



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:59 PM UTC

PDB ID : 2ISA / pdb_00002isa
Title : Crystal Structure of Vibrio salmonicida catalase
Authors : Riise, E.K.; Lorentzen, M.S.; Helland, R.; Smalas, A.O.; Leiros, H.K.S.; Willassen, N.P.
Deposited on : 2006-10-17
Resolution : 1.97 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

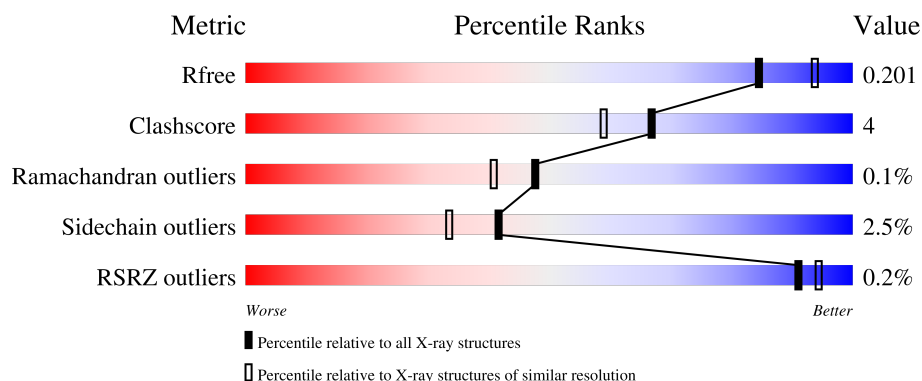
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	483	92% 7%
1	B	483	91% 8% .
1	C	483	90% 10% .
1	D	483	89% 10% .
1	E	483	92% 7% .

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Mol	Chain	Length	Quality of chain
1	F	483	 89%10% .
1	G	483	 91%8%
1	H	483	 90%9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35944 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.

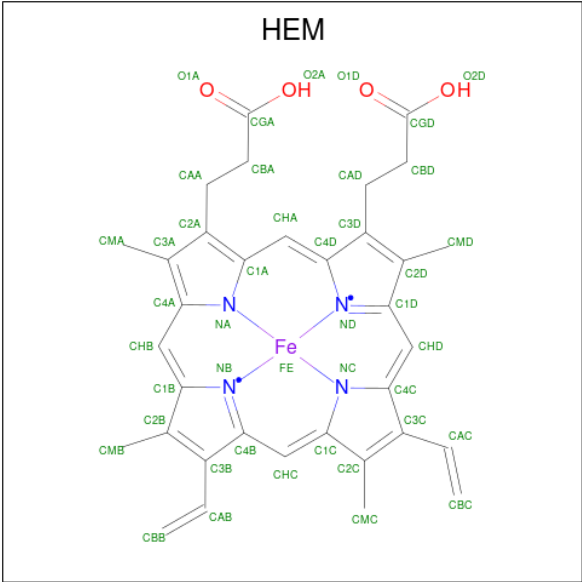
- Molecule 1 is a protein called Catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	3	0
			3871	2443	688	728	12			
1	B	482	Total	C	N	O	S	3	3	0
			3869	2442	688	727	12			
1	C	482	Total	C	N	O	S	3	3	0
			3869	2442	688	727	12			
1	D	482	Total	C	N	O	S	11	3	0
			3869	2442	688	727	12			
1	E	482	Total	C	N	O	S	6	2	0
			3868	2442	688	726	12			
1	F	482	Total	C	N	O	S	11	3	0
			3869	2442	688	727	12			
1	G	482	Total	C	N	O	S	7	2	0
			3868	2442	688	726	12			
1	H	482	Total	C	N	O	S	7	3	0
			3871	2443	688	728	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	OMT	MET	modified residue	UNP Q3LSM1
B	53	OMT	MET	modified residue	UNP Q3LSM1
C	53	OMT	MET	modified residue	UNP Q3LSM1
D	53	OMT	MET	modified residue	UNP Q3LSM1
E	53	OMT	MET	modified residue	UNP Q3LSM1
F	53	OMT	MET	modified residue	UNP Q3LSM1
G	53	OMT	MET	modified residue	UNP Q3LSM1
H	53	OMT	MET	modified residue	UNP Q3LSM1

- 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
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

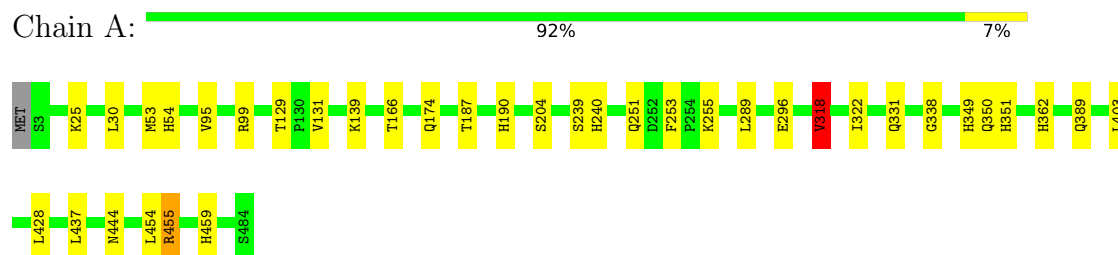
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	578	Total O 578 578	0	0
5	B	611	Total O 611 611	0	0
5	C	588	Total O 588 588	0	0
5	D	609	Total O 609 609	0	0
5	E	541	Total O 541 541	0	0
5	F	543	Total O 543 543	0	0
5	G	556	Total O 556 556	0	0
5	H	568	Total O 568 568	0	0

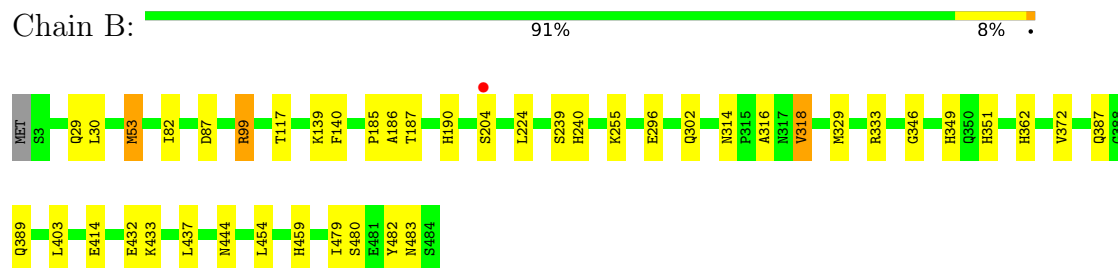
3 Residue-property plots [i](#)

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.

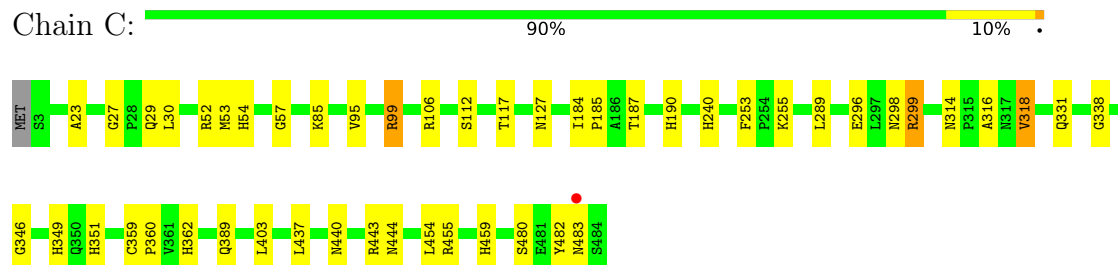
• Molecule 1: Catalase



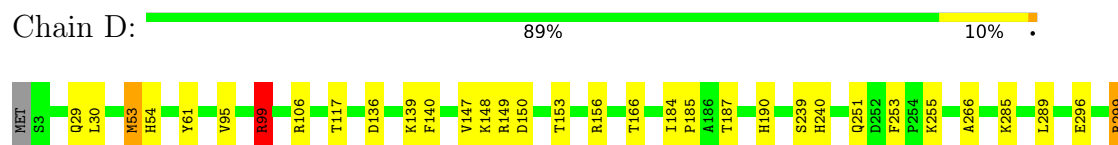
• Molecule 1: Catalase

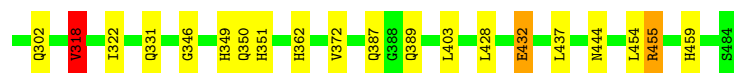


• Molecule 1: Catalase



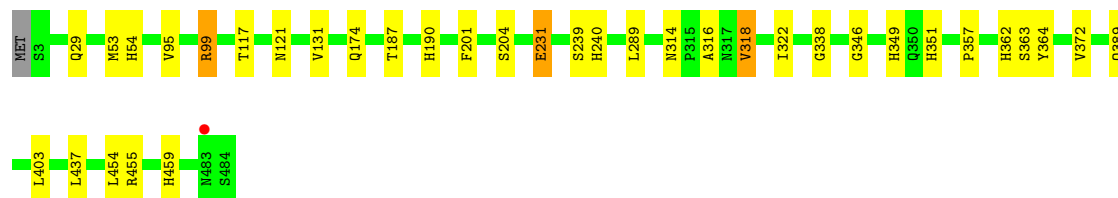
• Molecule 1: Catalase





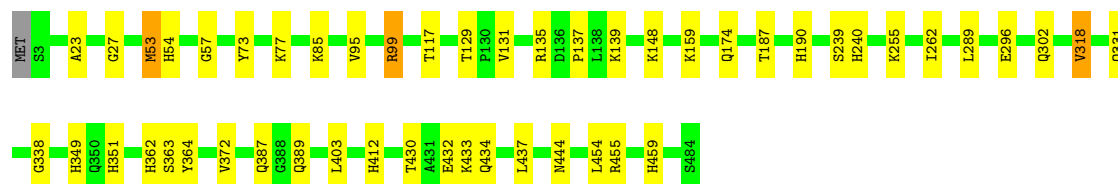
• Molecule 1: Catalase

Chain E: 92% 7%



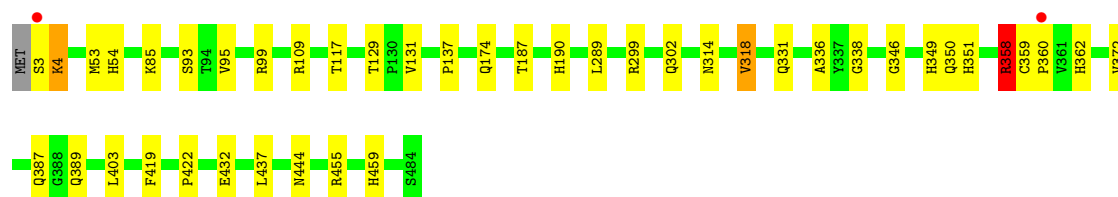
• Molecule 1: Catalase

Chain F: 89% 10%



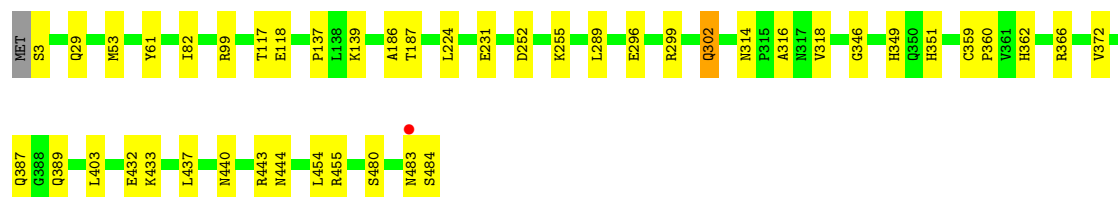
• Molecule 1: Catalase

Chain G: 91% 8%



• Molecule 1: Catalase

Chain H: 90% 9%



• Molecule 1: Catalase

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.15Å 217.76Å 99.28Å 90.00° 110.48° 90.00°	Depositor
Resolution (Å)	20.00 – 1.97 20.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-1.97) 96.9 (20.00-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.200 0.148 , 0.201	Depositor DCC
R_{free} test set	13407 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35944	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: GOL, HEM, CL, OMT

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	0.63	0/3989	0.83	3/5411 (0.1%)
1	B	0.64	0/3987	0.83	3/5408 (0.1%)
1	C	0.79	1/3987 (0.0%)	0.99	9/5408 (0.2%)
1	D	0.62	0/3987	0.84	8/5408 (0.1%)
1	E	0.68	1/3981 (0.0%)	0.83	3/5400 (0.1%)
1	F	0.60	1/3987 (0.0%)	0.88	8/5408 (0.1%)
1	G	1.31	4/3981 (0.1%)	0.94	12/5400 (0.2%)
1	H	0.64	1/3989 (0.0%)	0.92	6/5411 (0.1%)
All	All	0.77	8/31888 (0.0%)	0.89	52/43254 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	358	ARG	CZ-NH1	62.97	2.21	1.32
1	C	299	ARG	NE-CZ	-29.25	1.00	1.33
1	G	358	ARG	NE-CZ	28.71	1.64	1.33
1	G	358	ARG	CZ-NH2	21.18	1.60	1.33
1	E	231	GLU	CD-OE1	18.49	1.60	1.25
1	G	302	GLN	CG-CD	-7.40	1.33	1.52
1	H	231	GLU	CG-CD	6.90	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	302	GLN	CG-CD	-6.42	1.35	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ARG	NE-CZ-NH1	-25.44	96.06	121.50
1	C	299	ARG	NE-CZ-NH2	24.27	141.04	119.20
1	G	358	ARG	NH1-CZ-NH2	-19.80	93.57	119.30
1	C	299	ARG	CD-NE-CZ	16.81	147.94	124.40
1	F	302	GLN	CB-CG-CD	15.45	138.86	112.60
1	G	302	GLN	CB-CG-CD	15.44	138.84	112.60
1	F	302	GLN	CG-CD-NE2	14.21	137.72	116.40
1	G	302	GLN	CG-CD-NE2	13.32	136.39	116.40
1	H	99[A]	ARG	CA-C-N	-12.95	101.88	122.86
1	H	99[A]	ARG	C-N-CA	-12.95	101.88	122.86
1	H	99[B]	ARG	CA-C-N	-12.95	101.88	122.86
1	H	99[B]	ARG	C-N-CA	-12.95	101.88	122.86
1	E	231	GLU	OE1-CD-OE2	-11.60	95.07	122.90
1	H	302	GLN	CG-CD-NE2	-11.18	99.63	116.40
1	F	302	GLN	CG-CD-OE1	-10.60	99.61	120.80
1	G	358	ARG	NE-CZ-NH2	9.98	128.19	119.20
1	G	302	GLN	CG-CD-OE1	-9.77	101.25	120.80
1	D	302	GLN	CG-CD-NE2	-9.33	102.41	116.40
1	H	302	GLN	CG-CD-OE1	8.55	137.91	120.80
1	G	358	ARG	CD-NE-CZ	7.89	135.45	124.40
1	E	99[A]	ARG	N-CA-C	7.88	127.59	110.80
1	E	99[B]	ARG	N-CA-C	7.88	127.59	110.80
1	A	99[A]	ARG	N-CA-C	7.53	126.83	110.80
1	A	99[B]	ARG	N-CA-C	7.53	126.83	110.80
1	B	318	VAL	N-CA-CB	-7.47	103.83	112.34
1	B	99[A]	ARG	N-CA-C	-7.43	99.03	110.10
1	B	99[B]	ARG	N-CA-C	-7.43	99.03	110.10
1	C	99[A]	ARG	N-CA-C	7.42	126.61	110.80
1	C	99[B]	ARG	N-CA-C	7.42	126.61	110.80
1	G	358	ARG	NE-CZ-NH1	7.32	128.82	121.50
1	F	99[A]	ARG	N-CA-C	7.31	126.37	110.80
1	F	99[B]	ARG	N-CA-C	7.31	126.37	110.80
1	G	99[A]	ARG	N-CA-C	7.16	126.04	110.80
1	G	99[B]	ARG	N-CA-C	7.16	126.04	110.80
1	D	99[A]	ARG	N-CA-C	6.97	125.65	110.80
1	D	99[B]	ARG	N-CA-C	6.97	125.65	110.80
1	D	302	GLN	CG-CD-OE1	6.78	134.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	VAL	N-CA-CB	-6.28	105.18	112.34
1	G	4	LYS	N-CA-C	-6.09	105.14	113.30
1	D	299	ARG	CB-CG-CD	6.03	125.17	111.30
1	D	318	VAL	N-CA-CB	-5.87	105.38	112.07
1	F	318	VAL	CB-CA-C	5.84	119.64	111.70
1	A	318	VAL	N-CA-CB	-5.81	105.72	112.34
1	G	318	VAL	N-CA-CB	-5.71	105.83	112.34
1	C	482	TYR	CA-C-N	5.63	128.60	120.38
1	C	482	TYR	C-N-CA	5.63	128.60	120.38
1	G	336	ALA	N-CA-C	5.46	117.99	111.71
1	F	57	GLY	N-CA-C	5.33	119.40	110.56
1	F	318	VAL	N-CA-CB	-5.22	106.39	112.34
1	C	57	GLY	N-CA-C	5.15	119.11	110.56
1	D	136	ASP	CA-C-N	5.09	124.70	119.56
1	D	136	ASP	C-N-CA	5.09	124.70	119.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	ARG	Sidechain
1	E	231	GLU	Sidechain
1	G	358	ARG	Sidechain

