



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 19, 2023 – 01:02 AM EDT

PDB ID : 2ISA
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

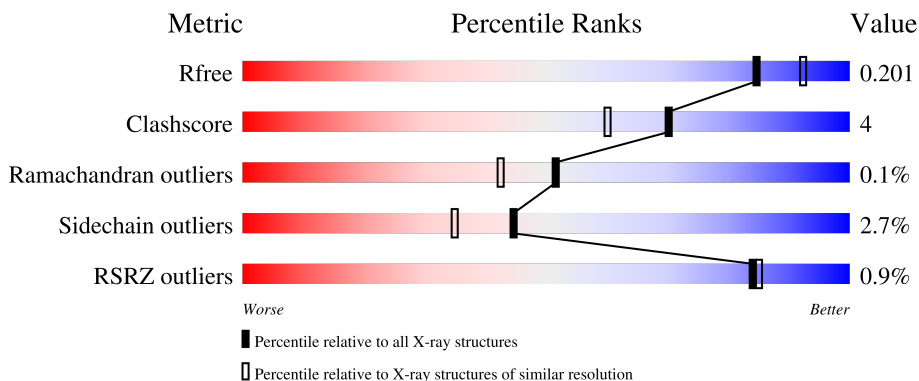
1 Overall quality at a glance i

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.



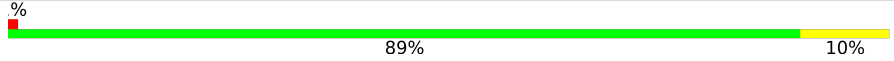
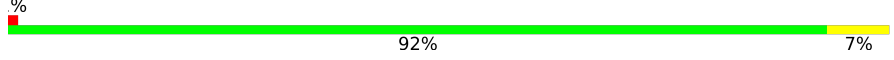
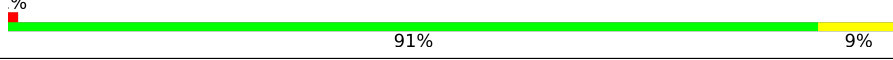
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	 91% 8%
1	B	483	 91% 9%
1	C	483	 90% 9% .
1	D	483	 89% 10% .
1	E	483	 93% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	483	 <p>% 89% 10%</p>
1	G	483	 <p>% 92% 7%</p>
1	H	483	 <p>% 91% 9%</p>

2 Entry composition [i](#)

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

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

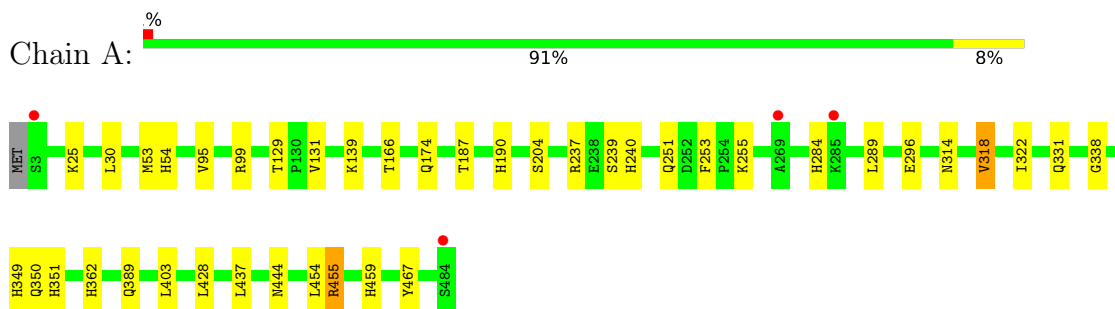
- Molecule 5 is water.

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

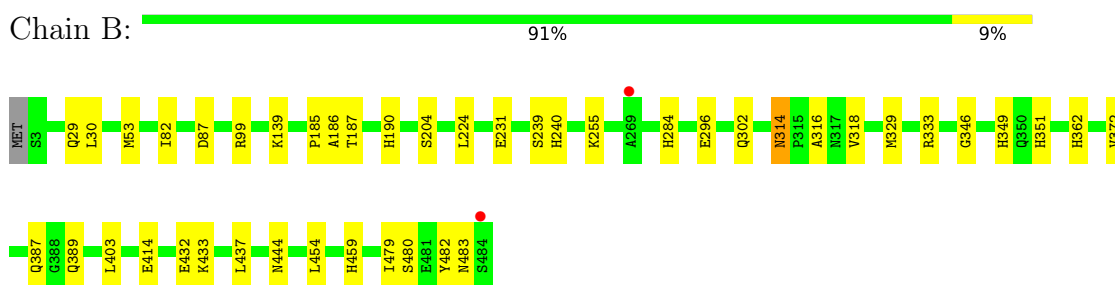
3 Residue-property plots

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.

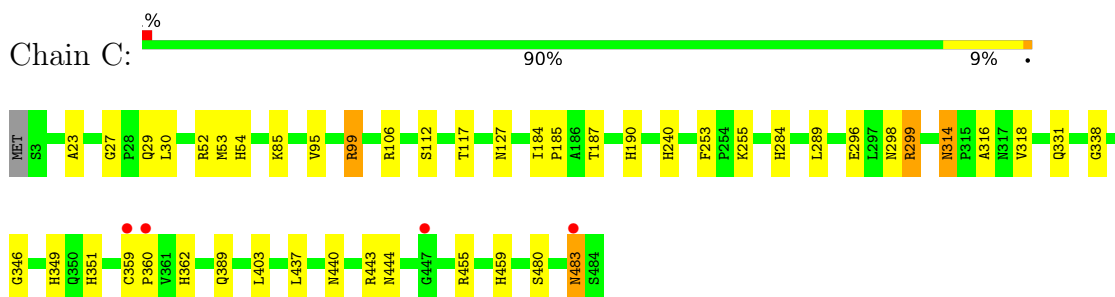
- Molecule 1: Catalase



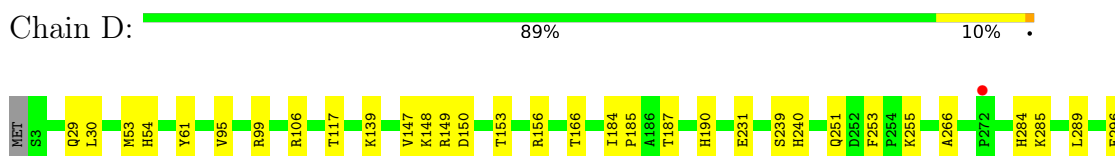
- Molecule 1: Catalase



- Molecule 1: Catalase

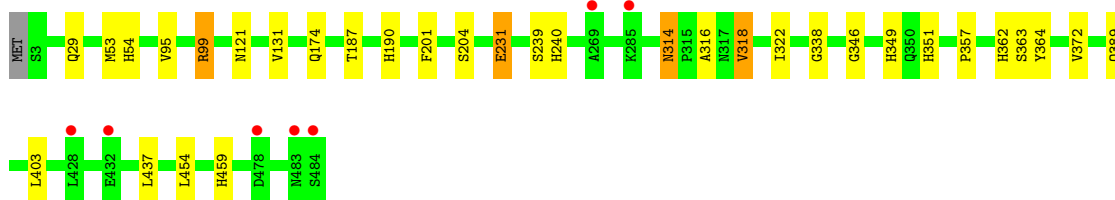
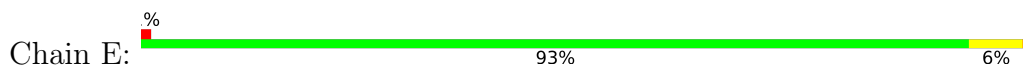


- Molecule 1: Catalase

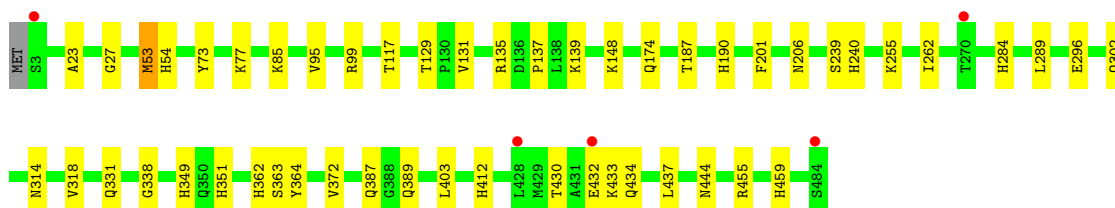
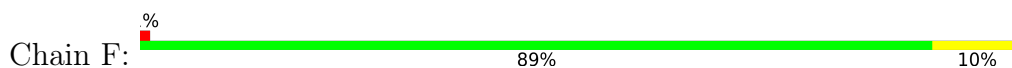




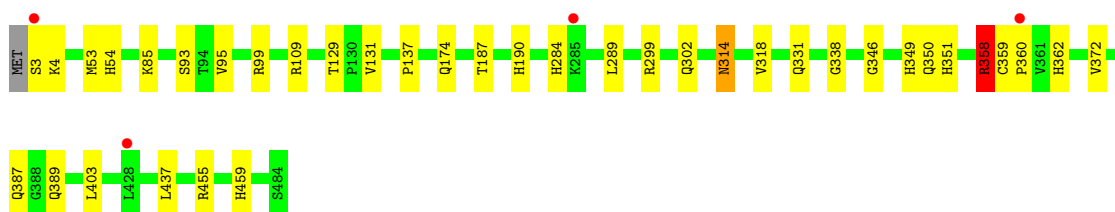
- Molecule 1: Catalase



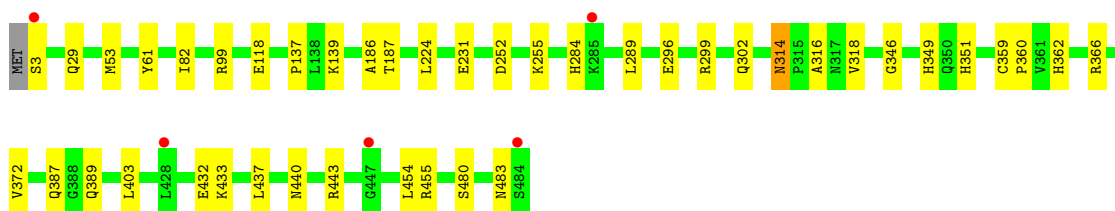
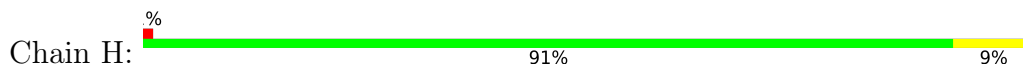
- Molecule 1: Catalase



- Molecule 1: Catalase



- 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 19.93 – 1.97	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-1.97) 96.5 (19.93-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.96Å)	Xtrriage
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 (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.027 for l,-k,h	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, OMT, GOL, HEM

