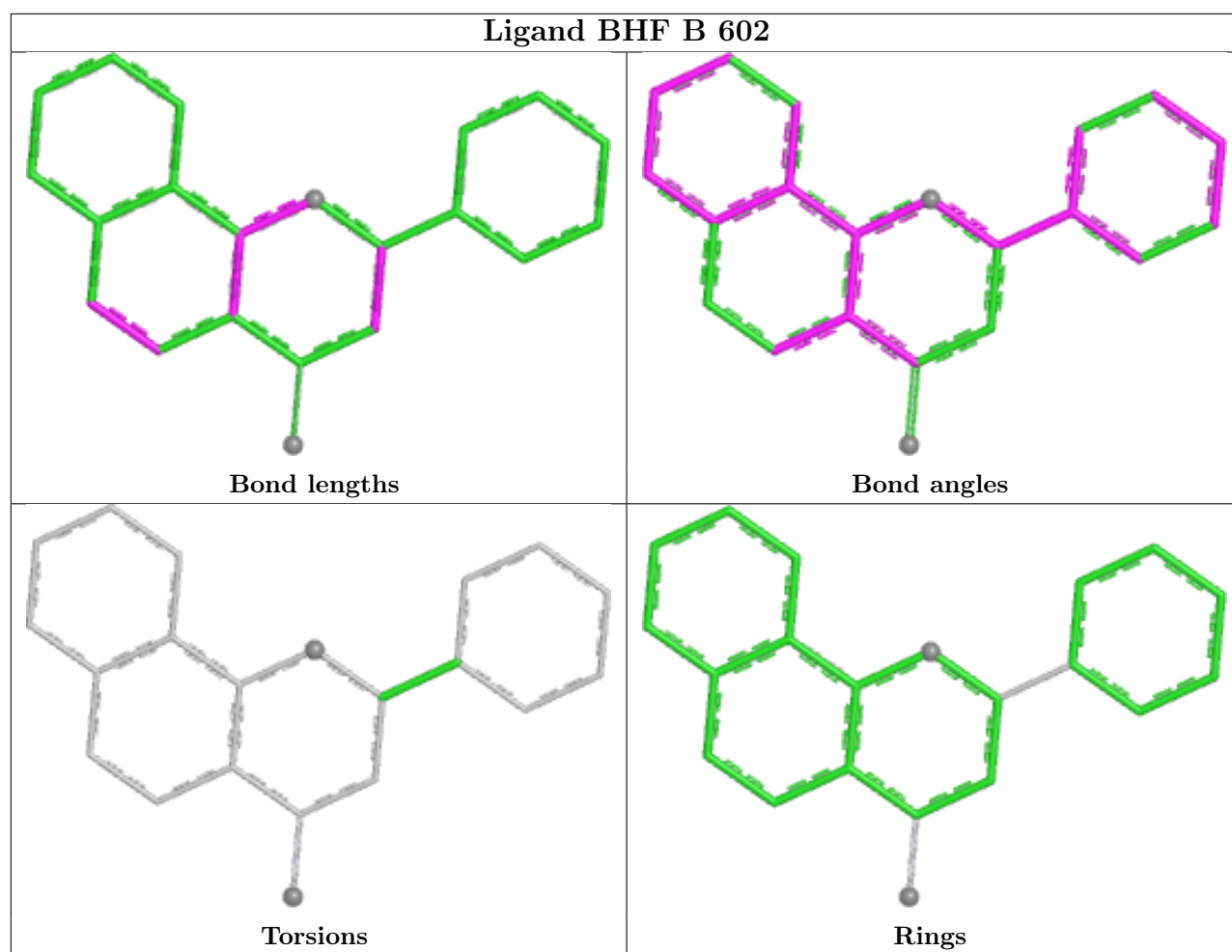
There are no ring outliers.