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	3871	0	3646	25	0
1	B	3869	0	3647	35	0
1	C	3869	0	3647	26	0
1	D	3869	0	3647	31	0
1	E	3868	0	3646	21	0
1	F	3869	0	3647	28	0
1	G	3868	0	3646	30	0
1	H	3871	0	3645	28	0
2	A	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	2	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
2	E	43	0	30	2	0
2	F	43	0	30	2	0
2	G	43	0	30	2	0
2	H	43	0	30	1	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
3	E	6	0	8	1	0
3	F	6	0	8	1	0
3	G	6	0	8	1	0
3	H	6	0	8	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	A	578	0	0	7	0
5	B	611	0	0	19	0
5	C	588	0	0	5	0
5	D	609	0	0	10	0
5	E	541	0	0	9	0
5	F	543	0	0	9	0
5	G	556	0	0	13	0
5	H	568	0	0	7	0
All	All	35944	0	29475	224	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 4.

All (224) 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:F:387:GLN:HG2	5:F:8755:HOH:O	1.46	1.10
1:B:432:GLU:HG2	5:B:6655:HOH:O	1.73	0.88
1:B:387:GLN:HG2	5:B:6834:HOH:O	1.76	0.84
1:C:362:HIS:HE1	1:C:389:GLN:OE1	1.63	0.81
1:A:362:HIS:HE1	1:A:389:GLN:OE1	1.65	0.78
1:D:387:GLN:HG2	5:D:5647:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:GLN:HG2	5:D:5568:HOH:O	1.84	0.77
1:G:362:HIS:HE1	1:G:389:GLN:OE1	1.70	0.74
1:D:255:LYS:HG2	1:D:296:GLU:HB3	1.70	0.72
2:E:486:HEM:HMB1	2:E:486:HEM:HBB2	1.72	0.72
2:B:486:HEM:HBB2	2:B:486:HEM:HMB1	1.72	0.71
2:C:485:HEM:HMB1	2:C:485:HEM:HBB2	1.71	0.71
1:A:318:VAL:HG13	1:A:322:ILE:O	1.91	0.70
1:B:362:HIS:HD2	5:B:6699:HOH:O	1.75	0.68
1:F:362:HIS:HE1	1:F:389:GLN:OE1	1.77	0.68
1:A:362:HIS:HD2	5:A:5565:HOH:O	1.77	0.68
1:B:82:ILE:HD13	5:B:6929:HOH:O	1.93	0.68
2:F:486:HEM:HMB1	2:F:486:HEM:HBB2	1.75	0.68
1:B:349:HIS:HE1	5:B:6527:HOH:O	1.78	0.67
1:B:362:HIS:HE1	1:B:389:GLN:OE1	1.77	0.67
1:H:362:HIS:HD2	5:H:7540:HOH:O	1.78	0.66
1:A:349:HIS:HE1	5:A:5532:HOH:O	1.78	0.66
1:A:318:VAL:CG1	1:A:322:ILE:O	2.44	0.66
1:C:85:LYS:HE2	5:C:5970:HOH:O	1.96	0.66
2:D:485:HEM:HMB1	2:D:485:HEM:HBB2	1.76	0.65
1:E:362:HIS:HE1	1:E:389:GLN:OE1	1.80	0.65
1:E:99[A]:ARG:O	5:E:5729:HOH:O	2.15	0.65
1:C:187:THR:OG1	1:C:190:HIS:HD2	1.80	0.64
1:B:433:LYS:HE2	5:B:6634:HOH:O	1.96	0.64
1:C:480:SER:HA	1:C:483:ASN:HB2	1.79	0.64
1:B:255:LYS:HG2	1:B:296:GLU:HB3	1.80	0.63
1:H:346:GLY:O	1:H:349:HIS:HD2	1.82	0.63
1:B:187:THR:OG1	1:B:190:HIS:HD2	1.81	0.63
1:B:87:ASP:HB3	5:B:6999:HOH:O	2.00	0.62
1:G:459:HIS:HD2	5:G:5609:HOH:O	1.82	0.62
1:B:351:HIS:HD2	5:B:6490:HOH:O	1.81	0.62
1:F:351:HIS:HD2	5:F:8538:HOH:O	1.80	0.62
1:D:362:HIS:HE1	1:D:389:GLN:OE1	1.83	0.61
1:G:359:CYS:HB2	1:G:360:PRO:HD2	1.83	0.61
1:B:459:HIS:HD2	5:B:6513:HOH:O	1.84	0.61
1:A:351:HIS:HD2	5:A:5581:HOH:O	1.84	0.60
1:C:351:HIS:HD2	5:C:5507:HOH:O	1.85	0.59
1:H:362:HIS:HE1	1:H:389:GLN:OE1	1.85	0.59
1:G:3:SER:O	5:G:6047:HOH:O	2.17	0.59
2:B:486:HEM:HBB2	2:B:486:HEM:CMB	2.32	0.58
1:E:349:HIS:HE1	5:E:5520:HOH:O	1.84	0.58
1:H:349:HIS:HE1	5:H:7546:HOH:O	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:THR:OG1	1:D:190:HIS:HD2	1.86	0.58
1:E:187:THR:OG1	1:E:190:HIS:HD2	1.86	0.58
1:H:139:LYS:HA	1:H:139:LYS:HE2	1.85	0.58
1:F:73:TYR:CD2	1:F:262:ILE:HD13	2.39	0.58
1:G:351:HIS:HD2	5:G:5536:HOH:O	1.86	0.58
1:C:359:CYS:HB2	1:C:360:PRO:HD2	1.86	0.57
2:A:486:HEM:HMB1	2:A:486:HEM:HBB2	1.86	0.57
1:A:331:GLN:NE2	1:B:29:GLN:H	2.02	0.56
1:F:139:LYS:HA	1:F:139:LYS:HE2	1.87	0.56
1:G:349:HIS:HE1	5:G:5511:HOH:O	1.88	0.56
1:H:433:LYS:HD2	5:H:7639:HOH:O	2.05	0.56
1:D:139:LYS:HA	1:D:139:LYS:HE2	1.87	0.56
1:G:137:PRO:HB3	2:G:485:HEM:HBB1	1.89	0.55
1:H:255:LYS:HG2	1:H:296:GLU:HB3	1.88	0.55
1:A:331:GLN:HE21	1:B:29:GLN:H	1.55	0.55
1:C:29:GLN:H	1:D:331:GLN:NE2	2.05	0.54
5:B:6692:HOH:O	1:H:82:ILE:HD13	2.07	0.54
1:B:139:LYS:HA	1:B:139:LYS:HE2	1.90	0.54
1:C:29:GLN:H	1:D:331:GLN:HE21	1.56	0.53
1:H:255:LYS:HG2	1:H:296:GLU:CB	2.39	0.53
1:F:187:THR:OG1	1:F:190:HIS:HD2	1.91	0.53
1:E:459:HIS:HD2	5:E:5717:HOH:O	1.92	0.53
1:B:433:LYS:HD2	5:B:6602:HOH:O	2.08	0.53
1:H:137:PRO:HB3	2:H:485:HEM:HBB1	1.89	0.53
1:F:85:LYS:NZ	5:F:8905:HOH:O	2.43	0.52
1:D:349:HIS:HE1	5:D:5518:HOH:O	1.93	0.52
1:E:351:HIS:HD2	5:E:5497:HOH:O	1.93	0.52
1:F:372:VAL:HG21	1:H:372:VAL:HG21	1.92	0.52
1:B:346:GLY:O	1:B:349:HIS:HD2	1.93	0.52
1:F:53:OMT:HE2	1:F:148:LYS:HE2	1.92	0.52
1:B:480:SER:HA	1:B:483:ASN:HD22	1.75	0.51
1:D:54:HIS:CE1	1:D:95:VAL:HG22	2.46	0.51
1:C:314:ASN:ND2	1:C:316:ALA:H	2.09	0.51
1:D:106:ARG:HA	1:D:184:ILE:HG12	1.93	0.51
1:F:53:OMT:CE	1:F:148:LYS:HE2	2.40	0.50
1:C:359:CYS:HB2	1:C:360:PRO:CD	2.41	0.50
1:A:338:GLY:HA3	3:A:5489:GOL:H2	1.93	0.50
1:G:131:VAL:HG23	1:G:174:GLN:HE21	1.76	0.50
1:A:239:SER:OG	1:A:240:HIS:HD2	1.95	0.50
1:G:54:HIS:CE1	1:G:95:VAL:HG22	2.47	0.50
1:A:139:LYS:HE2	1:A:139:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:HG2	1:A:296:GLU:HB3	1.95	0.49
1:C:185:PRO:O	1:C:240:HIS:HE1	1.95	0.49
1:B:387:GLN:HG2	5:B:6735:HOH:O	2.11	0.49
1:A:54:HIS:CE1	1:A:95:VAL:HG22	2.48	0.49
5:E:6001:HOH:O	1:G:350:GLN:HB3	2.11	0.49
1:B:351:HIS:HE1	5:B:7022:HOH:O	1.96	0.49
1:B:372:VAL:HG21	1:D:372:VAL:HG21	1.93	0.49
1:C:255:LYS:HG2	1:C:296:GLU:HB3	1.95	0.49
5:D:5963:HOH:O	1:H:82:ILE:HD11	2.12	0.49
1:C:346:GLY:O	1:C:349:HIS:HD2	1.96	0.48
1:B:351:HIS:CD2	5:B:6490:HOH:O	2.61	0.48
1:D:346:GLY:O	1:D:349:HIS:HD2	1.96	0.48
1:E:362:HIS:HD2	5:E:5598:HOH:O	1.96	0.48
1:F:77:LYS:HE2	5:F:8884:HOH:O	2.12	0.48
1:A:131:VAL:HG23	1:A:174:GLN:HE21	1.77	0.48
1:D:185:PRO:O	1:D:240:HIS:HE1	1.96	0.48
1:G:187:THR:OG1	1:G:190:HIS:HD2	1.97	0.48
1:F:137:PRO:HB3	2:F:486:HEM:HBB1	1.96	0.48
1:G:85:LYS:HE2	5:G:5872:HOH:O	2.14	0.48
1:F:459:HIS:HD2	5:F:8594:HOH:O	1.96	0.48
1:F:349:HIS:HE1	5:F:8604:HOH:O	1.96	0.48
1:H:346:GLY:O	1:H:349:HIS:CD2	2.66	0.48
1:C:349:HIS:HE1	5:C:5647:HOH:O	1.97	0.47
1:G:331:GLN:NE2	1:H:29:GLN:H	2.12	0.47
1:D:266:ALA:HB3	5:D:6037:HOH:O	2.14	0.47
1:E:54:HIS:CE1	1:E:95:VAL:HG22	2.50	0.47
1:A:350:GLN:HG2	5:A:5892:HOH:O	2.14	0.47
1:D:351:HIS:HD2	5:D:5515:HOH:O	1.97	0.47
2:E:486:HEM:HMC1	2:E:486:HEM:HBC2	1.96	0.47
5:E:5915:HOH:O	1:G:4:LYS:HE2	2.15	0.47
1:G:4:LYS:HA	5:G:6047:HOH:O	2.15	0.47
1:G:351:HIS:CD2	5:G:5536:HOH:O	2.62	0.47
2:A:486:HEM:HBB2	2:A:486:HEM:CMB	2.45	0.47
1:C:187:THR:OG1	1:C:190:HIS:CD2	2.65	0.47
1:E:131:VAL:HG23	1:E:174:GLN:HE21	1.79	0.47
1:C:127:ASN:CG	2:C:485:HEM:HAC	2.39	0.47
1:F:338:GLY:HA3	3:F:5494:GOL:H2	1.97	0.47
1:G:314:ASN:ND2	5:G:5580:HOH:O	2.48	0.47
1:C:331:GLN:NE2	1:D:29:GLN:H	2.14	0.46
1:F:433:LYS:HE2	5:F:8746:HOH:O	2.15	0.46
1:G:359:CYS:HB2	1:G:360:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:HIS:CD2	5:A:5581:HOH:O	2.64	0.46
1:F:255:LYS:HG2	1:F:296:GLU:HB3	1.98	0.46
1:H:351:HIS:HD2	5:H:7488:HOH:O	1.99	0.46
1:D:459:HIS:HE1	5:D:5750:HOH:O	1.99	0.46
1:D:53:OMT:HE3	1:D:140:PHE:CZ	2.51	0.46
1:A:459:HIS:HD2	5:A:5578:HOH:O	1.97	0.45
1:C:459:HIS:HD2	5:C:5534:HOH:O	1.99	0.45
1:F:430:THR:O	1:F:434:GLN:HG3	2.15	0.45
1:H:359:CYS:HB2	1:H:360:PRO:HD2	1.97	0.45
1:B:483:ASN:CG	5:B:6994:HOH:O	2.60	0.45
1:F:363:SER:O	1:F:364:TYR:HB3	2.16	0.45
1:B:82:ILE:CD1	5:B:6929:HOH:O	2.57	0.45
1:D:239:SER:OG	1:D:240:HIS:HD2	1.99	0.45
1:A:187:THR:OG1	1:A:190:HIS:HD2	1.99	0.45
5:B:6717:HOH:O	1:D:350:GLN:HB3	2.16	0.45
1:B:302:GLN:NE2	5:B:6797:HOH:O	2.50	0.45
1:C:52:ARG:HE	1:C:52:ARG:HA	1.82	0.45
1:F:54:HIS:CE1	1:F:95:VAL:HG22	2.52	0.45
1:F:239:SER:OG	1:F:240:HIS:HD2	1.99	0.45
1:A:30:LEU:HD23	1:D:30:LEU:HD23	1.98	0.45
1:D:318:VAL:HG13	1:D:322:ILE:O	2.16	0.44
1:H:314:ASN:C	1:H:314:ASN:HD22	2.25	0.44
1:D:432:GLU:HB3	5:D:5571:HOH:O	2.16	0.44
1:E:29:GLN:H	1:F:331:GLN:NE2	2.15	0.44
1:C:23:ALA:O	1:C:27:GLY:HA3	2.17	0.44
1:A:25:LYS:HD3	1:B:414:GLU:OE2	2.18	0.44
1:B:479:ILE:HA	1:B:482:TYR:CZ	2.52	0.44
2:C:485:HEM:HBB2	2:C:485:HEM:CMB	2.46	0.44
1:E:346:GLY:O	1:E:349:HIS:HD2	2.00	0.44
1:F:351:HIS:CD2	5:F:8538:HOH:O	2.61	0.44
1:H:314:ASN:ND2	1:H:316:ALA:H	2.16	0.44
1:E:314:ASN:C	1:E:314:ASN:HD22	2.26	0.44
1:C:106:ARG:HA	1:C:184:ILE:HG12	1.98	0.43
1:G:358:ARG:NH2	5:G:5918:HOH:O	2.51	0.43
1:H:387:GLN:NE2	5:H:7794:HOH:O	2.51	0.43
1:C:54:HIS:CE1	1:C:95:VAL:HG22	2.52	0.43
1:G:187:THR:OG1	1:G:190:HIS:CD2	2.71	0.43
1:H:480:SER:HA	1:H:483:ASN:HD22	1.84	0.43
1:A:318:VAL:HG11	1:A:322:ILE:O	2.18	0.43
1:G:346:GLY:O	1:G:349:HIS:HD2	2.01	0.43
1:G:331:GLN:HE21	1:H:29:GLN:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:HA	1:B:224:LEU:HG	2.01	0.43
1:B:239:SER:OG	1:B:240:HIS:HD2	2.02	0.43
1:E:372:VAL:HG21	1:G:372:VAL:HG21	2.01	0.42
1:G:362:HIS:HD2	5:G:5828:HOH:O	2.01	0.42
1:B:329:MET:O	1:B:333:ARG:HG3	2.20	0.42
1:D:150:ASP:HB3	1:D:153:THR:OG1	2.20	0.42
1:F:362:HIS:HD2	5:F:8617:HOH:O	2.03	0.42
1:B:314:ASN:ND2	1:B:316:ALA:H	2.17	0.42
1:C:338:GLY:HA3	3:C:5487:GOL:H2	2.01	0.42
2:G:485:HEM:CMB	2:G:485:HEM:HBB2	2.50	0.42
1:H:366:ARG:HA	1:H:366:ARG:HD2	1.90	0.42
1:A:251:GLN:HA	1:A:253:PHE:CE2	2.55	0.42
1:H:440:ASN:HD22	1:H:443:ARG:NH2	2.18	0.42
1:E:187:THR:OG1	1:E:190:HIS:CD2	2.69	0.42
1:G:387:GLN:NE2	5:G:5724:HOH:O	2.52	0.42
1:F:131:VAL:HG23	1:F:174:GLN:HE21	1.84	0.42
1:H:483:ASN:ND2	5:H:7874:HOH:O	2.53	0.41
1:A:166:THR:HB	1:A:455:ARG:HB3	2.02	0.41
1:H:118:GLU:HB2	5:H:7748:HOH:O	2.20	0.41
1:G:299:ARG:HD3	5:G:5873:HOH:O	2.20	0.41
1:H:61:TYR:HB2	1:H:299:ARG:HB3	2.01	0.41
1:B:30:LEU:HD23	1:C:30:LEU:HD23	2.03	0.41
1:D:61:TYR:HB2	1:D:299:ARG:HB3	2.03	0.41
1:F:23:ALA:O	1:F:27:GLY:HA3	2.21	0.41
1:G:93:SER:O	1:G:109:ARG:HA	2.20	0.41
1:C:253:PHE:CD2	1:C:298:ASN:HA	2.55	0.41
1:D:147:VAL:O	1:D:156:ARG:HD3	2.20	0.41
1:D:166:THR:HB	1:D:455:ARG:HB3	2.02	0.41
1:E:121:ASN:HD21	1:E:357:PRO:HA	1.86	0.41
1:E:314:ASN:ND2	1:E:316:ALA:H	2.19	0.41
1:F:135:ARG:HD2	1:F:412:HIS:ND1	2.35	0.41
1:F:159:LYS:C	1:F:159:LYS:HD3	2.46	0.41
1:H:186:ALA:HA	1:H:224:LEU:HG	2.02	0.41
1:B:53:OMT:HE3	1:B:140:PHE:CZ	2.56	0.41
1:E:318:VAL:HG13	1:E:322:ILE:O	2.20	0.41
1:E:338:GLY:HA3	3:E:5493:GOL:H2	2.02	0.41
1:D:148:LYS:HB3	1:D:149:ARG:H	1.79	0.41
1:D:387:GLN:CG	5:D:5647:HOH:O	2.54	0.41
1:A:255:LYS:HG2	1:A:296:GLU:CB	2.50	0.40
1:B:187:THR:OG1	1:B:190:HIS:CD2	2.67	0.40
1:C:440:ASN:HD22	1:C:443:ARG:NH2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:5719:HOH:O	1:H:252:ASP:HB2	2.21	0.40
1:E:459:HIS:HE1	5:E:5742:HOH:O	2.04	0.40
1:A:459:HIS:HE1	5:A:5883:HOH:O	2.03	0.40
1:E:239:SER:OG	1:E:240:HIS:HD2	2.04	0.40
1:G:338:GLY:HA3	3:G:5491:GOL:H2	2.03	0.40
1:B:185:PRO:O	1:B:240:HIS:HE1	2.05	0.40
1:E:363:SER:O	1:E:364:TYR:HB3	2.22	0.40
1:D:251:GLN:HA	1:D:253:PHE:CE2	2.56	0.40
1:G:3:SER:HA	5:G:5810:HOH:O	2.21	0.40
1:G:419:PHE:C	1:G:422:PRO:HD2	2.46	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	482/483 (100%)	466 (97%)	16 (3%)	0	100	100
1	B	482/483 (100%)	463 (96%)	17 (4%)	2 (0%)	30	20
1	C	482/483 (100%)	462 (96%)	20 (4%)	0	100	100
1	D	482/483 (100%)	465 (96%)	15 (3%)	2 (0%)	30	20
1	E	481/483 (100%)	463 (96%)	18 (4%)	0	100	100
1	F	482/483 (100%)	462 (96%)	18 (4%)	2 (0%)	30	20
1	G	481/483 (100%)	465 (97%)	16 (3%)	0	100	100
1	H	482/483 (100%)	465 (96%)	17 (4%)	0	100	100
All	All	3854/3864 (100%)	3711 (96%)	137 (4%)	6 (0%)	48	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	99[A]	ARG
1	F	99[B]	ARG
1	B	99[A]	ARG
1	B	99[B]	ARG
1	D	99[A]	ARG
1	D	99[B]	ARG

