



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:51 AM EDT

PDB ID : 4ENT / pdb_00004ent
Title : Structure of the S234A 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

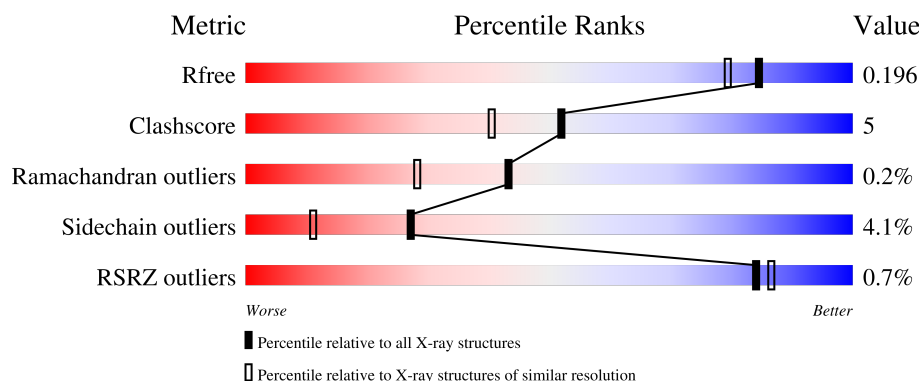
1 Overall quality at a glance

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 ≥ 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	% 85% 10% • •
1	B	753	% 82% 12% • •
1	C	753	% 81% 14% • •
1	D	753	% 83% 12% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HDD	A	801[A]	X	-	-	-
2	HDD	B	801[A]	X	-	-	-
2	HDD	C	801[A]	X	-	-	-
2	HDD	D	801[A]	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26312 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.

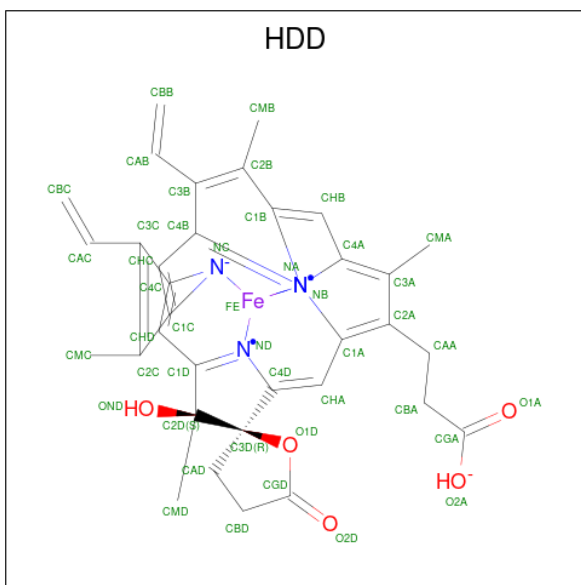
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	3	0
			5753	3652	1007	1082	12			
1	B	726	Total	C	N	O	S	0	0	0
			5740	3643	1004	1081	12			
1	C	726	Total	C	N	O	S	0	2	0
			5755	3654	1007	1082	12			
1	D	726	Total	C	N	O	S	0	2	0
			5749	3649	1005	1083	12			

There are 4 discrepancies between the modelled and reference sequences:

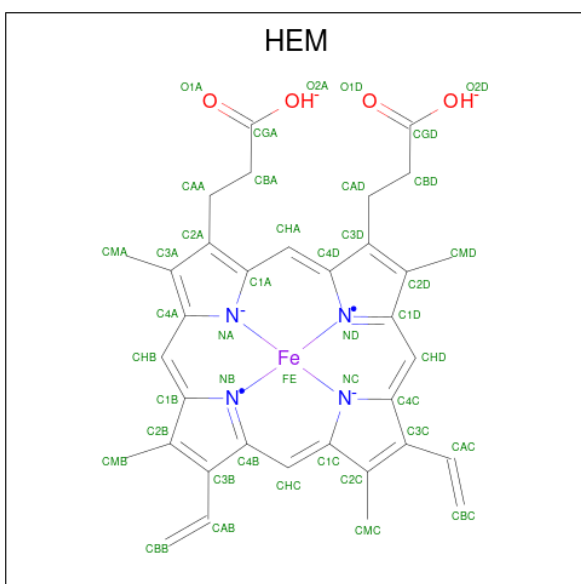
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	SER	engineered mutation	UNP P21179
B	234	ALA	SER	engineered mutation	UNP P21179
C	234	ALA	SER	engineered mutation	UNP P21179
D	234	ALA	SER	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
2	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
2	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
2	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	1

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

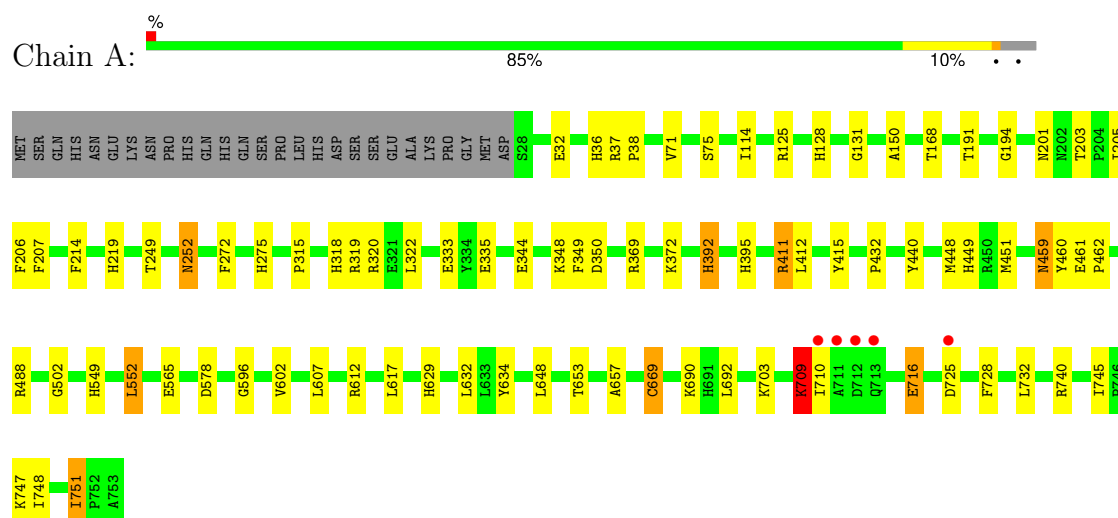
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	779	Total 779	O 779	0	0
4	B	679	Total 679	O 679	0	0
4	C	741	Total 741	O 741	0	0
4	D	768	Total 768	O 768	0	0

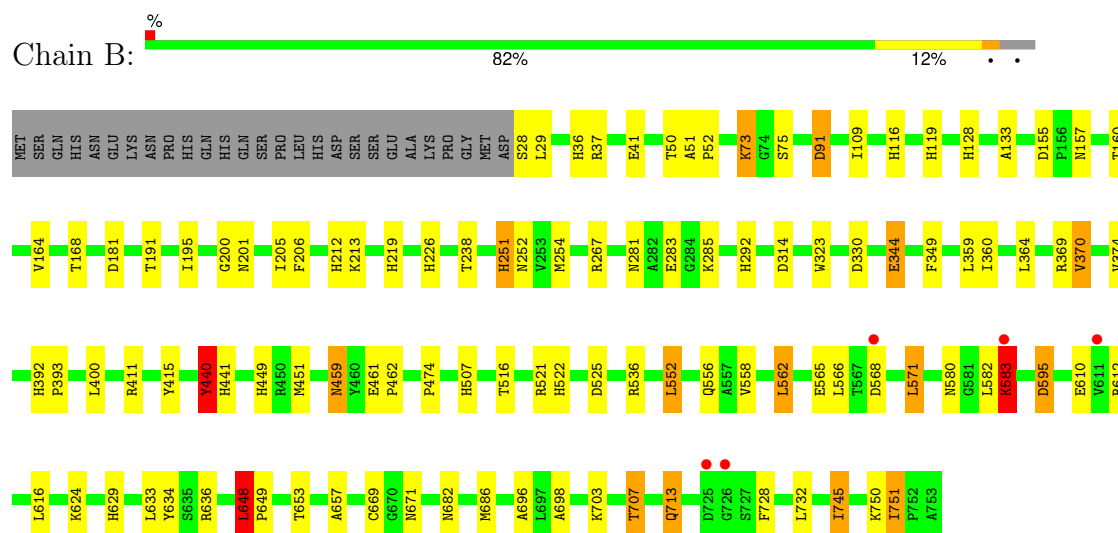
3 Residue-property plots

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.

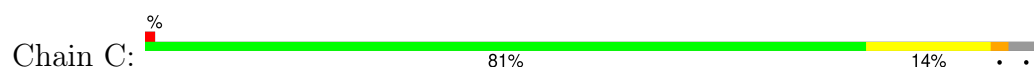
• Molecule 1: Catalase HP1I

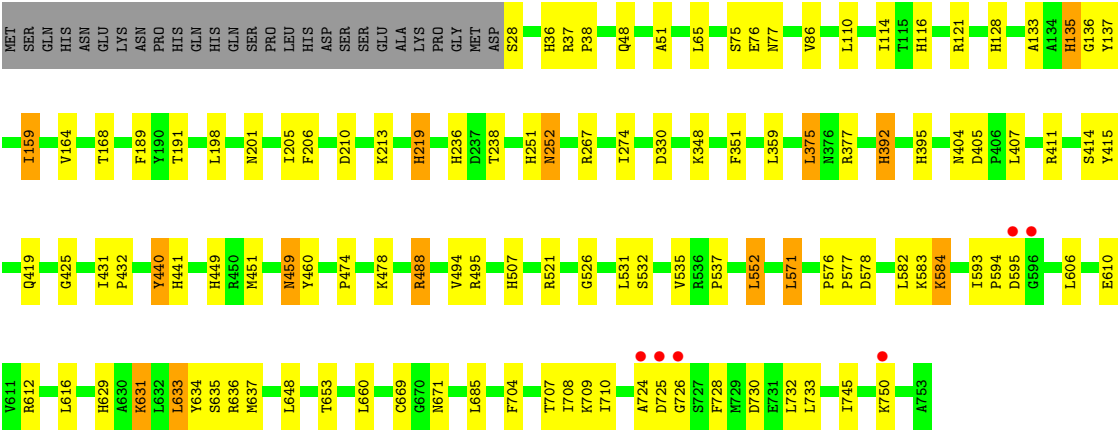


• Molecule 1: Catalase HP1I

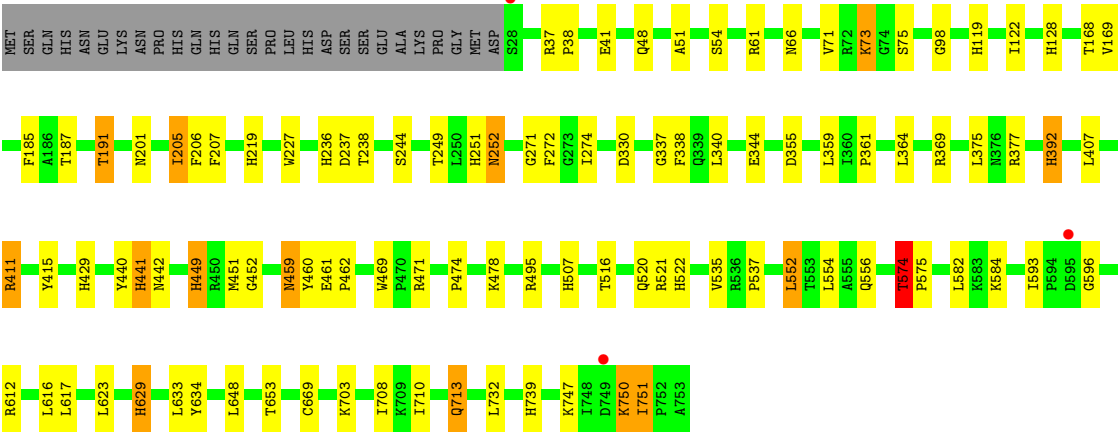
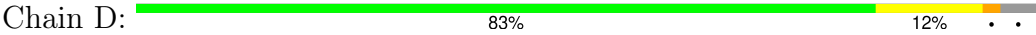