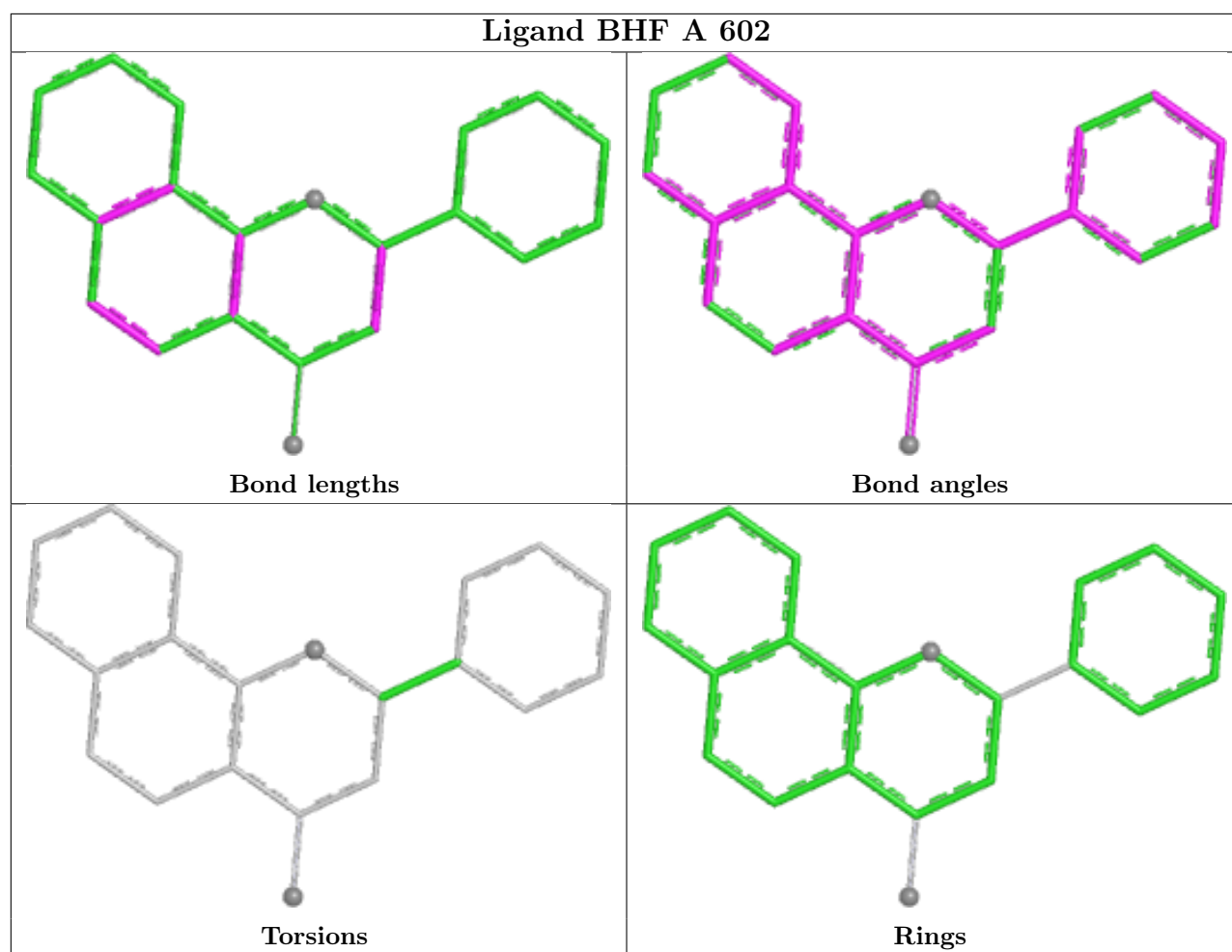
5 monomers are involved in 19 short contacts:

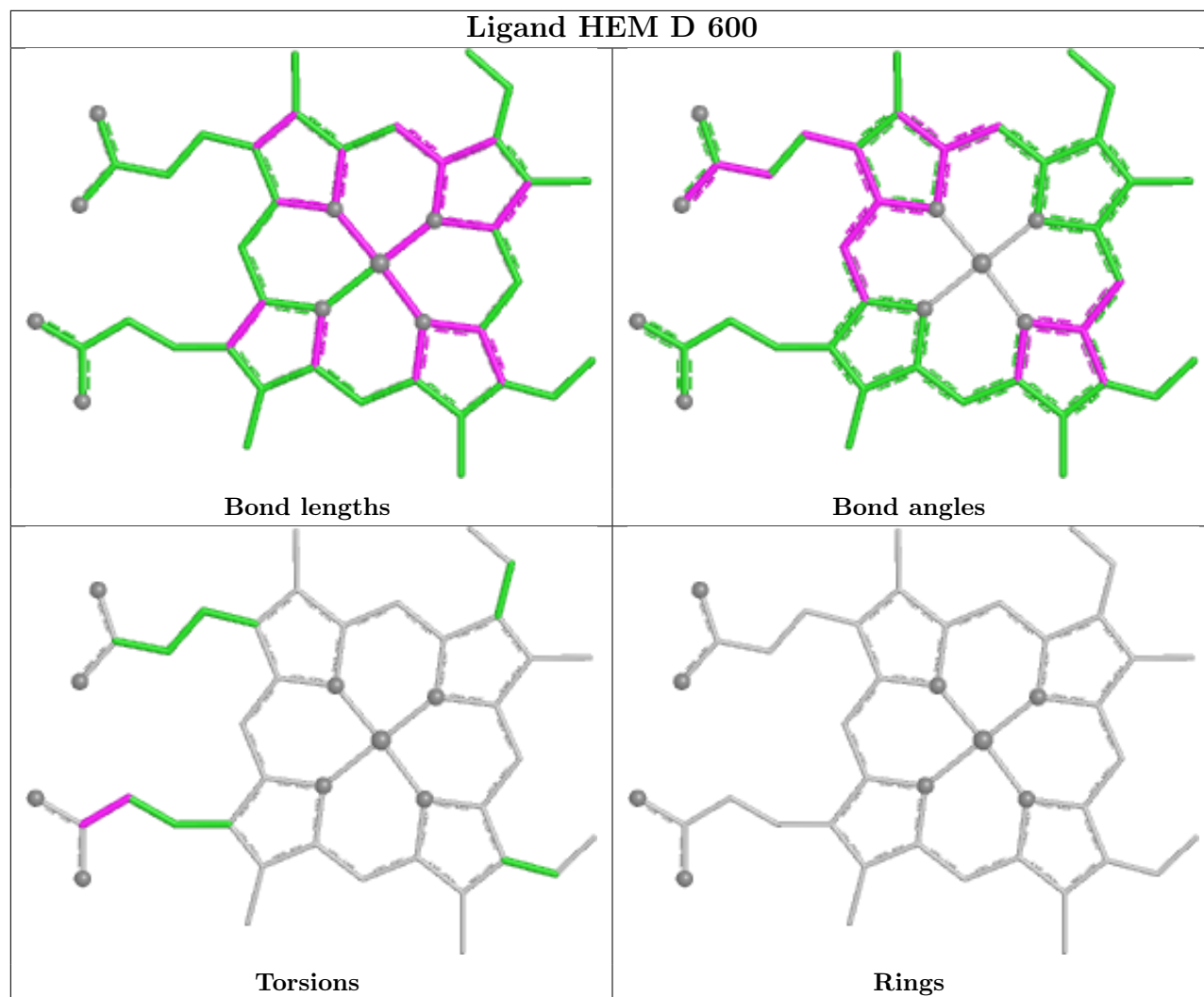
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	HEM	5	0
2	A	601	HEM	6	0
3	D	601	BHF	1	0
2	C	600	HEM	3	0
2	B	601	HEM	4	0