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 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	407/406 (100%)	397 (98%)	10 (2%)	42	33
1	B	407/406 (100%)	400 (98%)	7 (2%)	53	48
1	C	407/406 (100%)	396 (97%)	11 (3%)	39	31
1	D	407/406 (100%)	394 (97%)	13 (3%)	34	24
1	E	406/406 (100%)	397 (98%)	9 (2%)	45	38
1	F	407/406 (100%)	397 (98%)	10 (2%)	42	33
1	G	406/406 (100%)	396 (98%)	10 (2%)	42	33
1	H	407/406 (100%)	394 (97%)	13 (3%)	34	24
All	All	3254/3248 (100%)	3171 (97%)	83 (3%)	42	32

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	204	SER
1	A	289	LEU
1	A	318	VAL
1	A	403	LEU
1	A	428	LEU
1	A	437	LEU
1	A	444	ASN
1	A	454	LEU
1	A	455	ARG

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Mol	Chain	Res	Type
1	B	117	THR
1	B	204	SER
1	B	318	VAL
1	B	403	LEU
1	B	437	LEU
1	B	444	ASN
1	B	454	LEU
1	C	99[A]	ARG
1	C	99[B]	ARG
1	C	112	SER
1	C	117	THR
1	C	289	LEU
1	C	318	VAL
1	C	403	LEU
1	C	437	LEU
1	C	444	ASN
1	C	454	LEU
1	C	455	ARG
1	D	99[A]	ARG
1	D	99[B]	ARG
1	D	117	THR
1	D	285	LYS
1	D	289	LEU
1	D	318	VAL
1	D	403	LEU
1	D	428	LEU
1	D	432	GLU
1	D	437	LEU
1	D	444	ASN
1	D	454	LEU
1	D	455	ARG
1	E	117	THR
1	E	201	PHE
1	E	204	SER
1	E	289	LEU
1	E	318	VAL
1	E	403	LEU
1	E	437	LEU
1	E	454	LEU
1	E	455	ARG
1	F	117	THR
1	F	129	THR

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Mol	Chain	Res	Type
1	F	289	LEU
1	F	318	VAL
1	F	403	LEU
1	F	432	GLU
1	F	437	LEU
1	F	444	ASN
1	F	454	LEU
1	F	455	ARG
1	G	117	THR
1	G	129	THR
1	G	289	LEU
1	G	318	VAL
1	G	358	ARG
1	G	403	LEU
1	G	432	GLU
1	G	437	LEU
1	G	444	ASN
1	G	455	ARG
1	H	3	SER
1	H	117	THR
1	H	187	THR
1	H	289	LEU
1	H	302	GLN
1	H	318	VAL
1	H	403	LEU
1	H	432	GLU
1	H	437	LEU
1	H	444	ASN
1	H	454	LEU
1	H	455	ARG
1	H	484	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	32	GLN
1	A	121	ASN
1	A	174	GLN
1	A	190	HIS
1	A	218	GLN
1	A	223	ASN

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Mol	Chain	Res	Type
1	A	235	ASN
1	A	240	HIS
1	A	250	ASN
1	A	284	HIS
1	A	300	ASN
1	A	314	ASN
1	A	331	GLN
1	A	349	HIS
1	A	351	HIS
1	A	362	HIS
1	A	402	ASN
1	A	440	ASN
1	A	446	ASN
1	A	459	HIS
1	B	32	GLN
1	B	121	ASN
1	B	160	ASN
1	B	174	GLN
1	B	190	HIS
1	B	223	ASN
1	B	235	ASN
1	B	240	HIS
1	B	250	ASN
1	B	300	ASN
1	B	314	ASN
1	B	317	ASN
1	B	331	GLN
1	B	349	HIS
1	B	351	HIS
1	B	362	HIS
1	B	402	ASN
1	B	440	ASN
1	B	446	ASN
1	B	459	HIS
1	B	483	ASN
1	C	32	GLN
1	C	121	ASN
1	C	160	ASN
1	C	174	GLN
1	C	190	HIS
1	C	235	ASN
1	C	240	HIS

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Mol	Chain	Res	Type
1	C	250	ASN
1	C	300	ASN
1	C	314	ASN
1	C	317	ASN
1	C	331	GLN
1	C	349	HIS
1	C	351	HIS
1	C	362	HIS
1	C	402	ASN
1	C	440	ASN
1	C	459	HIS
1	D	32	GLN
1	D	121	ASN
1	D	160	ASN
1	D	190	HIS
1	D	218	GLN
1	D	223	ASN
1	D	240	HIS
1	D	250	ASN
1	D	300	ASN
1	D	314	ASN
1	D	317	ASN
1	D	331	GLN
1	D	349	HIS
1	D	351	HIS
1	D	362	HIS
1	D	402	ASN
1	D	440	ASN
1	D	459	HIS
1	E	21	GLN
1	E	121	ASN
1	E	174	GLN
1	E	190	HIS
1	E	218	GLN
1	E	235	ASN
1	E	240	HIS
1	E	250	ASN
1	E	284	HIS
1	E	300	ASN
1	E	302	GLN
1	E	314	ASN
1	E	317	ASN

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Mol	Chain	Res	Type
1	E	331	GLN
1	E	349	HIS
1	E	350	GLN
1	E	351	HIS
1	E	362	HIS
1	E	402	ASN
1	E	440	ASN
1	E	459	HIS
1	F	21	GLN
1	F	121	ASN
1	F	161	ASN
1	F	174	GLN
1	F	190	HIS
1	F	240	HIS
1	F	250	ASN
1	F	284	HIS
1	F	300	ASN
1	F	314	ASN
1	F	317	ASN
1	F	331	GLN
1	F	349	HIS
1	F	351	HIS
1	F	362	HIS
1	F	402	ASN
1	F	440	ASN
1	F	459	HIS
1	G	32	GLN
1	G	68	HIS
1	G	121	ASN
1	G	174	GLN
1	G	190	HIS
1	G	235	ASN
1	G	240	HIS
1	G	250	ASN
1	G	300	ASN
1	G	314	ASN
1	G	317	ASN
1	G	349	HIS
1	G	351	HIS
1	G	362	HIS
1	G	393	GLN
1	G	402	ASN

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Mol	Chain	Res	Type
1	G	440	ASN
1	G	459	HIS
1	H	32	GLN
1	H	121	ASN
1	H	160	ASN
1	H	174	GLN
1	H	190	HIS
1	H	235	ASN
1	H	240	HIS
1	H	250	ASN
1	H	251	GLN
1	H	284	HIS
1	H	300	ASN
1	H	314	ASN
1	H	317	ASN
1	H	349	HIS
1	H	351	HIS
1	H	362	HIS
1	H	402	ASN
1	H	440	ASN
1	H	446	ASN
1	H	459	HIS
1	H	483	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues 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
1	OMT	F	53	1	8,9,10	2.98	2 (25%)	6,12,14	2.49	2 (33%)
1	OMT	H	53	1	8,9,10	3.05	3 (37%)	6,12,14	1.95	2 (33%)
1	OMT	B	53	1	8,9,10	2.92	2 (25%)	6,12,14	2.48	2 (33%)
1	OMT	C	53	1	8,9,10	2.99	3 (37%)	6,12,14	3.01	4 (66%)
1	OMT	E	53	1	8,9,10	3.34	2 (25%)	6,12,14	2.42	3 (50%)
1	OMT	G	53	1	8,9,10	3.10	2 (25%)	6,12,14	2.32	2 (33%)
1	OMT	A	53	1	8,9,10	3.33	3 (37%)	6,12,14	2.79	3 (50%)
1	OMT	D	53	1	8,9,10	3.08	2 (25%)	6,12,14	3.09	3 (50%)