• Molecule 1: Catalase HP1I





● Molecule 1: Catalase HP1I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.46Å 133.05Å 122.19Å 90.00° 109.58° 90.00°	Depositor
Resolution (Å)	33.26 – 1.70 33.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (33.26-1.70) 98.1 (33.26-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.197 0.158 , 0.196	Depositor DCC
R_{free} test set	15289 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26312	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.47	21/5912 (0.4%)	1.26	16/8035 (0.2%)
1	B	1.45	33/5886 (0.6%)	1.25	23/8001 (0.3%)
1	C	1.41	21/5905 (0.4%)	1.22	16/8027 (0.2%)
1	D	1.48	34/5901 (0.6%)	1.25	17/8021 (0.2%)
All	All	1.45	109/23604 (0.5%)	1.25	72/32084 (0.2%)

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	HIS	ND1-CE1	8.67	1.41	1.32
1	B	251	HIS	ND1-CE1	7.48	1.40	1.32
1	C	441	HIS	ND1-CE1	7.32	1.39	1.32
1	A	203	THR	N-CA	7.00	1.51	1.45
1	D	522	HIS	ND1-CE1	6.97	1.39	1.32
1	D	474	PRO	CA-C	6.79	1.55	1.51
1	B	400	LEU	N-CA	6.58	1.53	1.45
1	D	274	ILE	N-CA	6.54	1.54	1.46
1	B	441	HIS	ND1-CE1	6.41	1.39	1.32
1	D	623	LEU	N-CA	6.33	1.53	1.46
1	C	210	ASP	N-CA	6.32	1.53	1.46
1	D	236	HIS	CG-CD2	6.30	1.42	1.35
1	C	136	GLY	N-CA	6.29	1.52	1.44
1	C	441	HIS	CG-CD2	6.17	1.42	1.35
1	C	236	HIS	CG-CD2	6.16	1.42	1.35
1	A	272	PHE	N-CA	6.12	1.53	1.46
1	B	160	THR	C-O	-6.07	1.17	1.24
1	B	449	HIS	CG-CD2	6.04	1.42	1.35
1	B	200	GLY	N-CA	6.03	1.50	1.44
1	B	212	HIS	ND1-CE1	5.97	1.38	1.32
1	A	322	LEU	C-O	5.96	1.30	1.24
1	D	377	ARG	CZ-NH1	5.96	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	375	LEU	N-CA	5.93	1.53	1.46
1	D	187	THR	N-CA	5.93	1.53	1.46
1	B	360	ILE	N-CA	5.88	1.50	1.46
1	A	131	GLY	C-O	5.88	1.30	1.24
1	A	219	HIS	CE1-NE2	5.87	1.38	1.32
1	B	449	HIS	CB-CG	5.86	1.58	1.50
1	B	441	HIS	CG-CD2	5.86	1.42	1.35
1	B	449	HIS	CE1-NE2	5.84	1.38	1.32
1	A	318	HIS	ND1-CE1	5.84	1.38	1.32
1	D	520	GLN	C-O	5.83	1.30	1.24
1	D	452	GLY	C-O	5.83	1.29	1.24
1	D	338	PHE	C-O	5.79	1.31	1.24
1	C	116	HIS	ND1-CE1	5.75	1.38	1.32
1	D	119	HIS	ND1-CE1	5.74	1.38	1.32
1	C	219	HIS	ND1-CE1	5.74	1.38	1.32
1	B	109	ILE	C-O	5.74	1.30	1.24
1	B	116	HIS	CG-CD2	5.71	1.42	1.35
1	A	194	GLY	C-O	5.71	1.28	1.23
1	B	226	HIS	CG-CD2	5.70	1.42	1.35
1	A	502	GLY	N-CA	5.68	1.53	1.45
1	B	116	HIS	ND1-CE1	5.65	1.38	1.32
1	B	119	HIS	CG-CD2	5.63	1.42	1.35
1	D	617	LEU	C-O	5.63	1.30	1.24
1	C	135	HIS	CG-CD2	5.61	1.42	1.35
1	D	244	SER	N-CA	5.61	1.53	1.46
1	D	429	HIS	ND1-CE1	5.58	1.38	1.32
1	B	323	TRP	CD2-CE2	5.58	1.50	1.41
1	D	392	HIS	ND1-CE1	5.58	1.38	1.32
1	D	219	HIS	CG-CD2	5.54	1.42	1.35
1	B	698	ALA	N-CA	5.54	1.52	1.46
1	D	355	ASP	CA-C	5.51	1.59	1.52
1	D	441	HIS	CE1-NE2	5.51	1.38	1.32
1	A	150	ALA	N-CA	5.50	1.53	1.46
1	B	522	HIS	CE1-NE2	5.50	1.38	1.32
1	D	219	HIS	CE1-NE2	5.47	1.38	1.32
1	D	54	SER	CA-C	5.47	1.60	1.52
1	D	739	HIS	N-CA	5.47	1.53	1.46
1	C	494	VAL	N-CA	5.43	1.52	1.46
1	C	251	HIS	ND1-CE1	5.41	1.38	1.32
1	C	36	HIS	CE1-NE2	5.40	1.38	1.32
1	D	271	GLY	C-O	5.40	1.30	1.23
1	A	315	PRO	CA-C	5.37	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	377	ARG	CZ-NH2	5.37	1.40	1.33
1	C	532	SER	N-CA	5.35	1.53	1.46
1	D	411	ARG	CA-CB	5.35	1.61	1.53
1	D	272	PHE	N-CA	5.34	1.52	1.46
1	B	226	HIS	ND1-CE1	5.34	1.37	1.32
1	C	236	HIS	CE1-NE2	5.33	1.37	1.32
1	A	214	PHE	C-O	-5.32	1.19	1.24
1	B	181	ASP	CB-CG	5.31	1.65	1.52
1	D	575	PRO	CA-C	5.31	1.54	1.51
1	B	374	VAL	C-O	-5.29	1.18	1.24
1	A	411	ARG	CZ-NH1	5.29	1.40	1.32
1	B	314	ASP	N-CA	5.29	1.51	1.46
1	D	449	HIS	ND1-CE1	5.26	1.37	1.32
1	B	251	HIS	CG-CD2	5.22	1.41	1.35
1	B	522	HIS	CG-CD2	5.19	1.41	1.35
1	C	86	VAL	N-CA	5.19	1.52	1.46
1	C	595	ASP	N-CA	5.19	1.51	1.46
1	C	189	PHE	N-CA	5.19	1.52	1.46
1	A	392	HIS	ND1-CE1	5.17	1.37	1.32
1	C	392	HIS	ND1-CE1	5.17	1.37	1.32
1	D	191	THR	CA-CB	5.16	1.61	1.53
1	D	442	ASN	C-O	5.16	1.28	1.24
1	C	526	GLY	N-CA	5.16	1.52	1.45
1	C	495	ARG	CZ-NH2	5.15	1.40	1.33
1	A	320	ARG	CZ-NH2	5.14	1.40	1.33
1	B	50	THR	C-O	5.13	1.30	1.23
1	A	629	HIS	ND1-CE1	5.13	1.37	1.32
1	A	629	HIS	CG-CD2	5.12	1.41	1.35
1	B	474	PRO	CA-C	5.12	1.54	1.51
1	A	125	ARG	N-CA	5.11	1.52	1.46
1	D	495	ARG	N-CA	5.09	1.54	1.46
1	B	522	HIS	ND1-CE1	5.09	1.37	1.32
1	B	292	HIS	ND1-CE1	5.09	1.37	1.32
1	A	412	LEU	N-CA	5.07	1.52	1.46
1	C	121	ARG	CZ-NH2	5.07	1.40	1.33
1	B	91	ASP	C-O	-5.07	1.17	1.24
1	B	157	ASN	C-O	-5.06	1.17	1.24
1	A	549	HIS	ND1-CE1	5.06	1.37	1.32
1	A	395	HIS	ND1-CE1	5.04	1.37	1.32
1	B	36	HIS	CG-CD2	5.04	1.41	1.35
1	D	251	HIS	CE1-NE2	5.04	1.37	1.32
1	D	629	HIS	ND1-CE1	5.04	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	395	HIS	CE1-NE2	5.02	1.37	1.32
1	B	440	TYR	CA-C	5.02	1.58	1.52
1	D	337	GLY	N-CA	5.01	1.50	1.45

