



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:29 PM UTC

PDB ID : 4ENV / pdb\_00004env  
Title : Structure of the S234I variant of E. coli KatE  
Authors : Loewen, P.C.; Jha, V.  
Deposited on : 2012-04-13  
Resolution : 1.70 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](mailto: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>.

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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

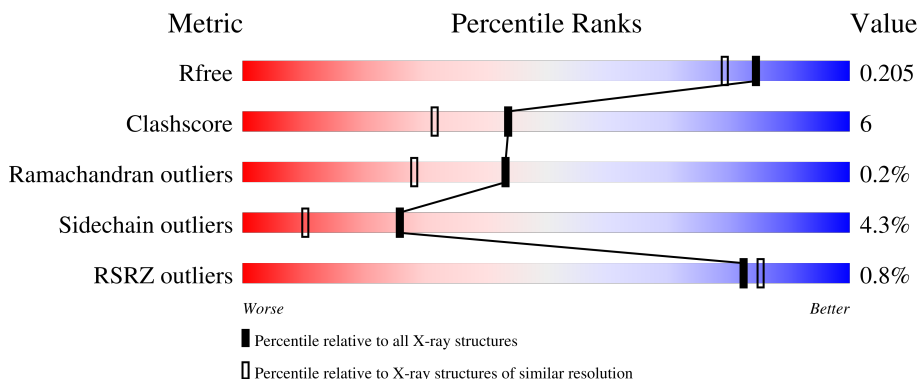
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



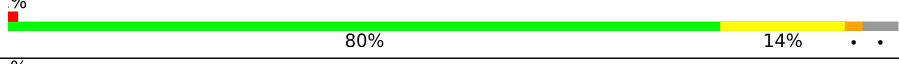

The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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  $\geq 3$ , 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	753	
1	B	753	
1	C	753	
1	D	753	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26342 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 HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5752	3654	1007	1079	12	0	2	0
1	B	726	5745	3649	1005	1079	12	0	1	0
1	C	726	5752	3654	1007	1079	12	0	2	0
1	D	726	5744	3648	1005	1079	12	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ILE	SER	engineered mutation	UNP P21179
B	234	ILE	SER	engineered mutation	UNP P21179
C	234	ILE	SER	engineered mutation	UNP P21179
D	234	ILE	SER	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>).



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

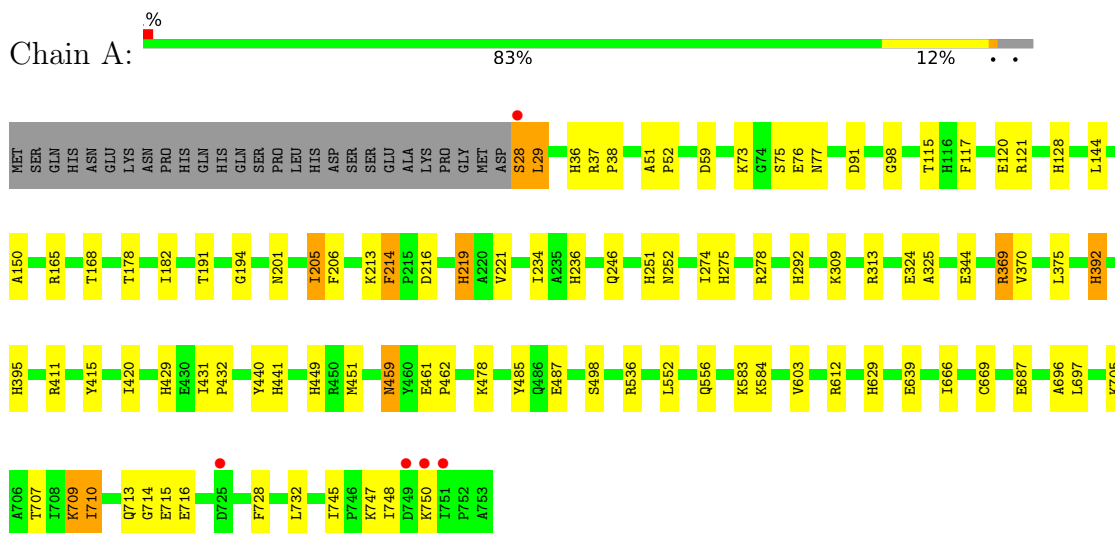
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	772	Total	O	0	0
			772	772		
4	B	695	Total	O	0	0
			695	695		
4	C	735	Total	O	0	0
			735	735		
4	D	799	Total	O	0	0
			799	799		

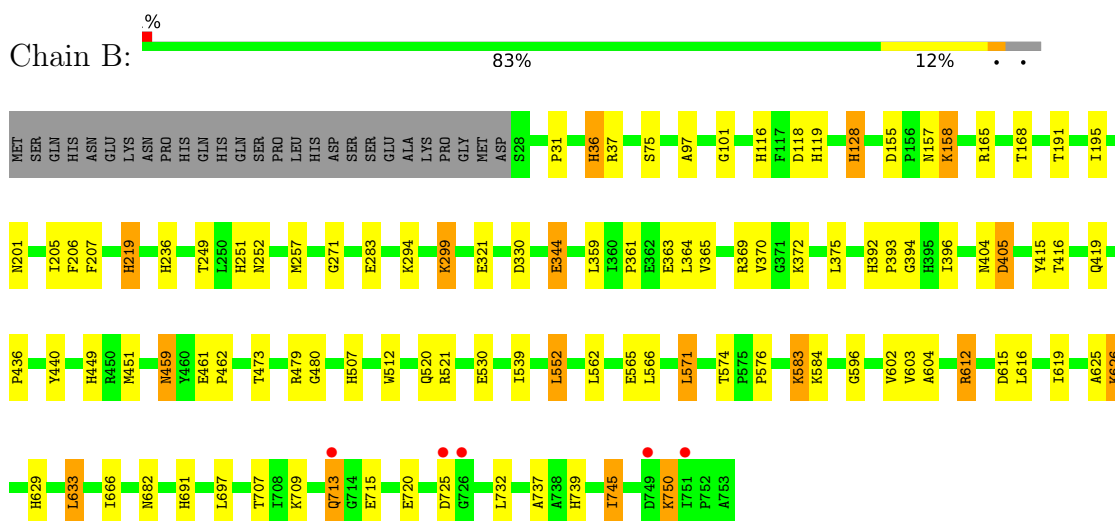
### 3 Residue-property plots

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.

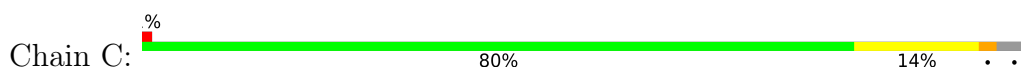
- Molecule 1: Catalase HPII

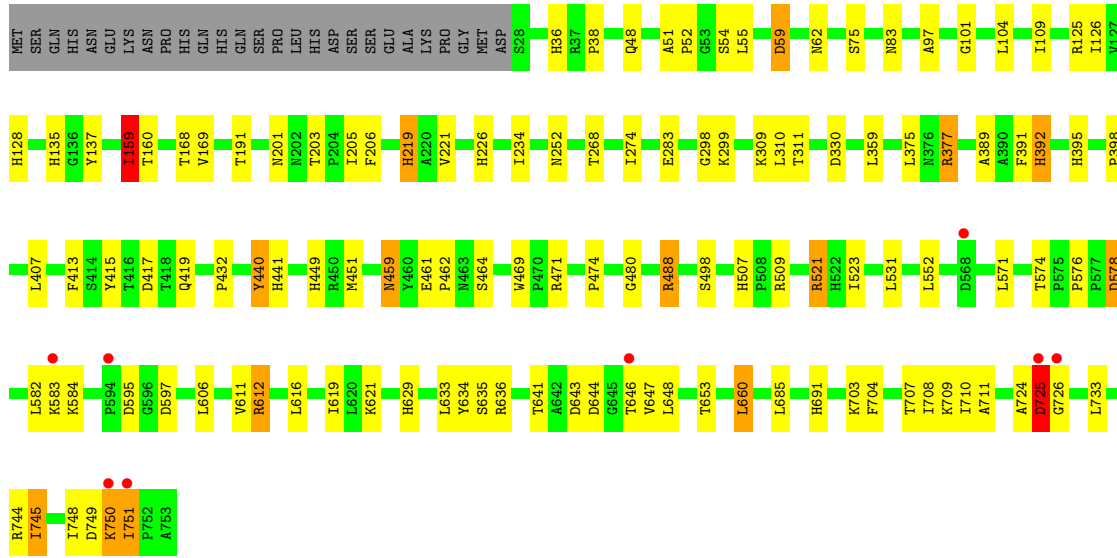


- Molecule 1: Catalase HPII

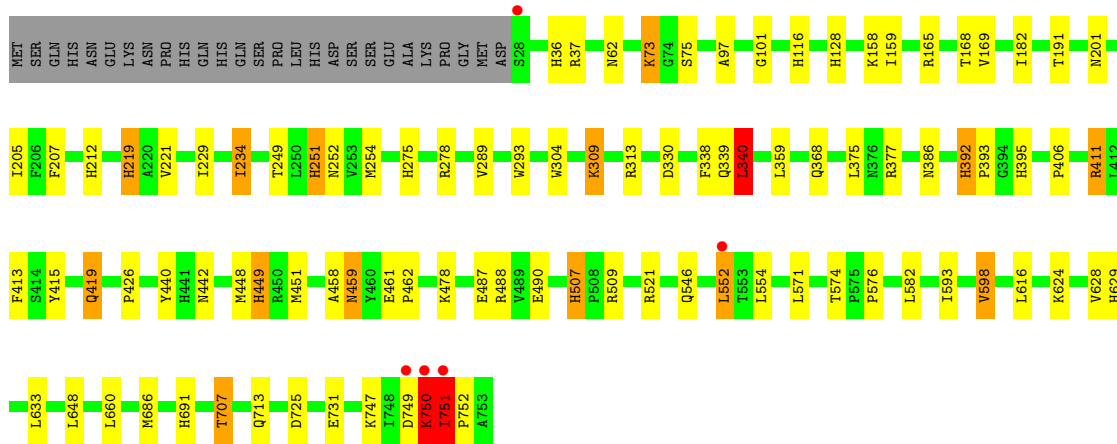
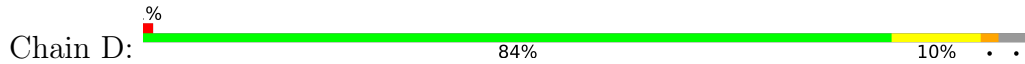


- Molecule 1: Catalase HPII





• Molecule 1: Catalase HPII



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.23Å 133.13Å 122.71Å 90.00° 109.39° 90.00°	Depositor
Resolution (Å)	32.12 – 1.70 32.12 – 1.70	Depositor EDS
% Data completeness (in resolution range)	79.5 (32.12-1.70) 79.5 (32.12-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 1.70Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.167 , 0.207 0.165 , 0.205	Depositor DCC
$R_{free}$ test set	12422 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.6	Xtrriage
Anisotropy	0.103	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26342	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HDD, 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	1.43	25/5916 (0.4%)	1.24	11/8043 (0.1%)
1	B	1.37	23/5905 (0.4%)	1.19	11/8028 (0.1%)
1	C	1.37	25/5916 (0.4%)	1.22	23/8043 (0.3%)
1	D	1.45	17/5905 (0.3%)	1.26	18/8028 (0.2%)
All	All	1.40	90/23642 (0.4%)	1.23	63/32142 (0.2%)