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	0.52	0/3989	0.63	2/5411 (0.0%)
1	B	0.54	1/3987 (0.0%)	0.61	0/5408
1	C	0.65	1/3987 (0.0%)	1.09	5/5408 (0.1%)
1	D	0.52	1/3987 (0.0%)	0.63	3/5408 (0.1%)
1	E	0.71	1/3981 (0.0%)	0.68	3/5400 (0.1%)
1	F	0.50	1/3987 (0.0%)	0.63	3/5408 (0.1%)
1	G	1.30	4/3981 (0.1%)	0.80	9/5400 (0.2%)
1	H	0.55	1/3989 (0.0%)	0.66	4/5411 (0.1%)
All	All	0.71	10/31888 (0.0%)	0.73	29/43254 (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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	358	ARG	CZ-NH1	67.58	2.21	1.33
1	E	231	GLU	CD-OE1	31.67	1.60	1.25
1	C	299	ARG	NE-CZ	-24.75	1.00	1.33
1	G	358	ARG	NE-CZ	24.29	1.64	1.33
1	G	358	ARG	CZ-NH2	21.48	1.60	1.33
1	H	231	GLU	CG-CD	11.56	1.69	1.51
1	G	302	GLN	CG-CD	-7.61	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	231	GLU	CG-CD	7.31	1.62	1.51
1	F	302	GLN	CG-CD	-6.54	1.35	1.51
1	D	231	GLU	CG-CD	5.42	1.60	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ARG	NE-CZ-NH1	-48.48	96.06	120.30
1	C	299	ARG	NE-CZ-NH2	41.48	141.04	120.30
1	E	231	GLU	OE1-CD-OE2	-23.53	95.07	123.30
1	G	358	ARG	NH1-CZ-NH2	-23.48	93.57	119.40
1	C	299	ARG	CD-NE-CZ	17.39	147.94	123.60
1	G	358	ARG	NE-CZ-NH1	17.04	128.82	120.30
1	G	358	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	F	302	GLN	CG-CD-OE1	-11.00	99.61	121.60
1	F	302	GLN	CB-CG-CD	10.48	138.86	111.60
1	G	302	GLN	CB-CG-CD	10.48	138.84	111.60
1	G	302	GLN	CG-CD-OE1	-10.17	101.25	121.60
1	H	99[A]	ARG	C-N-CA	-9.72	101.88	122.30
1	H	99[B]	ARG	C-N-CA	-9.72	101.88	122.30
1	F	302	GLN	CG-CD-NE2	8.76	137.72	116.70
1	G	358	ARG	CD-NE-CZ	8.46	135.45	123.60
1	G	302	GLN	CG-CD-NE2	8.20	136.39	116.70
1	H	302	GLN	CG-CD-OE1	8.15	137.91	121.60
1	H	302	GLN	CG-CD-NE2	-7.11	99.63	116.70
1	D	302	GLN	CG-CD-OE1	6.38	134.37	121.60
1	E	99[A]	ARG	N-CA-C	6.14	127.59	111.00
1	E	99[B]	ARG	N-CA-C	6.14	127.59	111.00
1	D	302	GLN	CG-CD-NE2	-5.96	102.41	116.70
1	A	99[A]	ARG	N-CA-C	5.86	126.83	111.00
1	A	99[B]	ARG	N-CA-C	5.86	126.83	111.00
1	C	99[A]	ARG	N-CA-C	5.78	126.61	111.00
1	C	99[B]	ARG	N-CA-C	5.78	126.61	111.00
1	G	99[A]	ARG	N-CA-C	5.57	126.04	111.00
1	G	99[B]	ARG	N-CA-C	5.57	126.04	111.00
1	D	299	ARG	CB-CG-CD	5.22	125.17	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	299	ARG	Sidechain

Continued on next page...

Continued from previous page...

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3871	0	3646	25	0
1	B	3869	0	3647	34	0
1	C	3869	0	3647	26	0
1	D	3869	0	3647	30	0
1	E	3868	0	3646	20	0
1	F	3869	0	3647	26	0
1	G	3868	0	3646	29	0
1	H	3871	0	3645	27	0
2	A	43	0	30	2	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	217	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 (217) 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
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:B:486:HEM:HBB2	2:B:486:HEM:HMB1	1.72	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:485:HEM:HBB2	2:D:485:HEM:HMB2	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
2:C:485:HEM:HMB2	2:C:485:HEM:HBB2	1.83	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
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
2:E:486:HEM:HMB2	2:E:486:HEM:HBB2	1.88	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:137:PRO:HB3	2:H:485:HEM:HBB1	1.89	0.53
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:85:LYS:NZ	5:F:8905:HOH:O	2.43	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
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: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: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
2:C:485:HEM:HBB2	2:C:485:HEM:CMB	2.46	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
2:F:486:HEM:HMB2	2:F:486:HEM:HBB2	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:127:ASN:CG	2:C:485:HEM:HAC	2.39	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
2:E:486:HEM:HBB2	2:E:486:HEM:CMB	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:186:ALA:HA	1:H:224:LEU:HG	2.02	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:B:483:ASN:CG	5:B:6994:HOH:O	2.60	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
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

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%)	34 22
1	C	482/483 (100%)	462 (96%)	20 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	482/483 (100%)	465 (96%)	15 (3%)	2 (0%)	34	22
1	E	481/483 (100%)	463 (96%)	18 (4%)	0	100	100
1	F	482/483 (100%)	462 (96%)	18 (4%)	2 (0%)	34	22
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%)	51	38

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 [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	407/406 (100%)	393 (97%)	14 (3%)	37	25
1	B	407/406 (100%)	399 (98%)	8 (2%)	55	48
1	C	407/406 (100%)	394 (97%)	13 (3%)	39	28
1	D	407/406 (100%)	395 (97%)	12 (3%)	42	31
1	E	406/406 (100%)	399 (98%)	7 (2%)	60	53
1	F	407/406 (100%)	394 (97%)	13 (3%)	39	28
1	G	406/406 (100%)	397 (98%)	9 (2%)	52	46
1	H	407/406 (100%)	396 (97%)	11 (3%)	44	35
All	All	3254/3248 (100%)	3167 (97%)	87 (3%)	44	35

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	THR
1	A	204	SER
1	A	237	ARG
1	A	284	HIS
1	A	289	LEU
1	A	314	ASN
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
1	A	467	TYR
1	B	204	SER
1	B	284	HIS
1	B	314	ASN
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	284	HIS
1	C	289	LEU
1	C	314	ASN
1	C	318	VAL
1	C	403	LEU
1	C	437	LEU
1	C	444	ASN
1	C	455	ARG
1	C	483	ASN
1	D	117	THR
1	D	284	HIS
1	D	285	LYS
1	D	289	LEU
1	D	314	ASN
1	D	318	VAL
1	D	403	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	428	LEU
1	D	432	GLU
1	D	437	LEU
1	D	454	LEU
1	D	455	ARG
1	E	201	PHE
1	E	204	SER
1	E	314	ASN
1	E	318	VAL
1	E	403	LEU
1	E	437	LEU
1	E	454	LEU
1	F	117	THR
1	F	129	THR
1	F	201	PHE
1	F	206	ASN
1	F	284	HIS
1	F	289	LEU
1	F	314	ASN
1	F	318	VAL
1	F	403	LEU
1	F	432	GLU
1	F	437	LEU
1	F	444	ASN
1	F	455	ARG
1	G	129	THR
1	G	284	HIS
1	G	289	LEU
1	G	314	ASN
1	G	318	VAL
1	G	358	ARG
1	G	403	LEU
1	G	437	LEU
1	G	455	ARG
1	H	3	SER
1	H	187	THR
1	H	284	HIS
1	H	289	LEU
1	H	314	ASN
1	H	318	VAL
1	H	403	LEU
1	H	432	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	437	LEU
1	H	454	LEU
1	H	455	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	121	ASN
1	A	160	ASN
1	A	174	GLN
1	A	190	HIS
1	A	240	HIS
1	A	250	ASN
1	A	284	HIS
1	A	300	ASN
1	A	314	ASN
1	A	317	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	459	HIS
1	B	32	GLN
1	B	121	ASN
1	B	160	ASN
1	B	174	GLN
1	B	190	HIS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	240	HIS
1	C	284	HIS
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	174	GLN
1	D	190	HIS
1	D	235	ASN
1	D	240	HIS
1	D	250	ASN
1	D	284	HIS
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	32	GLN
1	E	121	ASN
1	E	160	ASN
1	E	174	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	190	HIS
1	E	240	HIS
1	E	250	ASN
1	E	300	ASN
1	E	314	ASN
1	E	317	ASN
1	E	331	GLN
1	E	349	HIS
1	E	351	HIS
1	E	362	HIS
1	E	402	ASN
1	E	440	ASN
1	E	459	HIS
1	F	32	GLN
1	F	121	ASN
1	F	160	ASN
1	F	174	GLN
1	F	190	HIS
1	F	235	ASN
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	121	ASN
1	G	174	GLN
1	G	190	HIS
1	G	240	HIS
1	G	300	ASN
1	G	314	ASN
1	G	317	ASN
1	G	331	GLN
1	G	349	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	350	GLN
1	G	351	HIS
1	G	362	HIS
1	G	402	ASN
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	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	331	GLN
1	H	349	HIS
1	H	351	HIS
1	H	362	HIS
1	H	402	ASN
1	H	440	ASN
1	H	459	HIS
1	H	483	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	B	53	1	8,9,10	2.78	2 (25%)	6,12,14	2.30	2 (33%)
1	OMT	C	53	1	8,9,10	2.86	3 (37%)	6,12,14	2.89	4 (66%)
1	OMT	A	53	1	8,9,10	3.19	3 (37%)	6,12,14	2.60	3 (50%)
1	OMT	G	53	1	8,9,10	2.97	2 (25%)	6,12,14	2.12	2 (33%)
1	OMT	E	53	1	8,9,10	3.20	2 (25%)	6,12,14	2.23	3 (50%)
1	OMT	D	53	1	8,9,10	2.94	2 (25%)	6,12,14	2.96	3 (50%)
1	OMT	H	53	1	8,9,10	2.92	2 (25%)	6,12,14	1.77	2 (33%)
1	OMT	F	53	1	8,9,10	2.84	2 (25%)	6,12,14	2.25	2 (33%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	OMT	CG-SD	-8.54	1.67	1.78
1	A	53	OMT	CG-SD	-8.27	1.67	1.78
1	G	53	OMT	CG-SD	-7.87	1.68	1.78
1	D	53	OMT	CG-SD	-7.73	1.68	1.78
1	H	53	OMT	CG-SD	-7.69	1.68	1.78
1	F	53	OMT	CG-SD	-7.47	1.68	1.78
1	C	53	OMT	CG-SD	-7.36	1.68	1.78
1	B	53	OMT	CG-SD	-7.20	1.68	1.78
1	B	53	OMT	CE-SD	-2.63	1.65	1.75
1	F	53	OMT	CE-SD	-2.58	1.65	1.75
1	A	53	OMT	CE-SD	-2.35	1.66	1.75
1	A	53	OMT	CB-CG	2.18	1.54	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	53	OMT	CB-CG	2.16	1.54	1.52
1	C	53	OMT	CE-SD	-2.16	1.67	1.75
1	E	53	OMT	CE-SD	-2.15	1.67	1.75
1	D	53	OMT	CE-SD	-2.14	1.67	1.75
1	G	53	OMT	CE-SD	-2.03	1.67	1.75
1	H	53	OMT	CE-SD	-2.00	1.67	1.75

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	OMT	OD2-SD-CG	4.72	111.65	108.34
1	C	53	OMT	OD1-SD-CG	4.41	111.43	108.34
1	D	53	OMT	OD2-SD-OD1	-4.28	107.94	117.09
1	A	53	OMT	OD2-SD-OD1	-4.21	108.10	117.09
1	B	53	OMT	OD2-SD-OD1	-4.01	108.51	117.09
1	G	53	OMT	OD2-SD-OD1	-3.99	108.56	117.09
1	F	53	OMT	OD2-SD-OD1	-3.92	108.72	117.09
1	E	53	OMT	OD2-SD-OD1	-3.80	108.97	117.09
1	C	53	OMT	OD2-SD-OD1	-3.78	109.01	117.09
1	B	53	OMT	OD2-SD-CG	3.66	110.91	108.34
1	D	53	OMT	OD1-SD-CG	3.20	110.59	108.34
1	C	53	OMT	OD2-SD-CG	3.16	110.56	108.34
1	F	53	OMT	OD1-SD-CE	2.95	111.87	108.91
1	A	53	OMT	OD1-SD-CG	2.93	110.39	108.34
1	G	53	OMT	OD1-SD-CG	2.86	110.35	108.34
1	H	53	OMT	OD2-SD-OD1	-2.84	111.03	117.09
1	A	53	OMT	OD2-SD-CG	2.81	110.31	108.34
1	H	53	OMT	OD1-SD-CE	-2.40	106.49	108.91
1	C	53	OMT	OD1-SD-CE	-2.17	106.72	108.91
1	E	53	OMT	OD1-SD-CG	2.13	109.83	108.34
1	E	53	OMT	OD2-SD-CG	2.11	109.83	108.34

There are no chirality outliers.