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	LYS	CD-CE-NZ	7.97	137.40	111.90
1	B	583	LYS	N-CA-CB	-7.65	98.52	110.30
1	B	648	LEU	CA-C-N	7.52	127.95	119.83
1	B	648	LEU	C-N-CA	7.52	127.95	119.83
1	C	576	PRO	CA-C-N	-7.49	113.11	120.52
1	C	576	PRO	C-N-CA	-7.49	113.11	120.52
1	B	582	LEU	CA-C-N	7.16	132.86	120.68
1	B	582	LEU	C-N-CA	7.16	132.86	120.68
1	C	48	GLN	N-CA-C	-6.54	100.66	108.25
1	B	582	LEU	N-CA-C	6.41	119.06	109.25
1	A	38	PRO	CB-CA-C	-6.25	103.39	111.46
1	B	536	ARG	CA-C-N	-6.22	112.60	119.19
1	B	536	ARG	C-N-CA	-6.22	112.60	119.19
1	B	745	ILE	CA-C-N	-6.15	113.47	119.87
1	B	745	ILE	C-N-CA	-6.15	113.47	119.87
1	A	648	LEU	CA-C-N	-6.13	113.66	119.85
1	A	648	LEU	C-N-CA	-6.13	113.66	119.85
1	C	213	LYS	CD-CE-NZ	-6.12	92.32	111.90
1	A	37	ARG	CA-C-N	6.05	125.99	119.76
1	A	37	ARG	C-N-CA	6.05	125.99	119.76
1	A	748	ILE	N-CA-C	6.05	119.54	111.44
1	A	751	ILE	N-CA-CB	5.88	116.53	110.23
1	D	71	VAL	CB-CA-C	-5.78	104.57	110.93
1	B	370	VAL	CB-CA-C	5.75	116.29	110.65
1	C	631	LYS	CB-CA-C	5.74	119.32	110.14
1	D	41	GLU	N-CA-C	-5.66	101.69	108.25
1	C	375	LEU	CD1-CG-CD2	5.66	123.24	110.80
1	C	348	LYS	CA-CB-CG	-5.64	102.81	114.10
1	D	98	GLY	N-CA-C	-5.63	105.67	112.48
1	D	596	GLY	N-CA-C	5.61	117.92	111.36
1	A	350	ASP	CB-CA-C	5.60	120.34	110.37
1	B	41	GLU	CA-C-N	-5.57	114.19	119.76
1	B	41	GLU	C-N-CA	-5.57	114.19	119.76
1	A	348	LYS	N-CA-C	5.57	119.94	113.20
1	D	478	LYS	CB-CG-CD	5.56	124.09	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	431	ILE	N-CA-C	-5.53	103.53	108.95
1	C	414	SER	N-CA-C	5.51	116.97	111.07
1	B	657	ALA	CA-C-N	5.49	125.79	119.92
1	B	657	ALA	C-N-CA	5.49	125.79	119.92
1	B	370	VAL	CG1-CB-CG2	5.38	122.63	110.80
1	A	596	GLY	N-CA-C	5.33	117.59	111.36
1	A	745	ILE	CA-C-N	-5.32	113.56	119.19
1	A	745	ILE	C-N-CA	-5.32	113.56	119.19
1	D	122	ILE	CA-C-N	-5.31	114.29	119.76
1	D	122	ILE	C-N-CA	-5.31	114.29	119.76
1	D	516	THR	CA-C-N	-5.30	113.58	119.19
1	D	516	THR	C-N-CA	-5.30	113.58	119.19
1	D	237	ASP	N-CA-C	5.29	116.73	111.07
1	C	745	ILE	CA-C-N	-5.29	114.17	119.56
1	C	745	ILE	C-N-CA	-5.29	114.17	119.56
1	A	552	LEU	CB-CG-CD1	5.23	126.39	110.70
1	C	351	PHE	N-CA-C	-5.21	101.37	109.24
1	C	110	LEU	N-CA-C	-5.21	105.51	111.14
1	C	425	GLY	CA-C-N	5.21	126.23	120.45
1	C	425	GLY	C-N-CA	5.21	126.23	120.45
1	D	713	GLN	CB-CA-C	5.20	119.97	110.36
1	B	370	VAL	N-CA-CB	-5.19	105.11	112.12
1	A	657	ALA	CA-C-N	5.19	125.47	119.92
1	A	657	ALA	C-N-CA	5.19	125.47	119.92
1	D	377	ARG	CG-CD-NE	-5.16	100.66	112.00
1	B	595	ASP	CA-C-N	5.16	124.87	119.92
1	B	595	ASP	C-N-CA	5.16	124.87	119.92
1	C	474	PRO	O-C-N	5.15	123.68	121.31
1	B	516	THR	CA-C-N	-5.13	113.63	119.28
1	B	516	THR	C-N-CA	-5.13	113.63	119.28
1	A	71	VAL	N-CA-C	5.09	117.78	112.90
1	D	574	THR	CB-CA-C	5.09	116.74	109.26
1	B	349	PHE	CA-C-N	-5.08	113.83	122.56
1	B	349	PHE	C-N-CA	-5.08	113.83	122.56
1	D	244	SER	N-CA-C	-5.06	106.37	112.54
1	D	377	ARG	NH1-CZ-NH2	5.01	125.82	119.30
1	D	449	HIS	CB-CA-C	-5.00	104.83	111.63