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	474	PRO	CA-C	9.95	1.57	1.51
1	B	449	HIS	CE1-NE2	9.14	1.41	1.32
1	B	449	HIS	CG-CD2	8.03	1.44	1.35
1	C	135	HIS	CE1-NE2	7.91	1.40	1.32
1	B	219	HIS	CE1-NE2	7.82	1.40	1.32
1	A	275	HIS	CE1-NE2	7.50	1.40	1.32
1	A	178	THR	N-CA	7.25	1.54	1.46
1	C	203	THR	C-O	7.17	1.33	1.24
1	B	739	HIS	CG-CD2	6.90	1.43	1.35
1	B	158	LYS	C-O	6.73	1.31	1.24
1	D	507	HIS	N-CA	6.68	1.52	1.46
1	D	392	HIS	ND1-CE1	6.62	1.39	1.32
1	C	691	HIS	CG-CD2	6.60	1.43	1.35
1	A	395	HIS	CG-CD2	6.59	1.43	1.35
1	C	395	HIS	ND1-CE1	6.58	1.39	1.32
1	C	392	HIS	ND1-CE1	6.56	1.39	1.32
1	C	135	HIS	CG-CD2	6.50	1.43	1.35
1	D	458	ALA	C-O	6.36	1.31	1.23
1	A	275	HIS	ND1-CE1	6.33	1.38	1.32
1	C	59	ASP	CB-CG	6.31	1.67	1.52
1	B	449	HIS	ND1-CE1	6.29	1.38	1.32
1	D	36	HIS	CG-CD2	6.27	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	PHE	C-O	6.26	1.31	1.24
1	D	395	HIS	CG-CD2	6.26	1.42	1.35
1	C	725	ASP	CA-C	6.25	1.61	1.52
1	D	442	ASN	C-O	6.15	1.29	1.24
1	C	413	PHE	CA-C	6.12	1.60	1.52
1	D	254	MET	C-O	6.10	1.31	1.24
1	D	413	PHE	CA-C	6.02	1.60	1.52
1	D	251	HIS	CE1-NE2	5.94	1.38	1.32
1	A	216	ASP	C-O	5.93	1.30	1.24
1	B	165	ARG	CZ-NH1	5.91	1.41	1.32
1	A	214	PHE	C-O	-5.89	1.19	1.24
1	B	480	GLY	N-CA	5.85	1.50	1.44
1	A	236	HIS	ND1-CE1	5.76	1.38	1.32
1	B	128	HIS	ND1-CE1	5.72	1.38	1.32
1	D	212	HIS	ND1-CE1	5.68	1.38	1.32
1	B	36	HIS	CE1-NE2	5.67	1.38	1.32
1	A	697	LEU	N-CA	5.63	1.52	1.46
1	C	226	HIS	CG-CD2	5.62	1.42	1.35
1	C	391	PHE	N-CA	5.61	1.52	1.45
1	D	406	PRO	C-O	-5.60	1.17	1.24
1	A	441	HIS	CG-CD2	5.55	1.42	1.35
1	C	441	HIS	CE1-NE2	5.53	1.38	1.32
1	C	377	ARG	CZ-NH1	5.52	1.40	1.32
1	B	396	ILE	C-O	5.52	1.30	1.24
1	C	389	ALA	N-CA	5.51	1.52	1.46
1	B	36	HIS	CG-CD2	5.49	1.41	1.35
1	D	36	HIS	CE1-NE2	5.48	1.38	1.32
1	C	160	THR	C-O	-5.47	1.18	1.24
1	C	395	HIS	CE1-NE2	5.47	1.38	1.32
1	B	271	GLY	CA-C	-5.45	1.47	1.52
1	C	219	HIS	CE1-NE2	5.45	1.38	1.32
1	D	219	HIS	CG-CD2	5.43	1.41	1.35
1	D	293	TRP	CA-C	-5.42	1.46	1.52
1	A	251	HIS	ND1-CE1	5.41	1.38	1.32
1	A	629	HIS	ND1-CE1	5.41	1.38	1.32
1	B	365	VAL	C-O	-5.39	1.17	1.24
1	D	275	HIS	CE1-NE2	5.39	1.38	1.32
1	A	121	ARG	CZ-NH2	5.38	1.40	1.33
1	A	219	HIS	CE1-NE2	5.38	1.38	1.32
1	C	125	ARG	N-CA	5.36	1.52	1.46
1	C	36	HIS	CE1-NE2	5.33	1.37	1.32
1	C	311	THR	N-CA	5.32	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	HIS	CD2-NE2	-5.31	1.32	1.37
1	D	691	HIS	CG-CD2	5.30	1.41	1.35
1	A	150	ALA	N-CA	5.28	1.52	1.46
1	D	116	HIS	CG-ND1	-5.25	1.32	1.38
1	A	441	HIS	ND1-CE1	5.22	1.37	1.32
1	A	485	TYR	C-O	5.19	1.30	1.23
1	A	498	SER	CA-C	5.19	1.58	1.53
1	A	420	ILE	CA-CB	5.19	1.60	1.54
1	B	363	GLU	N-CA	5.18	1.52	1.46
1	A	246	GLN	N-CA	5.18	1.52	1.46
1	A	292	HIS	ND1-CE1	5.17	1.37	1.32
1	B	195	ILE	C-O	5.17	1.29	1.24
1	A	324	GLU	N-CA	5.17	1.52	1.46
1	B	479	ARG	CA-CB	5.17	1.61	1.53
1	B	691	HIS	ND1-CE1	5.16	1.37	1.32
1	A	392	HIS	ND1-CE1	5.16	1.37	1.32
1	C	395	HIS	CG-CD2	5.16	1.41	1.35
1	A	194	GLY	C-O	5.16	1.27	1.23
1	B	119	HIS	ND1-CE1	5.10	1.37	1.32
1	B	576	PRO	CA-C	5.08	1.56	1.52
1	C	464	SER	N-CA	5.07	1.52	1.46
1	C	619	ILE	N-CA	5.05	1.52	1.46
1	C	54	SER	N-CA	5.04	1.52	1.46
1	A	629	HIS	CG-CD2	5.03	1.41	1.35
1	B	219	HIS	CG-CD2	5.02	1.41	1.35
1	B	436	PRO	C-O	5.02	1.29	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	ILE	N-CA-C	-9.01	101.81	109.19
1	D	749	ASP	CA-C-N	8.95	137.81	121.70
1	D	749	ASP	C-N-CA	8.95	137.81	121.70
1	A	745	ILE	N-CA-CB	8.81	116.42	110.52
1	D	749	ASP	N-CA-C	7.42	123.61	111.37
1	C	498	SER	CA-C-N	-7.03	112.46	119.56
1	C	498	SER	C-N-CA	-7.03	112.46	119.56
1	D	749	ASP	CA-C-O	-6.93	113.15	120.92
1	C	159	ILE	CB-CG1-CD1	-6.68	99.78	113.80
1	C	48	GLN	CA-C-N	-6.53	113.25	119.85
1	C	48	GLN	C-N-CA	-6.53	113.25	119.85
1	B	574	THR	CA-C-N	6.52	124.42	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	THR	C-N-CA	6.52	124.42	119.66
1	B	745	ILE	CA-C-N	-6.51	112.98	119.56
1	B	745	ILE	C-N-CA	-6.51	112.98	119.56
1	D	707	THR	CB-CA-C	-6.50	100.00	110.79
1	A	709	LYS	CA-C-N	-6.40	114.86	122.93
1	A	709	LYS	C-N-CA	-6.40	114.86	122.93
1	C	523	ILE	N-CA-C	6.37	117.05	110.36
1	D	449	HIS	N-CA-C	-6.37	104.81	112.58
1	B	283	GLU	N-CA-C	6.22	120.34	112.87
1	C	474	PRO	CB-CA-C	-6.08	105.68	111.39
1	A	748	ILE	N-CA-C	6.06	119.56	111.44
1	D	751	ILE	N-CA-C	6.00	113.79	108.63
1	A	120	GLU	N-CA-C	5.79	117.59	111.28
1	D	340	LEU	CA-C-N	-5.76	117.84	122.85
1	D	340	LEU	C-N-CA	-5.76	117.84	122.85
1	A	325	ALA	N-CA-C	-5.75	105.09	111.36
1	C	126	ILE	CB-CA-C	-5.70	104.44	112.14
1	C	750	LYS	CA-C-N	-5.58	117.91	123.04
1	C	750	LYS	C-N-CA	-5.58	117.91	123.04
1	D	304	TRP	N-CA-C	5.56	117.02	111.07
1	A	98	GLY	N-CA-C	-5.52	105.72	112.68
1	B	539	ILE	N-CA-C	-5.52	105.14	110.72
1	A	431	ILE	N-CA-C	-5.48	103.58	108.95
1	D	411	ARG	N-CA-C	-5.48	105.31	111.28
1	C	474	PRO	O-C-N	5.43	123.81	121.31
1	C	595	ASP	CA-C-N	5.42	125.25	120.10
1	C	595	ASP	C-N-CA	5.42	125.25	120.10
1	A	536	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	294	LYS	CD-CE-NZ	-5.40	94.62	111.90
1	B	473	THR	CA-C-N	-5.39	115.73	119.66
1	B	473	THR	C-N-CA	-5.39	115.73	119.66
1	D	182	ILE	N-CA-C	-5.33	104.25	110.05
1	C	724	ALA	N-CA-C	5.31	117.59	109.62
1	A	115	THR	N-CA-C	-5.28	105.60	111.36
1	D	377	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	182	ILE	CA-C-O	-5.18	116.25	121.59
1	D	593	ILE	CA-C-N	5.15	125.44	119.93
1	D	593	ILE	C-N-CA	5.15	125.44	119.93
1	C	480	GLY	CA-C-N	5.11	124.95	120.10
1	C	480	GLY	C-N-CA	5.11	124.95	120.10
1	B	158	LYS	N-CA-C	5.08	116.47	109.15
1	C	574	THR	CA-C-N	-5.08	115.14	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	574	THR	C-N-CA	-5.08	115.14	120.38
1	C	745	ILE	CA-C-N	-5.06	114.45	119.56
1	C	745	ILE	C-N-CA	-5.06	114.45	119.56
1	D	234	ILE	N-CA-C	-5.06	107.82	112.83
1	C	109	ILE	N-CA-C	-5.05	105.92	110.82
1	B	405	ASP	O-C-N	5.02	125.39	121.47
1	C	611	VAL	N-CA-C	5.00	116.67	109.51
1	C	751	ILE	CB-CA-C	5.00	115.83	110.53
1	D	750	LYS	N-CA-CB	5.00	119.00	110.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5752	0	5591	61	1
1	B	5745	0	5584	67	1
1	C	5752	0	5591	75	1
1	D	5744	0	5584	70	0
2	A	44	0	31	4	0
2	B	44	0	31	1	0
2	C	44	0	31	2	0
2	D	44	0	31	3	0
3	A	43	0	30	15	0
3	B	43	0	30	7	0
3	C	43	0	30	12	0
3	D	43	0	30	10	0
4	A	772	0	0	11	0
4	B	695	0	0	12	1
4	C	735	0	0	19	0
4	D	799	0	0	16	0
All	All	26342	0	22594	278	2

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 6.

All (278) 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:C:392:HIS:ND1	1:C:415:TYR:CB	1.67	1.54
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.68	1.51
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.73	1.50
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.76	1.48
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.64	1.30
1:D:521:ARG:HD2	4:D:1642:HOH:O	1.36	1.25
1:D:546:GLN:HG3	4:D:1601:HOH:O	1.05	1.22
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.73	1.21
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.76	1.20
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.81	1.13
3:C:802[B]:HEM:HMC2	3:C:802[B]:HEM:HBC2	1.17	1.13
1:A:451:MET:HE2	1:C:451:MET:HE2	1.16	1.12
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.80	1.12
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.79	1.11
3:A:802[B]:HEM:HMC2	3:A:802[B]:HEM:HBC2	1.13	1.10
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.76	1.08
1:B:451:MET:HE2	1:D:451:MET:HE2	0.99	0.99
3:D:802[B]:HEM:HMC2	3:D:802[B]:HEM:HBC2	1.43	0.98
1:A:201:ASN:CG	3:A:802[B]:HEM:HMB2	1.89	0.97
1:B:451:MET:CE	1:D:451:MET:HE2	1.94	0.96
1:C:612:ARG:HH11	1:C:612:ARG:HG3	1.27	0.96
1:B:451:MET:HE2	1:D:451:MET:CE	1.94	0.96
4:B:1503:HOH:O	1:D:73:LYS:HD3	1.67	0.95
1:A:344:GLU:OE1	4:A:1588:HOH:O	1.84	0.95
1:B:416:THR:HG21	4:D:1528:HOH:O	1.64	0.95
1:A:369:ARG:HH21	1:A:369:ARG:HG3	1.28	0.94
1:C:725:ASP:HB2	1:C:726:GLY:C	1.93	0.94
1:D:731:GLU:OE2	4:D:1670:HOH:O	1.86	0.92
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:CMC	1.98	0.92
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.04	0.92
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.04	0.89
1:C:725:ASP:HB2	1:C:726:GLY:O	1.72	0.89
1:A:716:GLU:HG2	4:A:1647:HOH:O	1.74	0.88
3:A:802[B]:HEM:HMC2	3:A:802[B]:HEM:CBC	2.01	0.88
1:D:201:ASN:CG	3:D:802[B]:HEM:HMB2	1.99	0.87
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.04	0.87
3:D:802[B]:HEM:HBC2	3:D:802[B]:HEM:CMC	2.03	0.87
1:A:29:LEU:HD22	4:C:1476:HOH:O	1.75	0.85
1:B:157:ASN:HB2	4:B:1581:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASN:CG	3:C:802[B]:HEM:HMB2	2.06	0.81
1:A:369:ARG:HH21	1:A:369:ARG:CG	1.94	0.80
1:C:59:ASP:OD2	4:C:1498:HOH:O	1.99	0.80
1:C:629:HIS:HD2	4:C:1209:HOH:O	1.65	0.80
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:CMC	1.94	0.80
4:B:1503:HOH:O	1:D:73:LYS:CD	2.25	0.77
1:C:612:ARG:HH11	1:C:612:ARG:CG	1.96	0.77
1:C:621:LYS:HG2	4:C:1618:HOH:O	1.85	0.77
1:C:636:ARG:HD3	4:C:1540:HOH:O	1.85	0.77
1:D:221:VAL:CG2	1:D:234:ILE:HG22	2.15	0.77
1:C:392:HIS:ND1	1:C:415:TYR:HB3	1.96	0.75
1:C:597:ASP:OD1	4:C:1425:HOH:O	2.04	0.75
1:C:206:PHE:CG	3:C:802[B]:HEM:HAB	2.22	0.74
1:B:369:ARG:HG2	4:B:1306:HOH:O	1.87	0.73
1:D:751:ILE:HG12	1:D:752:PRO:HD2	1.69	0.72
1:D:488:ARG:NE	4:D:1586:HOH:O	2.03	0.72
1:D:488:ARG:NH2	4:D:1586:HOH:O	2.21	0.72
1:C:612:ARG:HG3	1:C:612:ARG:NH1	2.05	0.71
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.57	0.71
1:A:369:ARG:HD3	4:A:1495:HOH:O	1.91	0.70
1:A:639:GLU:HG3	4:A:1498:HOH:O	1.92	0.69
1:B:330:ASP:OD2	1:B:629:HIS:HE1	1.75	0.69
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.58	0.69
1:D:629:HIS:HD2	4:D:1260:HOH:O	1.74	0.69
1:C:578:ASP:HB2	1:C:582:LEU:O	1.93	0.69
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.60	0.68
1:A:710:ILE:HD11	1:A:714:GLY:HA2	1.76	0.68
1:D:368:GLN:OE1	4:D:1587:HOH:O	2.12	0.67
1:C:221:VAL:CG2	1:C:234:ILE:HG22	2.25	0.67
1:C:440:TYR:HD2	4:C:1375:HOH:O	1.78	0.66
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.77	0.66
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.26	0.66
1:C:521:ARG:CD	4:C:1440:HOH:O	2.44	0.65
1:C:330:ASP:OD2	1:C:629:HIS:HE1	1.80	0.65
1:A:201:ASN:CG	3:A:802[B]:HEM:CMB	2.67	0.65
1:B:201:ASN:CG	3:B:802[B]:HEM:HMB2	2.21	0.65
1:D:488:ARG:HH12	1:D:490:GLU:CD	2.06	0.64
1:A:369:ARG:HG3	1:A:369:ARG:NH2	2.04	0.64
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.63	0.64
1:C:488:ARG:HD3	4:C:1472:HOH:O	1.98	0.64
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:CG	3:A:802[B]:HEM:HAB	2.33	0.63
1:A:28:SER:O	1:A:28:SER:OG	2.15	0.63
1:C:407:LEU:HD23	3:C:802[B]:HEM:HBB1	1.81	0.62
1:A:344:GLU:HB3	4:A:1588:HOH:O	1.98	0.62
1:A:201:ASN:ND2	3:A:802[B]:HEM:CMB	2.63	0.61
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.82	0.61
1:D:201:ASN:CG	3:D:802[B]:HEM:CMB	2.74	0.61
3:D:802[B]:HEM:HMC2	3:D:802[B]:HEM:CBC	2.24	0.61
1:C:274:ILE:HD12	3:C:802[B]:HEM:HMB1	1.83	0.60
1:B:625:ALA:O	1:B:626:LYS:HE3	2.01	0.60
1:D:330:ASP:OD2	1:D:629:HIS:HE1	1.83	0.60
1:C:201:ASN:ND2	3:C:802[B]:HEM:CMB	2.65	0.60
1:D:415:TYR:O	1:D:419[B]:GLN:HG2	2.01	0.60
1:D:750:LYS:HD2	1:D:750:LYS:C	2.27	0.59
1:C:521:ARG:HD2	4:C:1440:HOH:O	2.02	0.59
1:B:201:ASN:CG	3:B:802[B]:HEM:CMB	2.76	0.59
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.18	0.58
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.58
2:C:801[A]:HDD:HBD2	4:C:1091:HOH:O	2.02	0.58
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.34	0.58
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.12	0.58
2:A:801[A]:HDD:HBD2	4:A:995:HOH:O	2.03	0.58
1:C:745:ILE:HD13	4:C:1570:HOH:O	2.03	0.58
1:C:725:ASP:HB2	1:C:726:GLY:CA	2.34	0.57
1:D:201:ASN:ND2	3:D:802[B]:HEM:CMB	2.68	0.57
1:C:52:PRO:HG2	1:C:55:LEU:HD12	1.87	0.57
1:B:392:HIS:CG	1:B:415:TYR:CB	2.78	0.57
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.02	0.57
1:D:490:GLU:OE2	4:D:1485:HOH:O	2.18	0.57
1:C:221:VAL:HG22	1:C:234:ILE:HG22	1.87	0.56
1:D:411:ARG:HG2	3:D:802[B]:HEM:C2C	2.40	0.56
1:A:369:ARG:CG	1:A:369:ARG:NH2	2.63	0.56
1:D:478:LYS:NZ	4:D:999:HOH:O	2.26	0.56
2:D:801[A]:HDD:HBD2	4:D:1141:HOH:O	2.05	0.56
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.71	0.55
1:C:206:PHE:CD1	3:C:802[B]:HEM:HAB	2.41	0.55
1:A:274:ILE:HD12	3:A:802[B]:HEM:HMB1	1.89	0.55
1:B:359:LEU:H	1:B:507:HIS:HD2	1.54	0.55
1:C:359:LEU:H	1:C:507:HIS:HD2	1.55	0.55
1:D:359:LEU:H	1:D:507:HIS:HD2	1.55	0.55
1:A:449[B]:HIS:HD2	4:C:1192:HOH:O	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:HIS:HD2	4:B:1162:HOH:O	1.89	0.54
1:A:710:ILE:CD1	1:A:714:GLY:HA2	2.36	0.54
1:C:704:PHE:O	1:C:707:THR:HG22	2.07	0.54
1:A:478:LYS:HG2	4:A:1370:HOH:O	2.08	0.54
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.90	0.54
3:C:802[B]:HEM:CMC	3:C:802[B]:HEM:CBC	2.76	0.54
1:C:359:LEU:H	1:C:507:HIS:CD2	2.26	0.54
1:B:583:LYS:NZ	1:B:583:LYS:H	2.05	0.53
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.43	0.53
1:D:165:ARG:HD3	2:D:801[A]:HDD:O2A	2.09	0.53
1:B:257:MET:SD	1:B:530:GLU:HG3	2.49	0.53
1:C:521:ARG:HG2	4:C:1570:HOH:O	2.09	0.53
1:B:361:PRO:HD2	1:B:364:LEU:HD12	1.90	0.52
1:C:38:PRO:HG2	1:C:51:ALA:HB2	1.90	0.52
1:B:206:PHE:CG	3:B:802[B]:HEM:HAB	2.45	0.52
1:B:626:LYS:HE3	1:B:626:LYS:HA	1.90	0.52
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.91	0.52
1:C:392:HIS:CE1	1:C:415:TYR:CB	2.57	0.52
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.17	0.52
1:D:449:HIS:CE1	4:D:1348:HOH:O	2.62	0.52
1:A:201:ASN:OD1	3:A:802[B]:HEM:HMB2	2.10	0.51
1:A:214:PHE:CD1	2:A:801[A]:HDD:HMC2	2.45	0.51
1:B:97:ALA:O	1:B:101:GLY:HA3	2.10	0.51
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.25	0.51
1:B:615:ASP:O	1:B:619:ILE:HG13	2.10	0.51
2:B:801[A]:HDD:HBD2	4:B:1042:HOH:O	2.10	0.51
1:B:713:GLN:NE2	1:B:713:GLN:H	2.10	0.50
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.27	0.50
1:C:725:ASP:CB	1:C:726:GLY:C	2.77	0.50
1:D:207:PHE:O	1:D:249:THR:HA	2.11	0.50
1:B:201:ASN:ND2	3:B:802[B]:HEM:HMB1	2.27	0.49
1:B:521:ARG:HH22	1:B:745:ILE:HD13	1.77	0.49
1:B:713:GLN:H	1:B:713:GLN:CD	2.21	0.49
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.27	0.49
1:D:449:HIS:HE1	4:D:1348:HOH:O	1.94	0.49
1:B:359:LEU:H	1:B:507:HIS:CD2	2.30	0.49
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.48	0.49
1:B:612:ARG:HB2	1:B:612:ARG:CZ	2.42	0.49
1:A:76:GLU:O	1:A:77:ASN:HB2	2.13	0.48
1:B:128:HIS:HA	1:B:168:THR:O	2.14	0.48
1:D:488:ARG:NH1	1:D:490:GLU:CD	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.95	0.48
1:A:705:LYS:HE3	1:A:710:ILE:CG1	2.44	0.47
1:D:221:VAL:HG22	1:D:234:ILE:HG22	1.94	0.47
1:A:128:HIS:HA	1:A:168:THR:O	2.14	0.47
1:A:461:GLU:HA	1:A:462:PRO:C	2.38	0.47
1:C:634:TYR:CG	1:C:635:SER:N	2.81	0.47
1:D:37:ARG:HD2	4:D:1444:HOH:O	2.14	0.47
1:A:313:ARG:NH1	1:D:309:LYS:HD2	2.30	0.47
1:C:509:ARG:HD3	1:C:576:PRO:HG2	1.97	0.47
1:C:745:ILE:O	1:C:748:ILE:HG12	2.15	0.47
1:B:201:ASN:ND2	3:B:802[B]:HEM:CMB	2.78	0.47
1:C:407:LEU:CD2	3:C:802[B]:HEM:HBB1	2.45	0.47
1:C:583:LYS:HB2	4:C:1373:HOH:O	2.14	0.47
1:A:201:ASN:ND2	3:A:802[B]:HEM:HMB2	2.23	0.46
1:B:521:ARG:NH2	1:B:521:ARG:HB3	2.30	0.46
1:A:309:LYS:NZ	1:A:687:GLU:OE2	2.37	0.46
1:B:155:ASP:OD2	4:B:1581:HOH:O	2.21	0.46
1:A:205:ILE:HD13	1:A:205:ILE:H	1.80	0.46
1:A:36:HIS:CD2	1:A:36:HIS:H	2.33	0.46
1:C:461:GLU:HA	1:C:462:PRO:C	2.40	0.46
1:D:392:HIS:CG	1:D:415:TYR:CB	2.82	0.46
1:A:36:HIS:HE1	4:A:1352:HOH:O	1.99	0.46
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.51	0.46
1:C:274:ILE:HD12	3:C:802[B]:HEM:CMB	2.47	0.46
1:D:201:ASN:ND2	3:D:802[B]:HEM:HMB1	2.31	0.46
1:A:583:LYS:O	1:A:584:LYS:HB3	2.14	0.45
2:A:801[A]:HDD:HBB1	2:A:801[A]:HDD:HMB1	1.98	0.45
4:B:1503:HOH:O	1:D:73:LYS:HG3	2.16	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
1:B:344:GLU:CD	1:B:344:GLU:H	2.25	0.45
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.98	0.45
1:C:711:ALA:HB1	4:C:1575:HOH:O	2.16	0.45
1:D:201:ASN:OD1	3:D:802[B]:HEM:HMB2	2.15	0.45
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.98	0.45
1:A:201:ASN:ND2	3:A:802[B]:HEM:HMB1	2.32	0.45
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.52	0.45
1:D:158:LYS:NZ	4:D:1656:HOH:O	2.43	0.45
1:C:309:LYS:HB3	1:C:660:LEU:HD21	2.00	0.44
1:D:598:VAL:HG13	1:D:628:VAL:HG22	1.98	0.44
1:B:566:LEU:HD23	4:B:1216:HOH:O	2.17	0.44
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:ASN:OD1	1:D:386:ASN:C	2.60	0.44
1:C:647:VAL:O	4:C:1488:HOH:O	2.20	0.44
3:A:802[B]:HEM:CMC	3:A:802[B]:HEM:CBC	2.73	0.44
1:B:201:ASN:OD1	3:B:802[B]:HEM:HMB2	2.17	0.44
1:D:201:ASN:ND2	3:D:802[B]:HEM:HMB2	2.30	0.44
1:D:552:LEU:HD11	1:D:571:LEU:HA	2.00	0.44
1:B:393:PRO:HD2	1:B:415:TYR:CD1	2.52	0.44
1:B:521:ARG:CG	1:B:521:ARG:HH21	2.31	0.44
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.53	0.44
1:A:221:VAL:CG2	1:A:234:ILE:HG22	2.48	0.44
1:B:596:GLY:HA3	1:B:737:ALA:O	2.18	0.44
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.53	0.44
1:D:686:MET:HE2	1:D:751:ILE:HD11	2.00	0.44
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.99	0.44
1:B:207:PHE:O	1:B:249:THR:HA	2.18	0.43
1:B:36:HIS:HD1	1:B:36:HIS:H	1.66	0.43
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.53	0.43
1:A:392:HIS:CE1	1:A:415:TYR:CB	2.68	0.43
1:D:221:VAL:HG23	1:D:234:ILE:HG22	1.97	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.34	0.43
1:A:411:ARG:HG2	3:A:802[B]:HEM:C2C	2.53	0.43
1:B:461:GLU:HA	1:B:462:PRO:C	2.42	0.43
1:B:566:LEU:N	1:B:566:LEU:HD22	2.34	0.43
1:B:709:LYS:HG3	1:B:750:LYS:HE3	2.00	0.43
4:B:1503:HOH:O	1:D:73:LYS:CG	2.60	0.43
1:D:725:ASP:OD1	1:D:725:ASP:C	2.62	0.43
1:B:31:PRO:HD2	1:B:36:HIS:HB3	2.01	0.43
1:B:299:LYS:HE2	4:B:991:HOH:O	2.18	0.43
1:A:91:ASP:OD2	1:C:461:GLU:OE1	2.37	0.43
2:D:801[A]:HDD:HMB1	2:D:801[A]:HDD:HBB1	2.01	0.42
2:C:801[A]:HDD:HMD3	2:C:801[A]:HDD:HAD2	1.76	0.42
1:D:448:MET:O	1:D:449:HIS:HB2	2.20	0.42
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.01	0.42
1:B:419[B]:GLN:HE22	3:B:802[B]:HEM:CGD	2.31	0.42
1:C:612:ARG:CG	1:C:612:ARG:NH1	2.67	0.42
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.54	0.42
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.54	0.42
1:A:29:LEU:HB2	4:C:1476:HOH:O	2.20	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:D:62:ASN:OD1	1:D:62:ASN:C	2.63	0.42
1:C:749:ASP:CG	4:C:1484:HOH:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:HD3	2:A:801[A]:HDD:O2A	2.20	0.41
1:C:643:ASP:OD1	1:C:644:ASP:N	2.53	0.41
1:A:51:ALA:HB1	1:A:52:PRO:HD2	2.02	0.41
4:A:1096:HOH:O	1:C:449[B]:HIS:HD2	2.01	0.41
4:A:1237:HOH:O	1:C:104:LEU:HB3	2.21	0.41
1:D:507:HIS:HE1	4:D:1112:HOH:O	2.03	0.41
1:A:715:GLU:CD	1:A:747:LYS:HE3	2.44	0.41
1:B:37:ARG:HD3	4:B:1542:HOH:O	2.21	0.41
1:C:97:ALA:O	1:C:101:GLY:HA3	2.21	0.41
1:C:634:TYR:O	1:C:653:THR:HA	2.20	0.41
1:D:289:VAL:HA	1:D:339:GLN:O	2.20	0.41
1:B:404:ASN:O	1:B:405:ASP:C	2.64	0.41
1:B:552:LEU:HD21	1:B:571:LEU:HD12	2.02	0.41
1:D:97:ALA:O	1:D:101:GLY:HA3	2.21	0.41
3:A:802[B]:HEM:HHA	3:A:802[B]:HEM:HAA2	1.94	0.41
1:B:118:ASP:OD2	1:C:417:ASP:OD2	2.38	0.41
1:B:512:TRP:CH2	1:B:520:GLN:HB3	2.56	0.41
1:B:697:LEU:O	1:B:720:GLU:HA	2.21	0.41
1:C:62:ASN:OD1	1:C:62:ASN:C	2.63	0.41
1:A:392:HIS:CG	1:A:415:TYR:CB	2.85	0.41
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.02	0.41
1:C:744:ARG:O	1:C:744:ARG:HG2	2.21	0.41
1:D:393:PRO:HD2	1:D:415:TYR:CD1	2.56	0.41
1:A:205:ILE:HD13	1:A:205:ILE:N	2.35	0.41
1:A:556:GLN:NE2	4:A:1482:HOH:O	2.54	0.40
1:D:461:GLU:HA	1:D:462:PRO:C	2.46	0.40
1:A:206:PHE:CD1	3:A:802[B]:HEM:HAB	2.56	0.40
1:C:725:ASP:CB	1:C:726:GLY:O	2.58	0.40
1:C:299:LYS:HB2	1:C:299:LYS:HE3	1.91	0.40
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.03	0.40
1:B:392:HIS:CD2	1:B:394:GLY:H	2.40	0.40
1:C:268:THR:HA	1:C:298:GLY:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASP:CB	4:B:1591:HOH:O[2_545]	2.07	0.13
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.19	0.01