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
1	OMT	F	53	1	-	4/7/8/10	-
1	OMT	H	53	1	-	5/7/8/10	-
1	OMT	B	53	1	-	3/7/8/10	-
1	OMT	C	53	1	-	4/7/8/10	-
1	OMT	E	53	1	-	3/7/8/10	-
1	OMT	G	53	1	-	2/7/8/10	-
1	OMT	A	53	1	-	3/7/8/10	-
1	OMT	D	53	1	-	3/7/8/10	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	OMT	CG-SD	-8.86	1.67	1.78
1	A	53	OMT	CG-SD	-8.58	1.67	1.78
1	G	53	OMT	CG-SD	-8.16	1.68	1.78
1	D	53	OMT	CG-SD	-8.01	1.68	1.78
1	H	53	OMT	CG-SD	-7.97	1.68	1.78
1	F	53	OMT	CG-SD	-7.74	1.68	1.78
1	C	53	OMT	CG-SD	-7.63	1.68	1.78
1	B	53	OMT	CG-SD	-7.46	1.68	1.78
1	B	53	OMT	CE-SD	-3.03	1.65	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	53	OMT	CE-SD	-2.98	1.65	1.75
1	A	53	OMT	CE-SD	-2.72	1.66	1.75
1	C	53	OMT	CE-SD	-2.50	1.67	1.75
1	E	53	OMT	CE-SD	-2.49	1.67	1.75
1	D	53	OMT	CE-SD	-2.48	1.67	1.75
1	G	53	OMT	CE-SD	-2.35	1.67	1.75
1	H	53	OMT	CE-SD	-2.32	1.67	1.75
1	A	53	OMT	CB-CG	2.30	1.54	1.52
1	C	53	OMT	CB-CG	2.28	1.54	1.52
1	H	53	OMT	CB-CG	2.01	1.54	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	OMT	OD2-SD-OD1	-4.95	107.94	117.22
1	A	53	OMT	OD2-SD-OD1	-4.86	108.10	117.22
1	B	53	OMT	OD2-SD-OD1	-4.64	108.51	117.22
1	G	53	OMT	OD2-SD-OD1	-4.62	108.56	117.22
1	D	53	OMT	OD2-SD-CG	4.60	111.65	108.33
1	F	53	OMT	OD2-SD-OD1	-4.53	108.72	117.22
1	E	53	OMT	OD2-SD-OD1	-4.40	108.97	117.22
1	C	53	OMT	OD2-SD-OD1	-4.38	109.01	117.22
1	C	53	OMT	OD1-SD-CG	4.30	111.43	108.33
1	B	53	OMT	OD2-SD-CG	3.57	110.91	108.33
1	H	53	OMT	OD2-SD-OD1	-3.30	111.03	117.22
1	F	53	OMT	OD1-SD-CE	3.23	111.87	108.87
1	D	53	OMT	OD1-SD-CG	3.14	110.59	108.33
1	C	53	OMT	OD2-SD-CG	3.10	110.56	108.33
1	A	53	OMT	OD1-SD-CG	2.87	110.39	108.33
1	G	53	OMT	OD1-SD-CG	2.80	110.35	108.33
1	A	53	OMT	OD2-SD-CG	2.75	110.31	108.33
1	H	53	OMT	OD1-SD-CE	-2.56	106.49	108.87
1	C	53	OMT	OD1-SD-CE	-2.31	106.72	108.87
1	E	53	OMT	OD1-SD-CG	2.09	109.83	108.33
1	E	53	OMT	OD2-SD-CG	2.08	109.83	108.33

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	53	OMT	CB-CG-SD-OD1
1	B	53	OMT	CB-CG-SD-OD1

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Mol	Chain	Res	Type	Atoms
1	C	53	OMT	O-C-CA-CB
1	C	53	OMT	CB-CG-SD-OD1
1	D	53	OMT	C-CA-CB-CG
1	D	53	OMT	CB-CG-SD-OD1
1	E	53	OMT	O-C-CA-CB
1	E	53	OMT	CB-CG-SD-OD1
1	F	53	OMT	O-C-CA-CB
1	F	53	OMT	CB-CG-SD-OD2
1	G	53	OMT	O-C-CA-CB
1	G	53	OMT	CB-CG-SD-OD1
1	H	53	OMT	C-CA-CB-CG
1	H	53	OMT	O-C-CA-CB
1	H	53	OMT	CB-CG-SD-OD1
1	E	53	OMT	CB-CG-SD-OD2
1	H	53	OMT	CB-CG-SD-OD2
1	A	53	OMT	N-CA-CB-CG
1	B	53	OMT	N-CA-CB-CG
1	C	53	OMT	N-CA-CB-CG
1	D	53	OMT	N-CA-CB-CG
1	F	53	OMT	N-CA-CB-CG
1	H	53	OMT	N-CA-CB-CG
1	A	53	OMT	C-CA-CB-CG
1	B	53	OMT	C-CA-CB-CG
1	C	53	OMT	C-CA-CB-CG
1	F	53	OMT	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	53	OMT	2	0
1	B	53	OMT	1	0
1	D	53	OMT	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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$
2	HEM	E	486	1	50,50,50	1.99	11 (22%)	67,82,82	1.41	8 (11%)
2	HEM	A	486	1	50,50,50	2.02	10 (20%)	67,82,82	1.38	7 (10%)
2	HEM	F	486	1	50,50,50	1.95	10 (20%)	67,82,82	1.39	5 (7%)
2	HEM	G	485	1	50,50,50	2.05	10 (20%)	67,82,82	1.52	11 (16%)
3	GOL	H	5492	-	5,5,5	0.31	0	5,5,5	0.53	0
3	GOL	G	5491	-	5,5,5	0.21	0	5,5,5	0.54	0
2	HEM	D	485	1	50,50,50	1.99	8 (16%)	67,82,82	1.45	9 (13%)
3	GOL	D	5488	-	5,5,5	0.33	0	5,5,5	0.54	0
3	GOL	E	5493	-	5,5,5	0.27	0	5,5,5	0.47	0
2	HEM	H	485	1	50,50,50	1.89	8 (16%)	67,82,82	1.40	7 (10%)
3	GOL	A	5489	-	5,5,5	0.27	0	5,5,5	0.53	0
2	HEM	B	486	1	50,50,50	1.92	9 (18%)	67,82,82	1.43	7 (10%)
3	GOL	B	5490	-	5,5,5	0.33	0	5,5,5	0.66	0
2	HEM	C	485	1	50,50,50	1.97	10 (20%)	67,82,82	1.45	9 (13%)
3	GOL	F	5494	-	5,5,5	0.33	0	5,5,5	0.56	0
3	GOL	C	5487	-	5,5,5	0.27	0	5,5,5	0.41	0

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
2	HEM	E	486	1	-	4/14/54/54	-
2	HEM	A	486	1	-	4/14/54/54	-
2	HEM	F	486	1	-	4/14/54/54	-
2	HEM	G	485	1	-	5/14/54/54	-
3	GOL	H	5492	-	-	0/4/4/4	-
3	GOL	G	5491	-	-	4/4/4/4	-
2	HEM	D	485	1	-	4/14/54/54	-
3	GOL	D	5488	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	5493	-	-	4/4/4/4	-
2	HEM	H	485	1	-	5/14/54/54	-
3	GOL	A	5489	-	-	4/4/4/4	-
2	HEM	B	486	1	-	4/14/54/54	-
3	GOL	B	5490	-	-	0/4/4/4	-
2	HEM	C	485	1	-	4/14/54/54	-
3	GOL	F	5494	-	-	4/4/4/4	-
3	GOL	C	5487	-	-	4/4/4/4	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	486	HEM	C3D-C2D	8.47	1.55	1.36
2	G	485	HEM	C3D-C2D	7.90	1.53	1.36
2	E	486	HEM	C3D-C2D	7.68	1.53	1.36
2	D	485	HEM	C3D-C2D	7.61	1.53	1.36
2	C	485	HEM	C3D-C2D	7.56	1.53	1.36
2	F	486	HEM	C3D-C2D	7.54	1.53	1.36
2	B	486	HEM	C3D-C2D	7.52	1.53	1.36
2	H	485	HEM	C3D-C2D	7.30	1.52	1.36
2	G	485	HEM	FE-NB	6.47	2.14	1.94
2	A	486	HEM	FE-NB	6.20	2.14	1.94
2	C	485	HEM	FE-ND	5.75	2.12	1.94
2	F	486	HEM	FE-NB	5.74	2.12	1.94
2	D	485	HEM	FE-ND	5.47	2.11	1.94
2	E	486	HEM	FE-NB	5.25	2.11	1.94
2	C	485	HEM	FE-NB	5.06	2.10	1.94
2	F	486	HEM	FE-NC	5.05	2.11	1.95
2	H	485	HEM	FE-ND	4.97	2.10	1.94
2	D	485	HEM	FE-NA	4.54	2.10	1.95
2	G	485	HEM	FE-NC	4.45	2.09	1.95
2	D	485	HEM	FE-NC	4.44	2.09	1.95
2	E	486	HEM	FE-NC	4.39	2.09	1.95
2	A	486	HEM	FE-ND	4.33	2.08	1.94
2	B	486	HEM	FE-NC	4.28	2.09	1.95
2	B	486	HEM	FE-NA	4.22	2.09	1.95
2	D	485	HEM	FE-NB	3.98	2.07	1.94
2	B	486	HEM	FE-ND	3.96	2.07	1.94
2	H	485	HEM	FE-NA	3.95	2.08	1.95
2	E	486	HEM	FE-ND	3.95	2.07	1.94
2	B	486	HEM	FE-NB	3.84	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	485	HEM	FE-ND	3.74	2.06	1.94
2	H	485	HEM	FE-NC	3.67	2.07	1.95
2	F	486	HEM	FE-NA	3.54	2.06	1.95
2	E	486	HEM	FE-NA	3.47	2.06	1.95
2	H	485	HEM	FE-NB	3.42	2.05	1.94
2	A	486	HEM	FE-NA	3.39	2.06	1.95
2	H	485	HEM	CAB-C3B	3.22	1.56	1.47
2	C	485	HEM	FE-NA	3.20	2.05	1.95
2	E	486	HEM	CAC-C3C	3.20	1.55	1.47
2	C	485	HEM	CAB-C3B	3.20	1.55	1.47
2	G	485	HEM	CAC-C3C	3.12	1.55	1.47
2	E	486	HEM	CAB-C3B	3.11	1.55	1.47
2	G	485	HEM	CAB-C3B	3.06	1.55	1.47
2	B	486	HEM	CAB-C3B	3.02	1.55	1.47
2	D	485	HEM	CAB-C3B	2.98	1.55	1.47
2	G	485	HEM	FE-NA	2.96	2.04	1.95
2	D	485	HEM	CAC-C3C	2.96	1.55	1.47
2	A	486	HEM	CAB-C3B	2.94	1.55	1.47
2	C	485	HEM	FE-NC	2.93	2.04	1.95
2	C	485	HEM	CAC-C3C	2.90	1.55	1.47
2	B	486	HEM	CAC-C3C	2.88	1.55	1.47
2	A	486	HEM	CAC-C3C	2.87	1.55	1.47
2	F	486	HEM	CAB-C3B	2.85	1.55	1.47
2	H	485	HEM	CAC-C3C	2.85	1.55	1.47
2	F	486	HEM	CAC-C3C	2.80	1.54	1.47
2	A	486	HEM	FE-NC	2.73	2.04	1.95
2	F	486	HEM	FE-ND	2.64	2.03	1.94
2	E	486	HEM	CMC-C2C	2.63	1.56	1.50
2	B	486	HEM	CMA-C3A	2.57	1.56	1.50
2	G	485	HEM	CMC-C2C	2.57	1.56	1.50
2	C	485	HEM	CMC-C2C	2.55	1.56	1.50
2	E	486	HEM	CMB-C2B	2.38	1.55	1.50
2	A	486	HEM	CMC-C2C	2.36	1.55	1.50
2	B	486	HEM	CMB-C2B	2.35	1.55	1.50
2	D	485	HEM	CMA-C3A	2.35	1.55	1.50
2	F	486	HEM	CMA-C3A	2.31	1.55	1.50
2	C	485	HEM	CMA-C3A	2.29	1.55	1.50
2	H	485	HEM	CMA-C3A	2.24	1.55	1.50
2	F	486	HEM	CMC-C2C	2.23	1.55	1.50
2	E	486	HEM	CMD-C2D	2.23	1.55	1.50
2	F	486	HEM	CMB-C2B	2.16	1.55	1.50
2	A	486	HEM	CMB-C2B	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	485	HEM	CMA-C3A	2.14	1.55	1.50
2	E	486	HEM	CMA-C3A	2.12	1.55	1.50
2	A	486	HEM	CMA-C3A	2.11	1.55	1.50
2	G	485	HEM	CMB-C2B	2.06	1.55	1.50
2	C	485	HEM	CMB-C2B	2.06	1.55	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	486	HEM	C4D-ND-C1D	6.28	112.64	105.21
2	G	485	HEM	C4D-ND-C1D	5.94	112.25	105.21
2	C	485	HEM	C4D-ND-C1D	5.89	112.18	105.21
2	B	486	HEM	C4D-ND-C1D	5.82	112.11	105.21
2	F	486	HEM	C4D-ND-C1D	5.75	112.01	105.21
2	E	486	HEM	C4D-ND-C1D	5.73	111.99	105.21
2	D	485	HEM	C4D-ND-C1D	5.57	111.80	105.21
2	H	485	HEM	C4D-ND-C1D	5.30	111.48	105.21
2	H	485	HEM	CBA-CAA-C2A	-3.76	102.13	112.53
2	G	485	HEM	CBA-CAA-C2A	-3.70	102.30	112.53
2	B	486	HEM	CBA-CAA-C2A	-3.62	102.52	112.53
2	A	486	HEM	CBA-CAA-C2A	-3.35	103.27	112.53
2	E	486	HEM	CBA-CAA-C2A	-3.35	103.28	112.53
2	F	486	HEM	CAD-CBD-CGD	-3.28	104.98	113.67
2	D	485	HEM	CBA-CAA-C2A	-3.21	103.67	112.53
2	C	485	HEM	CBA-CAA-C2A	-3.18	103.74	112.53
2	E	486	HEM	CAD-CBD-CGD	-3.07	105.53	113.67
2	C	485	HEM	CAD-CBD-CGD	-3.05	105.57	113.67
2	H	485	HEM	CAD-CBD-CGD	-3.04	105.59	113.67
2	F	486	HEM	CBA-CAA-C2A	-2.95	104.38	112.53
2	G	485	HEM	C1B-NB-C4B	2.90	108.64	105.21
2	D	485	HEM	C1B-NB-C4B	2.76	108.47	105.21
2	D	485	HEM	C3B-C2B-C1B	2.63	108.38	106.41
2	H	485	HEM	C1B-NB-C4B	2.59	108.28	105.21
2	A	486	HEM	CAD-CBD-CGD	-2.53	106.96	113.67
2	E	486	HEM	C2A-C1A-NA	-2.51	107.36	110.15
2	D	485	HEM	C2A-C1A-NA	-2.50	107.38	110.15
2	E	486	HEM	C1B-NB-C4B	2.49	108.16	105.21
2	C	485	HEM	C2A-C1A-NA	-2.49	107.39	110.15
2	D	485	HEM	CAD-CBD-CGD	-2.47	107.12	113.67
2	E	486	HEM	CMD-C2D-C1D	2.46	128.88	125.03
2	B	486	HEM	C1B-NB-C4B	2.43	108.09	105.21
2	A	486	HEM	O1A-CGA-CBA	-2.37	115.56	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	485	HEM	CMD-C2D-C1D	2.36	128.72	125.03
2	G	485	HEM	CAD-CBD-CGD	-2.35	107.42	113.67
2	B	486	HEM	CAD-CBD-CGD	-2.34	107.46	113.67
2	G	485	HEM	C3B-C4B-NB	-2.33	107.79	109.47
2	G	485	HEM	C2A-C1A-NA	-2.33	107.56	110.15
2	H	485	HEM	CHA-C4D-ND	2.33	127.25	124.37
2	C	485	HEM	C1B-NB-C4B	2.33	107.96	105.21
2	E	486	HEM	C3D-C4D-ND	-2.30	107.65	110.17
2	E	486	HEM	C1D-C2D-C3D	-2.29	104.57	106.98
2	G	485	HEM	C3B-C2B-C1B	2.23	108.08	106.41
2	B	486	HEM	C3B-C2B-C1B	2.22	108.08	106.41
2	B	486	HEM	C2A-C1A-NA	-2.22	107.69	110.15
2	A	486	HEM	O2A-CGA-CBA	2.19	120.92	114.00
2	G	485	HEM	CAD-C3D-C4D	2.18	128.50	124.70
2	C	485	HEM	C3B-C2B-C1B	2.18	108.05	106.41
2	C	485	HEM	O1D-CGD-CBD	-2.17	116.22	123.09
2	F	486	HEM	C3B-C2B-C1B	2.17	108.04	106.41
2	D	485	HEM	C2B-C1B-NB	-2.16	107.35	109.84
2	G	485	HEM	CHD-C4C-NC	2.16	126.81	124.45
2	C	485	HEM	C3D-C4D-ND	-2.14	107.82	110.17
2	B	486	HEM	C3B-C4B-NB	-2.13	107.94	109.47
2	A	486	HEM	C1B-NB-C4B	2.11	107.71	105.21
2	H	485	HEM	O2A-CGA-CBA	2.08	120.56	114.00
2	D	485	HEM	O1D-CGD-CBD	-2.07	116.52	123.09
2	D	485	HEM	C3B-C4B-NB	-2.07	107.98	109.47
2	C	485	HEM	CAD-C3D-C4D	2.06	128.29	124.70
2	H	485	HEM	C3B-C2B-C1B	2.06	107.95	106.41
2	F	486	HEM	C1B-NB-C4B	2.04	107.62	105.21
2	G	485	HEM	C3D-C4D-ND	-2.03	107.94	110.17
2	A	486	HEM	C2A-C1A-NA	-2.01	107.92	110.15