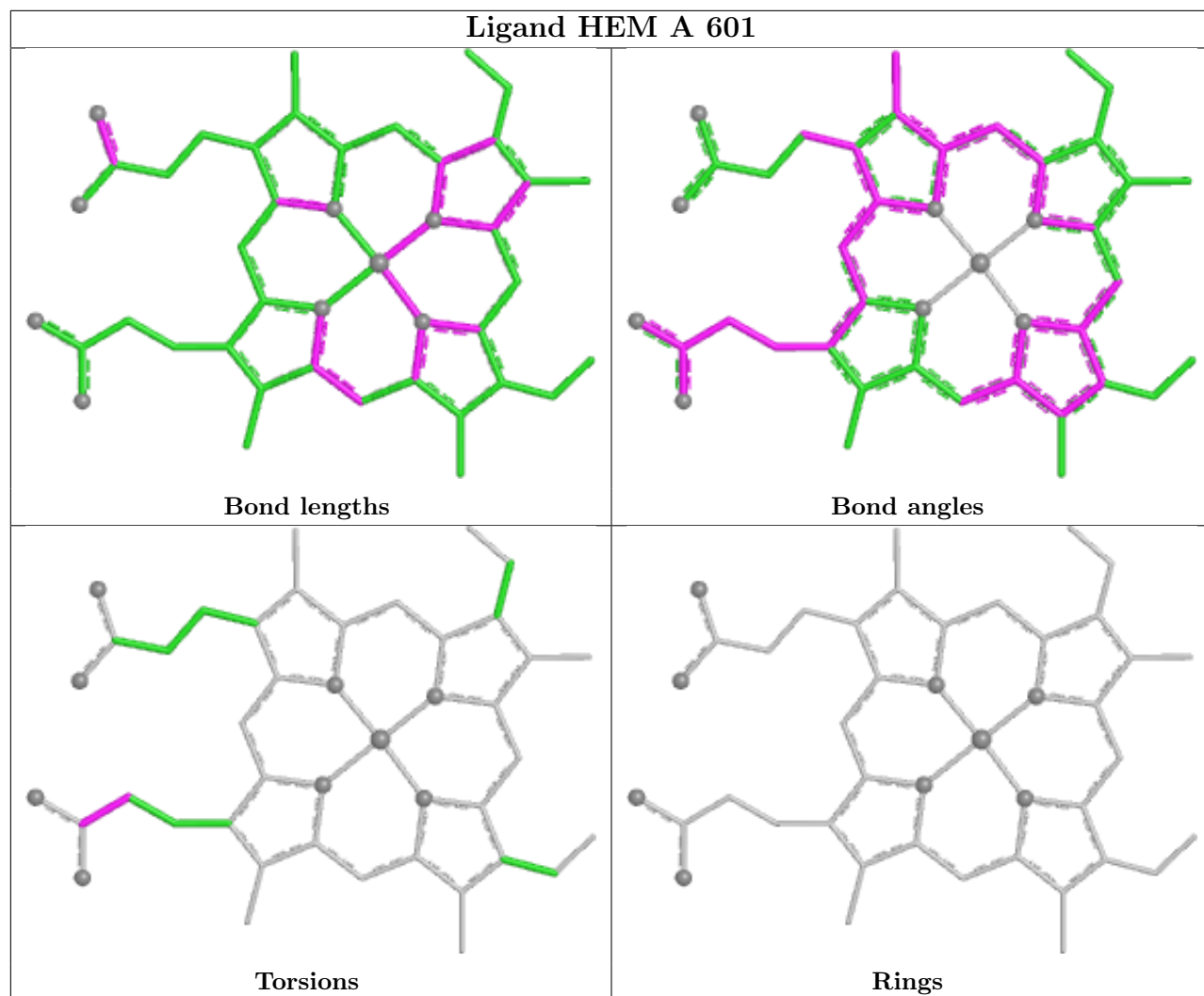
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