All (29) 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
1	C	53	OMT	O-C-CA-CB
1	C	53	OMT	CB-CG-SD-OD1
1	D	53	OMT	CB-CG-SD-OD1
1	E	53	OMT	O-C-CA-CB

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	H	485	1	41,50,50	1.88	6 (14%)	45,82,82	2.00	9 (20%)
3	GOL	A	5489	-	5,5,5	0.27	0	5,5,5	0.50	0
3	GOL	F	5494	-	5,5,5	0.32	0	5,5,5	0.52	0
3	GOL	D	5488	-	5,5,5	0.32	0	5,5,5	0.50	0
2	HEM	C	485	1	41,50,50	1.97	7 (17%)	45,82,82	2.00	12 (26%)
3	GOL	B	5490	-	5,5,5	0.32	0	5,5,5	0.63	0
3	GOL	C	5487	-	5,5,5	0.26	0	5,5,5	0.38	0
2	HEM	G	485	1	41,50,50	2.03	5 (12%)	45,82,82	2.08	11 (24%)
2	HEM	E	486	1	41,50,50	1.96	8 (19%)	45,82,82	1.95	9 (20%)
2	HEM	B	486	1	41,50,50	1.88	7 (17%)	45,82,82	1.98	7 (15%)
2	HEM	A	486	1	41,50,50	2.02	7 (17%)	45,82,82	1.96	9 (20%)
2	HEM	F	486	1	41,50,50	1.86	6 (14%)	45,82,82	2.00	10 (22%)
3	GOL	H	5492	-	5,5,5	0.30	0	5,5,5	0.49	0
3	GOL	G	5491	-	5,5,5	0.21	0	5,5,5	0.51	0
3	GOL	E	5493	-	5,5,5	0.26	0	5,5,5	0.45	0
2	HEM	D	485	1	41,50,50	1.89	6 (14%)	45,82,82	1.97	8 (17%)

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	H	485	1	-	4/12/54/54	-
3	GOL	A	5489	-	-	4/4/4/4	-
3	GOL	F	5494	-	-	4/4/4/4	-
3	GOL	D	5488	-	-	2/4/4/4	-
2	HEM	C	485	1	-	4/12/54/54	-
3	GOL	B	5490	-	-	0/4/4/4	-
3	GOL	C	5487	-	-	4/4/4/4	-
2	HEM	G	485	1	-	4/12/54/54	-
2	HEM	E	486	1	-	4/12/54/54	-
2	HEM	B	486	1	-	4/12/54/54	-
2	HEM	A	486	1	-	4/12/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	F	486	1	-	4/12/54/54	-
3	GOL	H	5492	-	-	0/4/4/4	-
3	GOL	G	5491	-	-	4/4/4/4	-
3	GOL	E	5493	-	-	4/4/4/4	-
2	HEM	D	485	1	-	4/12/54/54	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	486	HEM	C3D-C2D	8.60	1.55	1.36
2	G	485	HEM	C3D-C2D	8.02	1.53	1.36
2	E	486	HEM	C3D-C2D	7.81	1.53	1.36
2	D	485	HEM	C3D-C2D	7.74	1.53	1.36
2	C	485	HEM	C3D-C2D	7.68	1.53	1.36
2	F	486	HEM	C3D-C2D	7.66	1.53	1.36
2	B	486	HEM	C3D-C2D	7.64	1.53	1.36
2	H	485	HEM	C3D-C2D	7.42	1.52	1.36
2	G	485	HEM	C3C-C2C	-4.26	1.34	1.40
2	B	486	HEM	C3C-C2C	-4.07	1.34	1.40
2	E	486	HEM	C3C-CAC	3.96	1.55	1.47
2	E	486	HEM	C3C-C2C	-3.96	1.34	1.40
2	C	485	HEM	C3C-C2C	-3.89	1.35	1.40
2	G	485	HEM	C3C-CAC	3.86	1.55	1.47
2	A	486	HEM	C3C-C2C	-3.79	1.35	1.40
2	H	485	HEM	C3C-C2C	-3.74	1.35	1.40
2	F	486	HEM	C3C-C2C	-3.67	1.35	1.40
2	D	485	HEM	C3C-CAC	3.65	1.55	1.47
2	G	485	HEM	FE-NB	3.63	2.14	1.96
2	C	485	HEM	C3C-CAC	3.58	1.55	1.47
2	B	486	HEM	C3C-CAC	3.55	1.55	1.47
2	A	486	HEM	C3C-CAC	3.53	1.55	1.47
2	H	485	HEM	C3C-CAC	3.51	1.55	1.47
2	D	485	HEM	C3C-C2C	-3.47	1.35	1.40
2	A	486	HEM	FE-NB	3.46	2.14	1.96
2	F	486	HEM	C3C-CAC	3.44	1.54	1.47
2	C	485	HEM	FE-ND	3.18	2.12	1.96
2	F	486	HEM	FE-NB	3.18	2.12	1.96
2	H	485	HEM	CAB-C3B	3.14	1.56	1.47
2	C	485	HEM	CAB-C3B	3.12	1.55	1.47
2	E	486	HEM	CAB-C3B	3.03	1.55	1.47
2	D	485	HEM	FE-ND	3.01	2.11	1.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	485	HEM	CAB-C3B	2.98	1.55	1.47
2	B	486	HEM	CAB-C3B	2.94	1.55	1.47
2	D	485	HEM	CAB-C3B	2.91	1.55	1.47
2	E	486	HEM	FE-NB	2.87	2.11	1.96
2	A	486	HEM	CAB-C3B	2.86	1.55	1.47
2	F	486	HEM	CAB-C3B	2.78	1.55	1.47
2	C	485	HEM	FE-NB	2.75	2.10	1.96
2	H	485	HEM	FE-ND	2.70	2.10	1.96
2	C	485	HEM	CAA-C2A	2.49	1.55	1.52
2	A	486	HEM	FE-ND	2.30	2.08	1.96
2	E	486	HEM	CMB-C2B	2.29	1.55	1.50
2	B	486	HEM	CMB-C2B	2.27	1.55	1.50
2	E	486	HEM	CMD-C2D	2.14	1.55	1.50
2	B	486	HEM	CMA-C3A	2.12	1.56	1.51
2	D	485	HEM	FE-NB	2.08	2.07	1.96
2	F	486	HEM	CMB-C2B	2.08	1.55	1.50
2	A	486	HEM	CMB-C2B	2.07	1.55	1.50
2	B	486	HEM	FE-ND	2.07	2.07	1.96
2	E	486	HEM	FE-ND	2.06	2.07	1.96
2	H	485	HEM	CAA-C2A	2.03	1.55	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	486	HEM	C4D-ND-C1D	7.33	112.64	105.07
2	G	485	HEM	C4D-ND-C1D	6.94	112.25	105.07
2	C	485	HEM	C4D-ND-C1D	6.88	112.18	105.07
2	B	486	HEM	C4D-ND-C1D	6.81	112.11	105.07
2	F	486	HEM	C4D-ND-C1D	6.72	112.01	105.07
2	E	486	HEM	C4D-ND-C1D	6.70	111.99	105.07
2	D	485	HEM	C4D-ND-C1D	6.51	111.80	105.07
2	H	485	HEM	C4D-ND-C1D	6.21	111.48	105.07
2	H	485	HEM	CBA-CAA-C2A	-6.15	102.13	112.62
2	G	485	HEM	CBA-CAA-C2A	-6.05	102.30	112.62
2	B	486	HEM	CBA-CAA-C2A	-5.92	102.52	112.62
2	A	486	HEM	CBA-CAA-C2A	-5.48	103.27	112.62
2	E	486	HEM	CBA-CAA-C2A	-5.47	103.28	112.62
2	D	485	HEM	CBA-CAA-C2A	-5.25	103.67	112.62
2	C	485	HEM	CBA-CAA-C2A	-5.21	103.74	112.62
2	F	486	HEM	C4C-CHD-C1D	4.92	129.05	122.56
2	F	486	HEM	CBA-CAA-C2A	-4.83	104.38	112.62
2	G	485	HEM	C4C-CHD-C1D	4.35	128.29	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	485	HEM	C4C-CHD-C1D	4.06	127.92	122.56
2	F	486	HEM	CAD-CBD-CGD	-4.01	104.98	113.60
2	E	486	HEM	CAD-CBD-CGD	-3.75	105.53	113.60
2	B	486	HEM	C4C-CHD-C1D	3.75	127.50	122.56
2	C	485	HEM	CAD-CBD-CGD	-3.73	105.57	113.60
2	H	485	HEM	CAD-CBD-CGD	-3.72	105.59	113.60
2	G	485	HEM	C1B-NB-C4B	3.45	108.64	105.07
2	E	486	HEM	C4C-CHD-C1D	3.44	127.09	122.56
2	H	485	HEM	C4C-CHD-C1D	3.35	126.97	122.56
2	C	485	HEM	C4C-CHD-C1D	3.33	126.95	122.56
2	D	485	HEM	C1B-NB-C4B	3.29	108.47	105.07
2	A	486	HEM	C4C-CHD-C1D	3.21	126.79	122.56
2	H	485	HEM	C1B-NB-C4B	3.10	108.28	105.07
2	A	486	HEM	CAD-CBD-CGD	-3.09	106.96	113.60
2	D	485	HEM	CAD-CBD-CGD	-3.01	107.12	113.60
2	F	486	HEM	CMA-C3A-C4A	-3.01	123.84	128.46
2	E	486	HEM	C1B-NB-C4B	2.99	108.16	105.07
2	B	486	HEM	C1B-NB-C4B	2.92	108.09	105.07
2	G	485	HEM	CAD-CBD-CGD	-2.87	107.42	113.60
2	A	486	HEM	C4B-CHC-C1C	2.86	126.34	122.56
2	B	486	HEM	CAD-CBD-CGD	-2.86	107.46	113.60
2	C	485	HEM	C1B-NB-C4B	2.80	107.96	105.07
2	C	485	HEM	CMA-C3A-C4A	-2.75	124.23	128.46
2	H	485	HEM	CMA-C3A-C4A	-2.73	124.27	128.46
2	A	486	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
2	D	485	HEM	C3B-C2B-C1B	2.56	108.38	106.49
2	A	486	HEM	C1B-NB-C4B	2.55	107.71	105.07
2	E	486	HEM	CMD-C2D-C1D	2.52	128.88	125.04
2	F	486	HEM	C1B-NB-C4B	2.47	107.62	105.07
2	B	486	HEM	CMC-C2C-C3C	2.42	129.21	124.68
2	G	485	HEM	CMD-C2D-C1D	2.42	128.72	125.04
2	A	486	HEM	O1A-CGA-CBA	-2.34	115.56	123.08
2	H	485	HEM	CHA-C4D-ND	2.32	127.25	124.38
2	E	486	HEM	C1D-C2D-C3D	-2.27	104.57	106.96
2	E	486	HEM	C3D-C4D-ND	-2.26	107.65	110.17
2	G	485	HEM	C2C-C3C-C4C	2.23	108.45	106.90
2	G	485	HEM	CMA-C3A-C4A	-2.21	125.07	128.46
2	G	485	HEM	CAD-C3D-C4D	2.20	128.50	124.66
2	F	486	HEM	CMC-C2C-C3C	2.19	128.78	124.68
2	C	485	HEM	C4B-CHC-C1C	2.19	125.45	122.56
2	F	486	HEM	C2C-C3C-C4C	2.17	108.41	106.90
2	C	485	HEM	C2C-C3C-C4C	2.16	108.41	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	485	HEM	C3B-C2B-C1B	2.15	108.08	106.49
2	B	486	HEM	C3B-C2B-C1B	2.15	108.08	106.49
2	A	486	HEM	O2A-CGA-CBA	2.14	120.92	114.03
2	C	485	HEM	O1D-CGD-CBD	-2.14	116.22	123.08
2	G	485	HEM	C4B-CHC-C1C	2.12	125.36	122.56
2	C	485	HEM	C3B-C2B-C1B	2.11	108.05	106.49
2	C	485	HEM	C3D-C4D-ND	-2.10	107.82	110.17
2	D	485	HEM	C2B-C1B-NB	-2.10	107.35	109.84
2	F	486	HEM	C3B-C2B-C1B	2.09	108.04	106.49
2	C	485	HEM	CAD-C3D-C4D	2.08	128.29	124.66
2	F	486	HEM	CMA-C3A-C2A	2.07	128.85	124.94
2	D	485	HEM	O1D-CGD-CBD	-2.04	116.52	123.08
2	H	485	HEM	O2A-CGA-CBA	2.03	120.56	114.03
2	H	485	HEM	CMC-C2C-C3C	2.02	128.46	124.68
2	E	486	HEM	C4B-CHC-C1C	2.01	125.21	122.56