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	5753	0	5591	46	0
1	B	5740	0	5574	55	0
1	C	5755	0	5591	77	0
1	D	5749	0	5587	51	0
2	A	44	0	31	3	0
2	B	44	0	31	3	0
2	C	44	0	31	2	0
2	D	44	0	31	3	0
3	A	43	0	30	8	0
3	B	43	0	30	7	0
3	C	43	0	30	15	0
3	D	43	0	30	9	0
4	A	779	0	0	10	0
4	B	679	0	0	15	0
4	C	741	0	0	12	0
4	D	768	0	0	8	0
All	All	26312	0	22587	233	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 5.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.74	1.51
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.73	1.49
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.73	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.77	1.47
1:B:369:ARG:HG2	4:B:1296:HOH:O	1.26	1.32
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.73	1.23
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.83	1.15
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:HMC2	1.26	1.15
1:A:451:MET:HE2	1:C:451:MET:HE2	1.24	1.14
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.82	1.14
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.82	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.82	1.13
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.82	1.12
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.79	1.12
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.78	1.10
1:A:716:GLU:HG3	4:A:1647:HOH:O	1.50	1.10
4:B:1574:HOH:O	1:D:73:LYS:HD3	1.57	1.04
1:B:451:MET:HE2	1:D:451:MET:HE2	1.37	1.03
1:A:369:ARG:NH2	4:A:1179:HOH:O	1.96	0.99
1:C:267:ARG:HG3	4:C:1555:HOH:O	1.67	0.94
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.02	0.93
1:A:448:MET:HG3	1:A:449[A]:HIS:CD2	2.04	0.93
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.03	0.90
1:A:206:PHE:CD2	3:A:802[B]:HEM:HAB	2.08	0.88
1:B:267:ARG:HG3	4:B:1362:HOH:O	1.74	0.88
1:A:344:GLU:HB3	4:A:1587:HOH:O	1.75	0.87
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.08	0.86
3:D:802[B]:HEM:HBC2	3:D:802[B]:HEM:HMC2	1.55	0.85
2:A:801[A]:HDD:HBB1	2:A:801[A]:HDD:HMB1	1.58	0.85
1:C:201:ASN:CG	3:C:802[B]:HEM:HMB2	2.03	0.84
1:C:440:TYR:HD1	4:C:1374:HOH:O	1.60	0.83
1:C:725:ASP:HB3	1:C:726:GLY:C	2.02	0.83
1:C:725:ASP:HB3	1:C:726:GLY:CA	2.10	0.82
1:D:206:PHE:CG	3:D:802[B]:HEM:HAB	2.17	0.80
1:C:206:PHE:CG	3:C:802[B]:HEM:HAB	2.19	0.78
1:C:440:TYR:CD1	4:C:1374:HOH:O	2.36	0.77
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.66	0.77
4:B:1574:HOH:O	1:D:73:LYS:CD	2.18	0.77
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:CMC	2.06	0.76
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.69	0.74
1:A:449[A]:HIS:CG	1:C:449[A]:HIS:CG	2.62	0.73
1:D:703:LYS:HE2	4:D:1568:HOH:O	1.90	0.71
1:C:488:ARG:HD2	4:C:1460:HOH:O	1.90	0.71
1:A:206:PHE:CG	3:A:802[B]:HEM:HAB	2.25	0.71
1:B:206:PHE:CG	3:B:802[B]:HEM:HAB	2.26	0.71
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.57	0.70
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.74	0.70
1:C:636:ARG:NH1	4:C:1525:HOH:O	2.25	0.68
1:D:629:HIS:HD2	4:D:1255:HOH:O	1.77	0.68
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.61	0.68
1:C:206:PHE:CD2	3:C:802[B]:HEM:HAB	2.29	0.68
1:B:629:HIS:HD2	4:B:1160:HOH:O	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:LYS:HE2	1:D:751:ILE:HG22	1.75	0.67
1:A:448:MET:CG	1:A:449[A]:HIS:CD2	2.77	0.67
1:D:206:PHE:CD2	3:D:802[B]:HEM:HAB	2.29	0.67
1:A:709:LYS:N	1:A:709:LYS:HD3	2.09	0.67
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.63	0.66
1:B:28:SER:HA	4:B:1464:HOH:O	1.95	0.65
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.79	0.65
1:C:704:PHE:O	1:C:707:THR:HG22	1.95	0.65
1:D:201:ASN:CG	3:D:802[B]:HEM:HMB2	2.22	0.65
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.62	0.65
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.64	0.65
1:D:556:GLN:NE2	4:D:1571:HOH:O	2.31	0.63
1:B:201:ASN:CG	3:B:802[B]:HEM:HMB2	2.24	0.63
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.81	0.62
1:D:732:LEU:C	1:D:732:LEU:HD13	2.25	0.61
1:D:469:TRP:CE3	1:D:471:ARG:HG3	2.36	0.60
1:B:281:ASN:OD1	1:B:283:GLU:HG2	2.01	0.60
1:C:359:LEU:H	1:C:507:HIS:HD2	1.49	0.60
1:D:411:ARG:HG2	3:D:802[B]:HEM:C2C	2.36	0.60
1:A:449[B]:HIS:HD2	4:C:1195:HOH:O	1.83	0.60
1:A:612:ARG:HG3	4:A:1567:HOH:O	2.01	0.59
1:C:201:ASN:ND2	3:C:802[B]:HEM:CMB	2.66	0.59
1:B:359:LEU:H	1:B:507:HIS:HD2	1.50	0.59
1:C:578:ASP:HB2	1:C:582:LEU:O	2.03	0.58
1:A:690:LYS:HB2	1:A:751:ILE:HD11	1.86	0.58
1:C:137:TYR:HB2	1:C:159[A]:ILE:CD1	2.34	0.58
1:C:634:TYR:O	1:C:653:THR:HA	2.03	0.57
1:B:73:LYS:HD3	1:D:441:HIS:CD2	2.39	0.57
1:C:407:LEU:HD23	3:C:802[B]:HEM:HBB1	1.86	0.57
1:A:36:HIS:CD2	1:A:36:HIS:H	2.23	0.56
2:A:801[A]:HDD:HBB1	2:A:801[A]:HDD:CMB	2.34	0.56
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.88	0.56
1:A:201:ASN:CG	3:A:802[B]:HEM:HMB2	2.31	0.56
4:A:1097:HOH:O	1:C:449[B]:HIS:HD2	1.89	0.55
3:B:802[B]:HEM:HBC1	1:C:114:ILE:HD12	1.88	0.55
1:C:407:LEU:CD2	3:C:802[B]:HEM:HBB1	2.37	0.55
1:C:725:ASP:HB2	1:C:728:PHE:CB	2.36	0.55
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.88	0.55
1:C:583:LYS:HD2	4:C:1217:HOH:O	2.05	0.55
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.22	0.54
1:C:411:ARG:HG2	3:C:802[B]:HEM:C2C	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:HIS:HD2	4:C:1212:HOH:O	1.92	0.53
1:D:201:ASN:ND2	3:D:802[B]:HEM:HMB1	2.24	0.53
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:CMC	2.39	0.53
1:A:392:HIS:ND1	1:A:415:TYR:HB3	2.07	0.53
1:C:359:LEU:H	1:C:507:HIS:CD2	2.27	0.53
1:C:725:ASP:CB	1:C:726:GLY:HA3	2.39	0.53
1:C:725:ASP:CB	1:C:726:GLY:CA	2.83	0.52
1:D:201:ASN:CG	3:D:802[B]:HEM:CMB	2.82	0.52
1:A:725:ASP:H	1:A:728:PHE:HB3	1.73	0.52
1:B:206:PHE:CD2	3:B:802[B]:HEM:HAB	2.45	0.52
1:C:201:ASN:CG	3:C:802[B]:HEM:CMB	2.79	0.52
1:C:610:GLU:O	1:C:610:GLU:HG3	2.10	0.51
1:B:636:ARG:HA	4:B:1506:HOH:O	2.11	0.51
1:B:128:HIS:HA	1:B:168:THR:O	2.11	0.51
1:B:344:GLU:H	1:B:344:GLU:CD	2.18	0.51
1:C:725:ASP:HB3	1:C:726:GLY:HA3	1.87	0.50
1:A:201:ASN:CG	3:A:802[B]:HEM:CMB	2.84	0.50
1:B:37:ARG:NH1	4:B:1520:HOH:O	2.31	0.50
1:B:29:LEU:N	4:B:1464:HOH:O	2.26	0.50
2:C:801[A]:HDD:HBD2	4:C:1095:HOH:O	2.11	0.49
1:C:28:SER:HA	4:C:1635:HOH:O	2.11	0.49
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.94	0.49
1:A:451:MET:CE	1:C:451:MET:HE2	2.18	0.49
1:D:201:ASN:ND2	3:D:802[B]:HEM:CMB	2.75	0.49
1:C:274:ILE:HD12	3:C:802[B]:HEM:HMB1	1.94	0.49
2:B:801[A]:HDD:CMB	2:B:801[A]:HDD:HBB1	2.43	0.49
1:A:716:GLU:HG2	4:A:1304:HOH:O	2.12	0.48
1:C:610:GLU:HB3	1:C:671:ASN:HB2	1.95	0.48
1:A:448:MET:O	1:A:449[A]:HIS:HB2	2.13	0.48
2:D:801[A]:HDD:HBD2	4:D:1133:HOH:O	2.13	0.48
1:B:411:ARG:HG2	3:B:802[B]:HEM:C2C	2.48	0.48
1:C:404:ASN:O	1:C:405:ASP:C	2.55	0.48
1:C:392:HIS:CG	1:C:415:TYR:CB	2.85	0.47
1:C:725:ASP:HB2	1:C:728:PHE:HB2	1.96	0.47
1:D:703:LYS:CE	4:D:1568:HOH:O	2.56	0.47
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.97	0.47
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.30	0.47
1:D:128:HIS:HA	1:D:168:THR:O	2.14	0.47
3:B:802[B]:HEM:HBC2	3:B:802[B]:HEM:CMC	2.45	0.47
1:A:578:ASP:HB2	4:A:1657:HOH:O	2.15	0.47
1:D:461:GLU:HA	1:D:462:PRO:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:802[B]:HEM:HMC2	3:D:802[B]:HEM:CBC	2.37	0.46
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB1	2.30	0.46
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.51	0.46
1:B:267:ARG:HD2	4:B:1134:HOH:O	2.15	0.46
1:B:359:LEU:H	1:B:507:HIS:CD2	2.33	0.46
1:D:612:ARG:HD3	4:D:1559:HOH:O	2.15	0.46
2:A:801[A]:HDD:HBD2	4:A:997:HOH:O	2.15	0.46
4:A:1152:HOH:O	1:C:451:MET:HE1	2.16	0.46
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.51	0.46
1:A:128:HIS:HA	1:A:168:THR:O	2.16	0.45
1:C:725:ASP:OD1	1:C:726:GLY:HA3	2.15	0.45
1:A:411:ARG:HG2	3:A:802[B]:HEM:C2C	2.51	0.45
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.80	0.45
1:A:692:LEU:HB2	1:A:740:ARG:HB3	1.98	0.45
1:B:525:ASP:OD2	4:B:945:HOH:O	2.21	0.45
1:D:535:VAL:O	1:D:537:PRO:HD3	2.17	0.45
1:D:392:HIS:CG	1:D:415:TYR:CB	2.82	0.45
1:B:713:GLN:NE2	1:B:713:GLN:H	2.15	0.45
1:A:460:TYR:CE2	1:B:238:THR:HB	2.52	0.45
1:B:133:ALA:HA	1:B:164:VAL:O	2.17	0.44
3:C:802[B]:HEM:CMC	3:C:802[B]:HEM:CBC	2.83	0.44
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.67	0.44
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.98	0.44
1:C:411:ARG:HD2	3:C:802[B]:HEM:HBB2	2.00	0.44
1:A:349:PHE:CD1	1:A:349:PHE:N	2.86	0.44
1:B:634:TYR:O	1:B:653:THR:HA	2.17	0.44
1:C:460:TYR:CE2	1:D:238:THR:HB	2.53	0.44
1:C:552:LEU:HD21	1:C:571:LEU:CD1	2.45	0.44
1:A:114:ILE:HD12	2:D:801[A]:HDD:HBC2	1.99	0.44
1:B:583:LYS:H	1:B:583:LYS:HG2	0.96	0.44
1:C:725:ASP:HB2	1:C:728:PHE:HB3	1.98	0.43
1:A:459:ASN:HD22	1:A:459:ASN:H	1.66	0.43
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.53	0.43
1:A:369:ARG:NH2	1:A:369:ARG:HG3	2.34	0.43
1:A:612:ARG:NH1	1:A:669:OCS:OD3	2.51	0.43
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.43
1:B:254:MET:HE3	1:B:254:MET:HB3	1.89	0.43
1:B:459:ASN:H	1:B:459:ASN:HD22	1.67	0.43
1:C:76:GLU:O	1:C:77:ASN:HB2	2.18	0.43
1:D:634:TYR:O	1:D:653:THR:HA	2.19	0.43
1:A:319:ARG:HD3	1:D:227:TRP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HA	4:B:1563:HOH:O	2.18	0.43
1:B:610:GLU:HB3	1:B:671:ASN:HB2	2.01	0.43
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.67	0.43
1:C:535:VAL:O	1:C:537:PRO:HD3	2.18	0.43
1:B:364:LEU:HD11	1:B:580:ASN:HB2	2.01	0.43
1:D:361:PRO:HD2	1:D:364:LEU:HD12	1.99	0.43
1:A:461:GLU:HA	1:A:462:PRO:C	2.44	0.42
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB2	2.28	0.42
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:C:415:TYR:O	1:C:419:GLN:HG2	2.18	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:C:459:ASN:H	1:C:459:ASN:HD22	1.66	0.42
1:D:205:ILE:H	1:D:205:ILE:HD13	1.84	0.42
1:D:38:PRO:HG2	1:D:51:ALA:HB2	2.00	0.42
1:D:708:ILE:HG13	1:D:710:ILE:HG12	2.02	0.42
1:B:558:VAL:HG12	1:B:562:LEU:HD22	2.02	0.42
1:D:574:THR:HG23	4:D:1299:HOH:O	2.20	0.42
1:B:648:LEU:HA	1:B:649:PRO:HD2	1.67	0.42
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.01	0.42
1:C:634:TYR:CG	1:C:635:SER:N	2.88	0.42
4:B:1430:HOH:O	1:D:449:HIS:HD2	2.01	0.42
1:D:407:LEU:HD11	2:D:801[A]:HDD:HMC1	2.01	0.42
1:B:461:GLU:HA	1:B:462:PRO:C	2.44	0.42
1:C:577:PRO:HG2	4:C:1493:HOH:O	2.18	0.42
1:B:624:LYS:HD3	4:B:1513:HOH:O	2.20	0.41
1:C:488:ARG:NH1	4:C:1460:HOH:O	2.17	0.41
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.70	0.41
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.20	0.41
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:HMC2	2.02	0.41
1:B:51:ALA:HB1	1:B:52:PRO:HD2	2.02	0.41
1:C:440:TYR:CD2	1:C:440:TYR:C	2.98	0.41
1:C:274:ILE:HD12	2:C:801[A]:HDD:HMB3	2.02	0.41
1:D:37:ARG:HD2	4:D:1424:HOH:O	2.20	0.41
1:A:207:PHE:O	1:A:249:THR:HA	2.21	0.41
1:C:583:LYS:O	1:C:584:LYS:HB3	2.20	0.41
1:C:732:LEU:C	1:C:732:LEU:HD13	2.45	0.41
1:B:201:ASN:CG	3:B:802[B]:HEM:CMB	2.91	0.41
2:B:801[A]:HDD:HBD2	4:B:1043:HOH:O	2.20	0.41
1:A:369:ARG:HG3	1:A:369:ARG:HH21	1.86	0.41
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.38	0.41
1:B:440:TYR:CD2	1:B:440:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.36	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:D:552:LEU:HD22	1:D:552:LEU:HA	1.67	0.41
1:B:751:ILE:HD13	1:B:751:ILE:HG21	1.78	0.41
1:C:133:ALA:HA	1:C:164:VAL:O	2.21	0.41
1:C:238:THR:HB	1:D:460:TYR:CE2	2.56	0.41
1:C:137:TYR:HB2	1:C:159[A]:ILE:HD12	2.03	0.40
3:A:802[B]:HEM:HMC2	3:A:802[B]:HEM:CBC	2.51	0.40
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.57	0.40
2:B:801[A]:HDD:HBB1	2:B:801[A]:HDD:HMB3	2.02	0.40
1:D:359:LEU:H	1:D:507:HIS:HD2	1.67	0.40
1:A:488:ARG:NH2	4:A:1592:HOH:O	2.54	0.40
1:A:333:GLU:OE1	1:A:372:LYS:HE3	2.21	0.40
1:B:562:LEU:HA	1:C:637:MET:HB2	2.03	0.40
1:B:686:MET:HB3	1:B:751:ILE:HD11	2.03	0.40
1:C:65:LEU:HD21	1:C:135:HIS:CG	2.57	0.40
1:D:459:ASN:HD22	1:D:459:ASN:H	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	708 (98%)	15 (2%)	3 (0%)	30	16
1	B	723/753 (96%)	705 (98%)	17 (2%)	1 (0%)	48	31
1	C	725/753 (96%)	708 (98%)	15 (2%)	2 (0%)	36	22
1	D	725/753 (96%)	714 (98%)	10 (1%)	1 (0%)	48	31
All	All	2899/3012 (96%)	2835 (98%)	57 (2%)	7 (0%)	43	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	ILE
1	A	75	SER
1	A	709	LYS
1	B	75	SER
1	C	75	SER
1	C	724	ALA
1	D	75	SER