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5489	GOL	O1-C1-C2-C3
3	A	5489	GOL	C1-C2-C3-O3
3	C	5487	GOL	C1-C2-C3-O3
3	C	5487	GOL	O2-C2-C3-O3
3	D	5488	GOL	C1-C2-C3-O3
3	E	5493	GOL	C1-C2-C3-O3
3	F	5494	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	F	5494	GOL	C1-C2-C3-O3
3	F	5494	GOL	O2-C2-C3-O3
3	G	5491	GOL	O1-C1-C2-C3
3	G	5491	GOL	C1-C2-C3-O3
3	F	5494	GOL	O1-C1-C2-O2
3	C	5487	GOL	O1-C1-C2-C3
3	E	5493	GOL	O1-C1-C2-C3
3	A	5489	GOL	O2-C2-C3-O3
3	G	5491	GOL	O1-C1-C2-O2
3	G	5491	GOL	O2-C2-C3-O3
3	A	5489	GOL	O1-C1-C2-O2
3	E	5493	GOL	O2-C2-C3-O3
3	C	5487	GOL	O1-C1-C2-O2
3	D	5488	GOL	O2-C2-C3-O3
3	E	5493	GOL	O1-C1-C2-O2
2	A	486	HEM	CAD-CBD-CGD-O2D
2	F	486	HEM	CAD-CBD-CGD-O2D
2	C	485	HEM	CAD-CBD-CGD-O1D
2	H	485	HEM	CAD-CBD-CGD-O1D
2	F	486	HEM	CAD-CBD-CGD-O1D
2	G	485	HEM	CAD-CBD-CGD-O1D
2	H	485	HEM	CAD-CBD-CGD-O2D
2	A	486	HEM	CAD-CBD-CGD-O1D
2	C	485	HEM	CAD-CBD-CGD-O2D
2	D	485	HEM	CAD-CBD-CGD-O2D
2	G	485	HEM	CAD-CBD-CGD-O2D
2	B	486	HEM	CAD-CBD-CGD-O2D
2	E	486	HEM	CAD-CBD-CGD-O1D
2	F	486	HEM	CAA-CBA-CGA-O1A
2	A	486	HEM	CAA-CBA-CGA-O1A
2	E	486	HEM	CAD-CBD-CGD-O2D
2	C	485	HEM	CAA-CBA-CGA-O1A
2	G	485	HEM	CAA-CBA-CGA-O1A
2	D	485	HEM	CAA-CBA-CGA-O1A
2	D	485	HEM	CAD-CBD-CGD-O1D
2	B	486	HEM	CAD-CBD-CGD-O1D
2	C	485	HEM	CAA-CBA-CGA-O2A
2	A	486	HEM	CAA-CBA-CGA-O2A
2	F	486	HEM	CAA-CBA-CGA-O2A
2	H	485	HEM	CAA-CBA-CGA-O1A
2	D	485	HEM	CAA-CBA-CGA-O2A
2	G	485	HEM	CAA-CBA-CGA-O2A

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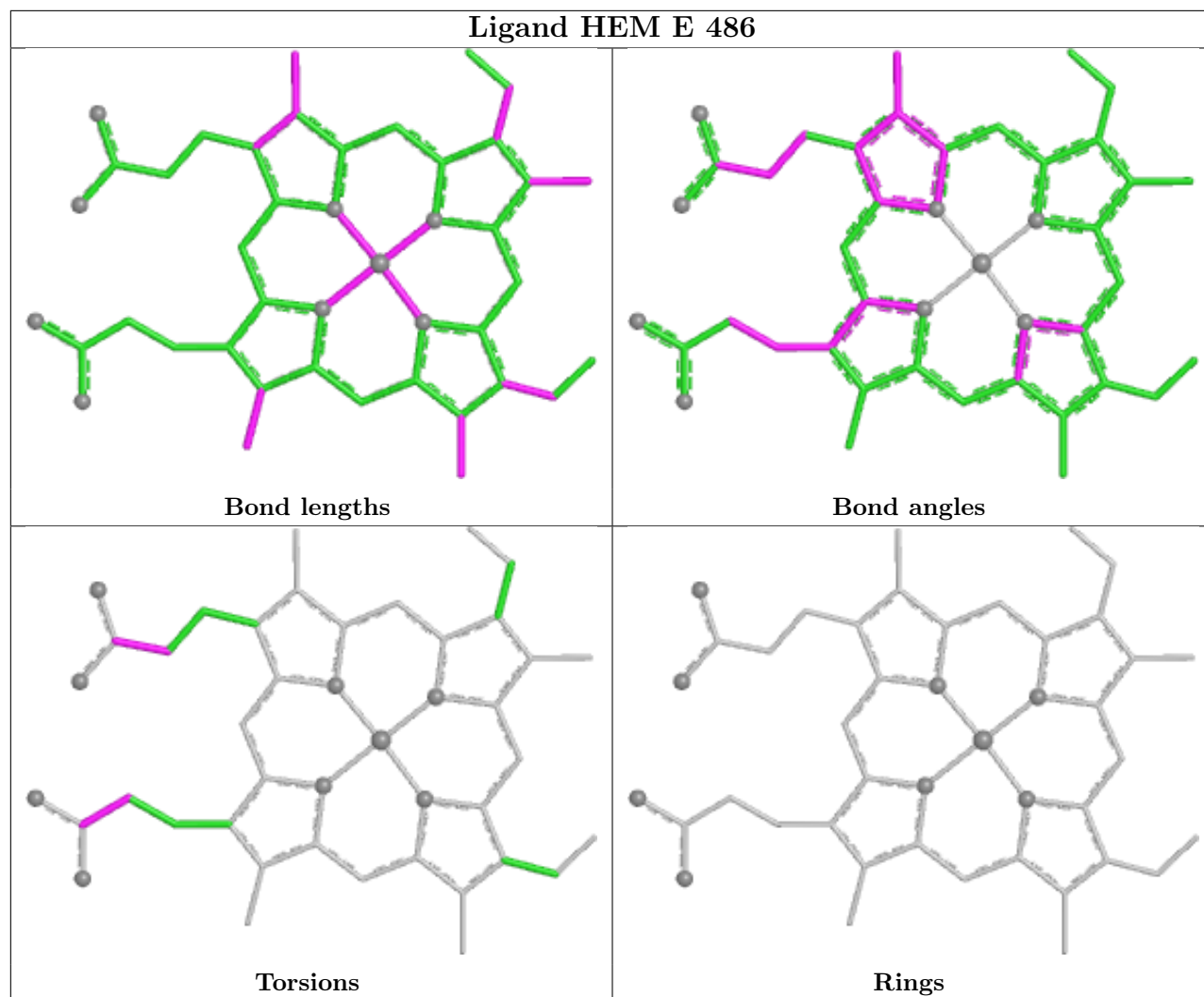
Mol	Chain	Res	Type	Atoms
2	B	486	HEM	CAA-CBA-CGA-O1A
2	E	486	HEM	CAA-CBA-CGA-O1A
2	E	486	HEM	CAA-CBA-CGA-O2A
2	B	486	HEM	CAA-CBA-CGA-O2A
2	H	485	HEM	CAA-CBA-CGA-O2A
2	G	485	HEM	C2C-C3C-CAC-CBC
2	H	485	HEM	C2C-C3C-CAC-CBC

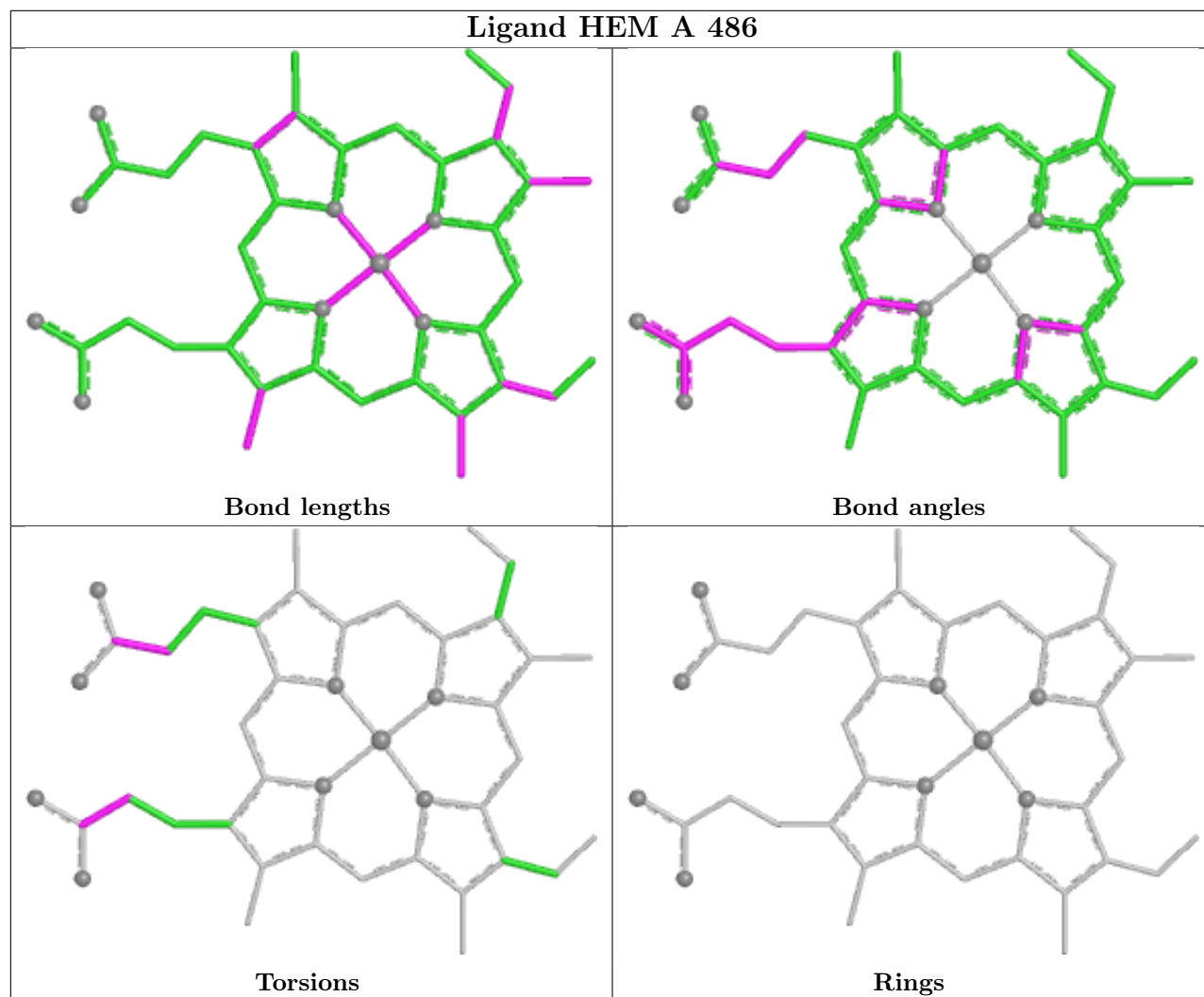
There are no ring outliers.