There are no chirality outliers.

All (54) 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	486	HEM	CAA-CBA-CGA-O1A
2	F	486	HEM	CAA-CBA-CGA-O1A
2	C	485	HEM	CAA-CBA-CGA-O1A
2	G	485	HEM	CAA-CBA-CGA-O1A
2	C	485	HEM	CAD-CBD-CGD-O1D
2	D	485	HEM	CAA-CBA-CGA-O1A
2	H	485	HEM	CAD-CBD-CGD-O1D
2	A	486	HEM	CAD-CBD-CGD-O2D
2	C	485	HEM	CAA-CBA-CGA-O2A
2	F	486	HEM	CAD-CBD-CGD-O1D
2	F	486	HEM	CAD-CBD-CGD-O2D
2	G	485	HEM	CAD-CBD-CGD-O1D
2	A	486	HEM	CAD-CBD-CGD-O1D
2	A	486	HEM	CAA-CBA-CGA-O2A
2	E	486	HEM	CAD-CBD-CGD-O1D
2	E	486	HEM	CAD-CBD-CGD-O2D
2	F	486	HEM	CAA-CBA-CGA-O2A
2	H	485	HEM	CAD-CBD-CGD-O2D
2	C	485	HEM	CAD-CBD-CGD-O2D
2	G	485	HEM	CAD-CBD-CGD-O2D
2	B	486	HEM	CAD-CBD-CGD-O2D
2	D	485	HEM	CAD-CBD-CGD-O2D
2	D	485	HEM	CAD-CBD-CGD-O1D
2	B	486	HEM	CAD-CBD-CGD-O1D
2	H	485	HEM	CAA-CBA-CGA-O1A
2	B	486	HEM	CAA-CBA-CGA-O1A
2	D	485	HEM	CAA-CBA-CGA-O2A
2	E	486	HEM	CAA-CBA-CGA-O1A
2	G	485	HEM	CAA-CBA-CGA-O2A
2	E	486	HEM	CAA-CBA-CGA-O2A
2	B	486	HEM	CAA-CBA-CGA-O2A
2	H	485	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

13 monomers are involved in 20 short contacts:

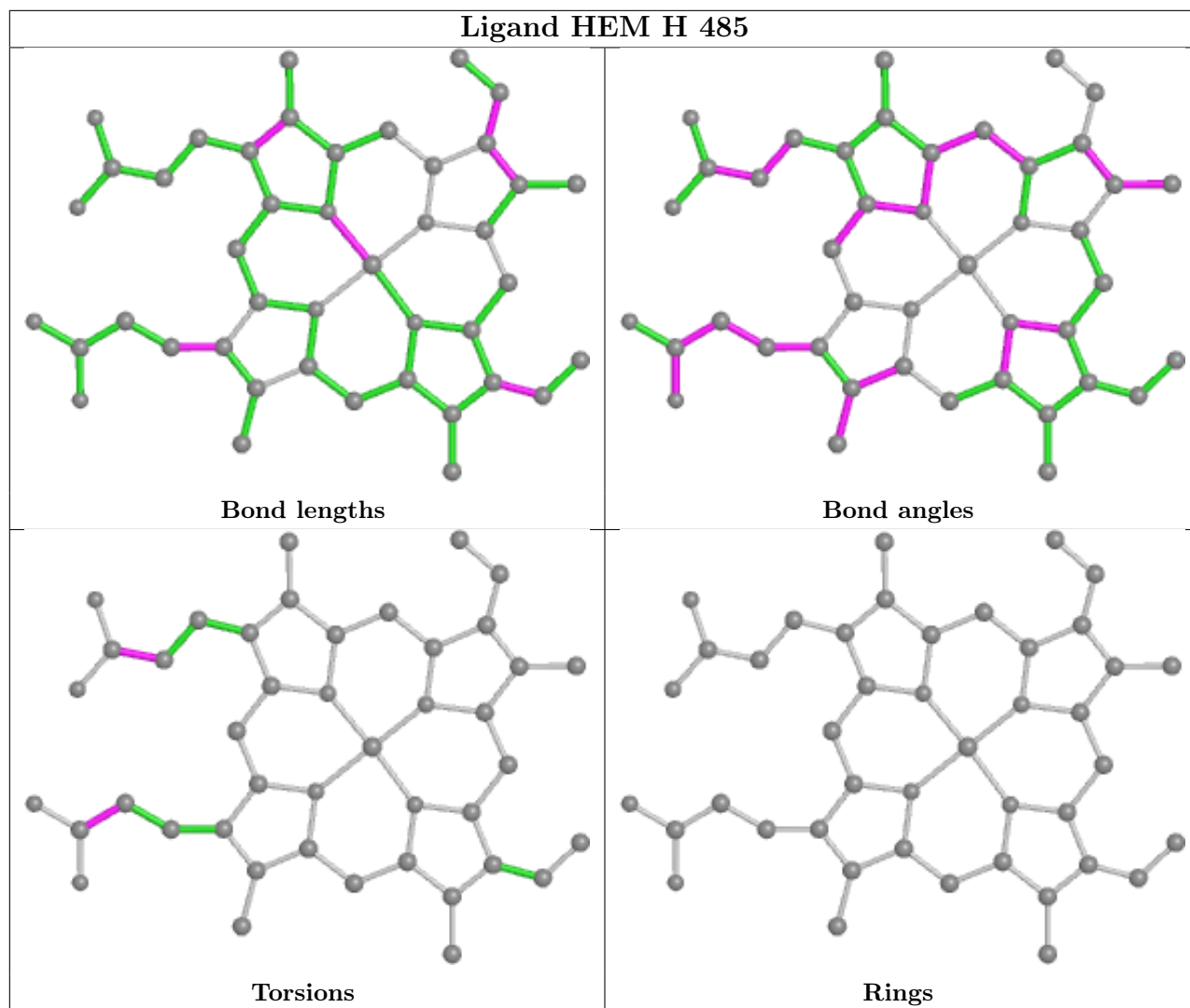
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	485	HEM	1	0
3	A	5489	GOL	1	0
3	F	5494	GOL	1	0
2	C	485	HEM	3	0
3	C	5487	GOL	1	0

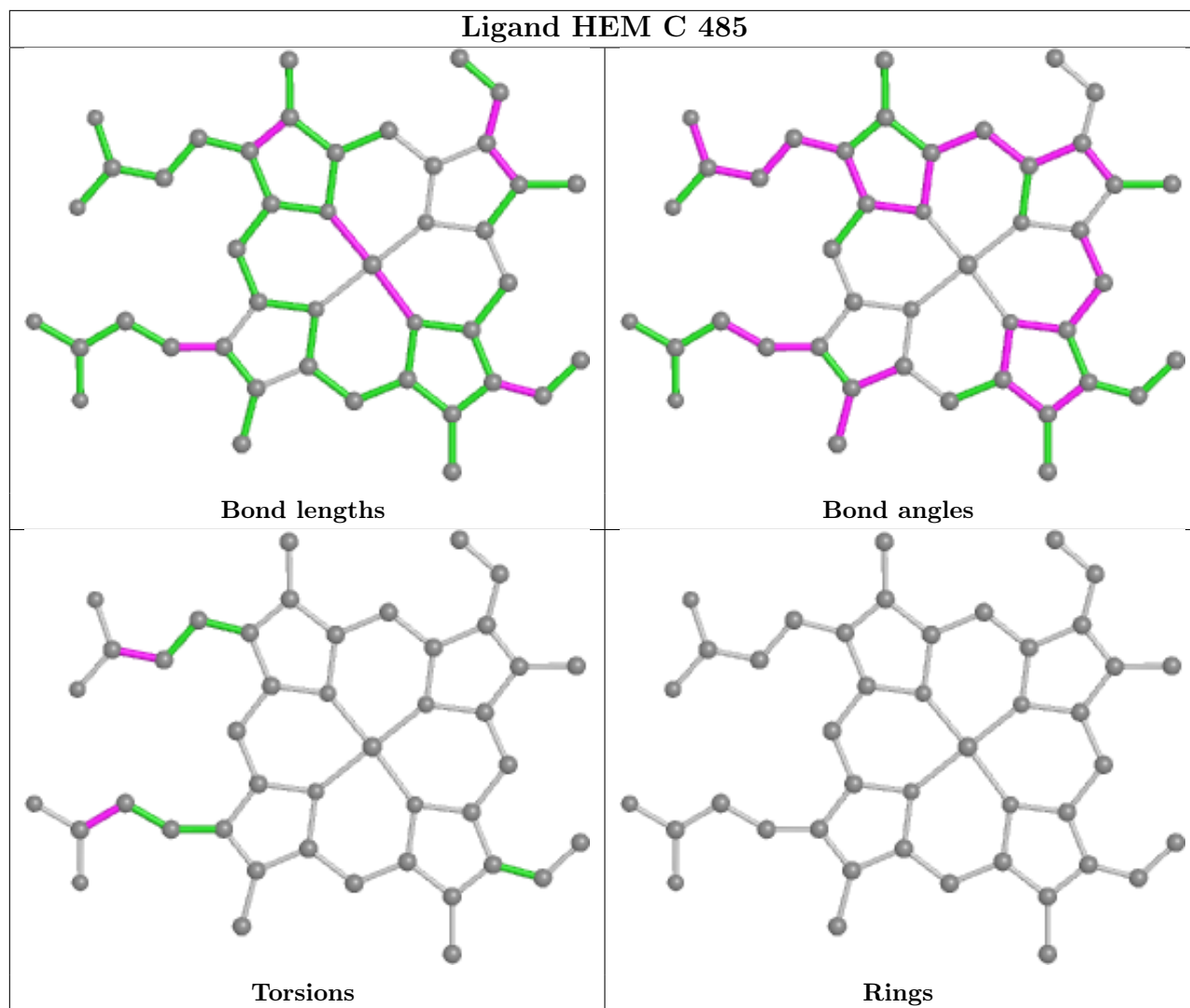
Continued on next page...