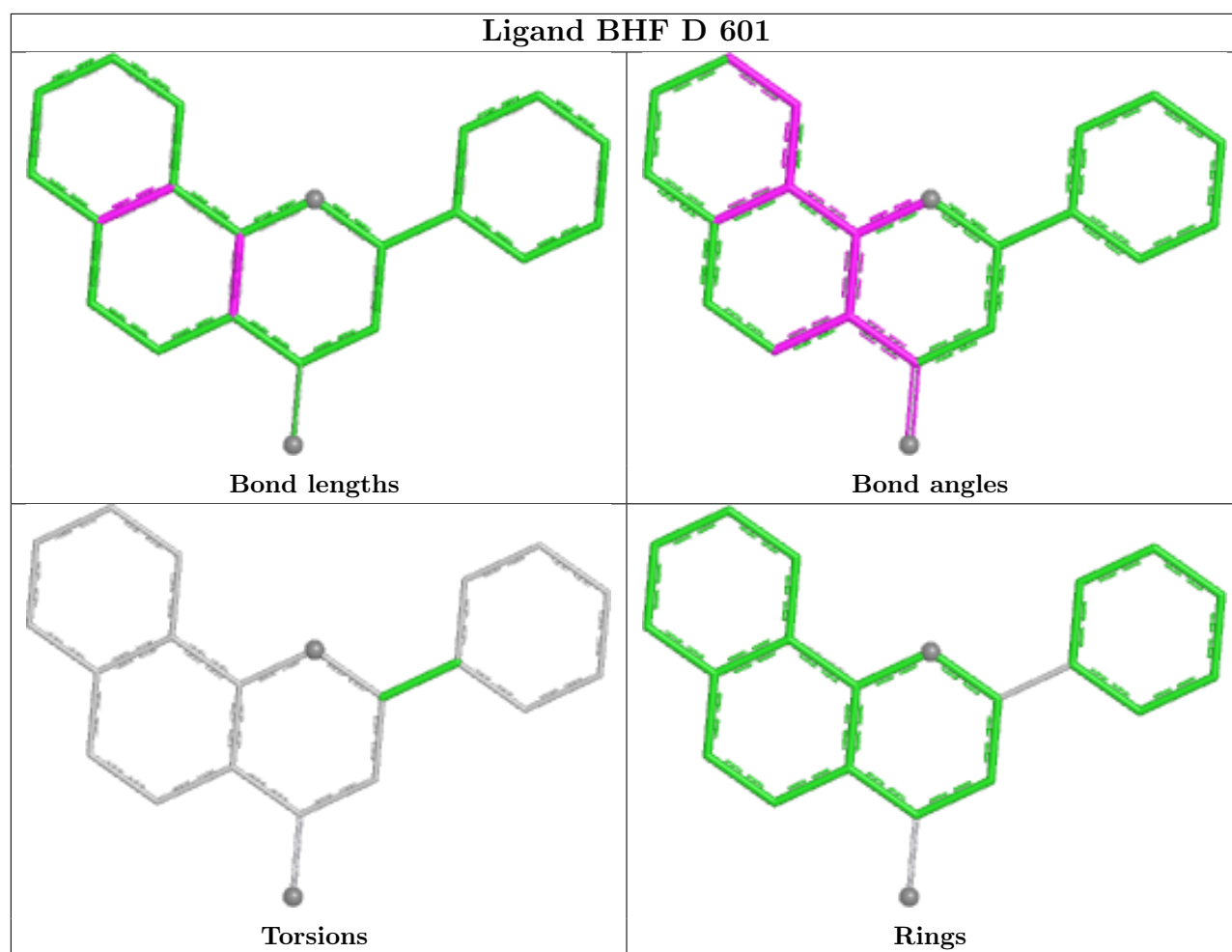


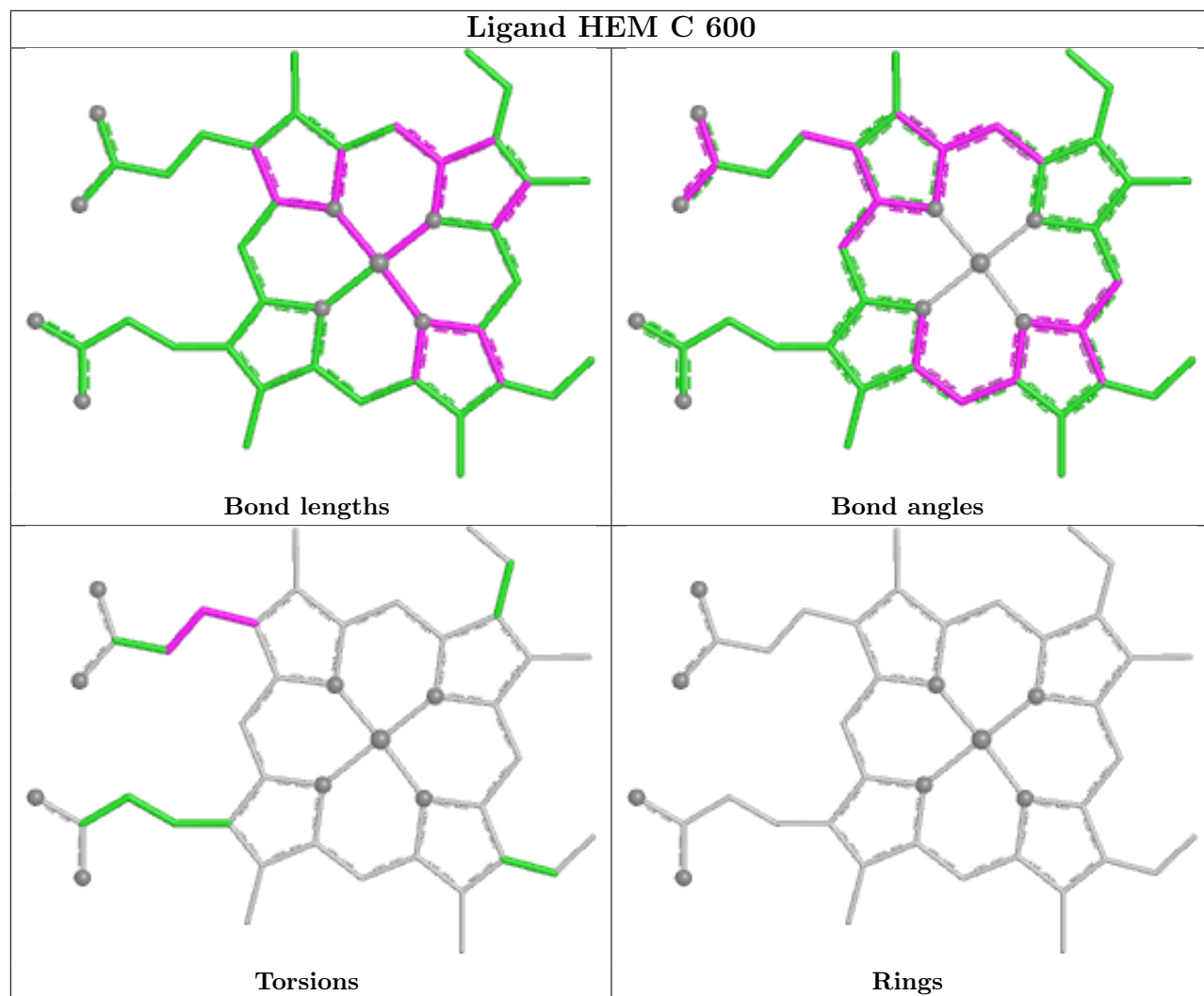


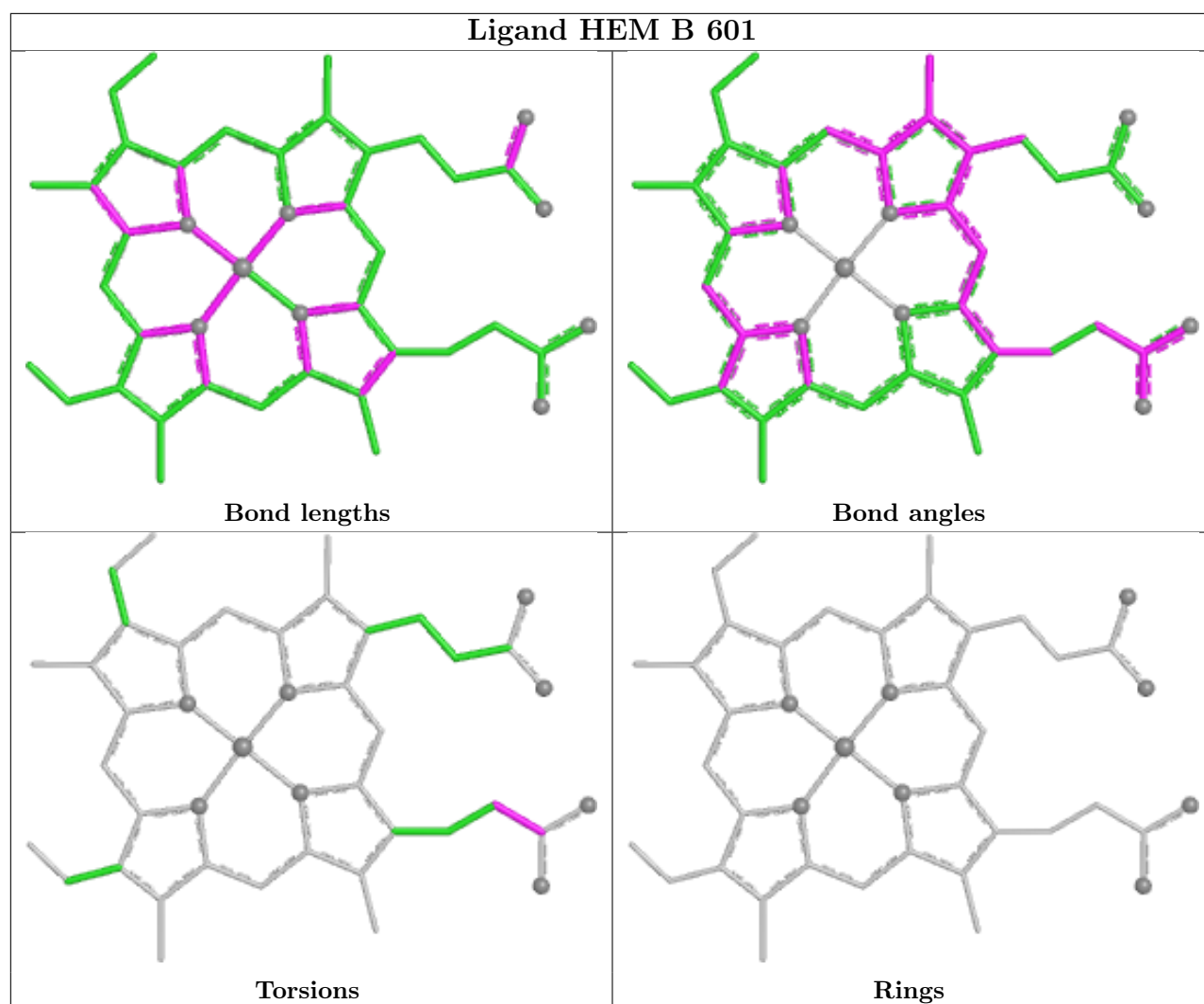












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	477/491 (97%)	-0.41	2 (0%) 88 86	31, 52, 91, 131	0
1	B	472/491 (96%)	-0.28	3 (0%) 85 83	35, 60, 100, 148	0
1	C	468/491 (95%)	0.27	11 (2%) 59 54	59, 90, 118, 146	0
1	D	467/491 (95%)	0.03	5 (1%) 78 74	51, 84, 117, 148	0
All	All	1884/1964 (95%)	-0.10	21 (1%) 78 74	31, 73, 113, 148	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	436	ASP	5.2
1	C	44	TRP	3.7
1	B	300	VAL	3.5
1	D	37	LEU	3.3
1	B	292	LYS	3.2
1	C	361	ASP	2.8
1	D	270	TYR	2.8
1	C	422	VAL	2.6
1	C	37	LEU	2.6
1	C	87	SER	2.4
1	C	222	ASN	2.4
1	C	226	GLU	2.3
1	A	311	VAL	2.3
1	C	220	LEU	2.2
1	D	512	SER	2.2
1	C	454	LYS	2.1
1	A	36	GLY	2.1
1	D	278	ILE	2.1
1	B	152	ALA	2.1
1	C	48	LEU	2.1
1	C	129	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