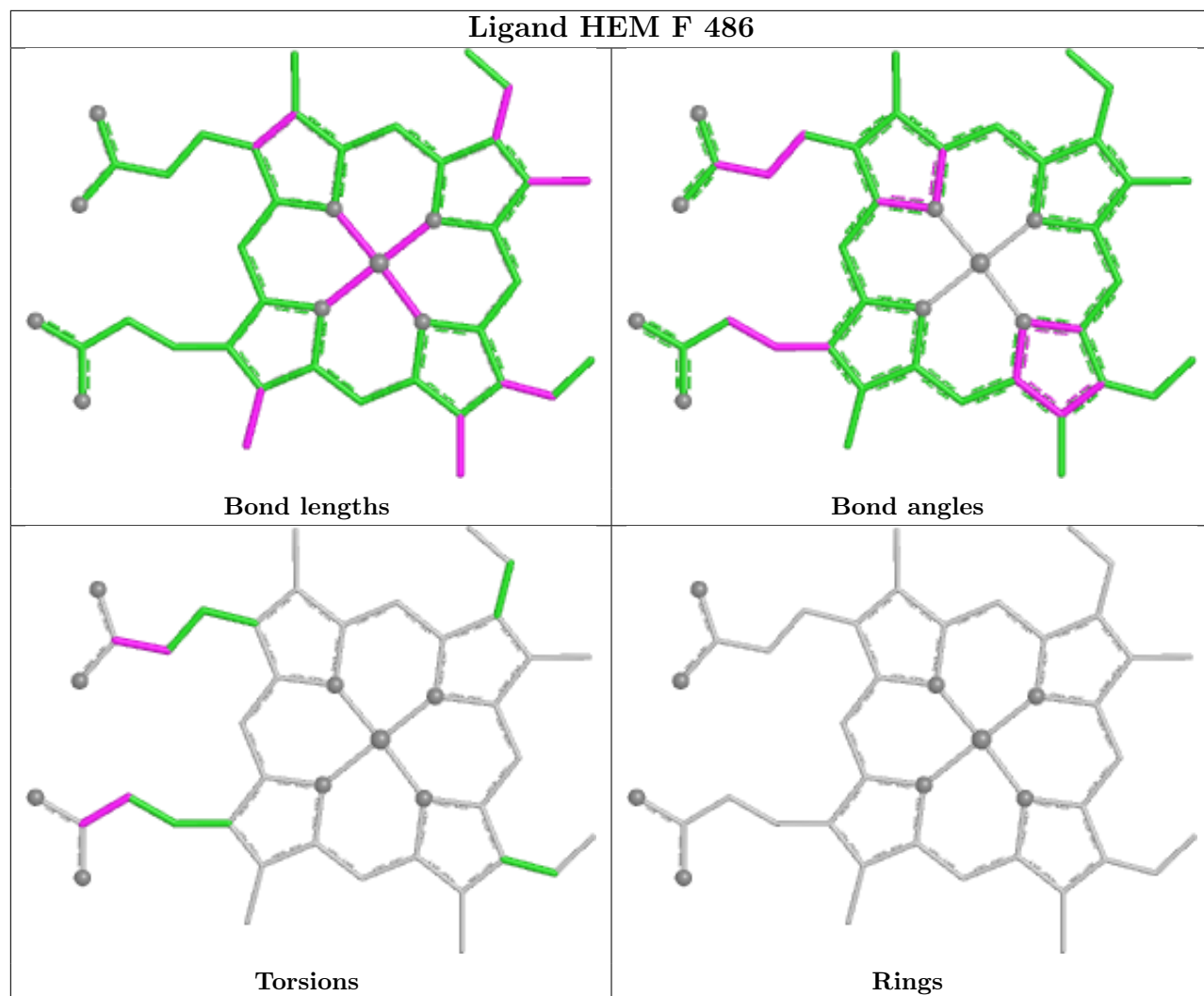
13 monomers are involved in 20 short contacts:

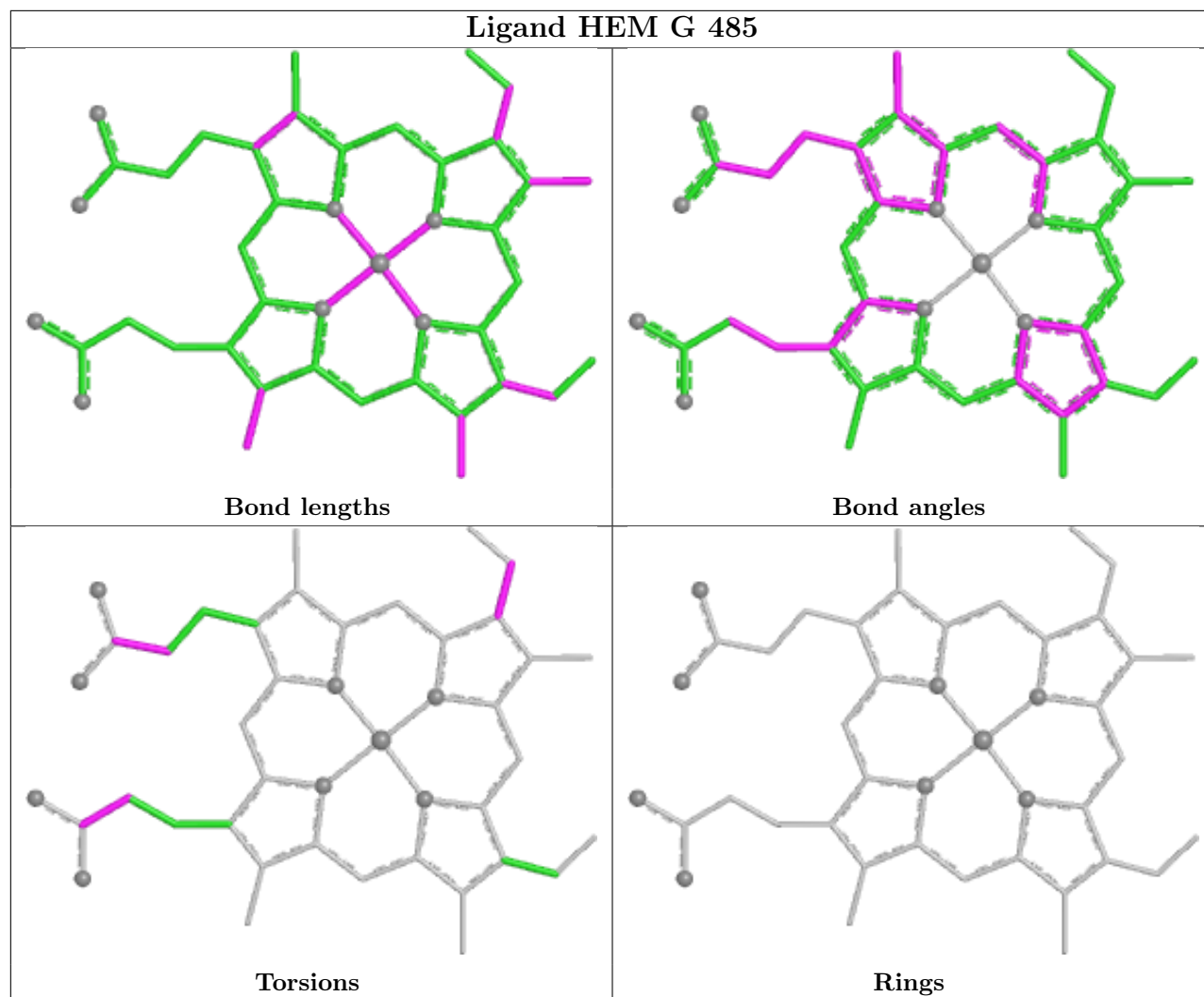
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	486	HEM	2	0
2	A	486	HEM	2	0
2	F	486	HEM	2	0
2	G	485	HEM	2	0
3	G	5491	GOL	1	0
2	D	485	HEM	1	0
3	E	5493	GOL	1	0
2	H	485	HEM	1	0
3	A	5489	GOL	1	0
2	B	486	HEM	2	0
2	C	485	HEM	3	0
3	F	5494	GOL	1	0
3	C	5487	GOL	1	0

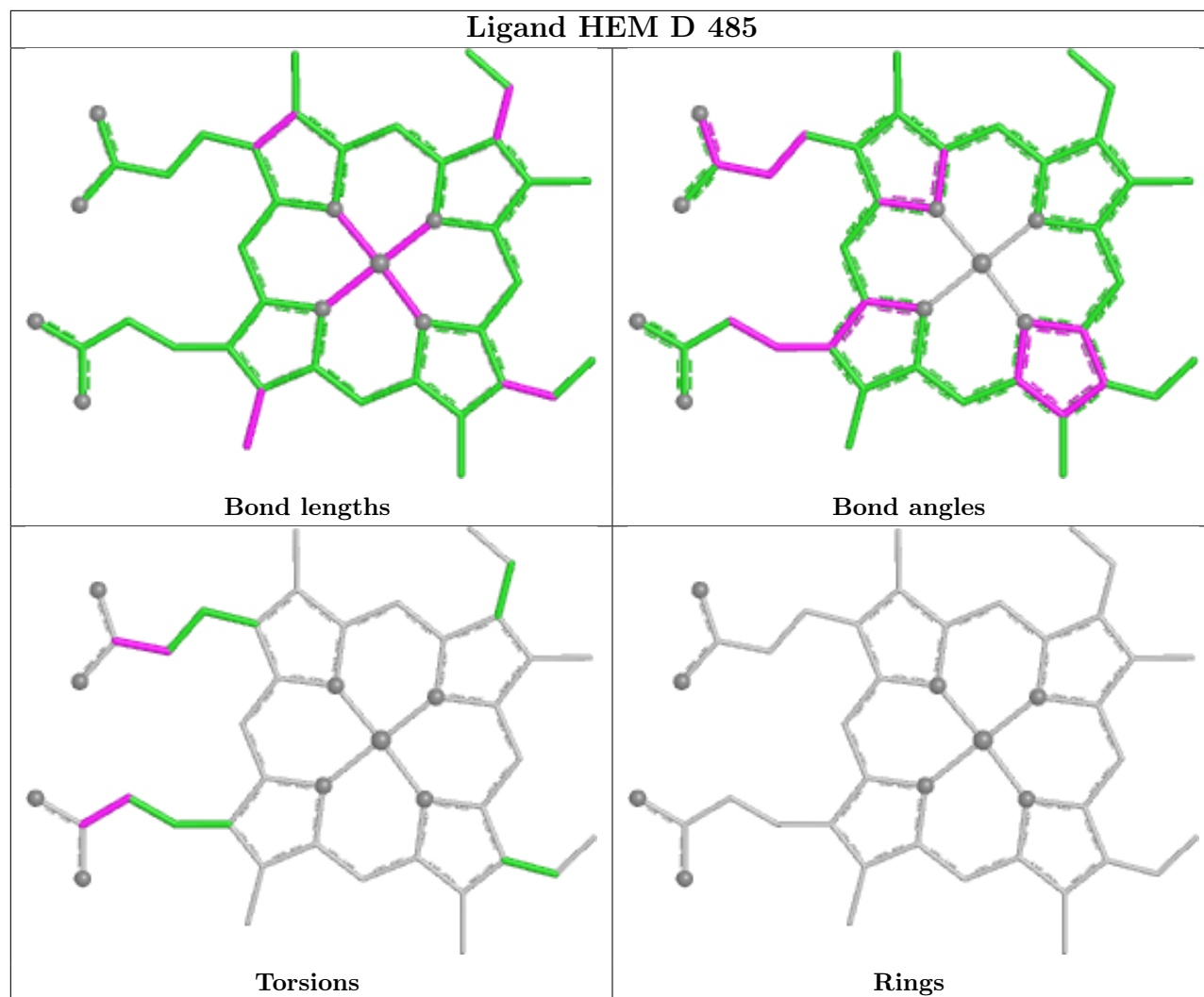
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