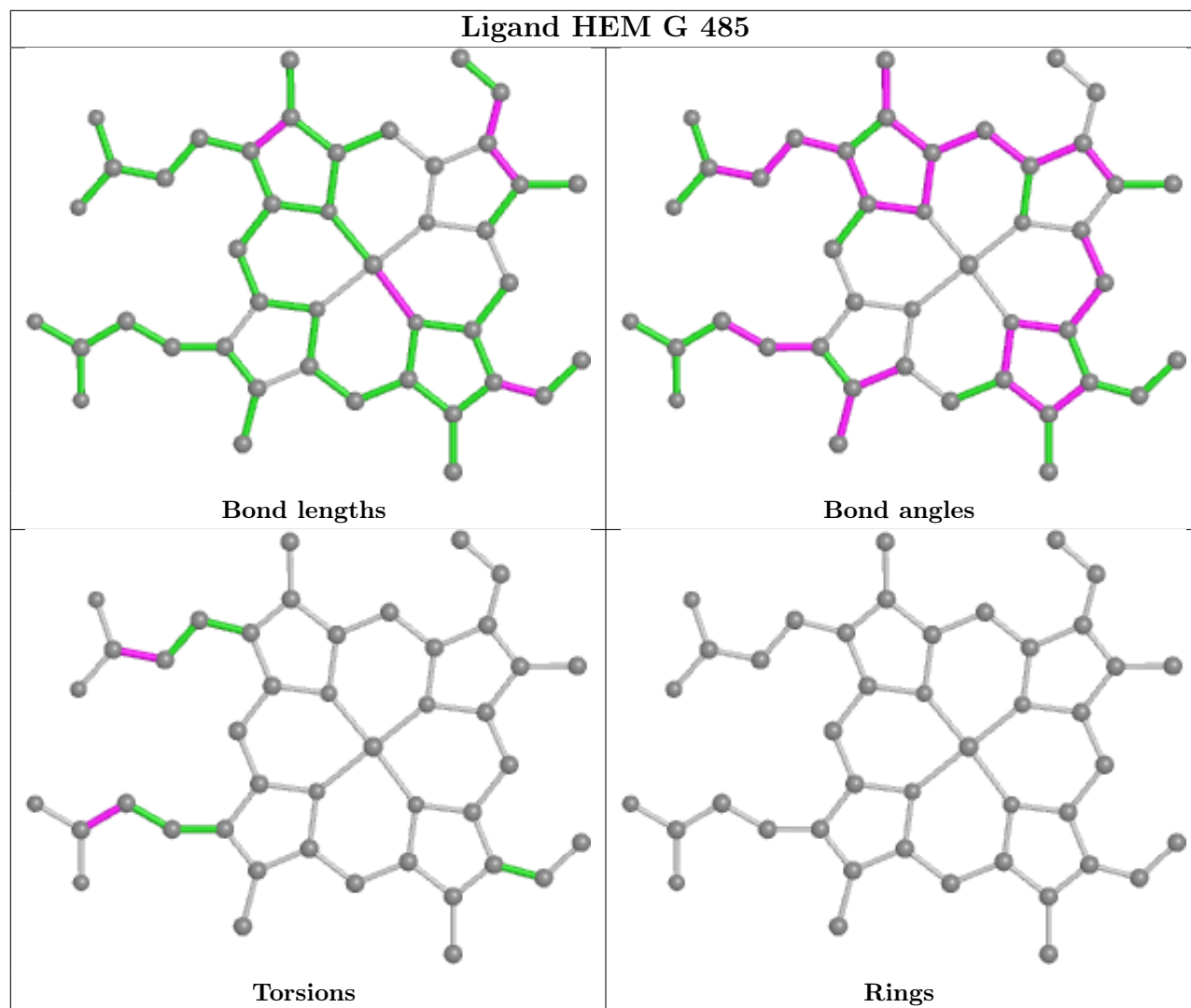
Continued from previous page...

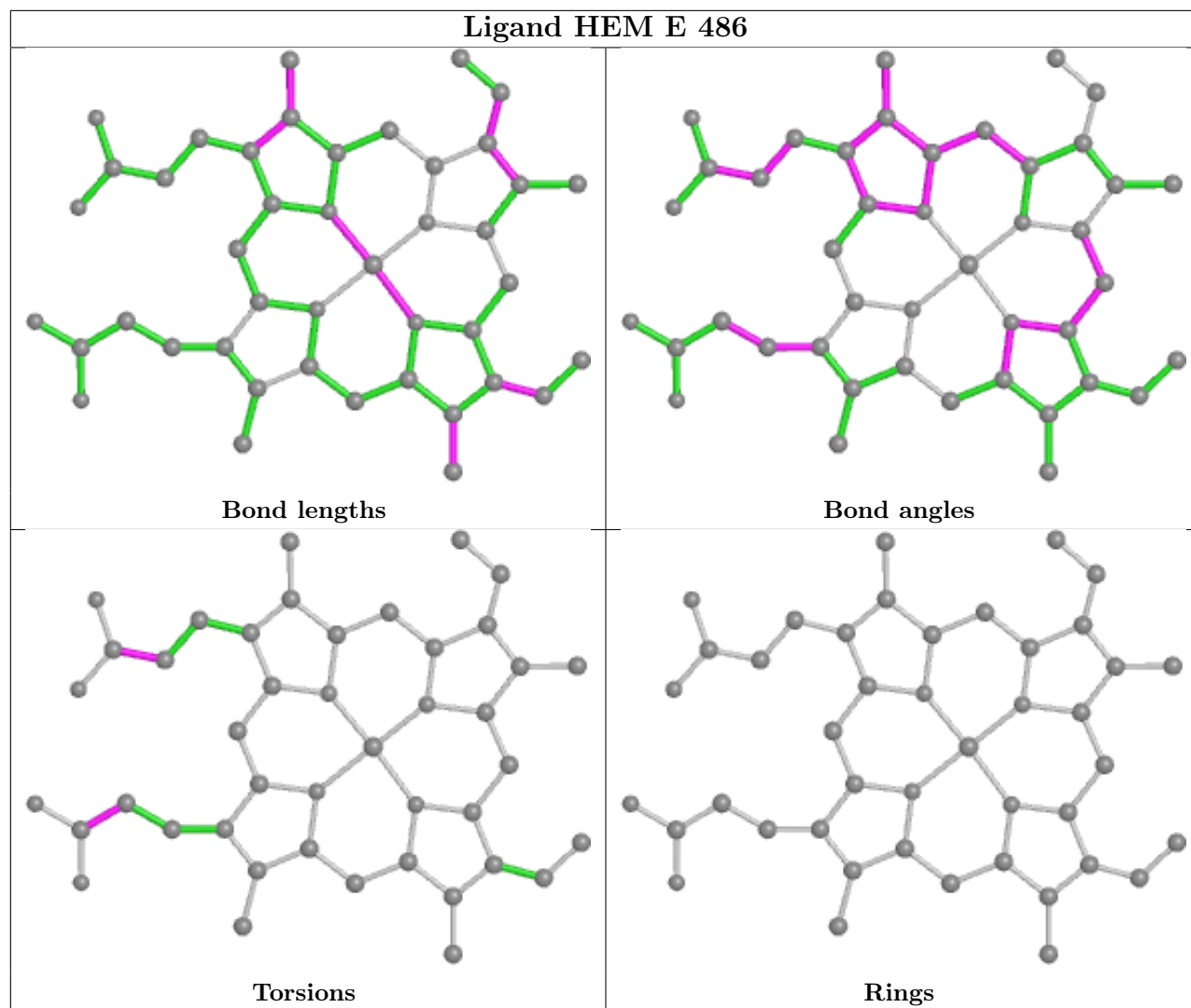
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	485	HEM	2	0
2	E	486	HEM	2	0
2	B	486	HEM	2	0
2	A	486	HEM	2	0
2	F	486	HEM	2	0
3	G	5491	GOL	1	0
3	E	5493	GOL	1	0
2	D	485	HEM	1	0

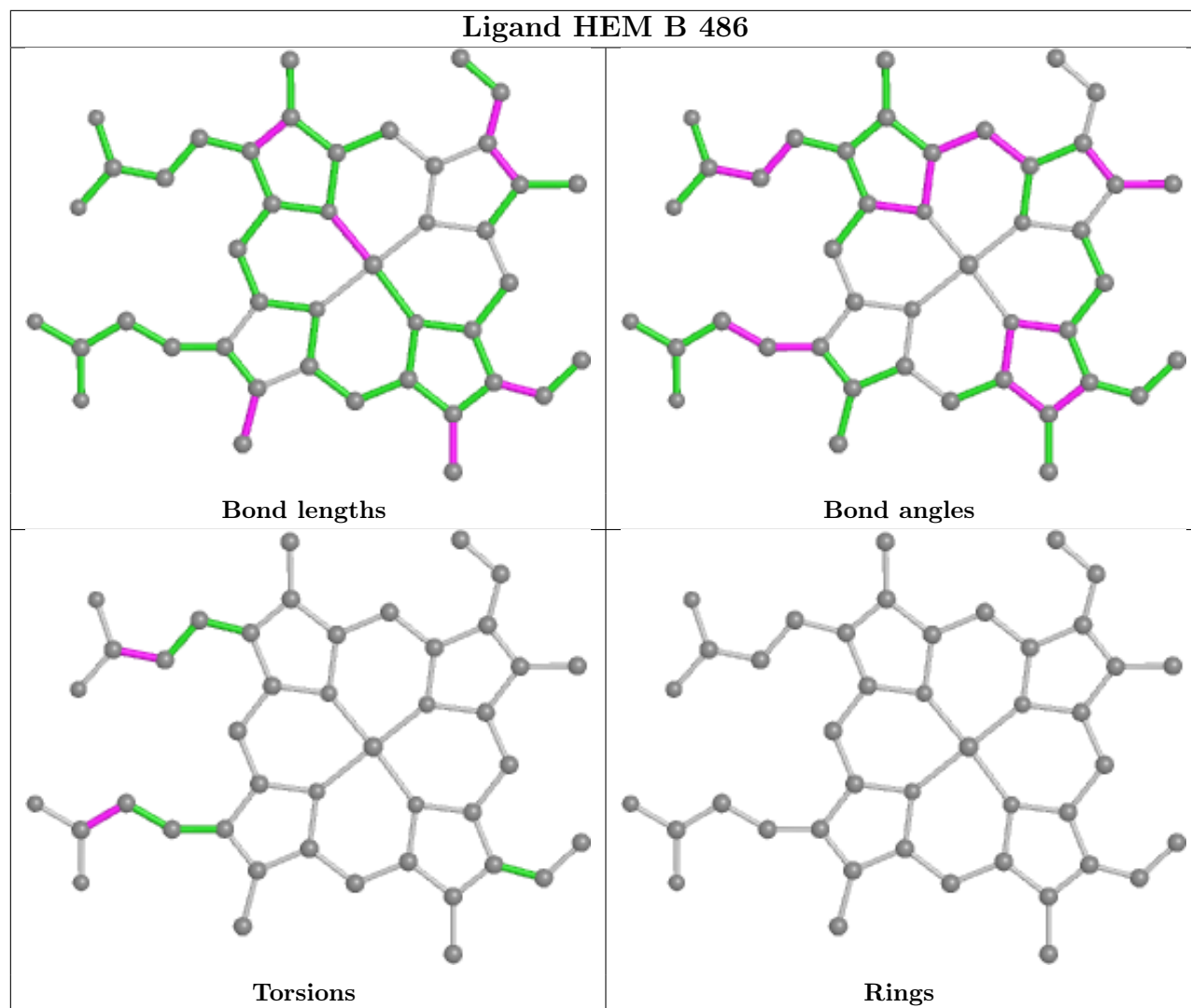
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