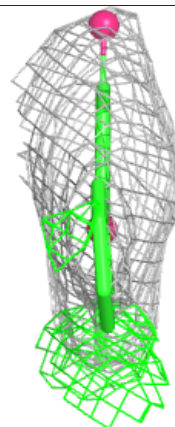
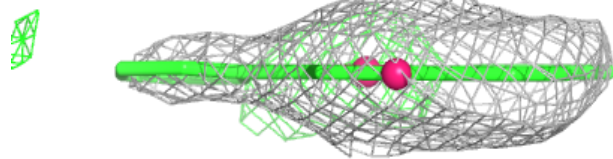
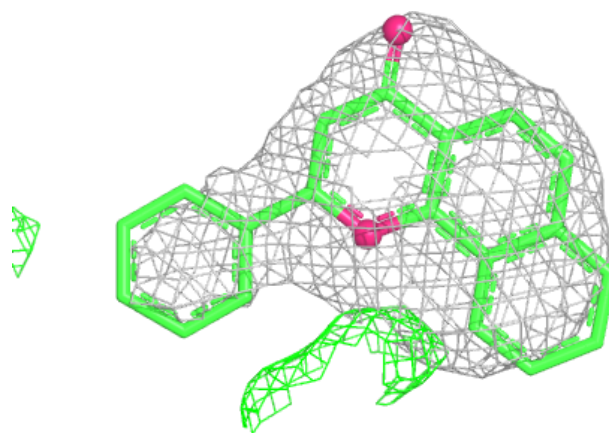
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NO3	B	603	4/4	0.81	0.24	51,68,73,86	0
4	NO3	A	604	4/4	0.83	0.15	64,66,70,101	0
4	NO3	A	603	4/4	0.84	0.12	103,103,111,118	0
3	BHF	D	601	21/21	0.90	0.16	94,106,115,121	0
3	BHF	B	602	21/21	0.90	0.13	58,62,67,79	0
3	BHF	A	602	21/21	0.92	0.13	43,55,72,81	0
3	BHF	C	601	21/21	0.93	0.17	88,104,120,122	0
2	HEM	C	600	43/43	0.98	0.07	43,56,80,103	0
2	HEM	D	600	43/43	0.98	0.06	40,53,73,80	0
2	HEM	B	601	43/43	0.98	0.06	36,46,54,60	0
2	HEM	A	601	43/43	0.99	0.05	32,38,44,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

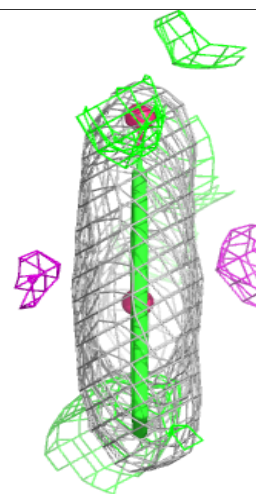
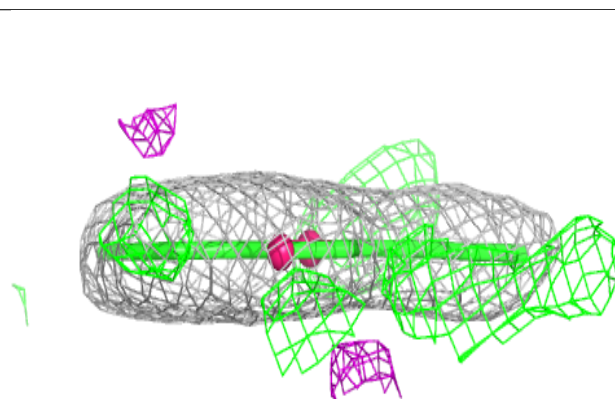
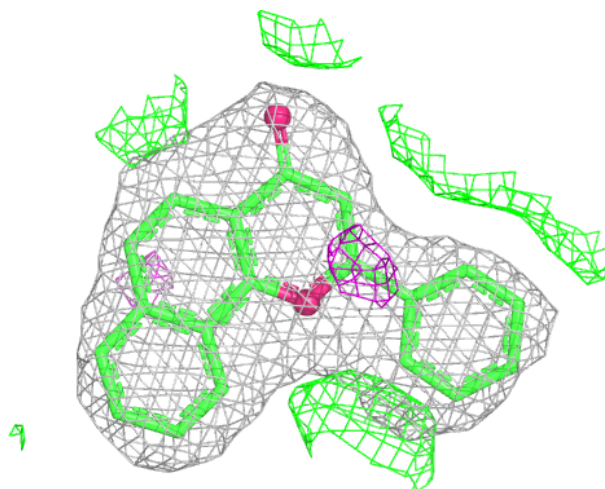
Electron density around BHF D 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