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/634 (96%)	596 (97%)	16 (3%)	40	23
1	B	609/634 (96%)	579 (95%)	30 (5%)	22	8
1	C	611/634 (96%)	581 (95%)	30 (5%)	22	8
1	D	611/634 (96%)	586 (96%)	25 (4%)	27	11
All	All	2443/2536 (96%)	2342 (96%)	101 (4%)	27	11

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	565	GLU
1	A	602	VAL
1	A	617	LEU
1	A	703	LYS
1	A	709	LYS
1	A	716	GLU
1	A	732	LEU

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Mol	Chain	Res	Type
1	A	747	LYS
1	B	73	LYS
1	B	155	ASP
1	B	191	THR
1	B	195	ILE
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	285	LYS
1	B	344	GLU
1	B	370	VAL
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	648	LEU
1	B	703	LYS
1	B	707	THR
1	B	713	GLN
1	B	732	LEU
1	B	750	LYS
1	B	751	ILE
1	C	37	ARG
1	C	159[A]	ILE
1	C	159[B]	ILE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	252	ASN
1	C	375	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR

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Mol	Chain	Res	Type
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	730	ASP
1	C	733	LEU
1	C	750	LYS
1	D	48	GLN
1	D	73	LYS
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	369	ARG
1	D	440	TYR
1	D	459	ASN
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	584	LYS
1	D	593	ILE
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS

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Mol	Chain	Res	Type
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	246	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	546	GLN
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	C	682	ASN
1	C	713	GLN
1	D	48	GLN
1	D	77	ASN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	OCS	A	669	1	6,8,9	1.78	1 (16%)	7,11,13	1.55	1 (14%)
1	OCS	D	669	1	6,8,9	2.10	2 (33%)	7,11,13	2.49	3 (42%)
1	OCS	C	669	1	6,8,9	1.69	1 (16%)	7,11,13	2.06	3 (42%)
1	OCS	B	669	1	6,8,9	2.17	1 (16%)	7,11,13	2.47	3 (42%)

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	OCS	A	669	1	-	3/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	C	669	1	-	3/4/7/9	-
1	OCS	B	669	1	-	1/4/7/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	OD2-SG	4.74	1.65	1.47
1	A	669	OCS	OD2-SG	4.16	1.62	1.47
1	D	669	OCS	OD2-SG	4.14	1.62	1.47
1	C	669	OCS	OD2-SG	3.87	1.61	1.47
1	D	669	OCS	CB-CA	2.35	1.55	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	669	OCS	OD1-SG-CB	5.38	114.79	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	5.18	114.49	106.76
1	C	669	OCS	OD2-SG-CB	3.21	112.17	105.97
1	A	669	OCS	OD3-SG-CB	-2.84	102.51	106.76
1	C	669	OCS	OD2-SG-OD3	-2.69	104.68	111.40
1	C	669	OCS	OD1-SG-CB	-2.50	103.03	106.76
1	D	669	OCS	OD3-SG-OD1	-2.42	105.97	113.82
1	B	669	OCS	OD3-SG-CB	-2.37	103.21	106.76
1	D	669	OCS	OD2-SG-OD3	2.32	117.21	111.40
1	B	669	OCS	OD2-SG-CB	-2.03	102.05	105.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD2
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD1
1	C	669	OCS	CA-CB-SG-OD2
1	C	669	OCS	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	669	OCS	1	0

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	B	801[A]	1,4	49,52,52	2.52	20 (40%)	62,89,89	2.73	20 (32%)
3	HEM	D	802[B]	1	50,50,50	2.67	22 (44%)	67,82,82	3.04	29 (43%)
2	HDD	D	801[A]	1	49,52,52	2.68	19 (38%)	62,89,89	2.64	22 (35%)
2	HDD	A	801[A]	1	49,52,52	2.60	22 (44%)	62,89,89	3.37	27 (43%)
3	HEM	C	802[B]	1	50,50,50	2.47	21 (42%)	67,82,82	3.30	35 (52%)
3	HEM	A	802[B]	1	50,50,50	2.52	22 (44%)	67,82,82	3.03	34 (50%)
3	HEM	B	802[B]	1	50,50,50	2.58	22 (44%)	67,82,82	2.77	30 (44%)
2	HDD	C	801[A]	1	49,52,52	2.32	19 (38%)	62,89,89	2.95	24 (38%)

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	B	801[A]	1,4	1/1/8/14	3/9/89/89	0/1/9/9
3	HEM	D	802[B]	1	-	4/14/54/54	-
2	HDD	D	801[A]	1	1/1/8/14	2/9/89/89	0/1/9/9
2	HDD	A	801[A]	1	1/1/8/14	3/9/89/89	0/1/9/9
3	HEM	C	802[B]	1	-	4/14/54/54	-
3	HEM	A	802[B]	1	-	4/14/54/54	-
3	HEM	B	802[B]	1	-	4/14/54/54	-
2	HDD	C	801[A]	1	1/1/8/14	2/9/89/89	0/1/9/9