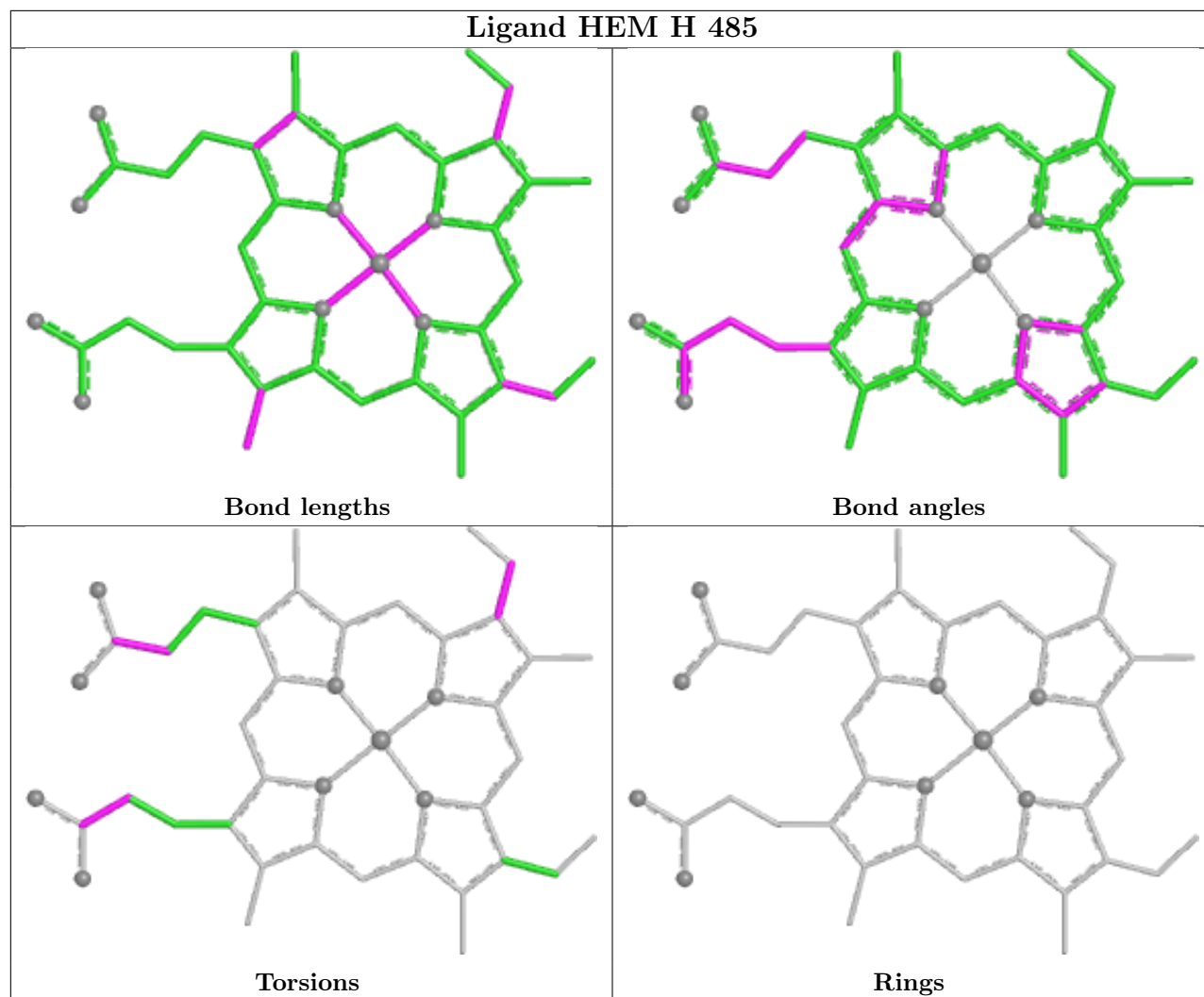


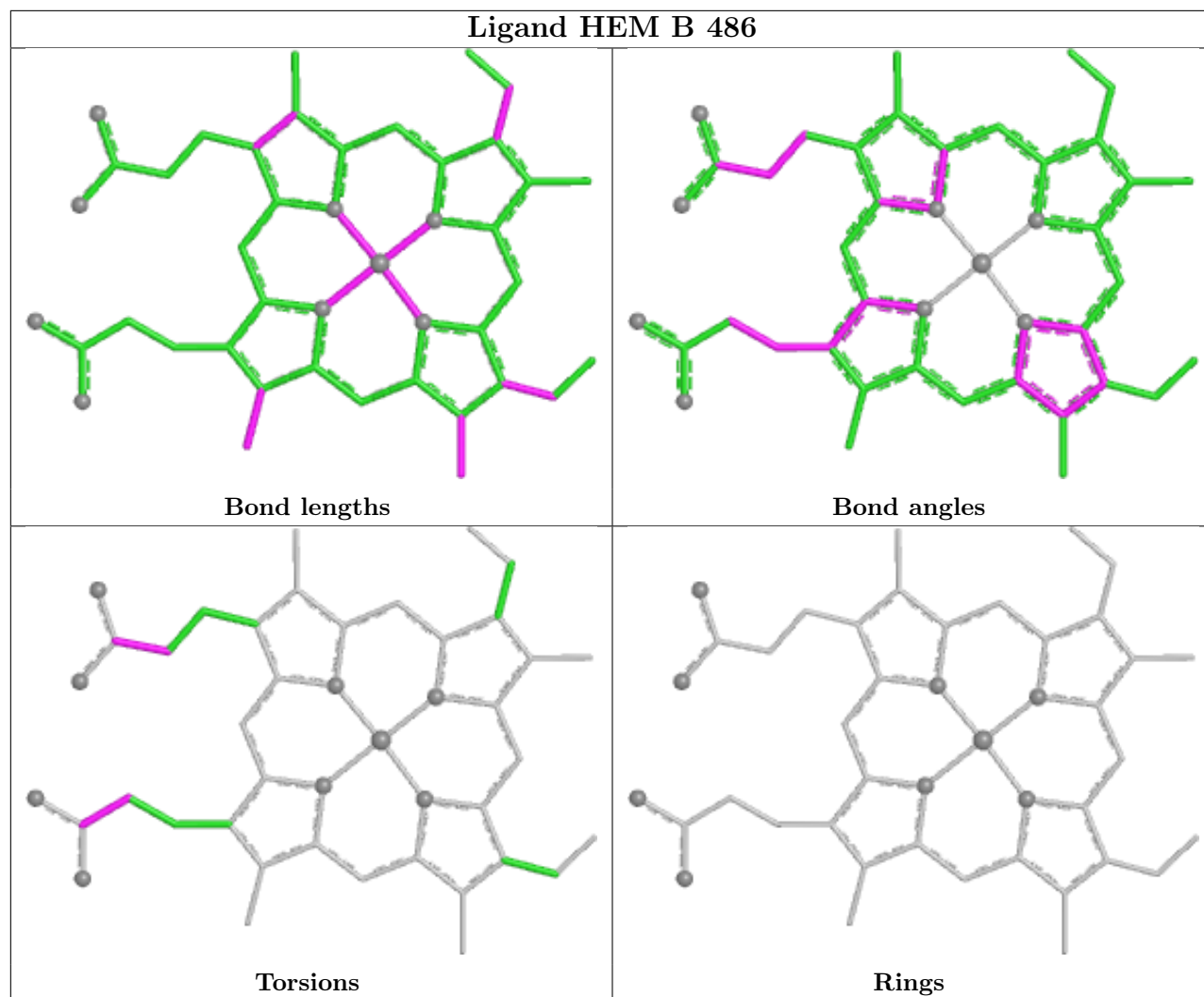


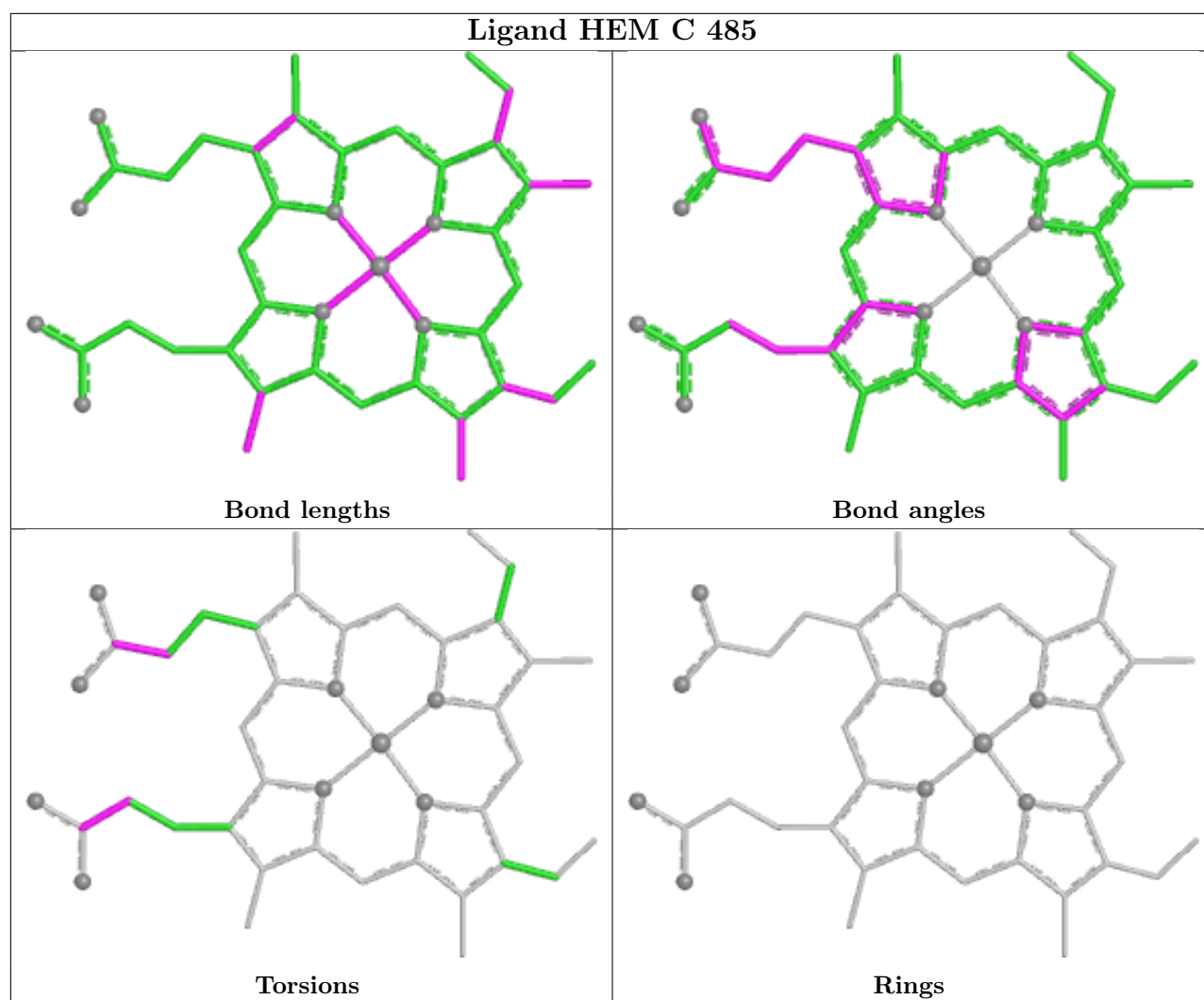












5.7 Other polymers [i](#)

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	481/483 (99%)	-0.78	0 100 100	5, 10, 20, 29	3 (0%)
1	B	481/483 (99%)	-0.72	1 (0%) 91 94	5, 11, 19, 30	4 (0%)
1	C	481/483 (99%)	-0.77	1 (0%) 91 94	4, 9, 20, 32	4 (0%)
1	D	481/483 (99%)	-0.73	0 100 100	4, 11, 21, 28	6 (1%)
1	E	481/483 (99%)	-0.60	1 (0%) 91 94	5, 13, 26, 36	4 (0%)
1	F	481/483 (99%)	-0.57	0 100 100	8, 14, 24, 32	6 (1%)
1	G	481/483 (99%)	-0.65	2 (0%) 88 92	6, 11, 23, 31	4 (0%)
1	H	481/483 (99%)	-0.64	1 (0%) 91 94	6, 12, 22, 32	5 (1%)
All	All	3848/3864 (99%)	-0.68	6 (0%) 91 94	4, 11, 22, 36	36 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	SER	6.7
1	C	483	ASN	2.7
1	B	204	SER	2.5
1	E	483	ASN	2.3
1	G	360	PRO	2.2
1	H	483	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	OMT	F	53	10/11	0.97	0.06	10,11,18,20	0
1	OMT	C	53	10/11	0.98	0.05	6,7,14,14	0
1	OMT	A	53	10/11	0.98	0.04	5,6,12,12	0
1	OMT	G	53	10/11	0.98	0.05	8,9,13,15	0
1	OMT	E	53	10/11	0.99	0.04	8,8,16,18	0
1	OMT	B	53	10/11	0.99	0.04	6,7,16,17	0
1	OMT	D	53	10/11	0.99	0.04	6,6,12,13	0
1	OMT	H	53	10/11	0.99	0.05	8,8,12,12	0

6.3 Carbohydrates [i](#)

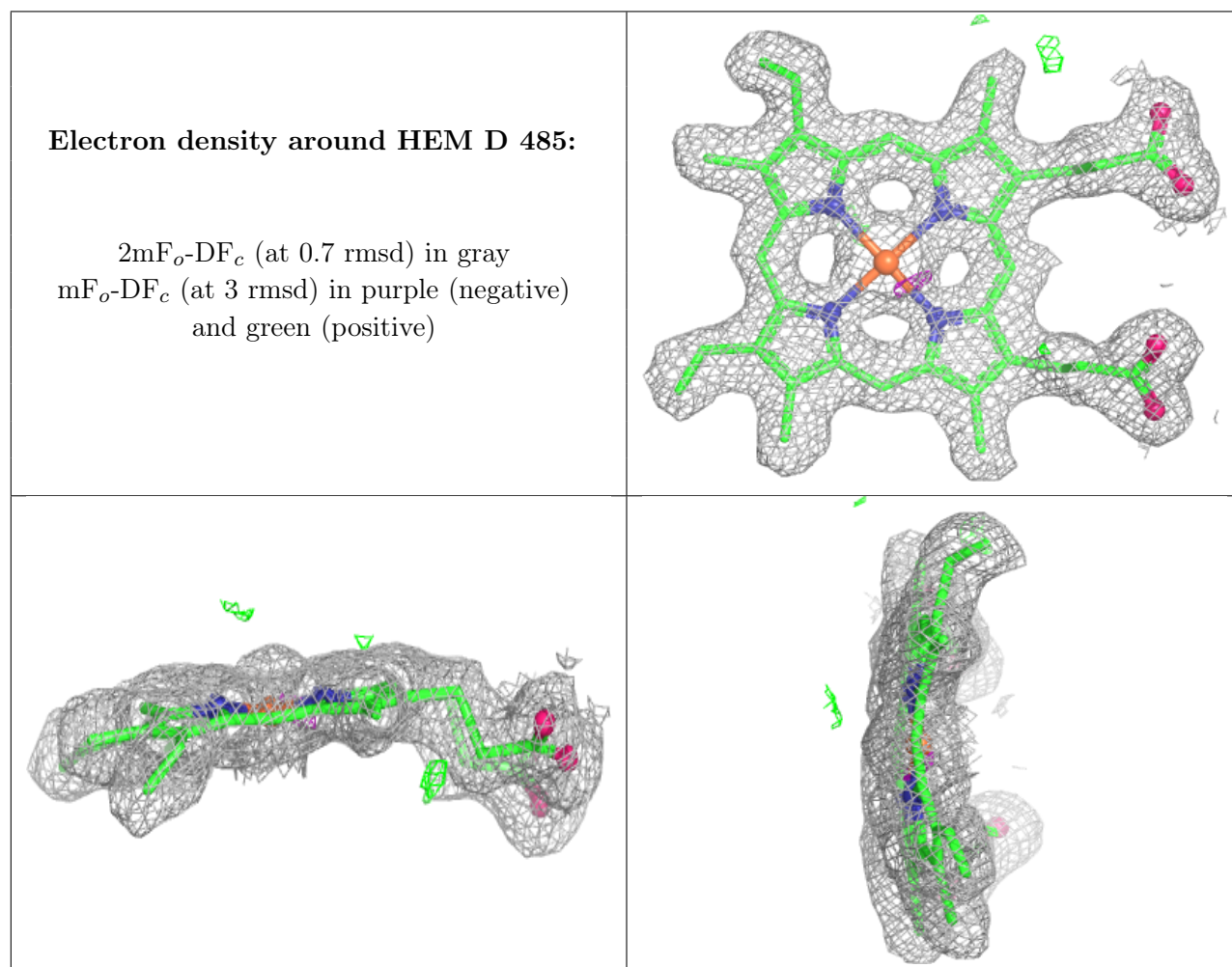
There are no oligosaccharides in this entry.

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.

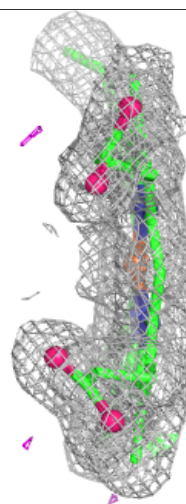
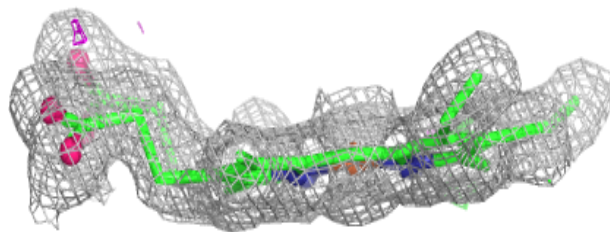
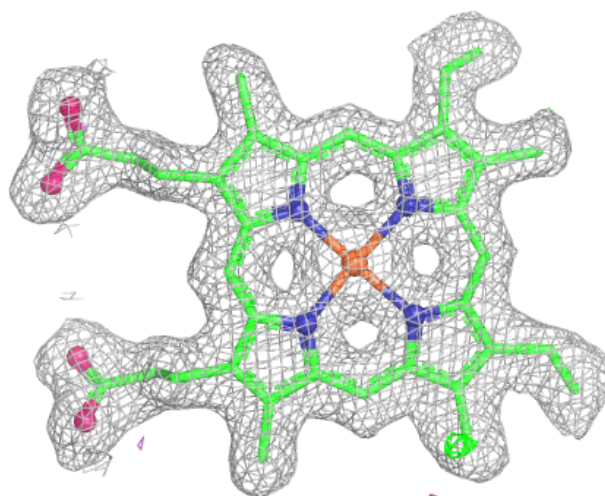
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	E	5493	6/6	0.86	0.11	18,21,22,22	0
3	GOL	G	5491	6/6	0.90	0.10	15,20,21,22	0
3	GOL	H	5492	6/6	0.90	0.09	18,21,22,25	0
3	GOL	D	5488	6/6	0.91	0.10	12,16,17,18	0
3	GOL	A	5489	6/6	0.92	0.09	10,17,18,18	0
3	GOL	C	5487	6/6	0.94	0.07	7,11,12,13	0
3	GOL	B	5490	6/6	0.95	0.07	13,17,17,20	0
3	GOL	F	5494	6/6	0.95	0.07	12,16,17,18	0
4	CL	H	7485	1/1	0.97	0.05	17,17,17,17	0
2	HEM	D	485	43/43	0.98	0.04	3,10,11,12	0
2	HEM	E	486	43/43	0.98	0.04	8,10,12,13	0
2	HEM	F	486	43/43	0.98	0.05	8,11,13,13	0
2	HEM	G	485	43/43	0.98	0.05	7,10,12,14	0
2	HEM	H	485	43/43	0.98	0.05	6,10,12,13	0
2	HEM	A	486	43/43	0.98	0.05	5,7,9,10	0
2	HEM	B	486	43/43	0.98	0.04	6,7,8,10	0
4	CL	B	6485	1/1	0.99	0.02	13,13,13,13	0
4	CL	D	5485	1/1	0.99	0.02	14,14,14,14	0
4	CL	F	8485	1/1	0.99	0.03	16,16,16,16	0
2	HEM	C	485	43/43	0.99	0.04	4,7,9,10	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.