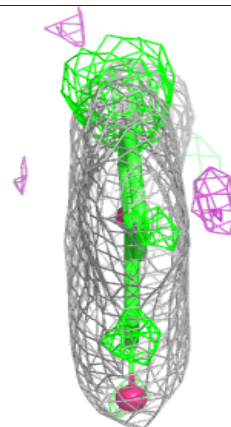
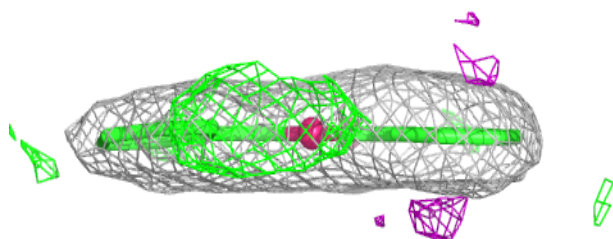
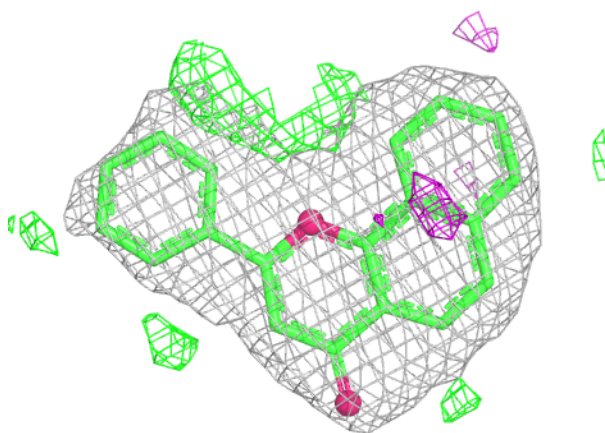
Electron density around BHF B 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

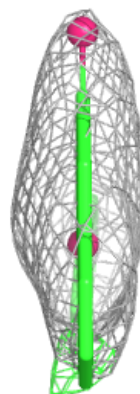
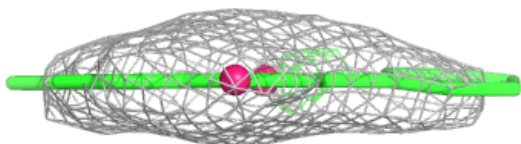
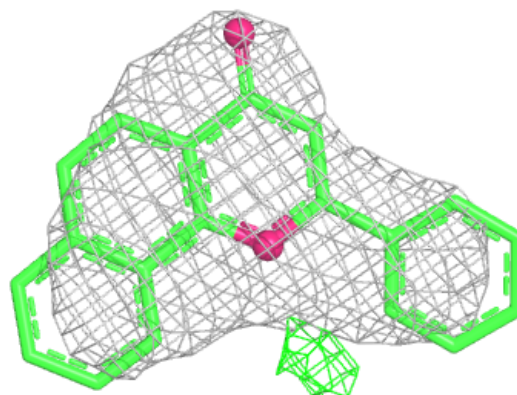


Electron density around BHF A 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

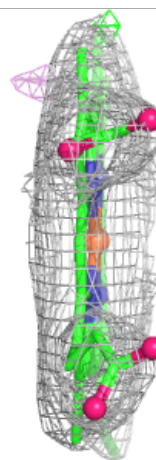
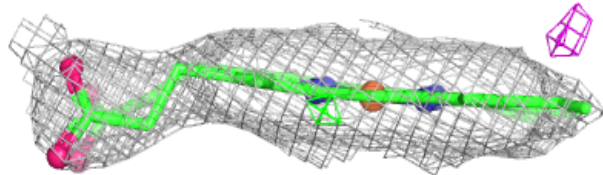
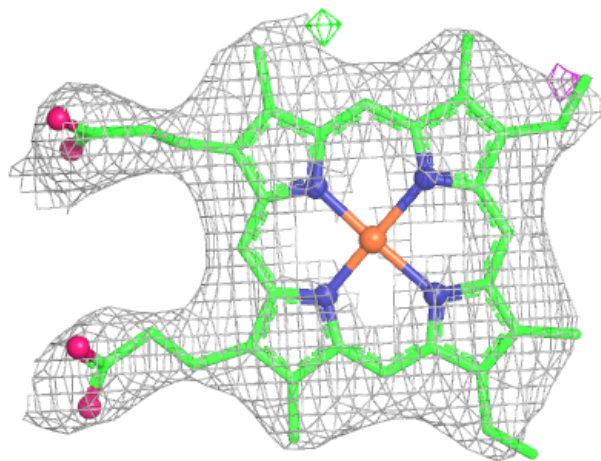
**Electron density around BHF C 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



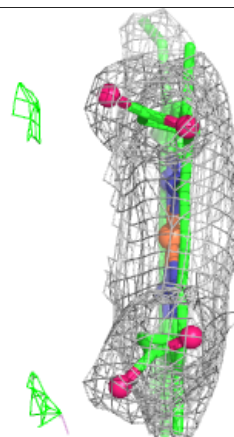
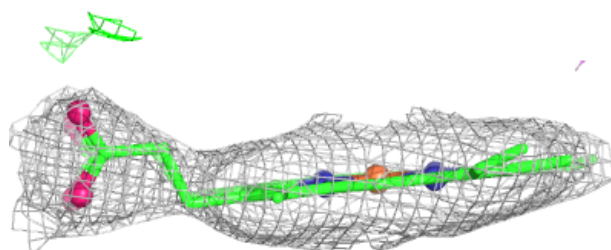
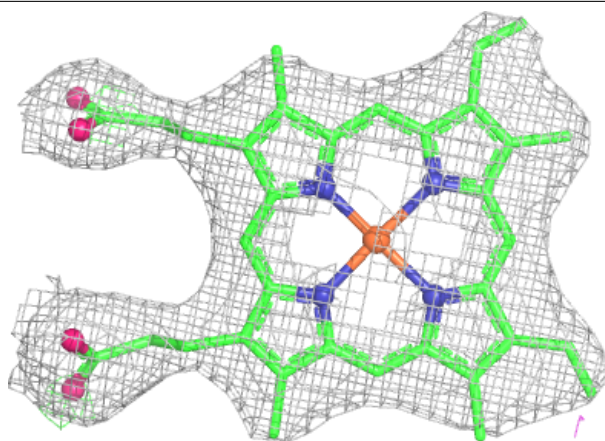
Electron density around HEM C 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