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801[A]	HDD	C1D-ND	9.40	1.41	1.35
2	A	801[A]	HDD	C1D-ND	8.49	1.40	1.35
2	B	801[A]	HDD	C1D-ND	6.94	1.39	1.35
3	D	802[B]	HEM	C1C-NC	5.97	1.50	1.39
3	C	802[B]	HEM	FE-ND	5.91	2.13	1.94
3	B	802[B]	HEM	FE-NB	5.75	2.12	1.94
2	D	801[A]	HDD	O1D-CGD	5.59	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802[B]	HEM	FE-NB	5.57	2.12	1.94
3	A	802[B]	HEM	C1C-NC	5.40	1.49	1.39
3	D	802[B]	HEM	FE-ND	5.17	2.10	1.94
3	A	802[B]	HEM	FE-NB	5.16	2.10	1.94
2	B	801[A]	HDD	FE-NC	5.07	2.11	1.95
3	A	802[B]	HEM	FE-ND	5.04	2.10	1.94
3	C	802[B]	HEM	FE-NB	5.04	2.10	1.94
2	C	801[A]	HDD	CHC-C1C	4.93	1.48	1.38
3	C	802[B]	HEM	C1C-NC	4.91	1.48	1.39
3	B	802[B]	HEM	FE-ND	4.88	2.09	1.94
3	D	802[B]	HEM	C1A-NA	4.86	1.48	1.39
3	D	802[B]	HEM	C3B-C2B	4.84	1.47	1.37
2	D	801[A]	HDD	C3B-C2B	4.80	1.46	1.37
2	B	801[A]	HDD	FE-NB	4.79	2.09	1.94
2	D	801[A]	HDD	C3C-C2C	4.70	1.46	1.37
2	A	801[A]	HDD	C4C-NC	-4.70	1.30	1.39
2	B	801[A]	HDD	CHC-C4B	4.63	1.49	1.39
3	D	802[B]	HEM	C4C-NC	4.62	1.48	1.39
3	B	802[B]	HEM	C1C-NC	4.57	1.48	1.39
3	B	802[B]	HEM	C4A-NA	4.55	1.48	1.39
2	D	801[A]	HDD	FE-NC	4.54	2.10	1.95
2	A	801[A]	HDD	CHD-C4C	4.54	1.47	1.38
3	D	802[B]	HEM	C3C-C2C	4.51	1.46	1.37
2	B	801[A]	HDD	C1B-NB	-4.49	1.32	1.40
3	A	802[B]	HEM	CHD-C4C	4.46	1.47	1.38
2	A	801[A]	HDD	CHB-C1B	4.43	1.47	1.38
3	B	802[B]	HEM	C4C-NC	4.32	1.47	1.39
3	A	802[B]	HEM	C1A-NA	4.31	1.47	1.39
3	B	802[B]	HEM	C1A-NA	4.31	1.47	1.39
2	A	801[A]	HDD	C3B-C2B	4.29	1.45	1.37
3	B	802[B]	HEM	C3C-C2C	4.20	1.45	1.37
2	A	801[A]	HDD	CHC-C4B	4.19	1.48	1.39
3	A	802[B]	HEM	CHA-C4D	4.15	1.46	1.38
3	C	802[B]	HEM	CHD-C4C	4.12	1.46	1.38
3	D	802[B]	HEM	C4A-NA	4.10	1.47	1.39
3	B	802[B]	HEM	CHD-C4C	4.09	1.46	1.38
2	D	801[A]	HDD	CHD-C4C	4.09	1.46	1.38
2	C	801[A]	HDD	C3C-C2C	4.08	1.45	1.37
2	C	801[A]	HDD	C1D-ND	4.07	1.38	1.35
2	A	801[A]	HDD	CHA-C1A	4.07	1.48	1.39
3	C	802[B]	HEM	C1A-NA	4.06	1.47	1.39
2	B	801[A]	HDD	CHA-C1A	4.04	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802[B]	HEM	CHA-C4D	4.04	1.46	1.38
2	D	801[A]	HDD	CHC-C4B	4.03	1.48	1.39
3	D	802[B]	HEM	C3D-C2D	4.00	1.45	1.36
3	A	802[B]	HEM	CHD-C1D	4.00	1.48	1.39
2	C	801[A]	HDD	C4A-NA	-3.99	1.32	1.39
3	D	802[B]	HEM	CHD-C1D	3.99	1.48	1.39
3	C	802[B]	HEM	CHD-C1D	3.97	1.48	1.39
2	C	801[A]	HDD	O1D-CGD	3.96	1.41	1.35
3	D	802[B]	HEM	CHD-C4C	3.96	1.46	1.38
2	C	801[A]	HDD	C4C-NC	-3.94	1.32	1.39
2	B	801[A]	HDD	CHD-C4C	3.94	1.46	1.38
3	C	802[B]	HEM	C3D-C2D	3.93	1.45	1.36
2	D	801[A]	HDD	CHB-C1B	3.93	1.46	1.38
2	C	801[A]	HDD	CHC-C4B	3.92	1.48	1.39
2	A	801[A]	HDD	FE-NA	3.87	2.07	1.95
3	C	802[B]	HEM	C3C-C2C	3.87	1.45	1.37
3	B	802[B]	HEM	C3D-C2D	3.79	1.44	1.36
2	A	801[A]	HDD	FE-NB	3.78	2.06	1.94
2	B	801[A]	HDD	C3C-C2C	3.77	1.44	1.37
3	D	802[B]	HEM	CHC-C4B	3.76	1.47	1.39
3	A	802[B]	HEM	C4C-NC	3.76	1.46	1.39
2	B	801[A]	HDD	C1A-NA	-3.74	1.32	1.39
3	C	802[B]	HEM	C4A-NA	3.73	1.46	1.39
3	A	802[B]	HEM	C4A-NA	3.69	1.46	1.39
2	A	801[A]	HDD	FE-NC	3.67	2.07	1.95
2	C	801[A]	HDD	CHD-C4C	3.63	1.45	1.38
3	A	802[B]	HEM	CHC-C1C	3.62	1.45	1.38
2	D	801[A]	HDD	FE-NB	3.61	2.06	1.94
2	C	801[A]	HDD	FE-NC	3.57	2.07	1.95
2	A	801[A]	HDD	O1D-CGD	3.56	1.41	1.35
3	A	802[B]	HEM	C3C-C2C	3.56	1.44	1.37
3	A	802[B]	HEM	C3D-C2D	3.54	1.44	1.36
3	C	802[B]	HEM	C4C-NC	3.50	1.46	1.39
3	B	802[B]	HEM	CHC-C4B	3.50	1.47	1.39
3	A	802[B]	HEM	C1B-NB	-3.45	1.34	1.40
2	C	801[A]	HDD	FE-NB	3.42	2.05	1.94
3	D	802[B]	HEM	CHA-C4D	3.42	1.45	1.38
3	B	802[B]	HEM	C3B-C2B	3.41	1.44	1.37
3	B	802[B]	HEM	CHA-C4D	3.40	1.45	1.38
2	B	801[A]	HDD	C4C-NC	-3.40	1.33	1.39
3	A	802[B]	HEM	C3B-C2B	3.40	1.44	1.37
2	C	801[A]	HDD	O1D-C3D	3.39	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801[A]	HDD	CHC-C1C	3.35	1.44	1.38
3	B	802[B]	HEM	CHD-C1D	3.34	1.46	1.39
3	D	802[B]	HEM	C1C-C2C	3.31	1.51	1.45
2	C	801[A]	HDD	C1A-NA	-3.30	1.33	1.39
3	C	802[B]	HEM	CHC-C1C	3.25	1.44	1.38
3	B	802[B]	HEM	CHA-C1A	3.24	1.46	1.39
2	B	801[A]	HDD	C3B-C2B	3.22	1.43	1.37
3	A	802[B]	HEM	CHC-C4B	3.21	1.46	1.39
3	C	802[B]	HEM	C3B-C2B	3.19	1.43	1.37
3	B	802[B]	HEM	CHB-C1B	3.17	1.44	1.38
3	B	802[B]	HEM	C1B-NB	-3.15	1.34	1.40
2	C	801[A]	HDD	CHB-C1B	3.15	1.44	1.38
2	C	801[A]	HDD	C3B-C2B	3.14	1.43	1.37
2	D	801[A]	HDD	CHA-C1A	3.13	1.46	1.39
2	C	801[A]	HDD	FE-NA	3.11	2.05	1.95
2	D	801[A]	HDD	FE-NA	3.06	2.05	1.95
3	B	802[B]	HEM	C4A-C3A	3.02	1.50	1.43
3	D	802[B]	HEM	CHC-C1C	3.02	1.44	1.38
3	C	802[B]	HEM	CHB-C4A	3.00	1.46	1.39
2	B	801[A]	HDD	CHB-C1B	2.99	1.44	1.38
3	A	802[B]	HEM	CHA-C1A	2.98	1.46	1.39
2	C	801[A]	HDD	CHA-C1A	2.93	1.46	1.39
3	B	802[B]	HEM	CHC-C1C	2.92	1.44	1.38
2	D	801[A]	HDD	CHB-C4A	2.88	1.45	1.39
3	A	802[B]	HEM	C1A-C2A	2.88	1.50	1.44
2	A	801[A]	HDD	C1B-NB	-2.87	1.35	1.40
2	D	801[A]	HDD	C1B-C2B	2.87	1.50	1.44
3	B	802[B]	HEM	C2A-C3A	2.86	1.46	1.38
2	A	801[A]	HDD	C4A-NA	-2.85	1.34	1.39
3	B	802[B]	HEM	C1A-C2A	2.80	1.50	1.44
3	C	802[B]	HEM	C4A-C3A	2.78	1.49	1.43
2	C	801[A]	HDD	CHB-C4A	2.77	1.45	1.39
3	C	802[B]	HEM	CHC-C4B	2.73	1.45	1.39
3	C	802[B]	HEM	C2A-C3A	2.71	1.46	1.38
3	C	802[B]	HEM	CHB-C1B	2.69	1.43	1.38
3	D	802[B]	HEM	CHA-C1A	2.64	1.45	1.39
2	D	801[A]	HDD	OND-C2D	2.63	1.47	1.42
2	A	801[A]	HDD	C1A-NA	-2.58	1.34	1.39
2	D	801[A]	HDD	C4A-NA	-2.57	1.34	1.39
2	A	801[A]	HDD	CMC-C2C	2.57	1.56	1.50
3	D	802[B]	HEM	C2A-C3A	2.56	1.45	1.38
3	A	802[B]	HEM	C4D-ND	-2.54	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801[A]	HDD	C1B-NB	-2.49	1.35	1.40
2	D	801[A]	HDD	C4C-NC	-2.49	1.34	1.39
2	B	801[A]	HDD	FE-NA	2.44	2.03	1.95
3	D	802[B]	HEM	C1B-NB	-2.43	1.36	1.40
2	A	801[A]	HDD	CHB-C4A	2.42	1.44	1.39
3	D	802[B]	HEM	C4D-ND	-2.40	1.36	1.40
2	B	801[A]	HDD	O1D-CGD	2.40	1.39	1.35
3	D	802[B]	HEM	CHB-C1B	2.40	1.43	1.38
3	D	802[B]	HEM	C4A-C3A	2.38	1.48	1.43
2	D	801[A]	HDD	C1A-NA	-2.36	1.35	1.39
3	B	802[B]	HEM	C4D-ND	-2.35	1.36	1.40
3	D	802[B]	HEM	C1A-C2A	2.32	1.49	1.44
2	C	801[A]	HDD	C4A-C3A	2.32	1.48	1.43
3	C	802[B]	HEM	CHA-C1A	2.30	1.44	1.39
3	A	802[B]	HEM	CHB-C4A	2.27	1.44	1.39
3	A	802[B]	HEM	C2A-C3A	2.27	1.44	1.38
2	C	801[A]	HDD	C2A-C3A	2.25	1.44	1.38
2	B	801[A]	HDD	C1C-NC	-2.20	1.35	1.39
3	C	802[B]	HEM	C4D-ND	-2.20	1.36	1.40
3	A	802[B]	HEM	CHB-C1B	2.19	1.42	1.38
2	B	801[A]	HDD	O1D-C3D	2.15	1.50	1.46
2	A	801[A]	HDD	C4A-C3A	2.14	1.48	1.43
2	D	801[A]	HDD	C2A-C3A	2.14	1.44	1.38
2	B	801[A]	HDD	C4A-C3A	2.14	1.48	1.43
2	A	801[A]	HDD	CHC-C1C	2.13	1.42	1.38
2	B	801[A]	HDD	C4A-NA	-2.12	1.35	1.39
3	B	802[B]	HEM	CHB-C4A	2.10	1.44	1.39
2	B	801[A]	HDD	C3D-C2D	-2.07	1.50	1.55
3	C	802[B]	HEM	C4B-NB	-2.06	1.34	1.38
2	A	801[A]	HDD	C2A-C3A	2.06	1.44	1.38
2	A	801[A]	HDD	C1B-C2B	2.05	1.48	1.44
3	A	802[B]	HEM	C4A-C3A	2.05	1.47	1.43
2	A	801[A]	HDD	C1C-C2C	2.04	1.49	1.45
2	A	801[A]	HDD	C3C-C2C	2.03	1.41	1.37