## 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	726/753 (96%)	705 (97%)	20 (3%)	1 (0%)	48	31
1	B	725/753 (96%)	702 (97%)	21 (3%)	2 (0%)	36	22
1	C	726/753 (96%)	708 (98%)	17 (2%)	1 (0%)	48	31
1	D	725/753 (96%)	708 (98%)	15 (2%)	2 (0%)	36	22
All	All	2902/3012 (96%)	2823 (97%)	73 (2%)	6 (0%)	43	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	D	750	LYS
1	C	75	SER
1	D	75	SER
1	A	75	SER
1	B	75	SER

### 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	613/636 (96%)	593 (97%)	20 (3%)	33	17
1	B	612/636 (96%)	586 (96%)	26 (4%)	26	11
1	C	613/636 (96%)	580 (95%)	33 (5%)	20	6
1	D	612/636 (96%)	586 (96%)	26 (4%)	26	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2450/2544 (96%)	2345 (96%)	105 (4%)	26 10

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	37	ARG
1	A	73	LYS
1	A	191	THR
1	A	205	ILE
1	A	213	LYS
1	A	252	ASN
1	A	369	ARG
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	707	THR
1	A	709	LYS
1	A	710	ILE
1	A	713	GLN
1	A	732	LEU
1	A	750	LYS
1	B	158	LYS
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	299	LYS
1	B	321	GLU
1	B	344	GLU
1	B	370	VAL
1	B	372	LYS
1	B	375	LEU
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	571	LEU
1	B	583	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	602	VAL
1	B	612	ARG
1	B	616	LEU
1	B	626	LYS
1	B	633	LEU
1	B	713	GLN
1	B	715	GLU
1	B	732	LEU
1	B	750	LYS
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	252	ASN
1	C	283	GLU
1	C	375	LEU
1	C	377	ARG
1	C	398	PRO
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	571	LEU
1	C	578	ASP
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	641	THR
1	C	646	THR
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	703	LYS
1	C	709	LYS
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE

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Mol	Chain	Res	Type
1	D	73	LYS
1	D	159	ILE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	309	LYS
1	D	340	LEU
1	D	375	LEU
1	D	419[A]	GLN
1	D	419[B]	GLN
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	624	LYS
1	D	633	LEU
1	D	648	LEU
1	D	707	THR
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	139	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	546	GLN
1	A	556	GLN
1	A	713	GLN
1	B	84	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS

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Mol	Chain	Res	Type
1	B	629	HIS
1	B	713	GLN
1	C	77	ASN
1	C	84	GLN
1	C	201	ASN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	546	GLN
1	C	629	HIS
1	C	682	ASN
1	C	713	GLN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	549	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN
1	D	682	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HDD	D	801[A]	1	46,52,52	2.16	12 (26%)	62,89,89	2.51	22 (35%)
3	HEM	D	802[B]	1	50,50,50	2.50	21 (42%)	67,82,82	3.00	36 (53%)
3	HEM	B	802[B]	1,4	50,50,50	2.45	24 (48%)	67,82,82	2.76	33 (49%)
3	HEM	C	802[B]	1	50,50,50	2.59	23 (46%)	67,82,82	3.13	35 (52%)
3	HEM	A	802[B]	1,4	50,50,50	2.52	21 (42%)	67,82,82	2.99	33 (49%)
2	HDD	A	801[A]	1,4	46,52,52	2.03	16 (34%)	62,89,89	2.57	21 (33%)
2	HDD	B	801[A]	1,4	46,52,52	2.27	17 (36%)	62,89,89	2.63	26 (41%)
2	HDD	C	801[A]	1,4	46,52,52	2.18	15 (32%)	62,89,89	2.21	21 (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
2	HDD	D	801[A]	1	-	4/9/89/89	0/1/9/9
3	HEM	D	802[B]	1	-	2/14/54/54	-
3	HEM	B	802[B]	1,4	-	4/14/54/54	-
3	HEM	C	802[B]	1	-	4/14/54/54	-
3	HEM	A	802[B]	1,4	-	4/14/54/54	-
2	HDD	A	801[A]	1,4	-	4/9/89/89	0/1/9/9
2	HDD	B	801[A]	1,4	-	4/9/89/89	0/1/9/9
2	HDD	C	801[A]	1,4	-	2/9/89/89	0/1/9/9