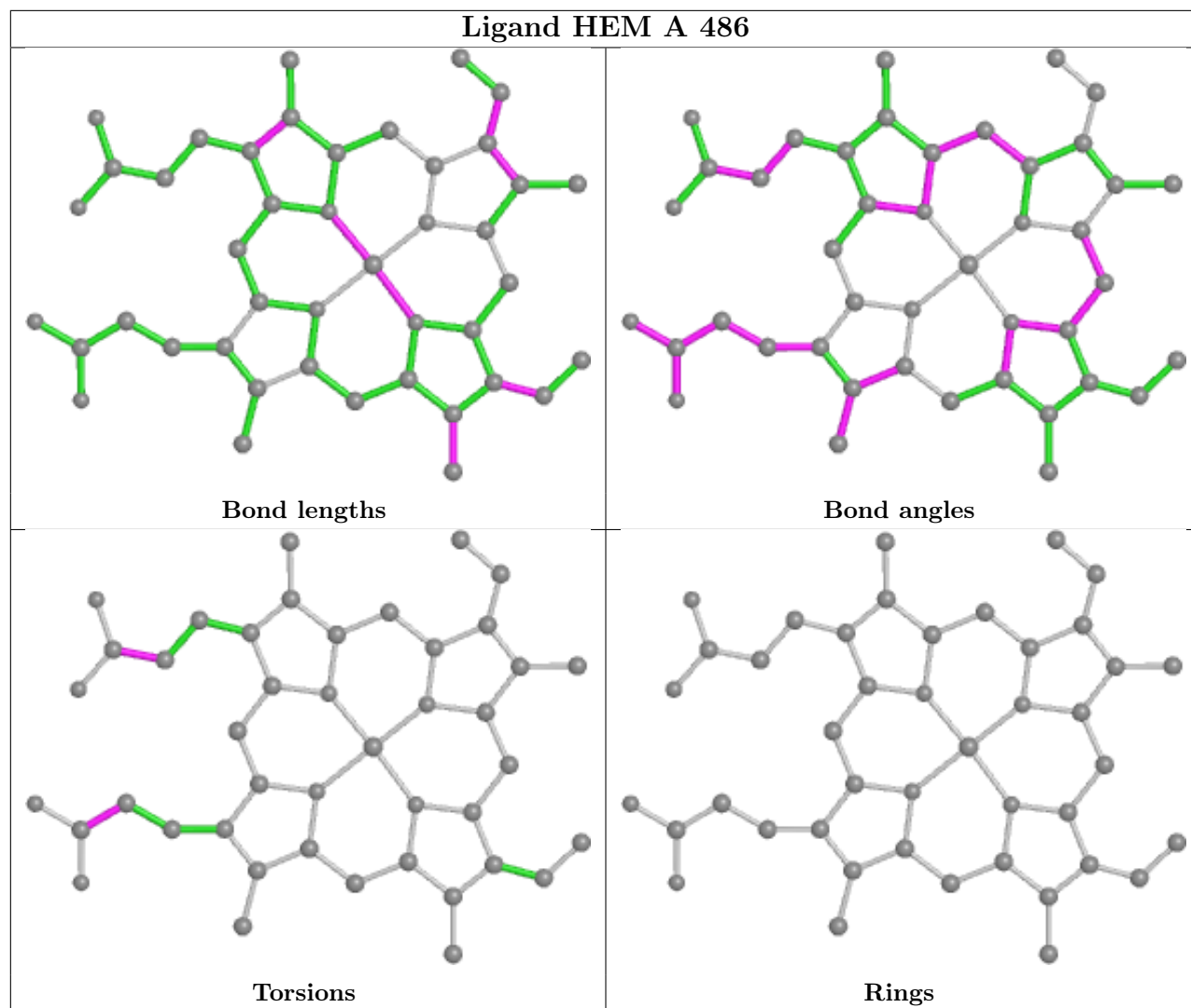


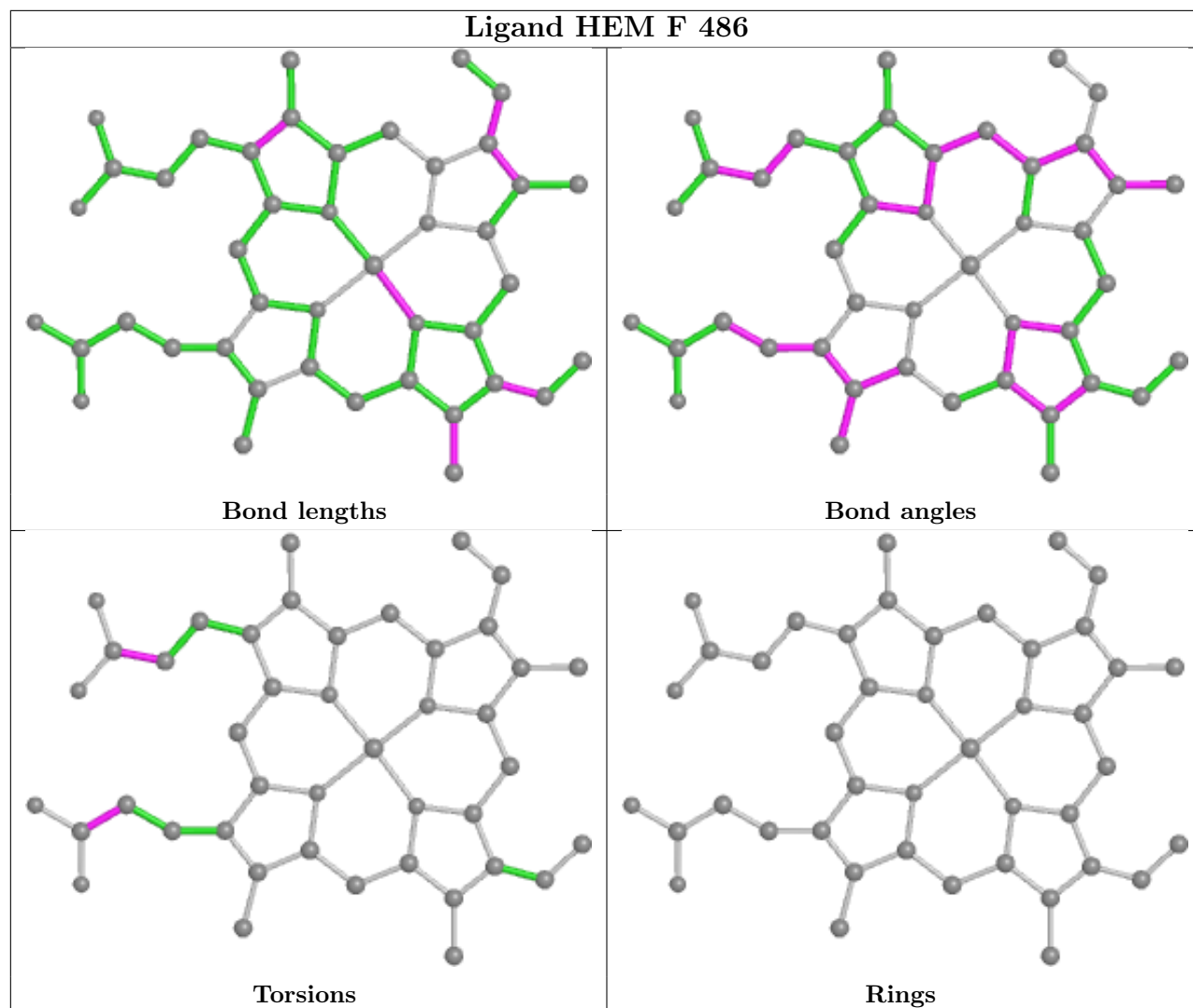


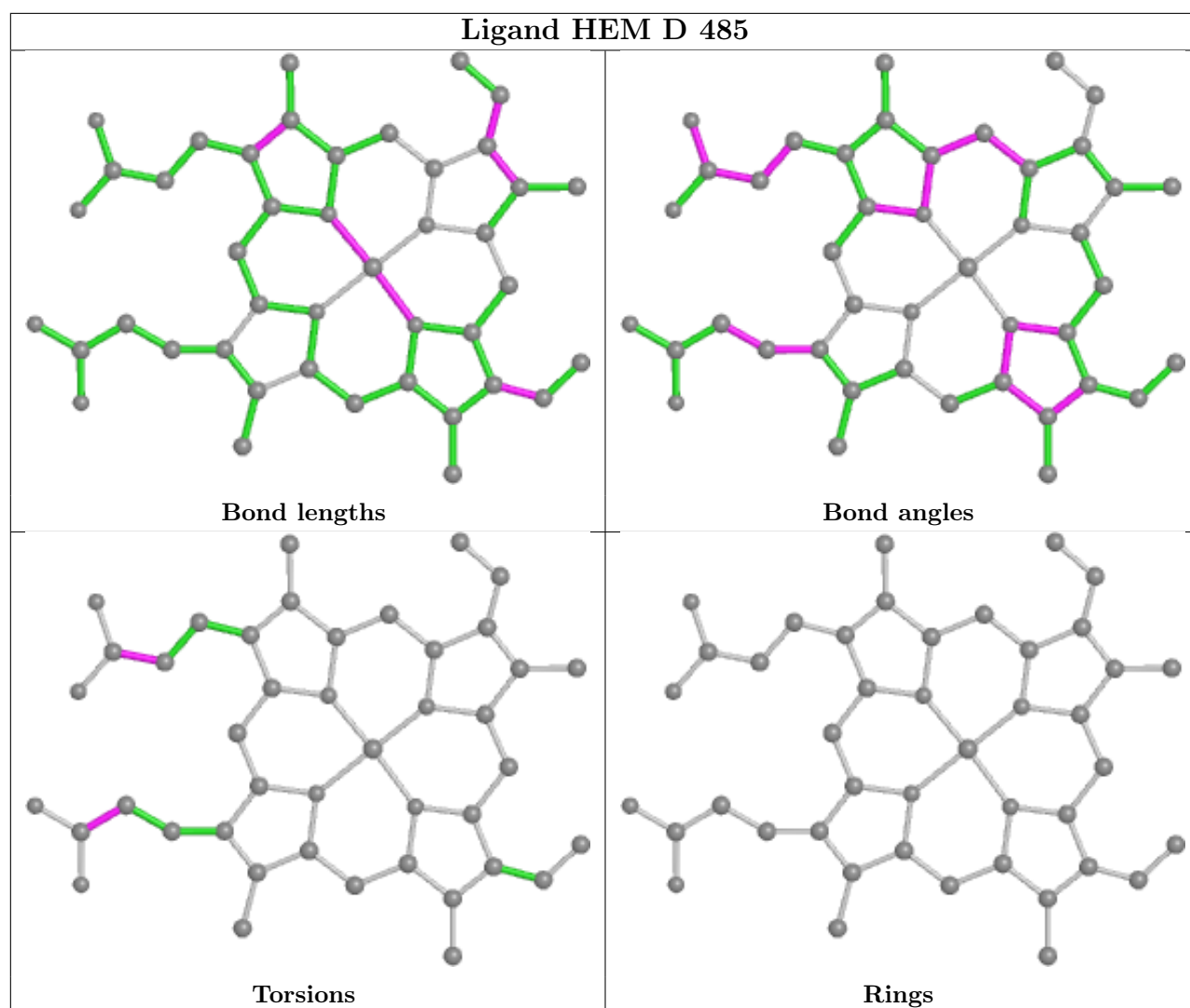












5.7 Other polymers [i](#)

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%)	-0.60	4 (0%) 86 87	5, 10, 20, 29	0
1	B	481/483 (99%)	-0.57	2 (0%) 92 93	5, 11, 19, 30	1 (0%)
1	C	481/483 (99%)	-0.65	4 (0%) 86 87	4, 9, 20, 32	1 (0%)
1	D	481/483 (99%)	-0.54	2 (0%) 92 93	4, 11, 21, 28	3 (0%)
1	E	481/483 (99%)	-0.45	7 (1%) 73 75	5, 13, 26, 36	2 (0%)
1	F	481/483 (99%)	-0.42	5 (1%) 82 83	8, 14, 24, 32	3 (0%)
1	G	481/483 (99%)	-0.51	4 (0%) 86 87	6, 11, 24, 31	2 (0%)
1	H	481/483 (99%)	-0.50	5 (1%) 82 83	6, 12, 22, 32	3 (0%)
All	All	3848/3864 (99%)	-0.53	33 (0%) 84 85	4, 11, 22, 36	15 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	3	SER	6.3
1	H	428	LEU	3.1
1	G	360	PRO	3.0
1	E	428	LEU	3.0
1	E	269	ALA	3.0
1	A	285	LYS	2.9
1	C	483	ASN	2.9
1	F	3	SER	2.9
1	F	428	LEU	2.7
1	E	432	GLU	2.7
1	G	285	LYS	2.7
1	A	269	ALA	2.6
1	H	285	LYS	2.5
1	C	447	GLY	2.5
1	E	483	ASN	2.4
1	A	3	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	484	SER	2.4
1	D	484	SER	2.4
1	C	360	PRO	2.3
1	E	478	ASP	2.3
1	B	269	ALA	2.3
1	H	3	SER	2.3
1	H	447	GLY	2.2
1	H	484	SER	2.2
1	C	359	CYS	2.2
1	E	484	SER	2.1
1	A	484	SER	2.1
1	B	484	SER	2.1
1	E	285	LYS	2.1
1	G	428	LEU	2.1
1	F	270	THR	2.0
1	D	272	PRO	2.0
1	F	432	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	OMT	F	53	10/11	0.97	0.07	10,11,18,20	0
1	OMT	B	53	10/11	0.98	0.06	6,7,16,17	0
1	OMT	C	53	10/11	0.98	0.06	6,7,14,14	0
1	OMT	D	53	10/11	0.98	0.06	6,6,12,13	0
1	OMT	A	53	10/11	0.98	0.06	5,6,12,12	0