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801[A]	HDD	C3B-C2B-C1B	-10.47	98.55	106.41
2	A	801[A]	HDD	C3D-O1D-CGD	10.10	120.56	111.14
3	C	802[B]	HEM	C3B-C2B-C1B	-10.02	98.88	106.41
3	A	802[B]	HEM	C3B-C2B-C1B	-9.97	98.92	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801[A]	HDD	O1D-CGD-O2D	9.85	129.11	120.81
2	B	801[A]	HDD	C3B-C2B-C1B	-9.74	99.10	106.41
3	A	802[B]	HEM	C2B-C1B-NB	9.64	120.92	109.84
2	A	801[A]	HDD	O1D-CGD-O2D	9.31	128.66	120.81
3	D	802[B]	HEM	C3B-C2B-C1B	-9.02	99.64	106.41
2	A	801[A]	HDD	C3C-C2C-C1C	-8.99	98.54	107.05
2	B	801[A]	HDD	O1D-CGD-O2D	8.53	127.99	120.81
3	D	802[B]	HEM	C2B-C1B-NB	8.21	119.28	109.84
2	D	801[A]	HDD	C3B-C2B-C1B	-8.01	100.40	106.41
2	A	801[A]	HDD	C3B-C2B-C1B	-7.85	100.51	106.41
3	C	802[B]	HEM	C3B-C4B-NB	7.57	114.91	109.47
3	C	802[B]	HEM	C2B-C1B-NB	7.50	118.46	109.84
2	B	801[A]	HDD	C3C-C2C-C1C	-7.25	100.19	107.05
3	B	802[B]	HEM	C3B-C2B-C1B	-7.23	100.98	106.41
3	C	802[B]	HEM	C3D-C4D-ND	7.22	118.09	110.17
2	C	801[A]	HDD	C2B-C1B-NB	7.14	118.04	109.84
2	A	801[A]	HDD	C3B-C4B-NB	6.90	114.42	109.47
2	D	801[A]	HDD	O1D-CGD-O2D	6.89	126.61	120.81
2	D	801[A]	HDD	C3C-C2C-C1C	-6.80	100.61	107.05
2	A	801[A]	HDD	O1D-CGD-CBD	-6.78	103.99	110.17
3	B	802[B]	HEM	C2B-C1B-NB	6.77	117.63	109.84
2	D	801[A]	HDD	CBD-CAD-C3D	6.26	112.91	103.98
2	A	801[A]	HDD	C2B-C1B-NB	6.22	116.99	109.84
3	C	802[B]	HEM	C3C-C2C-C1C	-6.14	101.23	107.05
2	B	801[A]	HDD	C2B-C1B-NB	6.13	116.89	109.84
3	C	802[B]	HEM	C2D-C1D-ND	5.98	116.81	109.90
3	A	802[B]	HEM	C3B-C4B-NB	5.90	113.71	109.47
3	D	802[B]	HEM	C4C-NC-C1C	-5.74	96.47	105.82
3	D	802[B]	HEM	C3C-C2C-C1C	-5.67	101.68	107.05
2	C	801[A]	HDD	OND-C2D-CMD	-5.65	98.53	109.45
3	D	802[B]	HEM	CMC-C2C-C1C	5.55	134.50	124.73
2	C	801[A]	HDD	C3C-C2C-C1C	-5.52	101.83	107.05
3	B	802[B]	HEM	C2D-C1D-ND	5.46	116.21	109.90
3	B	802[B]	HEM	C3C-C2C-C1C	-5.38	101.95	107.05
3	D	802[B]	HEM	C2D-C1D-ND	5.31	116.04	109.90
3	D	802[B]	HEM	C3B-C4B-NB	5.30	113.27	109.47
3	B	802[B]	HEM	C4C-NC-C1C	-5.29	97.20	105.82
3	B	802[B]	HEM	C2A-C1A-NA	5.27	116.00	110.15
3	A	802[B]	HEM	C3C-C2C-C1C	-5.25	102.08	107.05
3	D	802[B]	HEM	CAA-CBA-CGA	-5.23	99.81	113.67
2	D	801[A]	HDD	C3D-O1D-CGD	5.18	115.97	111.14
2	A	801[A]	HDD	OND-C2D-CMD	-5.10	99.58	109.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802[B]	HEM	C3B-C4B-NB	5.09	113.12	109.47
2	A	801[A]	HDD	CMC-C2C-C1C	4.93	133.41	124.73
2	B	801[A]	HDD	O1D-CGD-CBD	-4.85	105.75	110.17
3	A	802[B]	HEM	C3D-C4D-ND	4.80	115.43	110.17
3	B	802[B]	HEM	C2C-C1C-NC	4.71	118.35	109.64
3	C	802[B]	HEM	CHC-C1C-C2C	-4.71	115.69	125.49
3	D	802[B]	HEM	C3D-C4D-ND	4.67	115.30	110.17
3	C	802[B]	HEM	C4D-ND-C1D	-4.60	99.76	105.21
3	D	802[B]	HEM	CHC-C1C-NC	-4.55	119.50	124.45
2	B	801[A]	HDD	CAA-CBA-CGA	-4.55	101.61	113.67
3	A	802[B]	HEM	C4C-NC-C1C	-4.52	98.46	105.82
3	B	802[B]	HEM	C3D-C4D-ND	4.50	115.11	110.17
3	A	802[B]	HEM	C1B-NB-C4B	-4.49	99.89	105.21
3	A	802[B]	HEM	C2D-C1D-ND	4.48	115.08	109.90
3	C	802[B]	HEM	C2A-C1A-NA	4.45	115.09	110.15
3	D	802[B]	HEM	C4A-NA-C1A	-4.43	98.60	105.82
3	B	802[B]	HEM	C4A-NA-C1A	-4.41	98.62	105.82
3	C	802[B]	HEM	CHA-C4D-C3D	-4.37	117.17	125.23
3	C	802[B]	HEM	C4C-NC-C1C	-4.32	98.79	105.82
3	D	802[B]	HEM	C2C-C1C-NC	4.24	117.48	109.64
3	C	802[B]	HEM	C2C-C1C-NC	4.23	117.46	109.64
2	A	801[A]	HDD	CBD-CAD-C3D	4.19	109.95	103.98
3	B	802[B]	HEM	C1D-C2D-C3D	-4.17	102.59	106.98
3	C	802[B]	HEM	C1D-C2D-C3D	-4.10	102.67	106.98
2	A	801[A]	HDD	CAA-CBA-CGA	-4.10	102.80	113.67
2	B	801[A]	HDD	C2C-C1C-NC	4.07	117.16	109.64
3	D	802[B]	HEM	CHB-C1B-C2B	-4.06	115.42	126.95
2	D	801[A]	HDD	OND-C2D-CMD	-4.02	101.67	109.45
3	D	802[B]	HEM	C1D-C2D-C3D	-4.02	102.75	106.98
3	C	802[B]	HEM	C1B-NB-C4B	-3.99	100.48	105.21
3	B	802[B]	HEM	CHD-C1D-C2D	-3.95	118.79	125.03
2	A	801[A]	HDD	CMB-C2B-C1B	3.93	131.18	125.03
3	C	802[B]	HEM	CBB-CAB-C3B	-3.89	108.08	127.53
2	C	801[A]	HDD	C3B-C4B-NB	3.87	112.24	109.47
3	B	802[B]	HEM	CHC-C1C-C2C	-3.86	117.45	125.49
3	A	802[B]	HEM	CHB-C1B-C2B	-3.86	115.99	126.95
2	D	801[A]	HDD	C4A-C3A-C2A	-3.83	102.44	106.82
2	D	801[A]	HDD	C2C-C1C-NC	3.74	116.56	109.64
3	C	802[B]	HEM	CMD-C2D-C1D	3.73	130.87	125.03
3	D	802[B]	HEM	C3A-C4A-NA	3.70	116.07	110.14
3	A	802[B]	HEM	CBB-CAB-C3B	-3.69	109.10	127.53
3	A	802[B]	HEM	C2C-C1C-NC	3.66	116.42	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801[A]	HDD	C3D-O1D-CGD	3.66	114.55	111.14
2	C	801[A]	HDD	C4A-C3A-C2A	-3.64	102.65	106.82
3	A	802[B]	HEM	CAA-C2A-C1A	3.64	132.04	124.94
2	B	801[A]	HDD	OND-C2D-CMD	-3.63	102.44	109.45
3	D	802[B]	HEM	C2A-C1A-NA	3.61	114.16	110.15
3	C	802[B]	HEM	CAA-CBA-CGA	-3.58	104.18	113.67
3	A	802[B]	HEM	C1C-CHC-C4B	-3.57	118.44	126.02
2	A	801[A]	HDD	O1D-C3D-CAD	-3.57	96.46	103.06
3	A	802[B]	HEM	C4A-NA-C1A	-3.55	100.03	105.82
3	D	802[B]	HEM	CBD-CAD-C3D	-3.55	102.71	112.53
2	D	801[A]	HDD	C2B-C1B-NB	3.55	113.92	109.84
2	D	801[A]	HDD	CMB-C2B-C1B	3.53	130.55	125.03
3	C	802[B]	HEM	C4A-NA-C1A	-3.53	100.07	105.82
3	B	802[B]	HEM	CBD-CAD-C3D	-3.53	102.79	112.53
3	A	802[B]	HEM	C1D-C2D-C3D	-3.50	103.30	106.98
3	C	802[B]	HEM	CMC-C2C-C1C	3.45	130.81	124.73
3	C	802[B]	HEM	CMB-C2B-C1B	3.44	130.41	125.03
3	C	802[B]	HEM	C4C-C3C-C2C	3.43	109.78	106.81
2	C	801[A]	HDD	C2D-C1D-CHD	-3.41	117.91	123.28
2	D	801[A]	HDD	CHC-C1C-NC	-3.39	120.77	124.45
2	D	801[A]	HDD	CMC-C2C-C1C	3.37	130.65	124.73
2	D	801[A]	HDD	C4D-ND-C1D	-3.36	101.33	105.27
2	A	801[A]	HDD	C2A-C1A-NA	3.36	113.88	110.15
2	D	801[A]	HDD	C2D-C1D-CHD	-3.36	117.99	123.28
2	B	801[A]	HDD	C2D-C1D-CHD	-3.35	118.00	123.28
2	A	801[A]	HDD	C2C-C1C-NC	3.34	115.81	109.64
3	B	802[B]	HEM	CBB-CAB-C3B	-3.33	110.90	127.53
2	C	801[A]	HDD	CAA-CBA-CGA	-3.32	104.85	113.67
3	C	802[B]	HEM	C1C-CHC-C4B	-3.30	119.00	126.02
2	D	801[A]	HDD	CHD-C4C-NC	-3.28	120.88	124.45
2	C	801[A]	HDD	O1D-CGD-CBD	-3.24	107.21	110.17
3	A	802[B]	HEM	CHA-C4D-C3D	-3.23	119.27	125.23
2	B	801[A]	HDD	C4A-C3A-C2A	-3.20	103.15	106.82
2	C	801[A]	HDD	C2A-C1A-NA	3.20	113.70	110.15
3	A	802[B]	HEM	CAA-CBA-CGA	-3.15	105.30	113.67
2	C	801[A]	HDD	CHB-C1B-NB	-3.15	120.47	124.37
3	D	802[B]	HEM	C4A-CHB-C1B	-3.15	118.83	126.25
3	A	802[B]	HEM	CHC-C1C-C2C	-3.15	118.94	125.49
3	A	802[B]	HEM	CMC-C2C-C1C	3.12	130.23	124.73
3	C	802[B]	HEM	C4D-C3D-C2D	-3.11	102.36	106.89
2	B	801[A]	HDD	C3D-O1D-CGD	3.10	114.04	111.14
3	A	802[B]	HEM	CMD-C2D-C1D	3.09	129.86	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802[B]	HEM	CHA-C1A-C2A	-3.09	118.53	125.30
3	B	802[B]	HEM	C4C-CHD-C1D	-3.07	119.49	126.02
3	D	802[B]	HEM	CHD-C1D-C2D	-3.07	120.18	125.03
3	B	802[B]	HEM	CHB-C1B-C2B	-3.06	118.26	126.95
3	D	802[B]	HEM	CHD-C4C-C3C	-3.05	120.06	125.21
3	C	802[B]	HEM	C1A-CHA-C4D	-3.05	119.07	126.25
2	B	801[A]	HDD	CHB-C1B-NB	-3.04	120.61	124.37
3	A	802[B]	HEM	CBD-CAD-C3D	-3.02	104.18	112.53
2	C	801[A]	HDD	C2C-C1C-NC	2.99	115.17	109.64
2	C	801[A]	HDD	CBD-CAD-C3D	2.98	108.24	103.98
3	A	802[B]	HEM	C2A-C1A-NA	2.97	113.45	110.15
3	A	802[B]	HEM	C3A-C4A-NA	2.97	114.90	110.14
3	B	802[B]	HEM	C3A-C4A-NA	2.95	114.88	110.14
3	D	802[B]	HEM	C1B-NB-C4B	-2.93	101.74	105.21
3	C	802[B]	HEM	CHB-C4A-C3A	-2.87	119.10	127.43
3	D	802[B]	HEM	CHB-C4A-C3A	-2.87	119.10	127.43
3	B	802[B]	HEM	C1C-CHC-C4B	-2.86	119.94	126.02
2	D	801[A]	HDD	CAA-CBA-CGA	-2.86	106.09	113.67
3	C	802[B]	HEM	CHC-C4B-C3B	-2.84	119.40	125.07
2	C	801[A]	HDD	CMB-C2B-C1B	2.84	129.47	125.03
3	C	802[B]	HEM	C4C-CHD-C1D	-2.84	119.99	126.02
3	B	802[B]	HEM	CHD-C4C-C3C	-2.81	120.47	125.21
3	A	802[B]	HEM	C1A-CHA-C4D	-2.80	119.66	126.25
2	A	801[A]	HDD	CHB-C1B-NB	-2.80	120.91	124.37
3	D	802[B]	HEM	CMD-C2D-C1D	2.79	129.39	125.03
3	A	802[B]	HEM	C4C-C3C-C2C	2.76	109.21	106.81
3	A	802[B]	HEM	O2D-CGD-CBD	2.74	122.67	114.00
3	C	802[B]	HEM	CHB-C1B-NB	-2.74	120.98	124.37
2	C	801[A]	HDD	C4C-C3C-C2C	-2.72	104.46	106.81
3	D	802[B]	HEM	C4D-ND-C1D	-2.71	101.99	105.21
2	C	801[A]	HDD	C1B-NB-C4B	-2.71	102.00	105.21
3	C	802[B]	HEM	CHD-C1D-C2D	-2.70	120.77	125.03
3	A	802[B]	HEM	CHB-C4A-C3A	-2.69	119.61	127.43
2	C	801[A]	HDD	CMC-C2C-C1C	2.68	129.45	124.73
2	C	801[A]	HDD	CHC-C1C-C2C	-2.68	119.91	125.49
2	A	801[A]	HDD	C1B-NB-C4B	-2.67	102.04	105.21
3	B	802[B]	HEM	C4D-ND-C1D	-2.63	102.09	105.21
2	B	801[A]	HDD	C2A-C1A-NA	2.62	113.06	110.15
2	B	801[A]	HDD	CBA-CAA-C2A	-2.61	105.31	112.53
2	A	801[A]	HDD	CHC-C4B-NB	-2.60	121.62	124.42
3	A	802[B]	HEM	C4D-ND-C1D	-2.57	102.17	105.21
3	C	802[B]	HEM	CBD-CAD-C3D	-2.56	105.46	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801[A]	HDD	C4A-C3A-C2A	-2.56	103.89	106.82
3	B	802[B]	HEM	CHA-C4D-C3D	-2.53	120.57	125.23
2	A	801[A]	HDD	C2D-C1D-CHD	-2.51	119.33	123.28
2	D	801[A]	HDD	O1D-CGD-CBD	-2.49	107.90	110.17
2	D	801[A]	HDD	C1C-CHC-C4B	2.47	131.28	126.02
3	A	802[B]	HEM	C4C-CHD-C1D	-2.45	120.80	126.02
2	B	801[A]	HDD	CHD-C4C-NC	-2.43	121.81	124.45
2	C	801[A]	HDD	CMA-C3A-C4A	2.42	129.11	125.42
2	D	801[A]	HDD	CMA-C3A-C2A	2.40	130.71	125.62
3	B	802[B]	HEM	CHA-C1A-C2A	-2.38	120.09	125.30
2	A	801[A]	HDD	CMD-C2D-C3D	2.36	121.33	115.11
2	B	801[A]	HDD	CHC-C1C-C2C	-2.36	120.58	125.49
3	B	802[B]	HEM	CHB-C4A-C3A	-2.35	120.60	127.43
2	D	801[A]	HDD	C3B-C4B-NB	2.34	111.15	109.47
3	B	802[B]	HEM	C1B-NB-C4B	-2.33	102.44	105.21
3	D	802[B]	HEM	CHA-C1A-C2A	-2.33	120.19	125.30
2	C	801[A]	HDD	O2A-CGA-CBA	2.33	121.35	114.00
3	D	802[B]	HEM	CMB-C2B-C3B	2.31	134.03	128.43
3	B	802[B]	HEM	C4A-CHB-C1B	-2.31	120.81	126.25
2	A	801[A]	HDD	C1A-C2A-C3A	-2.31	103.29	106.87
3	D	802[B]	HEM	C4D-C3D-C2D	-2.30	103.55	106.89
3	C	802[B]	HEM	CHB-C1B-C2B	-2.28	120.45	126.95
2	A	801[A]	HDD	C4C-C3C-C2C	2.26	108.78	106.81
3	A	802[B]	HEM	CHD-C1D-C2D	-2.26	121.47	125.03
2	B	801[A]	HDD	CHB-C4A-C3A	-2.24	120.92	127.43
3	C	802[B]	HEM	CBC-CAC-C3C	-2.24	116.35	127.53
2	D	801[A]	HDD	O1D-C3D-CAD	-2.22	98.95	103.06
3	B	802[B]	HEM	O2D-CGD-CBD	2.22	121.00	114.00
2	B	801[A]	HDD	CHC-C1C-NC	-2.20	122.06	124.45
2	A	801[A]	HDD	CHC-C1C-C2C	-2.18	120.96	125.49
3	C	802[B]	HEM	CHC-C1C-NC	2.17	126.82	124.45
3	B	802[B]	HEM	O1D-CGD-CBD	-2.16	116.26	123.09
3	C	802[B]	HEM	C3A-C4A-NA	2.15	113.59	110.14
3	B	802[B]	HEM	CMD-C2D-C3D	2.12	131.89	126.15
3	B	802[B]	HEM	C4D-C3D-C2D	-2.11	103.81	106.89
3	A	802[B]	HEM	O1D-CGD-CBD	-2.11	116.40	123.09
2	C	801[A]	HDD	C3A-C4A-NA	2.11	113.52	110.14
3	A	802[B]	HEM	CAA-C2A-C3A	-2.09	122.39	127.07
2	C	801[A]	HDD	CHB-C4A-C3A	-2.08	121.38	127.43
3	D	802[B]	HEM	C4A-C3A-C2A	-2.08	104.43	106.82
3	A	802[B]	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
2	A	801[A]	HDD	C3A-C4A-NA	2.07	113.46	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[B]	HEM	C4A-CHB-C1B	-2.05	121.42	126.25
2	A	801[A]	HDD	CBC-CAC-C3C	-2.05	117.30	127.53
2	B	801[A]	HDD	CMB-C2B-C1B	2.03	128.21	125.03
3	D	802[B]	HEM	CAA-C2A-C1A	2.02	128.88	124.94
2	D	801[A]	HDD	C3A-C4A-NA	2.02	113.37	110.14
2	B	801[A]	HDD	OND-C2D-C3D	-2.01	105.74	110.46
2	A	801[A]	HDD	CBA-CAA-C2A	-2.01	106.97	112.53