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801[A]	HDD	CHC-C4B	6.07	1.50	1.38
3	A	802[B]	HEM	FE-ND	6.05	2.13	1.94
3	C	802[B]	HEM	FE-NB	5.87	2.13	1.94
3	C	802[B]	HEM	FE-ND	5.65	2.12	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801[A]	HDD	CHC-C4B	5.51	1.49	1.38
3	C	802[B]	HEM	C1C-NC	5.35	1.49	1.39
3	A	802[B]	HEM	C1C-NC	5.20	1.49	1.39
3	D	802[B]	HEM	FE-ND	5.13	2.10	1.94
3	D	802[B]	HEM	FE-NB	5.08	2.10	1.94
3	B	802[B]	HEM	FE-ND	5.07	2.10	1.94
2	D	801[A]	HDD	CHC-C4B	5.02	1.48	1.38
2	D	801[A]	HDD	CHB-C1B	4.96	1.48	1.38
2	B	801[A]	HDD	CHB-C1B	4.90	1.48	1.38
3	C	802[B]	HEM	C4C-NC	4.84	1.48	1.39
3	B	802[B]	HEM	FE-NB	4.80	2.09	1.94
3	C	802[B]	HEM	C3D-C2D	4.74	1.47	1.36
2	D	801[A]	HDD	O1D-CGD	4.70	1.43	1.35
3	D	802[B]	HEM	C1A-NA	4.70	1.48	1.39
2	B	801[A]	HDD	C3B-C2B	4.69	1.46	1.37
3	D	802[B]	HEM	C1C-NC	4.69	1.48	1.39
3	D	802[B]	HEM	C4C-NC	4.55	1.48	1.39
2	A	801[A]	HDD	CHC-C4B	4.53	1.47	1.38
3	D	802[B]	HEM	CHA-C4D	4.51	1.47	1.38
3	A	802[B]	HEM	C4A-NA	4.46	1.48	1.39
2	D	801[A]	HDD	C3B-C2B	4.46	1.46	1.37
2	C	801[A]	HDD	CHC-C1C	4.45	1.49	1.39
3	D	802[B]	HEM	C4A-NA	4.40	1.47	1.39
2	C	801[A]	HDD	O1D-CGD	4.26	1.42	1.35
2	C	801[A]	HDD	CHB-C4A	4.26	1.49	1.39
2	B	801[A]	HDD	CHB-C4A	4.24	1.48	1.39
3	A	802[B]	HEM	CHC-C1C	4.20	1.46	1.38
2	A	801[A]	HDD	CHA-C1A	4.18	1.48	1.39
2	A	801[A]	HDD	O1D-CGD	4.18	1.42	1.35
2	D	801[A]	HDD	CHB-C4A	4.14	1.48	1.39
3	D	802[B]	HEM	CHD-C4C	4.13	1.46	1.38
3	B	802[B]	HEM	C4A-NA	4.10	1.47	1.39
3	C	802[B]	HEM	C3C-C2C	4.09	1.45	1.37
3	A	802[B]	HEM	C1A-NA	4.09	1.47	1.39
2	A	801[A]	HDD	CHB-C1B	4.08	1.46	1.38
3	A	802[B]	HEM	C3C-C2C	4.06	1.45	1.37
3	D	802[B]	HEM	C3D-C2D	4.05	1.45	1.36
3	A	802[B]	HEM	C4C-NC	4.03	1.47	1.39
3	B	802[B]	HEM	CHD-C4C	4.01	1.46	1.38
3	B	802[B]	HEM	C3C-C2C	3.97	1.45	1.37
3	A	802[B]	HEM	FE-NB	3.95	2.07	1.94
3	B	802[B]	HEM	C1C-NC	3.86	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801[A]	HDD	O1D-CGD	3.82	1.41	1.35
3	A	802[B]	HEM	C3D-C2D	3.81	1.45	1.36
2	C	801[A]	HDD	CHB-C1B	3.80	1.45	1.38
3	C	802[B]	HEM	C1A-NA	3.79	1.46	1.39
3	A	802[B]	HEM	CHB-C1B	3.76	1.46	1.38
2	D	801[A]	HDD	CHD-C4C	3.76	1.47	1.39
3	B	802[B]	HEM	C1B-NB	-3.72	1.33	1.40
3	B	802[B]	HEM	C1A-NA	3.72	1.46	1.39
3	C	802[B]	HEM	CHD-C4C	3.68	1.45	1.38
3	D	802[B]	HEM	C3C-C2C	3.64	1.44	1.37
3	D	802[B]	HEM	CHD-C1D	3.64	1.47	1.39
3	B	802[B]	HEM	C3B-C2B	3.63	1.44	1.37
3	A	802[B]	HEM	CHD-C1D	3.59	1.47	1.39
3	B	802[B]	HEM	CHA-C4D	3.57	1.45	1.38
3	C	802[B]	HEM	CHA-C4D	3.55	1.45	1.38
3	B	802[B]	HEM	C4C-NC	3.50	1.46	1.39
3	C	802[B]	HEM	CHD-C1D	3.49	1.47	1.39
3	A	802[B]	HEM	C1B-NB	-3.49	1.34	1.40
3	C	802[B]	HEM	CHB-C4A	3.49	1.47	1.39
2	A	801[A]	HDD	C3B-C2B	3.46	1.44	1.37
2	C	801[A]	HDD	C4A-NA	-3.44	1.33	1.39
2	B	801[A]	HDD	CHD-C4C	3.42	1.47	1.39
2	C	801[A]	HDD	CHA-C1A	3.41	1.47	1.39
3	A	802[B]	HEM	CHC-C4B	3.40	1.46	1.39
3	C	802[B]	HEM	C4A-NA	3.35	1.45	1.39
2	B	801[A]	HDD	CHA-C1A	3.33	1.46	1.39
3	C	802[B]	HEM	CHC-C1C	3.31	1.44	1.38
3	B	802[B]	HEM	CHC-C4B	3.29	1.46	1.39
2	D	801[A]	HDD	C1C-C2C	3.27	1.50	1.43
3	A	802[B]	HEM	CHA-C4D	3.23	1.45	1.38
3	C	802[B]	HEM	CHB-C1B	3.23	1.45	1.38
2	A	801[A]	HDD	CHB-C4A	3.23	1.46	1.39
3	C	802[B]	HEM	C4A-C3A	3.22	1.50	1.43
3	B	802[B]	HEM	CHD-C1D	3.22	1.46	1.39
2	B	801[A]	HDD	C4C-NC	-3.21	1.33	1.39
2	C	801[A]	HDD	C3B-C2B	3.20	1.43	1.37
2	B	801[A]	HDD	C2A-C3A	3.17	1.47	1.38
3	B	802[B]	HEM	C3D-C2D	3.13	1.43	1.36
3	B	802[B]	HEM	C4D-ND	-3.11	1.34	1.40
2	C	801[A]	HDD	C1A-NA	-3.10	1.33	1.39
3	D	802[B]	HEM	C3B-C2B	3.08	1.43	1.37
3	D	802[B]	HEM	CHC-C1C	3.05	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802[B]	HEM	C2A-C3A	3.04	1.46	1.38
3	D	802[B]	HEM	CHB-C1B	3.02	1.44	1.38
2	C	801[A]	HDD	CHD-C4C	3.01	1.46	1.39
3	C	802[B]	HEM	C2A-C3A	3.01	1.46	1.38
3	B	802[B]	HEM	CHC-C1C	2.99	1.44	1.38
2	A	801[A]	HDD	CHC-C1C	2.94	1.46	1.39
2	C	801[A]	HDD	C2A-C3A	2.84	1.46	1.38
2	B	801[A]	HDD	CHC-C1C	2.83	1.45	1.39
2	B	801[A]	HDD	C1A-NA	-2.82	1.34	1.39
2	C	801[A]	HDD	C1B-NB	-2.81	1.34	1.39
2	D	801[A]	HDD	C4B-NB	-2.80	1.34	1.39
3	B	802[B]	HEM	CHB-C1B	2.79	1.44	1.38
3	C	802[B]	HEM	C4D-ND	-2.75	1.35	1.40
2	A	801[A]	HDD	C1C-C2C	2.75	1.49	1.43
3	D	802[B]	HEM	CHC-C4B	2.74	1.45	1.39
3	A	802[B]	HEM	CHD-C4C	2.70	1.43	1.38
3	C	802[B]	HEM	CHC-C4B	2.69	1.45	1.39
2	A	801[A]	HDD	CHD-C4C	2.63	1.45	1.39
3	B	802[B]	HEM	CHB-C4A	2.60	1.45	1.39
2	C	801[A]	HDD	C4A-C3A	2.59	1.49	1.43
3	A	802[B]	HEM	C2A-C3A	2.58	1.45	1.38
2	B	801[A]	HDD	C1C-C2C	2.57	1.49	1.43
2	D	801[A]	HDD	C2A-C3A	2.56	1.45	1.38
3	A	802[B]	HEM	C1C-C2C	2.54	1.50	1.45
3	C	802[B]	HEM	CHA-C1A	2.51	1.45	1.39
2	B	801[A]	HDD	C4A-NA	-2.49	1.34	1.39
3	A	802[B]	HEM	CHB-C4A	2.47	1.45	1.39
2	D	801[A]	HDD	C1C-NC	-2.46	1.35	1.39
3	D	802[B]	HEM	CHB-C4A	2.46	1.44	1.39
2	A	801[A]	HDD	C1A-C2A	2.44	1.49	1.44
3	D	802[B]	HEM	C1B-NB	-2.41	1.36	1.40
3	B	802[B]	HEM	CHA-C1A	2.41	1.44	1.39
3	D	802[B]	HEM	CHA-C1A	2.38	1.44	1.39
3	B	802[B]	HEM	C4A-C3A	2.37	1.48	1.43
2	D	801[A]	HDD	CHC-C1C	2.37	1.44	1.39
2	B	801[A]	HDD	C4A-C3A	2.36	1.48	1.43
3	D	802[B]	HEM	C2A-C3A	2.35	1.45	1.38
2	A	801[A]	HDD	C1B-C2B	2.32	1.49	1.45
2	A	801[A]	HDD	C4C-NC	-2.31	1.35	1.39
3	C	802[B]	HEM	C1B-NB	-2.29	1.36	1.40
3	C	802[B]	HEM	C1A-C2A	2.29	1.49	1.44
2	C	801[A]	HDD	C4C-NC	-2.28	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802[B]	HEM	C4D-ND	-2.27	1.36	1.40
3	C	802[B]	HEM	C1D-C2D	2.27	1.49	1.44
3	A	802[B]	HEM	C3B-C2B	2.26	1.41	1.37
2	D	801[A]	HDD	CHA-C1A	2.26	1.44	1.39
3	B	802[B]	HEM	C1D-ND	-2.25	1.34	1.38
2	B	801[A]	HDD	C1B-NB	-2.25	1.35	1.39
2	A	801[A]	HDD	C4A-NA	-2.20	1.35	1.39
3	A	802[B]	HEM	C4A-C3A	2.20	1.48	1.43
2	A	801[A]	HDD	O1A-CGA	2.17	1.29	1.22
3	A	802[B]	HEM	CHA-C1A	2.15	1.44	1.39
2	A	801[A]	HDD	OND-C2D	2.15	1.46	1.42
3	B	802[B]	HEM	C1A-C2A	2.12	1.48	1.44
2	B	801[A]	HDD	C3D-C2D	-2.09	1.50	1.55
2	A	801[A]	HDD	C3B-C4B	2.08	1.49	1.46
3	C	802[B]	HEM	C1B-C2B	2.06	1.48	1.44
3	D	802[B]	HEM	C1C-C2C	2.06	1.49	1.45
2	B	801[A]	HDD	C3C-C4C	2.06	1.48	1.42
2	C	801[A]	HDD	CMB-C2B	-2.04	1.46	1.50
3	B	802[B]	HEM	C1D-C2D	2.00	1.48	1.44