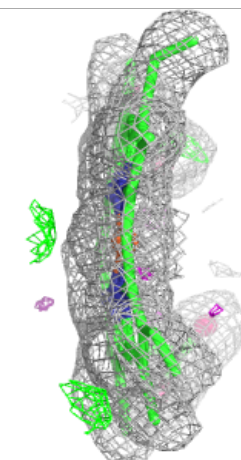
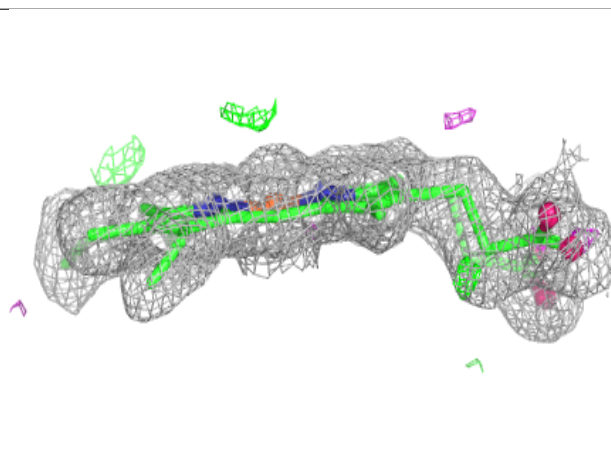
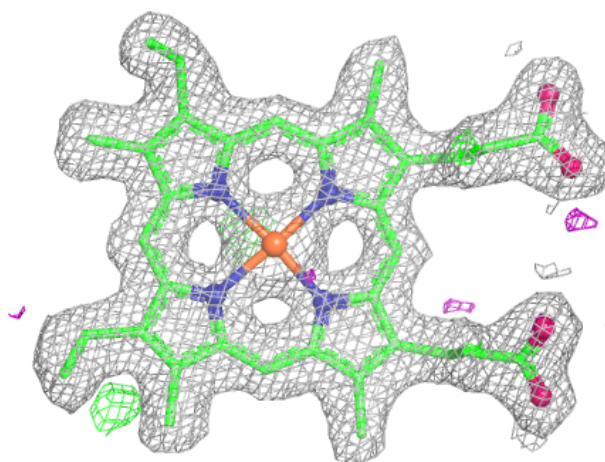
Electron density around HEM E 486:

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



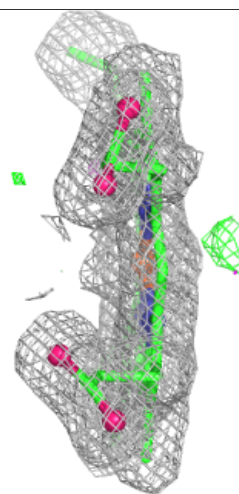
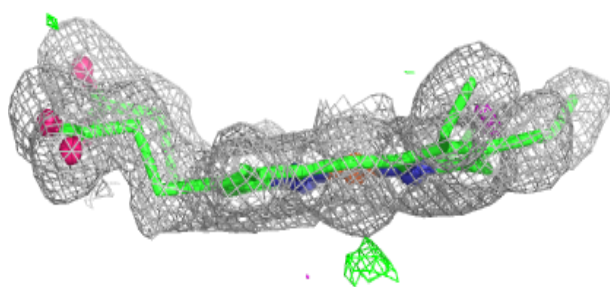
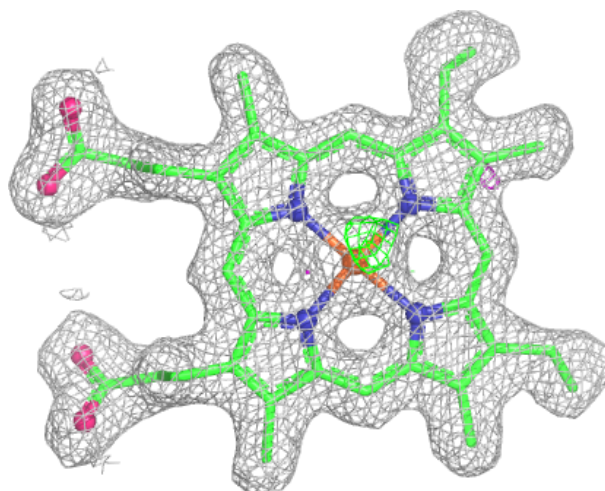
Electron density around HEM F 486:

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



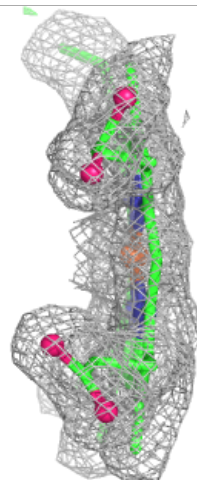
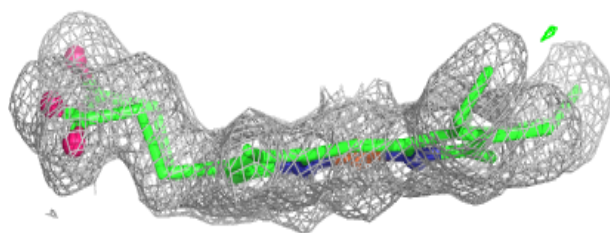
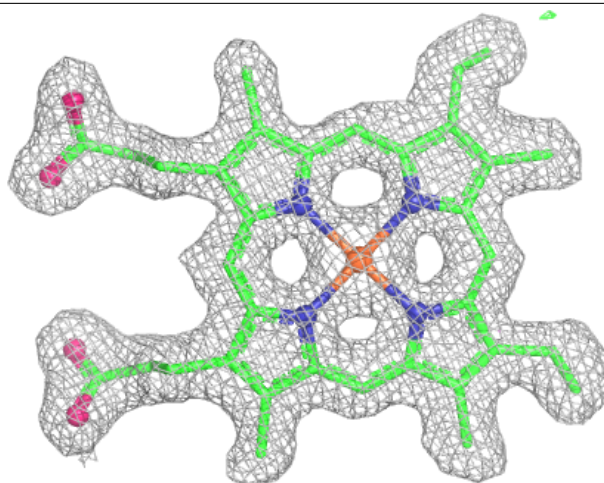
Electron density around HEM G 485:

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



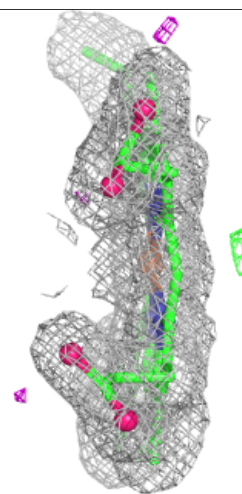
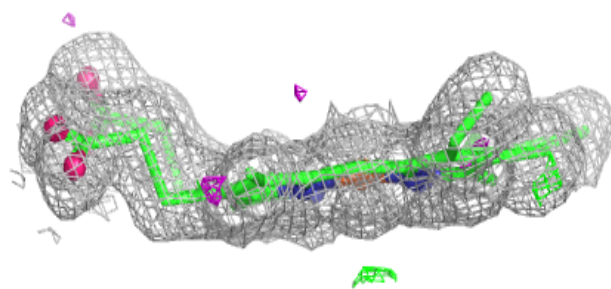
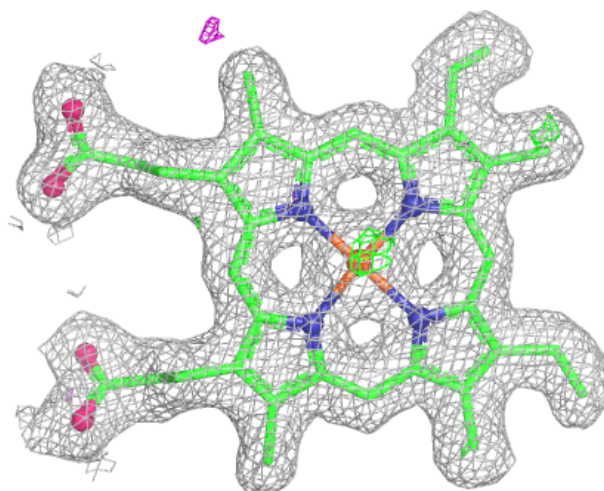
Electron density around HEM H 485:

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



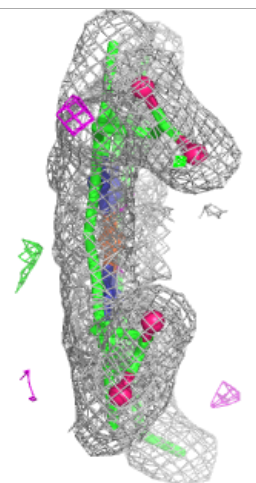
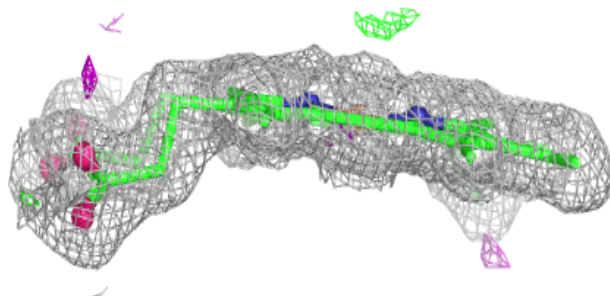
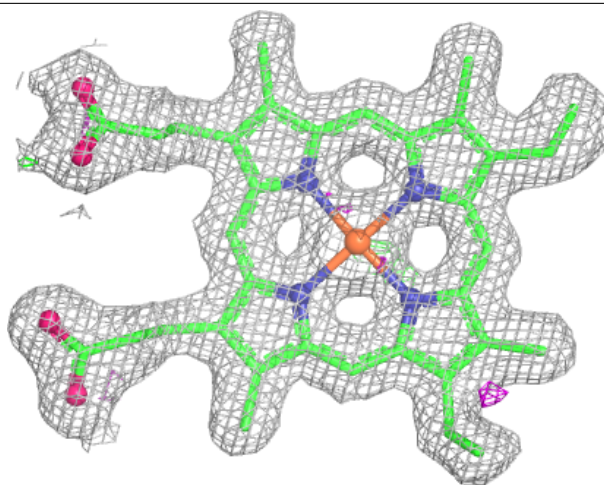
Electron density around HEM A 486:

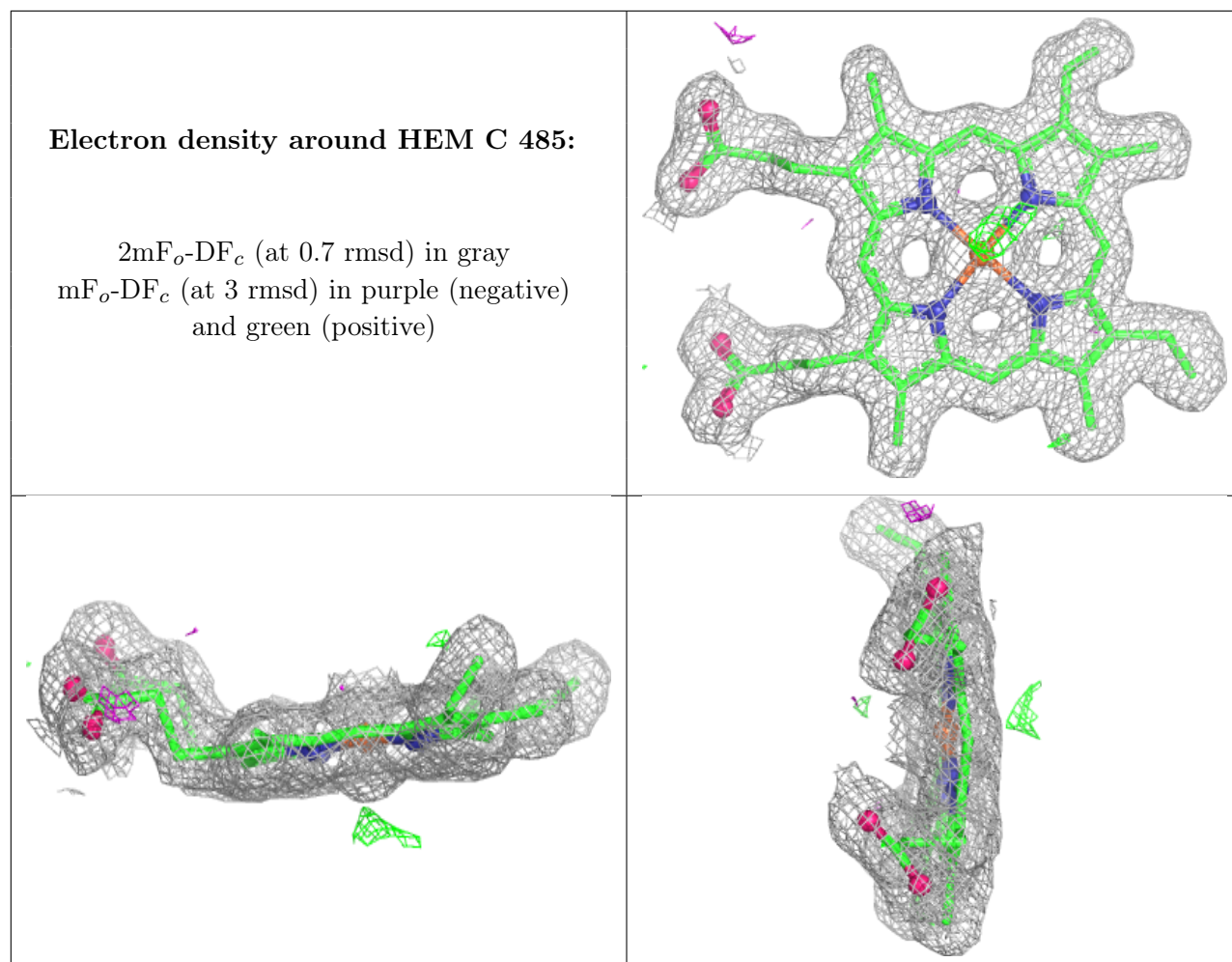
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 486:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.