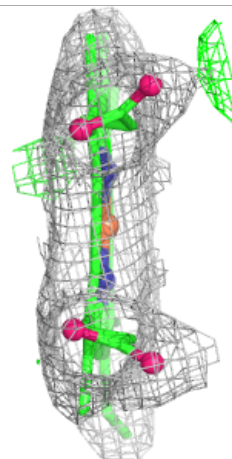
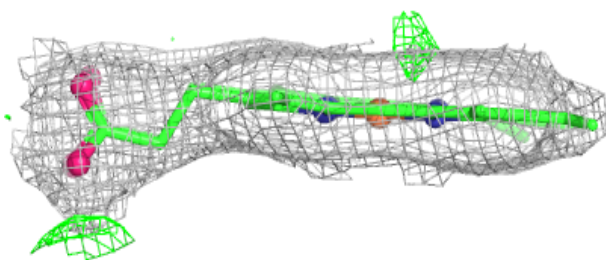
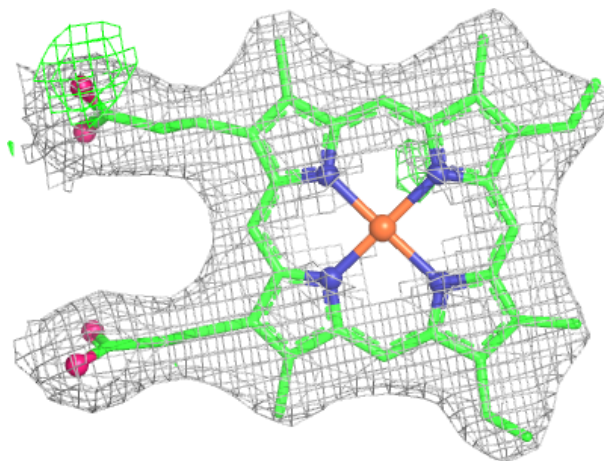
Electron density around HEM D 600:

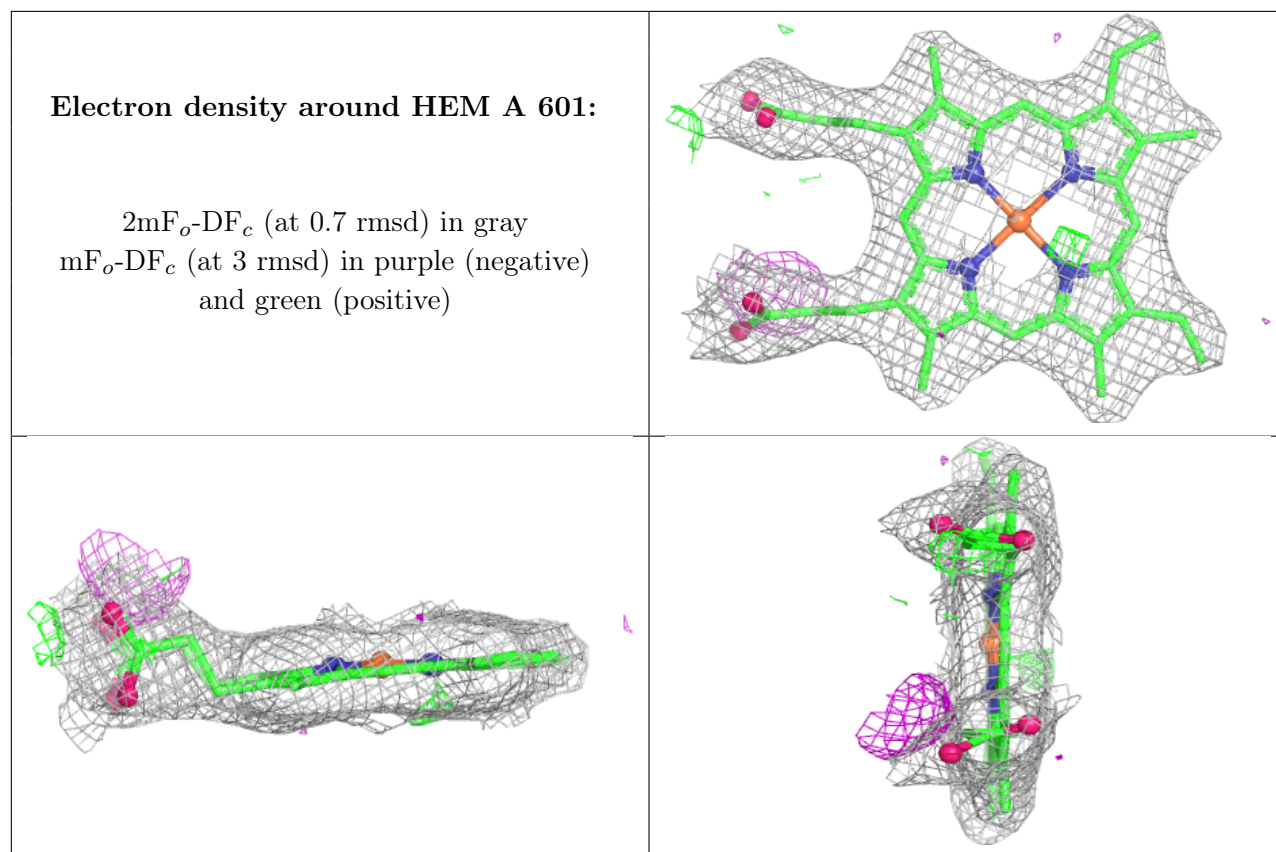
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.