All (227) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802[B]	HEM	C3B-C4B-NB	8.33	115.45	109.47
3	A	802[B]	HEM	C3D-C4D-ND	8.14	119.09	110.17
3	A	802[B]	HEM	C2D-C1D-ND	7.89	119.02	109.90
3	C	802[B]	HEM	C3B-C4B-NB	7.74	115.03	109.47
2	D	801[A]	HDD	C3C-C4C-NC	7.50	116.12	109.80
2	D	801[A]	HDD	C3B-C2B-C1B	-7.27	100.17	107.05
3	C	802[B]	HEM	C3B-C2B-C1B	-7.11	101.07	106.41
2	B	801[A]	HDD	O1D-CGD-O2D	7.08	126.78	120.81
2	B	801[A]	HDD	C3C-C2C-C1C	-7.08	98.83	107.17
3	A	802[B]	HEM	C3B-C2B-C1B	-7.00	101.16	106.41
2	A	801[A]	HDD	C3D-O1D-CGD	6.86	117.53	111.14
3	D	802[B]	HEM	C2B-C1B-NB	6.67	117.51	109.84
3	B	802[B]	HEM	C2B-C1B-NB	6.49	117.31	109.84
3	C	802[B]	HEM	C3D-C4D-ND	6.49	117.28	110.17
3	A	802[B]	HEM	C4D-ND-C1D	-6.40	97.62	105.21
3	C	802[B]	HEM	C2D-C1D-ND	6.07	116.92	109.90
3	D	802[B]	HEM	CAA-CBA-CGA	-5.98	97.80	113.67
3	C	802[B]	HEM	C2B-C1B-NB	5.92	116.65	109.84
2	A	801[A]	HDD	C3B-C2B-C1B	-5.92	101.45	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801[A]	HDD	C3C-C2C-C1C	-5.87	100.25	107.17
2	A	801[A]	HDD	O1D-CGD-O2D	5.78	125.68	120.81
3	B	802[B]	HEM	C3B-C4B-NB	5.76	113.60	109.47
3	D	802[B]	HEM	C3D-C4D-ND	5.67	116.39	110.17
3	B	802[B]	HEM	C2D-C1D-ND	5.64	116.42	109.90
2	B	801[A]	HDD	C3D-O1D-CGD	5.61	116.37	111.14
2	C	801[A]	HDD	C3C-C2C-C1C	-5.54	100.64	107.17
3	A	802[B]	HEM	C1D-C2D-C3D	-5.50	101.20	106.98
3	B	802[B]	HEM	C3B-C2B-C1B	-5.47	102.30	106.41
3	C	802[B]	HEM	CMB-C2B-C1B	5.46	133.57	125.03
2	B	801[A]	HDD	OND-C2D-CMD	-5.44	98.94	109.45
2	A	801[A]	HDD	CBD-CAD-C3D	5.39	111.66	103.98
3	C	802[B]	HEM	C3C-C2C-C1C	-5.36	101.97	107.05
3	B	802[B]	HEM	C3D-C4D-ND	5.34	116.02	110.17
3	D	802[B]	HEM	C3C-C2C-C1C	-5.22	102.11	107.05
2	D	801[A]	HDD	CMC-C2C-C1C	5.20	133.33	125.42
3	D	802[B]	HEM	C2D-C1D-ND	5.13	115.83	109.90
3	C	802[B]	HEM	C1D-C2D-C3D	-5.07	101.65	106.98
3	D	802[B]	HEM	C4C-NC-C1C	-5.06	97.57	105.82
2	D	801[A]	HDD	C3C-C2C-C1C	-5.04	101.23	107.17
3	A	802[B]	HEM	C2B-C1B-NB	4.96	115.55	109.84
3	B	802[B]	HEM	CAA-CBA-CGA	-4.93	100.59	113.67
3	C	802[B]	HEM	C4C-NC-C1C	-4.92	97.79	105.82
3	B	802[B]	HEM	C3C-C2C-C1C	-4.92	102.39	107.05
2	C	801[A]	HDD	C3B-C2B-C1B	-4.84	102.47	107.05
2	C	801[A]	HDD	CBD-CAD-C3D	4.83	110.87	103.98
2	A	801[A]	HDD	C3C-C4C-NC	4.72	113.78	109.80
3	C	802[B]	HEM	C1C-CHC-C4B	-4.72	115.99	126.02
3	D	802[B]	HEM	C3B-C2B-C1B	-4.71	102.88	106.41
2	B	801[A]	HDD	C3B-C2B-C1B	-4.70	102.60	107.05
2	B	801[A]	HDD	CMC-C2C-C1C	4.69	132.56	125.42
3	B	802[B]	HEM	C1D-C2D-C3D	-4.68	102.05	106.98
3	A	802[B]	HEM	CHD-C1D-C2D	-4.67	117.65	125.03
2	B	801[A]	HDD	C2D-C1D-CHD	-4.63	117.07	124.27
3	A	802[B]	HEM	C3C-C2C-C1C	-4.63	102.67	107.05
3	A	802[B]	HEM	CMC-C2C-C1C	4.61	132.84	124.73
3	C	802[B]	HEM	CHC-C1C-C2C	-4.59	115.94	125.49
2	D	801[A]	HDD	CBD-CAD-C3D	4.56	110.49	103.98
2	C	801[A]	HDD	OND-C2D-CMD	-4.55	100.66	109.45
3	C	802[B]	HEM	C2C-C1C-NC	4.54	118.04	109.64
3	C	802[B]	HEM	CHC-C4B-C3B	-4.54	116.02	125.07
3	B	802[B]	HEM	CHC-C1C-C2C	-4.52	116.09	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801[A]	HDD	C3D-O1D-CGD	4.52	115.36	111.14
2	A	801[A]	HDD	OND-C2D-CMD	-4.48	100.79	109.45
3	D	802[B]	HEM	CHC-C1C-C2C	-4.43	116.27	125.49
2	B	801[A]	HDD	C2C-C1C-NC	4.37	117.14	110.14
3	D	802[B]	HEM	C1D-C2D-C3D	-4.37	102.39	106.98
2	D	801[A]	HDD	C2C-C1C-NC	4.31	117.06	110.14
2	C	801[A]	HDD	C4A-C3A-C2A	-4.30	101.89	106.82
3	A	802[B]	HEM	C2A-C1A-NA	4.23	114.85	110.15
2	B	801[A]	HDD	CBD-CAD-C3D	4.18	109.94	103.98
3	D	802[B]	HEM	C1B-NB-C4B	-4.05	100.41	105.21
3	D	802[B]	HEM	C4B-C3B-C2B	-4.00	103.60	107.28
3	D	802[B]	HEM	CMC-C2C-C1C	4.00	131.76	124.73
3	A	802[B]	HEM	CAA-CBA-CGA	-3.98	103.10	113.67
3	B	802[B]	HEM	CHB-C1B-C2B	-3.95	115.73	126.95
3	C	802[B]	HEM	CHC-C4B-NB	3.93	128.65	124.42
2	A	801[A]	HDD	C2C-C1C-NC	3.88	116.36	110.14
3	D	802[B]	HEM	C2C-C1C-NC	3.86	116.77	109.64
3	A	802[B]	HEM	C4C-NC-C1C	-3.83	99.57	105.82
2	C	801[A]	HDD	C2D-C1D-CHD	-3.83	118.31	124.27
2	A	801[A]	HDD	CAA-CBA-CGA	-3.83	103.52	113.67
2	A	801[A]	HDD	CAA-C2A-C1A	3.82	132.41	124.94
3	C	802[B]	HEM	C1B-NB-C4B	-3.82	100.68	105.21
3	A	802[B]	HEM	C4A-NA-C1A	-3.82	99.60	105.82
3	B	802[B]	HEM	C4C-NC-C1C	-3.81	99.62	105.82
2	A	801[A]	HDD	CMC-C2C-C1C	3.79	131.19	125.42
3	C	802[B]	HEM	C2A-C1A-NA	3.78	114.35	110.15
2	D	801[A]	HDD	OND-C2D-CMD	-3.77	102.16	109.45
2	D	801[A]	HDD	C2D-C1D-CHD	-3.77	118.41	124.27
2	A	801[A]	HDD	C2B-C1B-NB	3.75	116.56	109.64
3	C	802[B]	HEM	CHA-C4D-C3D	-3.74	118.34	125.23
3	B	802[B]	HEM	C2C-C1C-NC	3.73	116.54	109.64
2	B	801[A]	HDD	C4A-C3A-C2A	-3.71	102.57	106.82
2	B	801[A]	HDD	C2A-C1A-NA	3.70	114.25	110.15
3	B	802[B]	HEM	CHD-C1D-C2D	-3.65	119.26	125.03
2	B	801[A]	HDD	O1D-CGD-CBD	-3.64	106.85	110.17
3	B	802[B]	HEM	C4A-NA-C1A	-3.64	99.88	105.82
3	A	802[B]	HEM	CMB-C2B-C1B	3.64	130.72	125.03
2	A	801[A]	HDD	C2D-C1D-CHD	-3.62	118.64	124.27
3	A	802[B]	HEM	CHA-C4D-C3D	-3.62	118.55	125.23
3	A	802[B]	HEM	CHA-C1A-C2A	-3.62	117.39	125.30
3	D	802[B]	HEM	C1C-CHC-C4B	-3.57	118.43	126.02
2	C	801[A]	HDD	CMC-C2C-C1C	3.56	130.84	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801[A]	HDD	CAA-CBA-CGA	-3.52	104.34	113.67
3	B	802[B]	HEM	C4B-C3B-C2B	-3.51	104.06	107.28
3	C	802[B]	HEM	CAA-CBA-CGA	-3.50	104.39	113.67
3	B	802[B]	HEM	C2A-C1A-NA	3.47	114.00	110.15
3	C	802[B]	HEM	CHD-C1D-ND	-3.43	120.74	124.42
2	B	801[A]	HDD	CMA-C3A-C2A	3.42	132.88	125.62
2	C	801[A]	HDD	C3D-O1D-CGD	3.41	114.32	111.14
2	A	801[A]	HDD	CHB-C1B-C2B	-3.39	118.43	125.49
3	D	802[B]	HEM	C4A-CHB-C1B	-3.39	118.28	126.25
2	C	801[A]	HDD	C2C-C1C-NC	3.37	115.54	110.14
3	C	802[B]	HEM	CBB-CAB-C3B	-3.36	110.74	127.53
3	D	802[B]	HEM	CHB-C1B-C2B	-3.33	117.49	126.95
3	D	802[B]	HEM	C4A-NA-C1A	-3.31	100.42	105.82
3	C	802[B]	HEM	C4D-ND-C1D	-3.31	101.29	105.21
2	D	801[A]	HDD	C2B-C1B-NB	3.30	115.74	109.64
2	C	801[A]	HDD	C3C-C4C-NC	3.30	112.57	109.80
3	B	802[B]	HEM	CHA-C4D-C3D	-3.28	119.17	125.23
3	D	802[B]	HEM	CBD-CAD-C3D	-3.28	103.47	112.53
2	C	801[A]	HDD	C2A-C1A-NA	3.26	113.77	110.15
3	B	802[B]	HEM	C4A-CHB-C1B	-3.26	118.59	126.25
3	D	802[B]	HEM	CHD-C1D-C2D	-3.25	119.89	125.03
2	B	801[A]	HDD	CAA-CBA-CGA	-3.24	105.08	113.67
2	D	801[A]	HDD	CHD-C1D-ND	3.23	128.74	124.28
3	D	802[B]	HEM	C4C-CHD-C1D	-3.22	119.18	126.02
3	D	802[B]	HEM	CHA-C4D-C3D	-3.21	119.31	125.23
3	B	802[B]	HEM	C1C-CHC-C4B	-3.20	119.22	126.02
3	B	802[B]	HEM	C3A-C4A-NA	3.19	115.26	110.14
2	B	801[A]	HDD	CMB-C2B-C1B	3.18	130.33	124.73
2	D	801[A]	HDD	CAA-C2A-C1A	3.18	131.15	124.94
2	C	801[A]	HDD	C2B-C1B-NB	3.18	115.51	109.64
3	B	802[B]	HEM	CHB-C4A-C3A	-3.17	118.24	127.43
3	D	802[B]	HEM	CHD-C4C-C3C	-3.09	119.99	125.21
2	B	801[A]	HDD	C3C-C4C-NC	3.07	112.39	109.80
3	D	802[B]	HEM	CHB-C4A-C3A	-3.06	118.55	127.43
3	D	802[B]	HEM	C4D-ND-C1D	-3.00	101.65	105.21
2	C	801[A]	HDD	CMA-C3A-C2A	3.00	131.99	125.62
3	A	802[B]	HEM	CBB-CAB-C3B	-2.99	112.59	127.53
3	A	802[B]	HEM	C4C-CHD-C1D	-2.98	119.68	126.02
3	A	802[B]	HEM	CHB-C1B-C2B	-2.96	118.53	126.95
2	C	801[A]	HDD	C3A-C4A-NA	2.95	114.87	110.14
3	C	802[B]	HEM	C4C-C3C-C2C	2.93	109.35	106.81
2	C	801[A]	HDD	O1D-CGD-O2D	2.93	123.28	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[B]	HEM	C4A-CHB-C1B	-2.93	119.37	126.25
3	B	802[B]	HEM	C4D-ND-C1D	-2.90	101.77	105.21
3	A	802[B]	HEM	C2C-C1C-NC	2.88	114.96	109.64
3	C	802[B]	HEM	C4D-C3D-C2D	-2.88	102.70	106.89
3	D	802[B]	HEM	CHC-C4B-C3B	-2.86	119.36	125.07
2	B	801[A]	HDD	CHD-C1D-ND	2.85	128.22	124.28
2	D	801[A]	HDD	C2A-C1A-NA	2.85	113.31	110.15
2	A	801[A]	HDD	O1D-CGD-CBD	-2.85	107.58	110.17
2	A	801[A]	HDD	CAD-CBD-CGD	-2.83	100.27	104.48
3	B	802[B]	HEM	CMD-C2D-C3D	2.82	133.79	126.15
2	D	801[A]	HDD	CHD-C4C-NC	-2.81	118.76	123.86
3	A	802[B]	HEM	CMD-C2D-C1D	2.80	129.41	125.03
3	C	802[B]	HEM	C4A-NA-C1A	-2.79	101.27	105.82
3	B	802[B]	HEM	CBD-CAD-C3D	-2.78	104.83	112.53
2	B	801[A]	HDD	CHC-C1C-C2C	-2.76	119.41	127.43
2	D	801[A]	HDD	C3D-C4D-CHA	-2.76	116.13	124.14
2	D	801[A]	HDD	C4C-C3C-C2C	-2.74	103.90	107.30
3	A	802[B]	HEM	C4D-C3D-C2D	-2.73	102.92	106.89
2	D	801[A]	HDD	C4C-NC-C1C	-2.71	101.41	105.82
2	A	801[A]	HDD	O1D-C3D-CAD	-2.70	98.06	103.06
3	C	802[B]	HEM	CBD-CAD-C3D	-2.68	105.13	112.53
2	C	801[A]	HDD	CAA-C2A-C1A	2.62	130.07	124.94
3	A	802[B]	HEM	CHD-C4C-C3C	-2.61	120.81	125.21
3	C	802[B]	HEM	CAA-C2A-C1A	2.58	129.99	124.94
3	A	802[B]	HEM	C3B-C4B-NB	2.58	111.32	109.47
2	D	801[A]	HDD	CHB-C1B-NB	-2.56	121.67	124.45
3	B	802[B]	HEM	CMB-C2B-C3B	2.56	134.62	128.43
3	A	802[B]	HEM	C4C-C3C-C2C	2.55	109.02	106.81
3	D	802[B]	HEM	C3A-C4A-NA	2.55	114.22	110.14
3	C	802[B]	HEM	CMD-C2D-C3D	2.53	133.00	126.15
3	C	802[B]	HEM	CHB-C1B-NB	-2.53	121.24	124.37
3	B	802[B]	HEM	CMA-C3A-C2A	2.53	130.98	125.62
3	C	802[B]	HEM	CHD-C4C-C3C	-2.51	120.97	125.21
2	A	801[A]	HDD	C2A-C1A-NA	2.50	112.93	110.15
2	D	801[A]	HDD	O1D-CGD-O2D	2.50	122.92	120.81
3	A	802[B]	HEM	C1A-CHA-C4D	-2.50	120.37	126.25
2	B	801[A]	HDD	C2B-C1B-NB	2.49	114.24	109.64
3	D	802[B]	HEM	C1A-CHA-C4D	-2.45	120.48	126.25
2	A	801[A]	HDD	C1A-C2A-C3A	-2.44	103.10	106.87
2	B	801[A]	HDD	C3A-C4A-NA	2.42	114.02	110.14
3	D	802[B]	HEM	C4D-C3D-C2D	-2.38	103.42	106.89
3	B	802[B]	HEM	CHC-C1C-NC	2.38	127.04	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802[B]	HEM	CMC-C2C-C1C	2.37	128.90	124.73
2	C	801[A]	HDD	C3D-C4D-CHA	-2.37	117.27	124.14
2	C	801[A]	HDD	CHB-C4A-C3A	-2.35	120.59	127.43
3	B	802[B]	HEM	C4D-C3D-C2D	-2.35	103.47	106.89
3	C	802[B]	HEM	CBC-CAC-C3C	-2.33	115.88	127.53
3	C	802[B]	HEM	CHB-C4A-C3A	-2.33	120.67	127.43
3	D	802[B]	HEM	CMB-C2B-C1B	2.31	128.64	125.03
3	B	802[B]	HEM	C4C-CHD-C1D	-2.30	121.12	126.02
3	B	802[B]	HEM	C4A-C3A-C2A	-2.29	104.19	106.82
3	D	802[B]	HEM	C4C-C3C-C2C	2.28	108.80	106.81
3	B	802[B]	HEM	C1B-NB-C4B	-2.27	102.52	105.21
3	D	802[B]	HEM	CHA-C1A-C2A	-2.26	120.36	125.30
3	A	802[B]	HEM	CHC-C1C-C2C	-2.25	120.80	125.49
2	B	801[A]	HDD	C4B-C3B-C2B	-2.24	104.87	106.81
3	C	802[B]	HEM	CAD-C3D-C2D	2.22	132.03	127.87
3	A	802[B]	HEM	CBD-CAD-C3D	-2.22	106.39	112.53
3	A	802[B]	HEM	CHB-C4A-C3A	-2.22	120.98	127.43
2	B	801[A]	HDD	CHB-C4A-C3A	-2.21	121.00	127.43
3	A	802[B]	HEM	CBC-CAC-C3C	-2.21	116.50	127.53
2	B	801[A]	HDD	C3D-C4D-CHA	-2.19	117.79	124.14
3	C	802[B]	HEM	C4C-CHD-C1D	-2.18	121.39	126.02
3	A	802[B]	HEM	C3A-C4A-NA	2.17	113.62	110.14
2	D	801[A]	HDD	C1A-C2A-C3A	-2.16	103.52	106.87
2	B	801[A]	HDD	C1A-C2A-C3A	-2.16	103.52	106.87
3	D	802[B]	HEM	CHC-C1C-NC	2.15	126.80	124.45
2	B	801[A]	HDD	CHB-C1B-NB	-2.15	122.11	124.45
3	B	802[B]	HEM	CBB-CAB-C3B	-2.14	116.85	127.53
3	A	802[B]	HEM	CHA-C1A-NA	2.13	127.72	123.86
2	C	801[A]	HDD	CBA-CAA-C2A	-2.12	106.66	112.53
2	C	801[A]	HDD	CHB-C1B-NB	-2.11	122.16	124.45
2	B	801[A]	HDD	CHD-C4C-NC	-2.10	120.05	123.86
3	B	802[B]	HEM	CAD-C3D-C2D	2.09	131.78	127.87
2	A	801[A]	HDD	CMA-C3A-C2A	2.08	130.04	125.62
3	D	802[B]	HEM	CMD-C2D-C3D	2.05	131.68	126.15
2	D	801[A]	HDD	CMA-C3A-C4A	2.04	128.52	125.42
2	A	801[A]	HDD	C4B-NB-C1B	-2.04	102.50	105.82
3	D	802[B]	HEM	C2A-C1A-NA	2.03	112.41	110.15
3	C	802[B]	HEM	CAC-C3C-C2C	-2.03	121.83	128.43
2	D	801[A]	HDD	CMB-C2B-C1B	2.03	128.30	124.73
3	D	802[B]	HEM	O1A-CGA-CBA	-2.02	116.67	123.09

There are no chirality outliers.

All (28) torsion outliers are listed below:

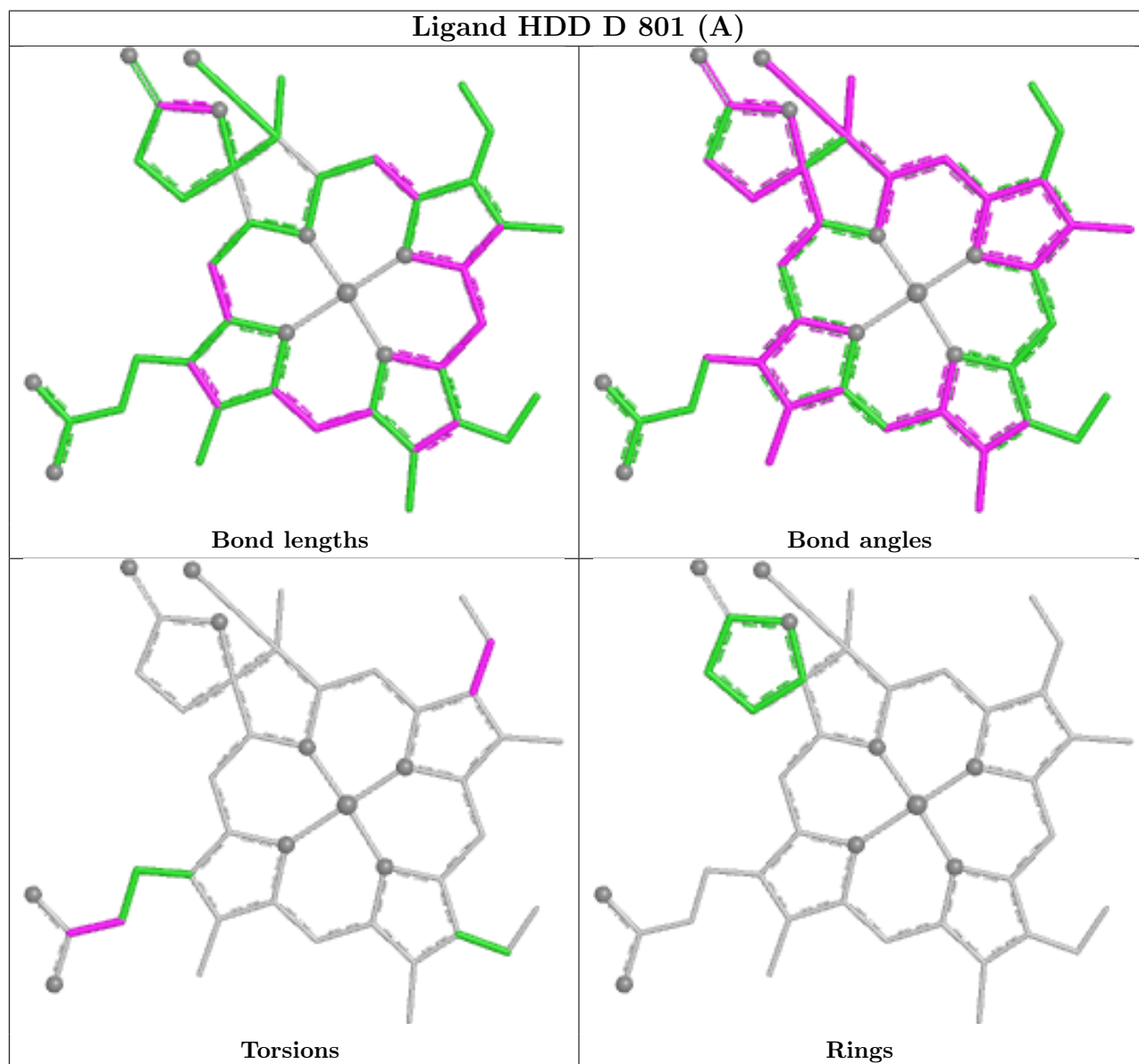
Mol	Chain	Res	Type	Atoms
3	A	802[B]	HEM	C2B-C3B-CAB-CBB
3	A	802[B]	HEM	C4B-C3B-CAB-CBB
3	C	802[B]	HEM	C2B-C3B-CAB-CBB
3	C	802[B]	HEM	C4B-C3B-CAB-CBB
2	A	801[A]	HDD	C4C-C3C-CAC-CBC
2	A	801[A]	HDD	C2C-C3C-CAC-CBC
2	B	801[A]	HDD	C4C-C3C-CAC-CBC
2	D	801[A]	HDD	C4C-C3C-CAC-CBC
3	B	802[B]	HEM	C2B-C3B-CAB-CBB
2	D	801[A]	HDD	C2C-C3C-CAC-CBC
2	A	801[A]	HDD	CAA-CBA-CGA-O1A
2	B	801[A]	HDD	CAA-CBA-CGA-O1A
2	C	801[A]	HDD	CAA-CBA-CGA-O1A
3	C	802[B]	HEM	CAA-CBA-CGA-O1A
2	C	801[A]	HDD	CAA-CBA-CGA-O2A
2	D	801[A]	HDD	CAA-CBA-CGA-O1A
3	D	802[B]	HEM	CAA-CBA-CGA-O2A
2	B	801[A]	HDD	C2C-C3C-CAC-CBC
2	A	801[A]	HDD	CAA-CBA-CGA-O2A
2	D	801[A]	HDD	CAA-CBA-CGA-O2A
2	B	801[A]	HDD	CAA-CBA-CGA-O2A
3	B	802[B]	HEM	CAA-CBA-CGA-O2A
3	C	802[B]	HEM	CAA-CBA-CGA-O2A
3	D	802[B]	HEM	CAA-CBA-CGA-O1A
3	B	802[B]	HEM	CAA-CBA-CGA-O1A
3	B	802[B]	HEM	C4B-C3B-CAB-CBB
3	A	802[B]	HEM	CAA-CBA-CGA-O2A
3	A	802[B]	HEM	CAA-CBA-CGA-O1A

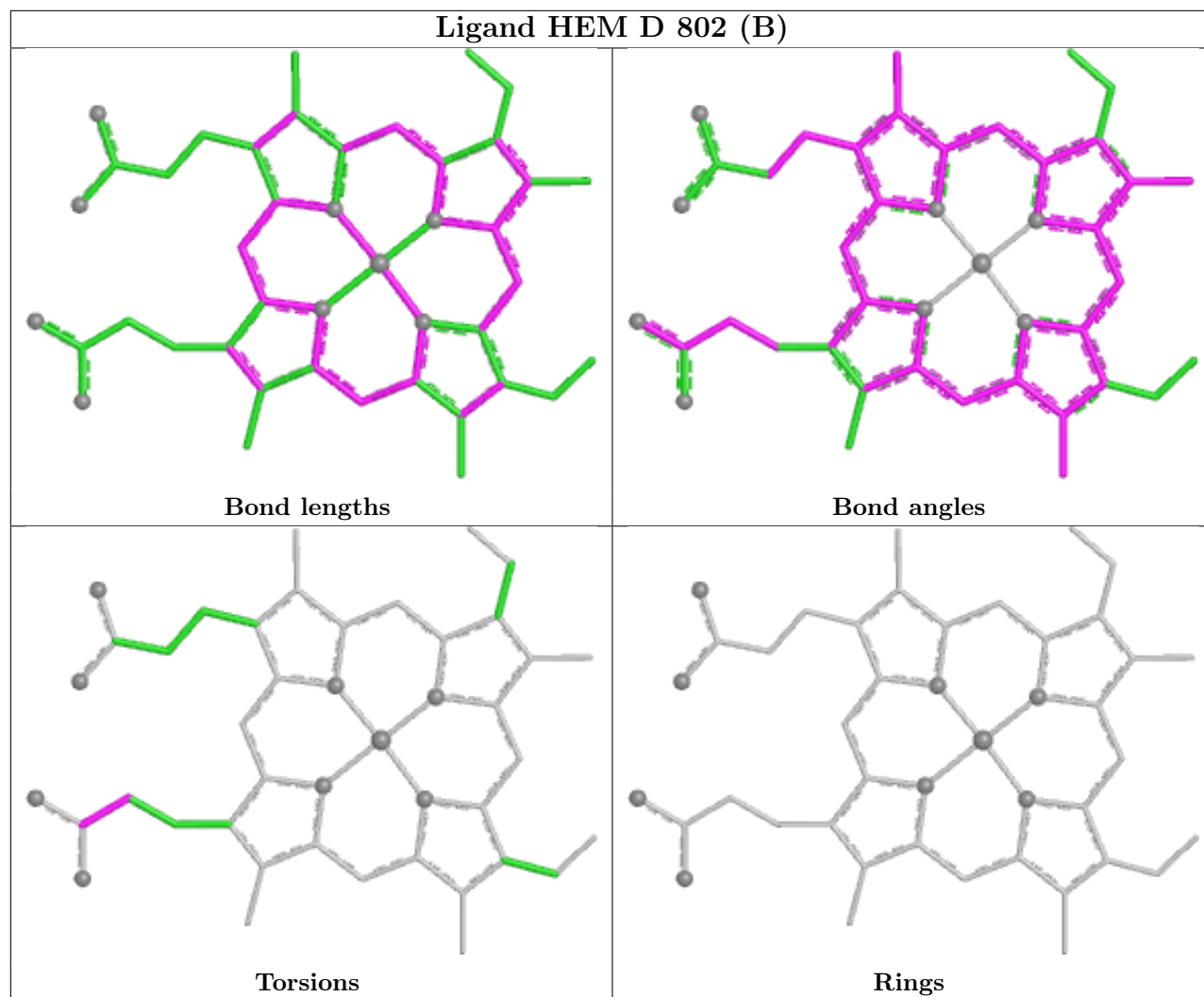
There are no ring outliers.

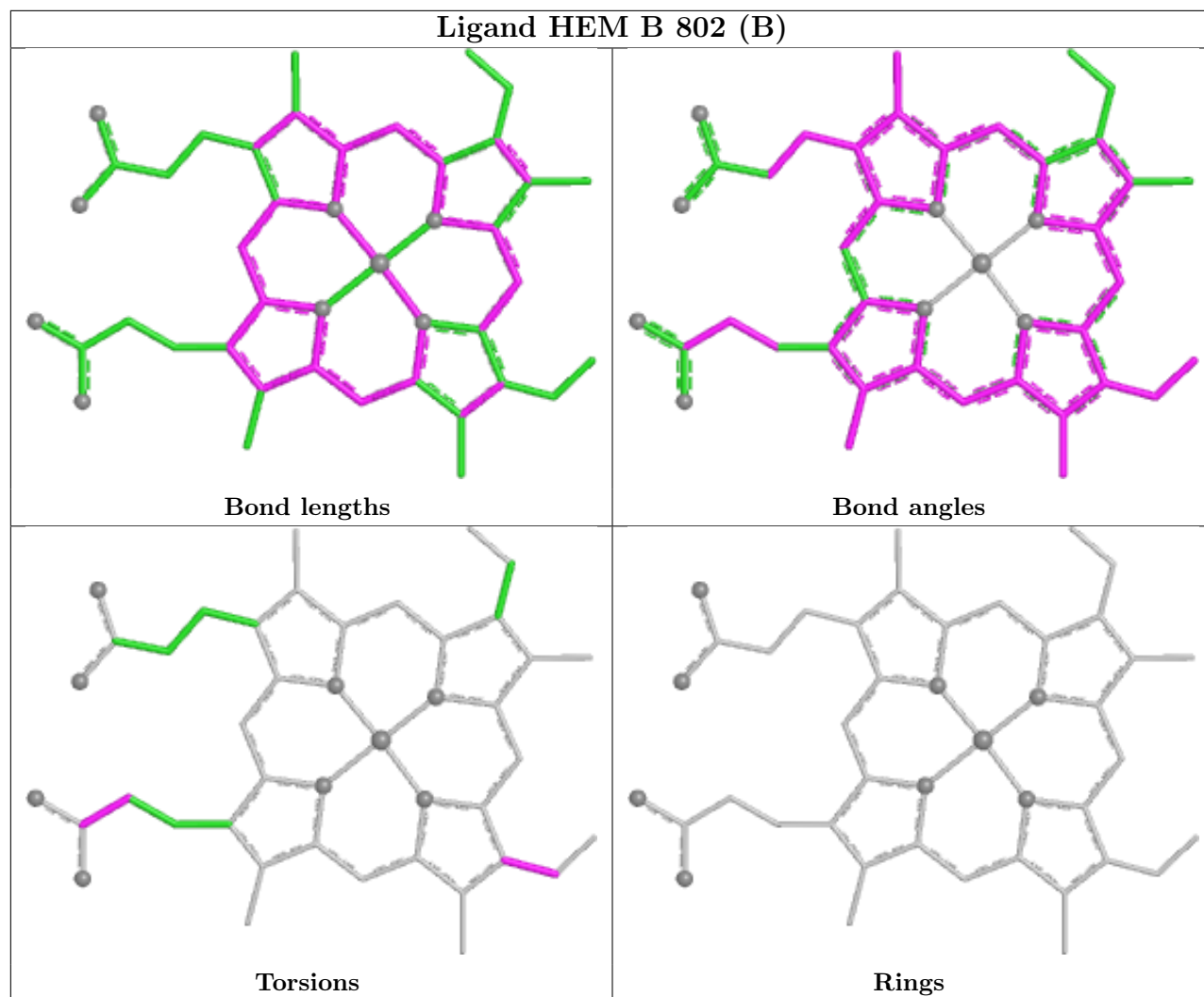
8 monomers are involved in 54 short contacts:

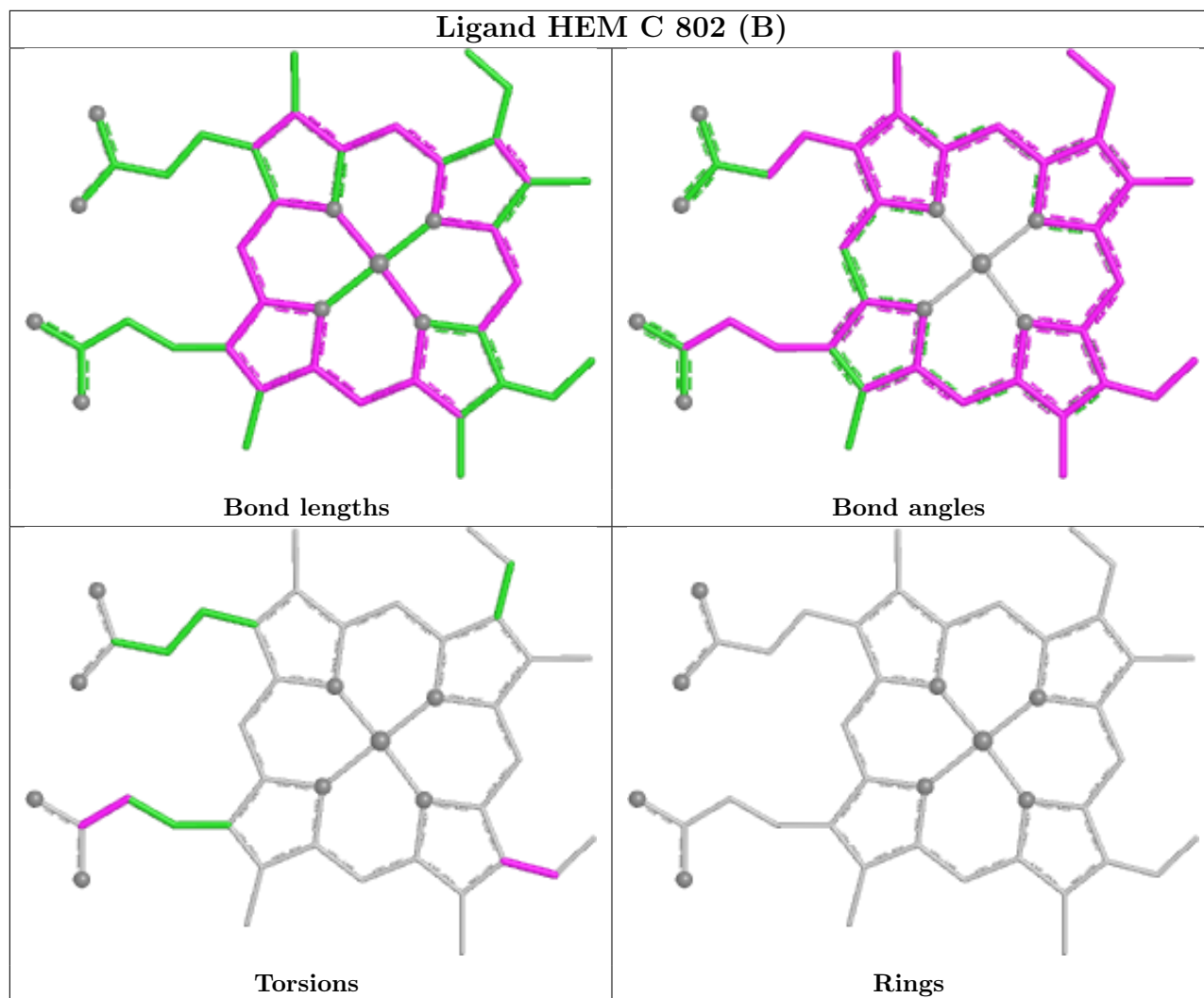
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801[A]	HDD	3	0
3	D	802[B]	HEM	10	0
3	B	802[B]	HEM	7	0
3	C	802[B]	HEM	12	0
3	A	802[B]	HEM	15	0
2	A	801[A]	HDD	4	0
2	B	801[A]	HDD	1	0
2	C	801[A]	HDD	2	0