1	OMT	G	53	10/11	0.98	0.07	8,9,13,15	0
1	OMT	E	53	10/11	0.99	0.05	8,8,16,18	0
1	OMT	H	53	10/11	0.99	0.05	8,8,12,12	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

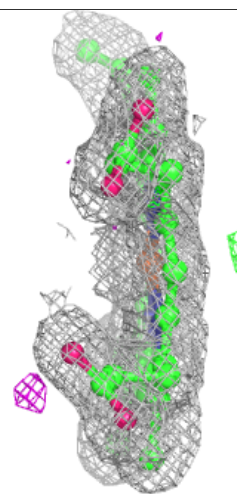
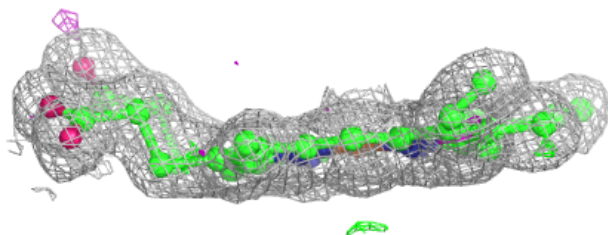
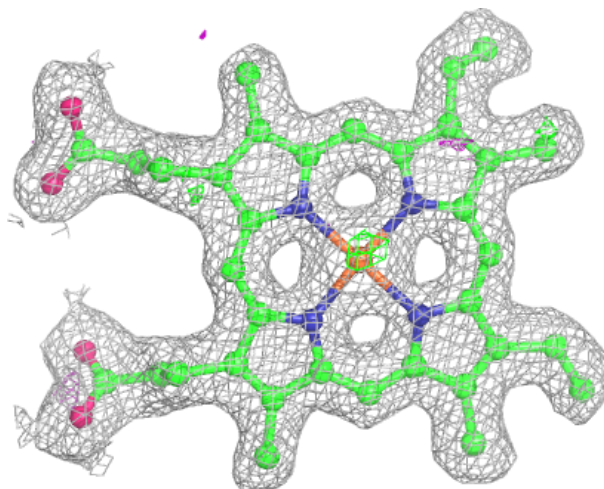
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	E	5493	6/6	0.88	0.13	18,21,22,22	0
3	GOL	H	5492	6/6	0.89	0.11	18,21,22,25	0
3	GOL	G	5491	6/6	0.90	0.13	15,20,21,22	0
3	GOL	D	5488	6/6	0.93	0.10	12,16,17,18	0
3	GOL	A	5489	6/6	0.94	0.11	10,17,18,18	0
3	GOL	B	5490	6/6	0.94	0.10	13,17,17,20	0
3	GOL	C	5487	6/6	0.95	0.10	7,11,12,13	0
3	GOL	F	5494	6/6	0.95	0.09	12,16,17,18	0
2	HEM	A	486	43/43	0.98	0.07	5,7,9,10	0
2	HEM	B	486	43/43	0.98	0.07	6,7,8,10	0
2	HEM	C	485	43/43	0.98	0.07	4,7,9,10	0
2	HEM	D	485	43/43	0.98	0.07	3,10,11,12	0
2	HEM	E	486	43/43	0.98	0.07	8,10,12,13	0
2	HEM	F	486	43/43	0.98	0.08	8,11,13,13	0
2	HEM	G	485	43/43	0.98	0.08	7,10,12,14	0
2	HEM	H	485	43/43	0.98	0.08	6,10,12,13	0
4	CL	H	7485	1/1	0.98	0.04	17,17,17,17	0
4	CL	D	5485	1/1	0.99	0.04	14,14,14,14	0
4	CL	F	8485	1/1	0.99	0.03	16,16,16,16	0
4	CL	B	6485	1/1	0.99	0.04	13,13,13,13	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.

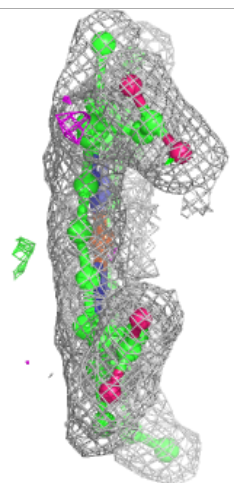
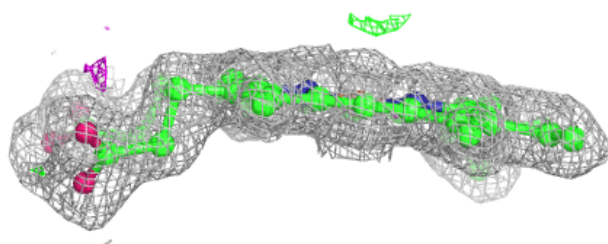
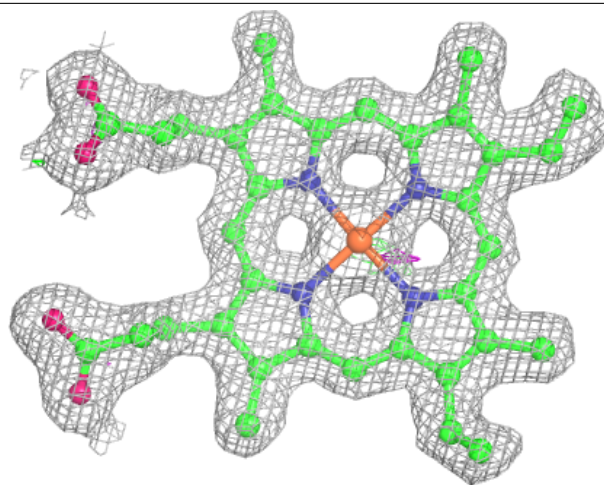
Electron density around HEM A 486:

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



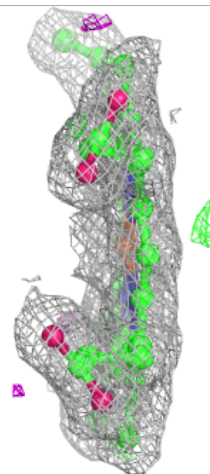
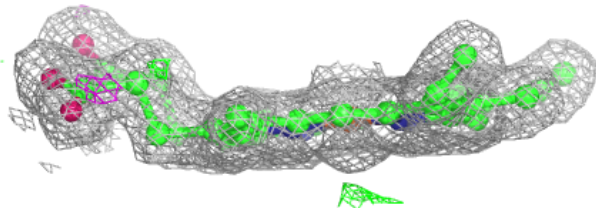
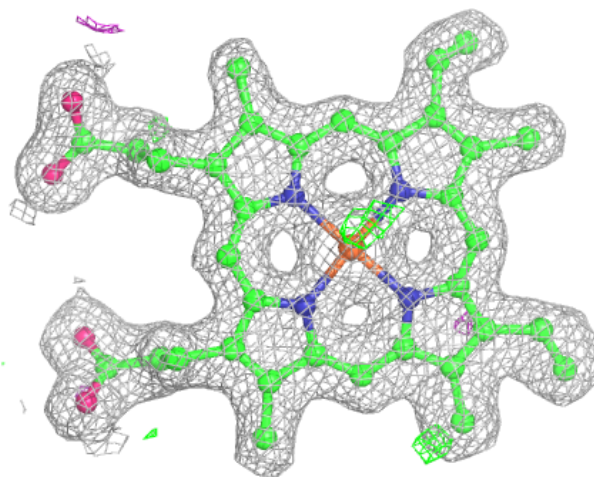
Electron density around HEM B 486:

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



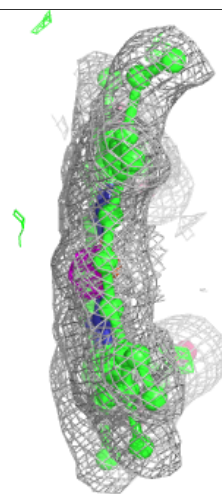
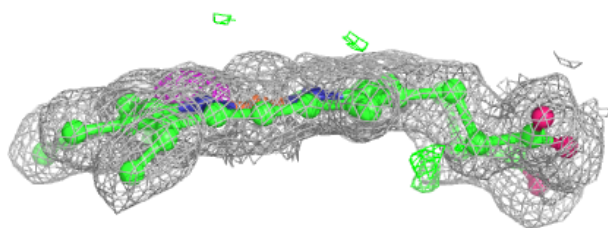
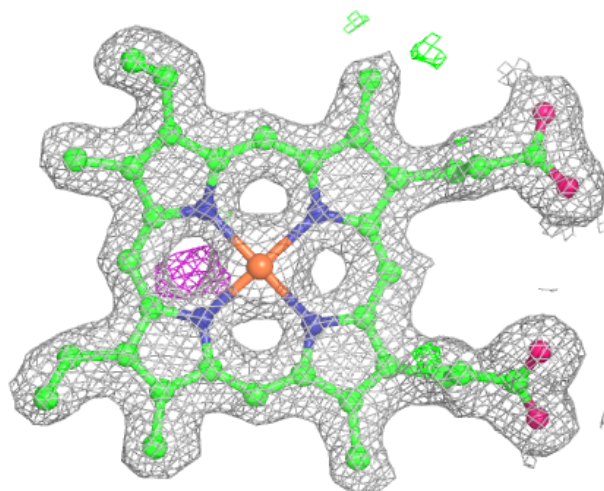
Electron density around HEM C 485:

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



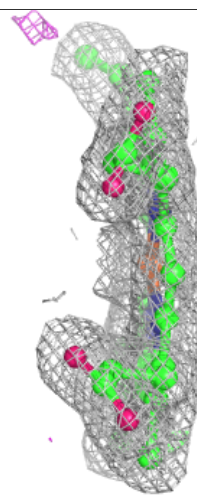
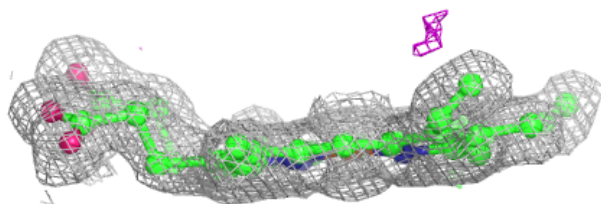
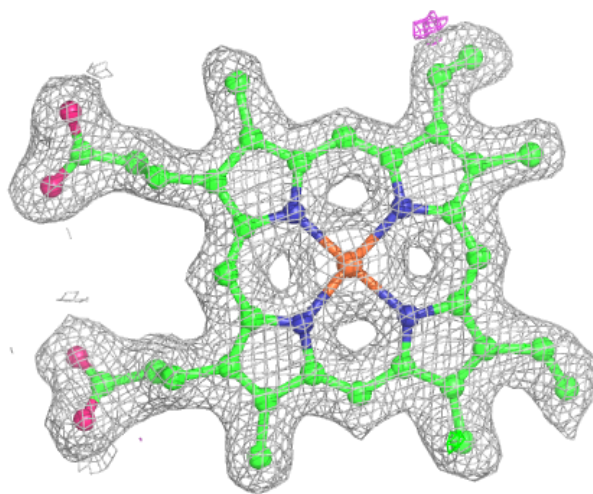
Electron density around HEM D 485:

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



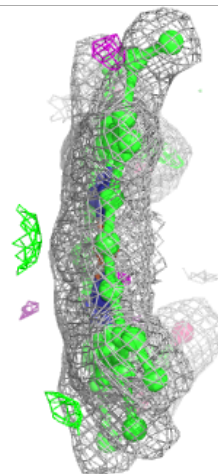
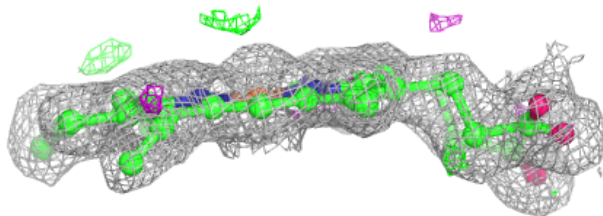
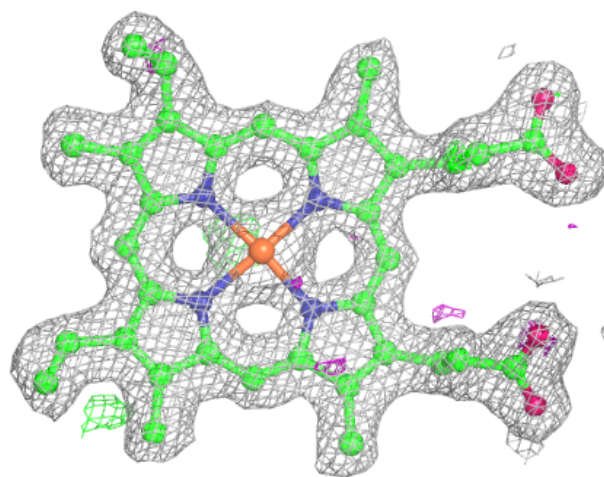
Electron density around HEM E 486:

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



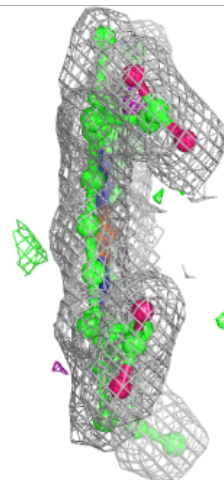
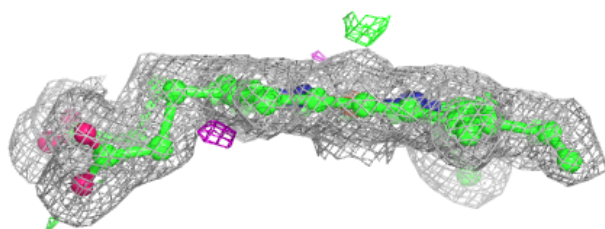
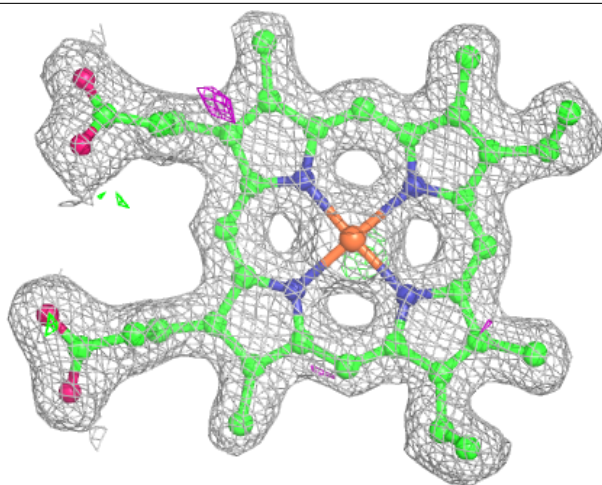
Electron density around HEM F 486:

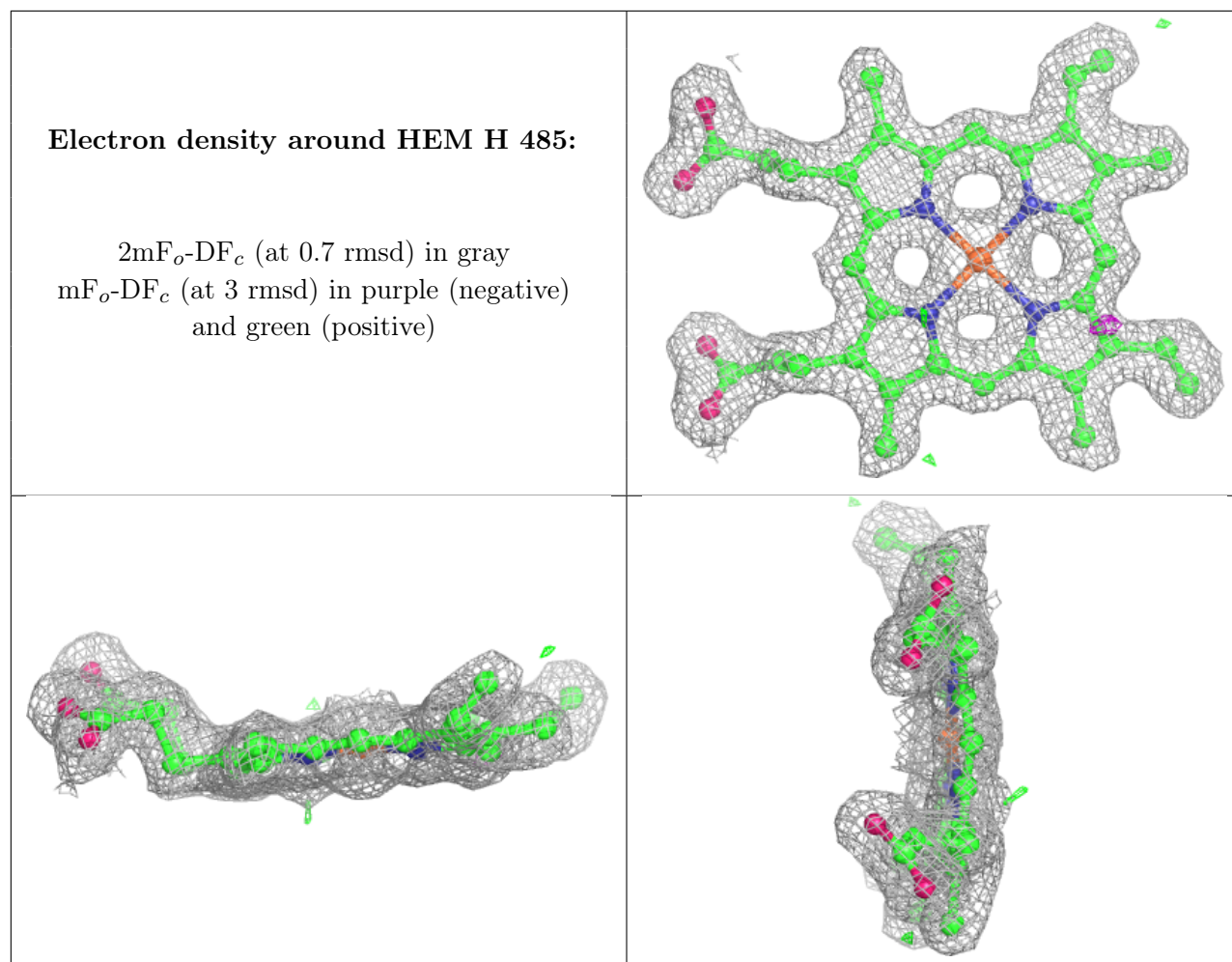
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.