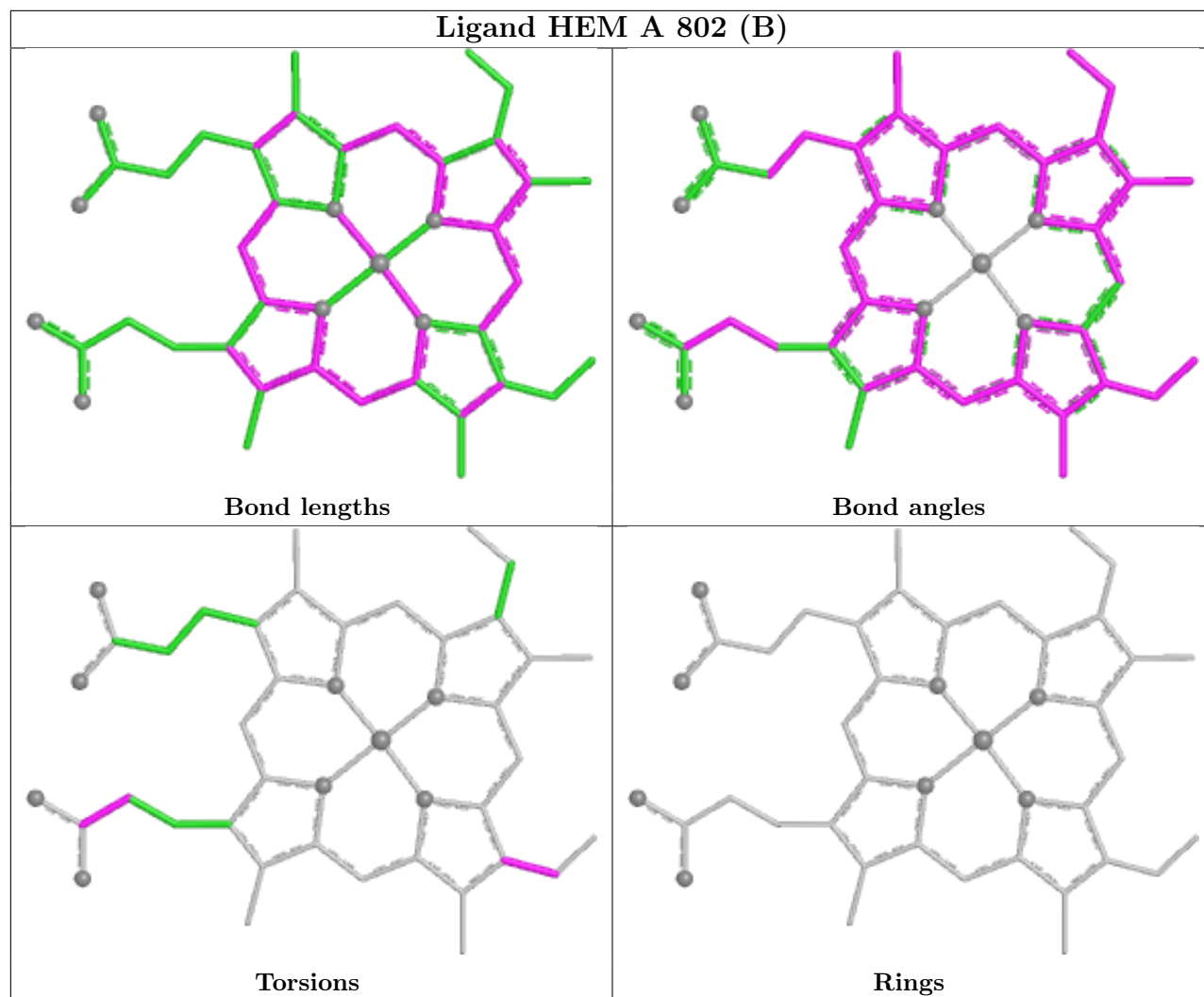
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

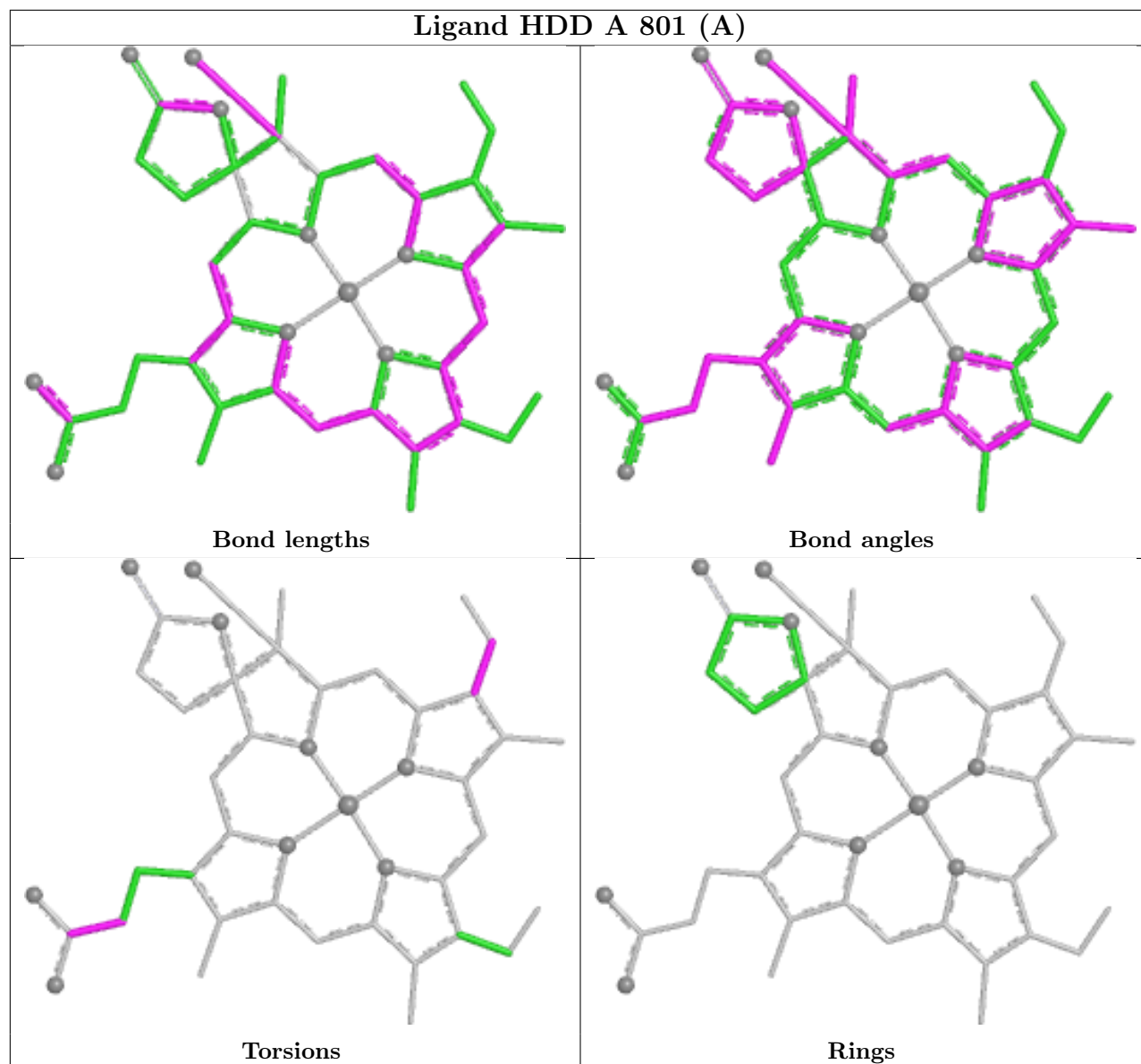


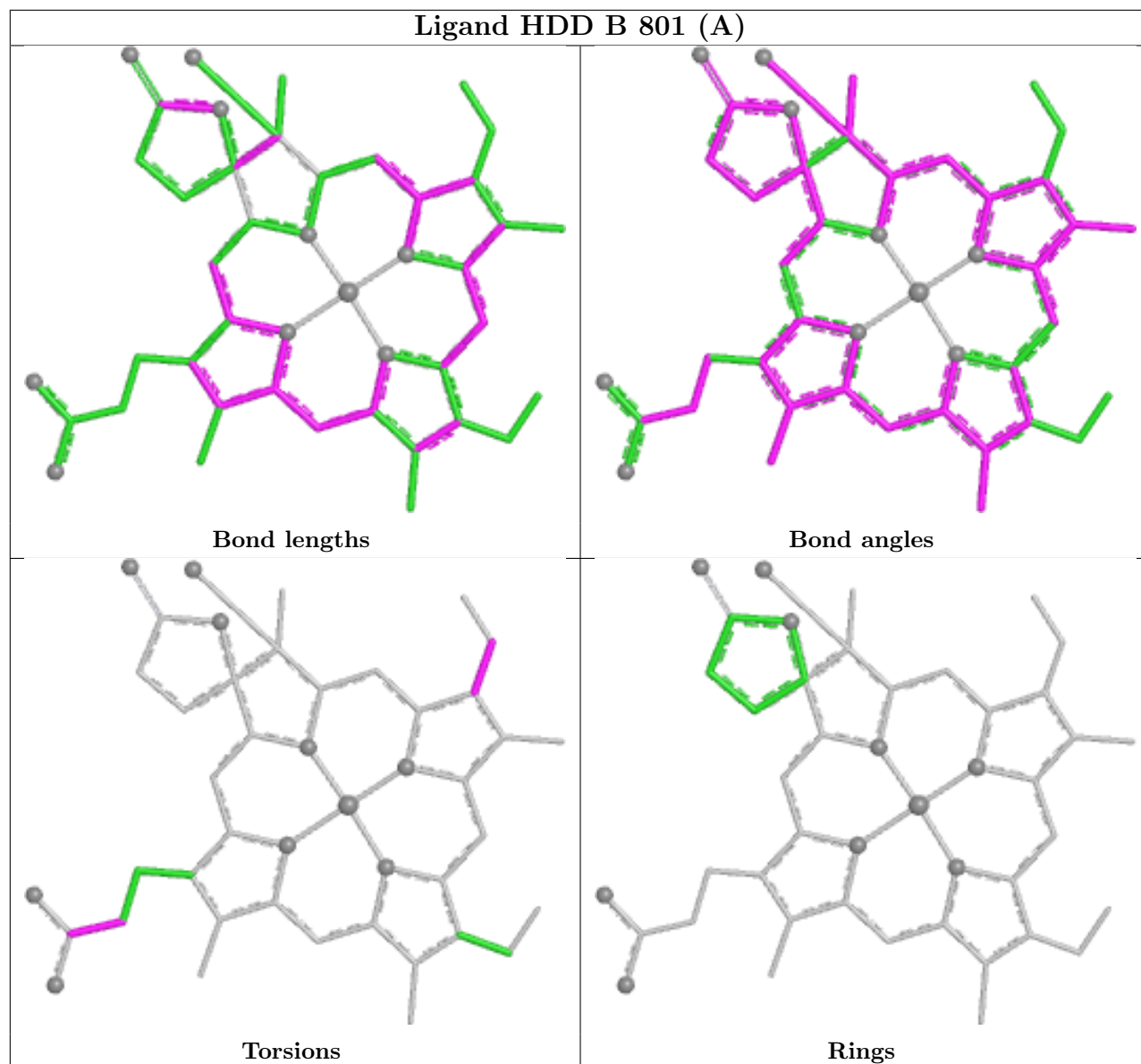


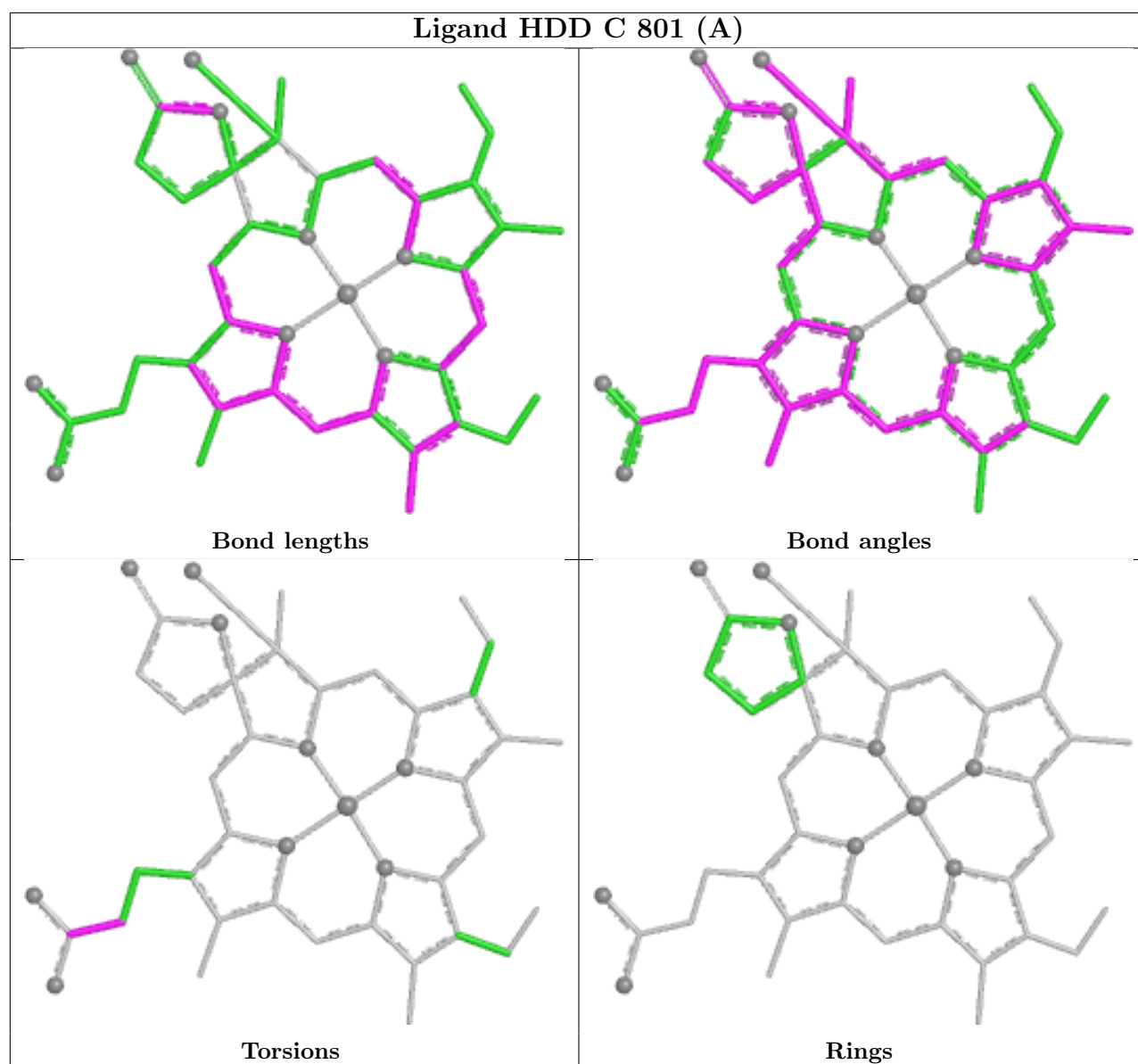












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	726/753 (96%)	-0.49	5 (0%) 84 86	5, 12, 28, 57	3 (0%)
1	B	726/753 (96%)	-0.34	5 (0%) 84 86	6, 13, 35, 56	2 (0%)
1	C	726/753 (96%)	-0.36	8 (1%) 78 81	6, 14, 35, 60	3 (0%)
1	D	726/753 (96%)	-0.50	5 (0%) 84 86	5, 12, 28, 50	2 (0%)
All	All	2904/3012 (96%)	-0.42	23 (0%) 82 85	5, 13, 32, 60	10 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	4.4
1	B	725	ASP	4.1
1	B	726	GLY	3.8
1	B	751	ILE	3.7
1	C	750	LYS	3.3
1	A	751	ILE	2.9
1	C	751	ILE	2.7
1	D	751	ILE	2.5
1	D	750	LYS	2.5
1	A	725	ASP	2.5
1	D	28	SER	2.5
1	B	713	GLN	2.4
1	C	594	PRO	2.3
1	A	749	ASP	2.3
1	B	749	ASP	2.3
1	C	726	GLY	2.1
1	D	552	LEU	2.1
1	C	646	THR	2.1
1	C	583	LYS	2.1
1	C	725	ASP	2.1
1	C	568	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	749	ASP	2.1
1	A	750	LYS	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

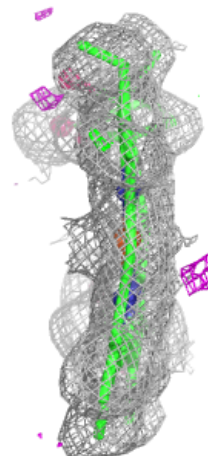
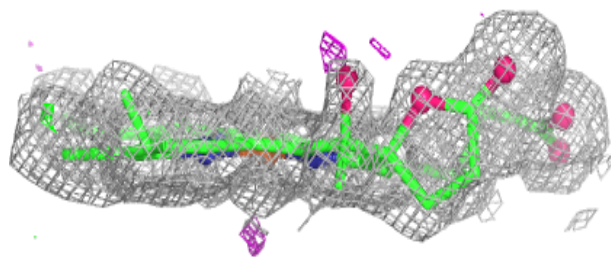
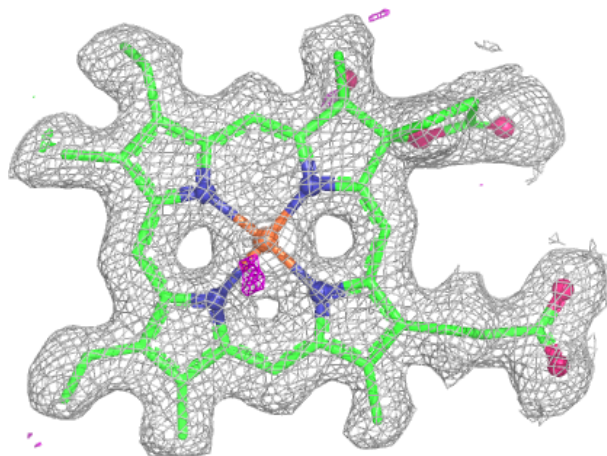
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HDD	A	801[A]	44/44	0.97	0.06	6,8,11,12	44
2	HDD	B	801[A]	44/44	0.97	0.06	7,9,11,12	44
2	HDD	C	801[A]	44/44	0.97	0.06	7,8,12,14	44
3	HEM	A	802[B]	43/43	0.97	0.06	6,6,7,8	43
2	HDD	D	801[A]	44/44	0.98	0.05	6,7,11,12	44
3	HEM	B	802[B]	43/43	0.98	0.06	5,7,8,8	43
3	HEM	C	802[B]	43/43	0.98	0.05	6,7,8,9	43
3	HEM	D	802[B]	43/43	0.98	0.06	4,5,6,7	43

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.

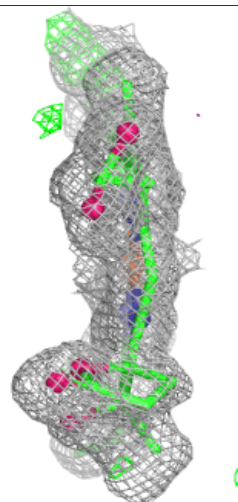
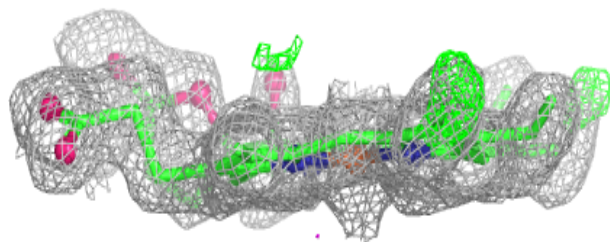
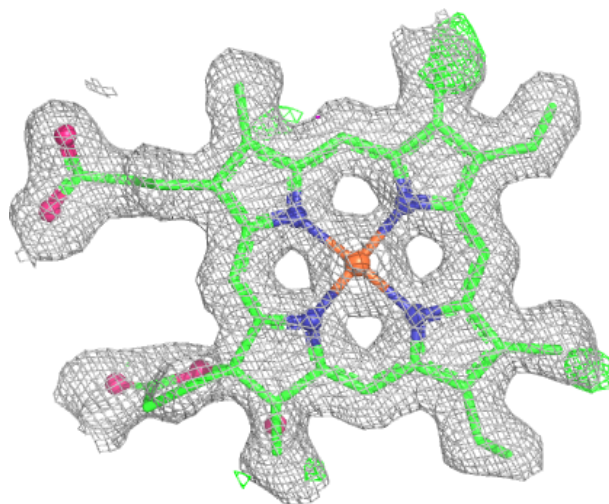
**Electron density around HDD A 801 (A):**

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



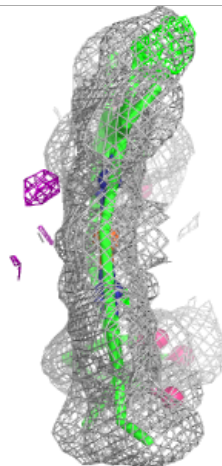
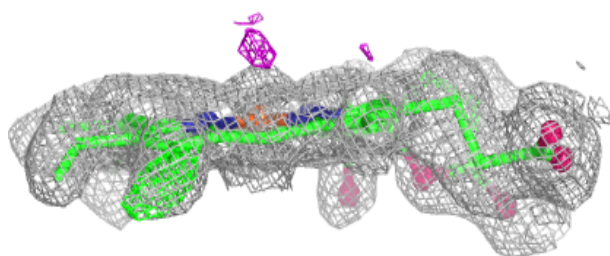
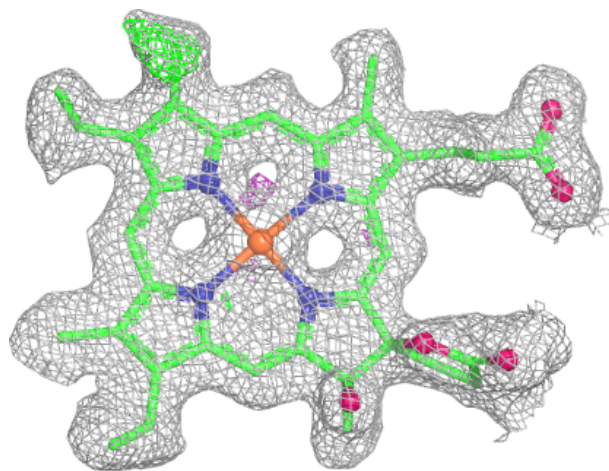
**Electron density around HDD B 801 (A):**

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



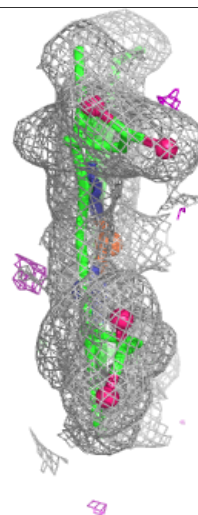
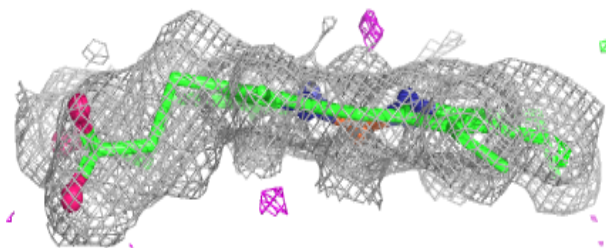
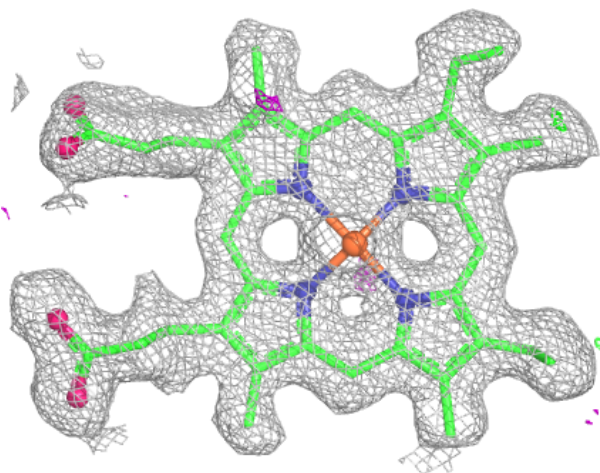
**Electron density around HDD C 801 (A):**

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



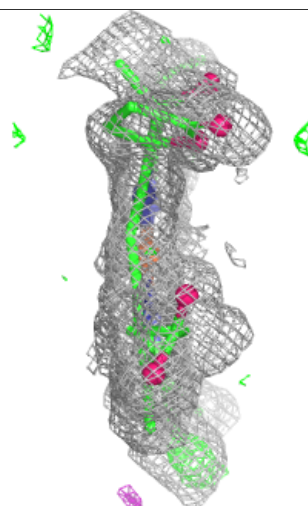
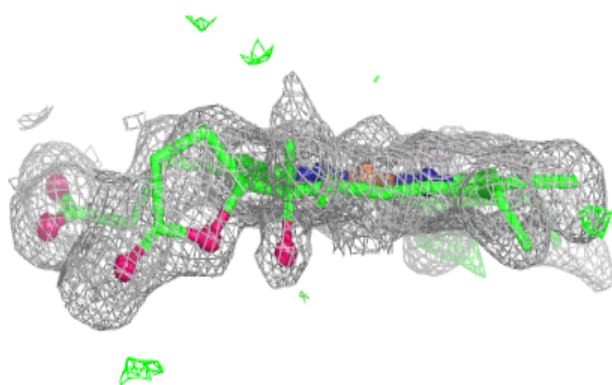
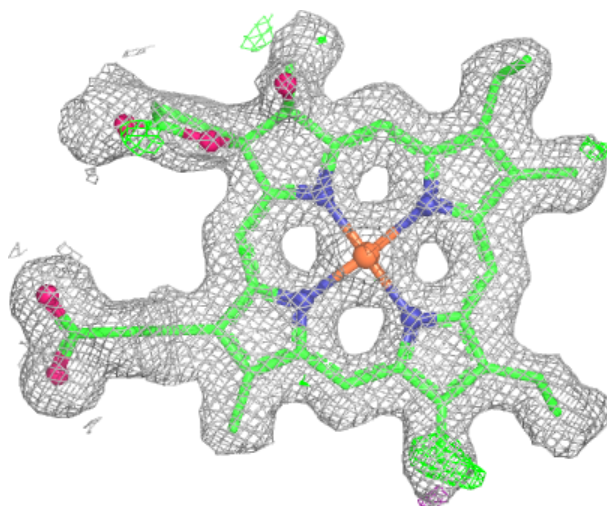
**Electron density around HEM A 802 (B):**

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



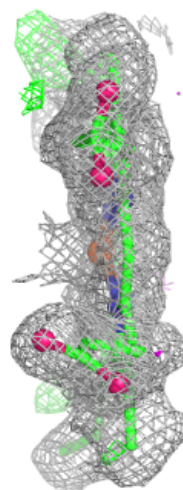
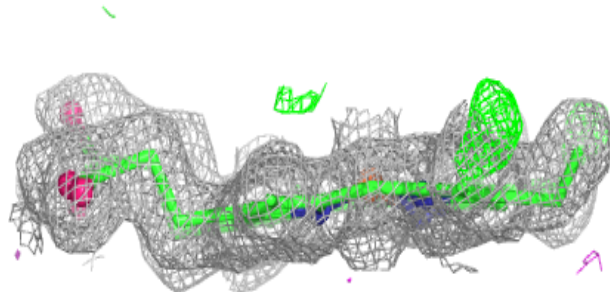
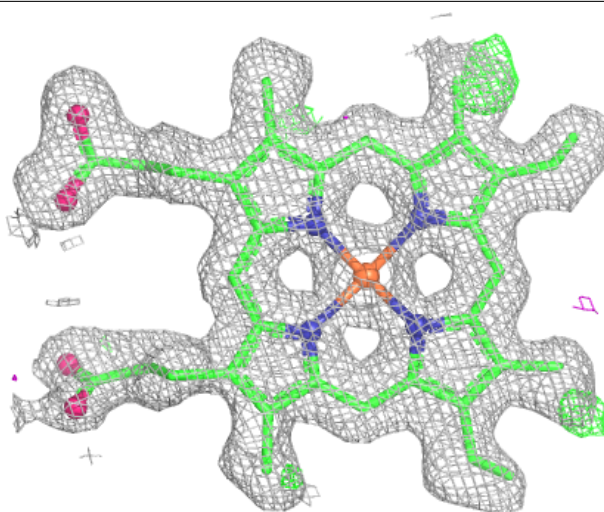
**Electron density around HDD D 801 (A):**

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



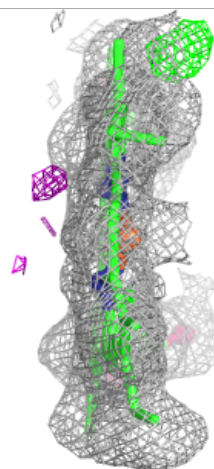
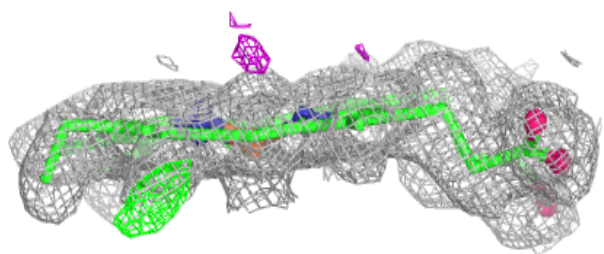
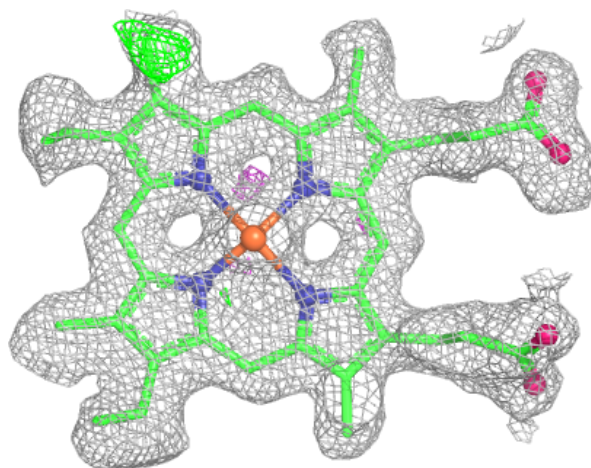
**Electron density around HEM B 802 (B):**

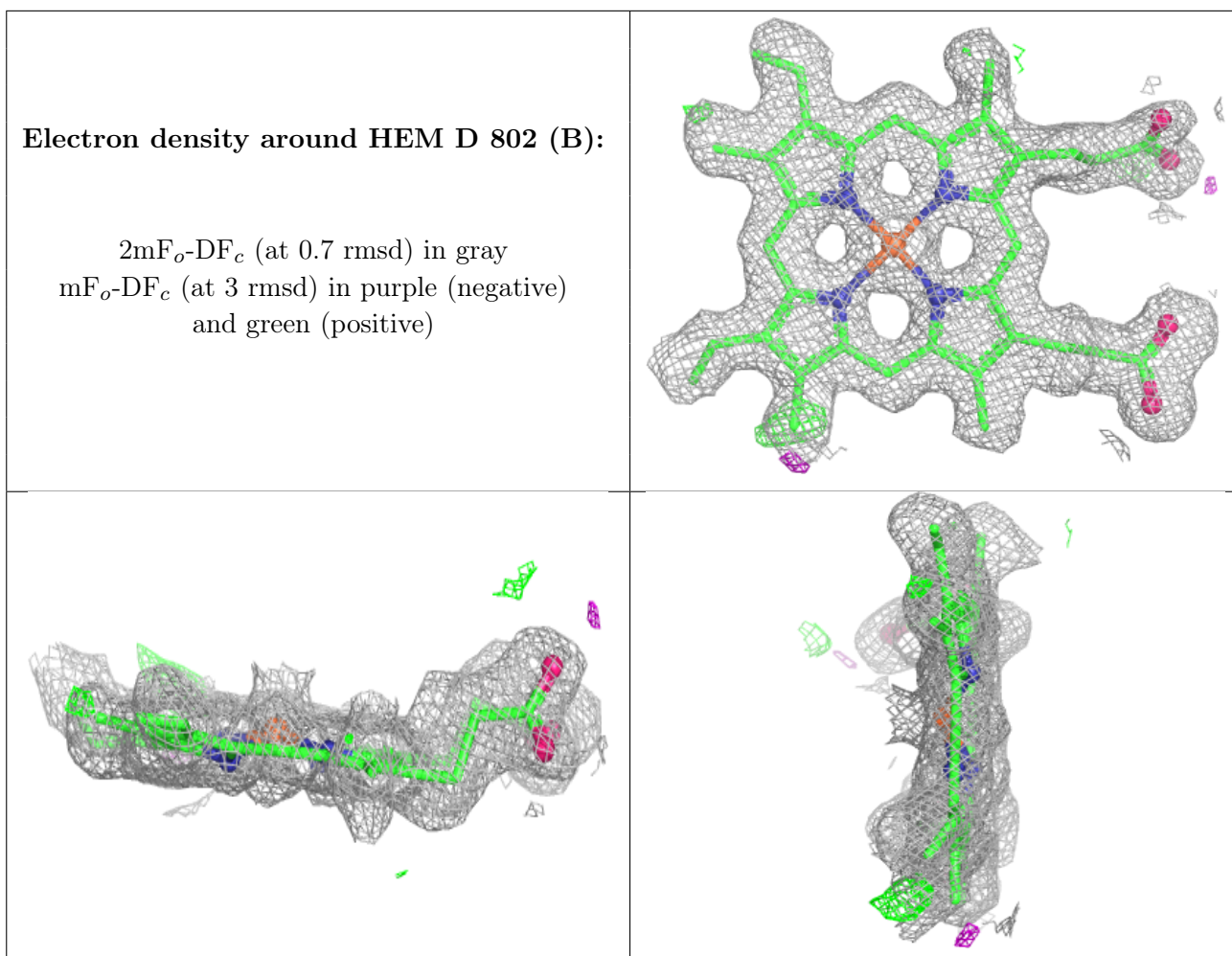
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 802 (B):**

$2mF_o-DF_c$  (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.