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801[A]	HDD	NC
2	B	801[A]	HDD	NC
2	C	801[A]	HDD	NC
2	D	801[A]	HDD	NC

All (26) 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	B	802[B]	HEM	C2B-C3B-CAB-CBB
3	C	802[B]	HEM	C2B-C3B-CAB-CBB
3	D	802[B]	HEM	C2B-C3B-CAB-CBB
3	B	802[B]	HEM	C4B-C3B-CAB-CBB
3	D	802[B]	HEM	C4B-C3B-CAB-CBB
3	C	802[B]	HEM	C4B-C3B-CAB-CBB
2	A	801[A]	HDD	CAA-CBA-CGA-O1A
2	C	801[A]	HDD	CAA-CBA-CGA-O1A
3	D	802[B]	HEM	CAA-CBA-CGA-O2A
3	B	802[B]	HEM	CAA-CBA-CGA-O2A
2	D	801[A]	HDD	CAA-CBA-CGA-O2A
2	A	801[A]	HDD	CAA-CBA-CGA-O2A
3	C	802[B]	HEM	CAA-CBA-CGA-O2A
3	A	802[B]	HEM	CAA-CBA-CGA-O2A
2	D	801[A]	HDD	CAA-CBA-CGA-O1A
3	A	802[B]	HEM	CAA-CBA-CGA-O1A
3	B	802[B]	HEM	CAA-CBA-CGA-O1A
3	C	802[B]	HEM	CAA-CBA-CGA-O1A
2	B	801[A]	HDD	CAA-CBA-CGA-O1A
3	D	802[B]	HEM	CAA-CBA-CGA-O1A
2	C	801[A]	HDD	CAA-CBA-CGA-O2A

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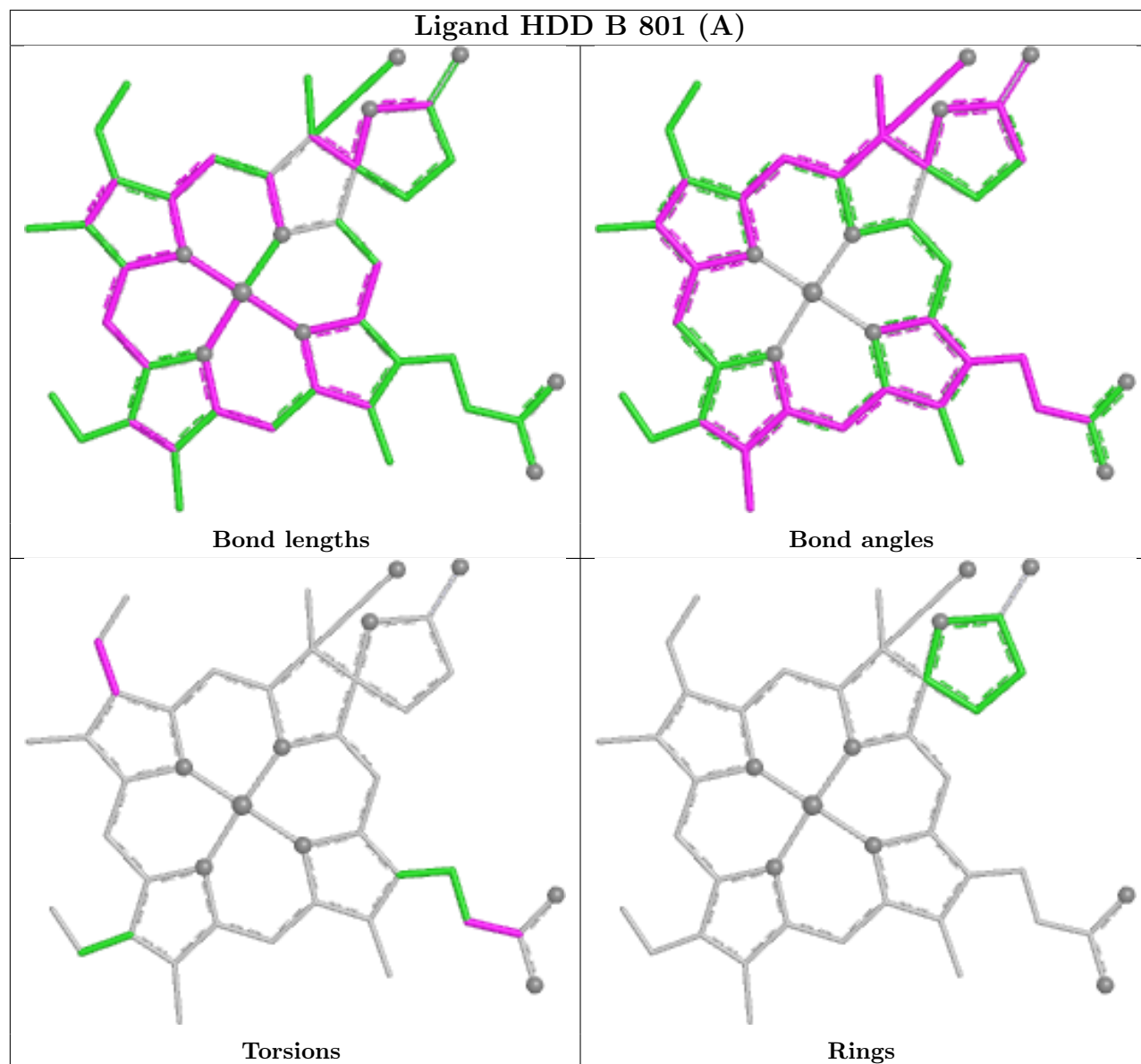
Mol	Chain	Res	Type	Atoms
2	B	801[A]	HDD	CAA-CBA-CGA-O2A
2	A	801[A]	HDD	C2C-C3C-CAC-CBC
2	B	801[A]	HDD	C4C-C3C-CAC-CBC

There are no ring outliers.

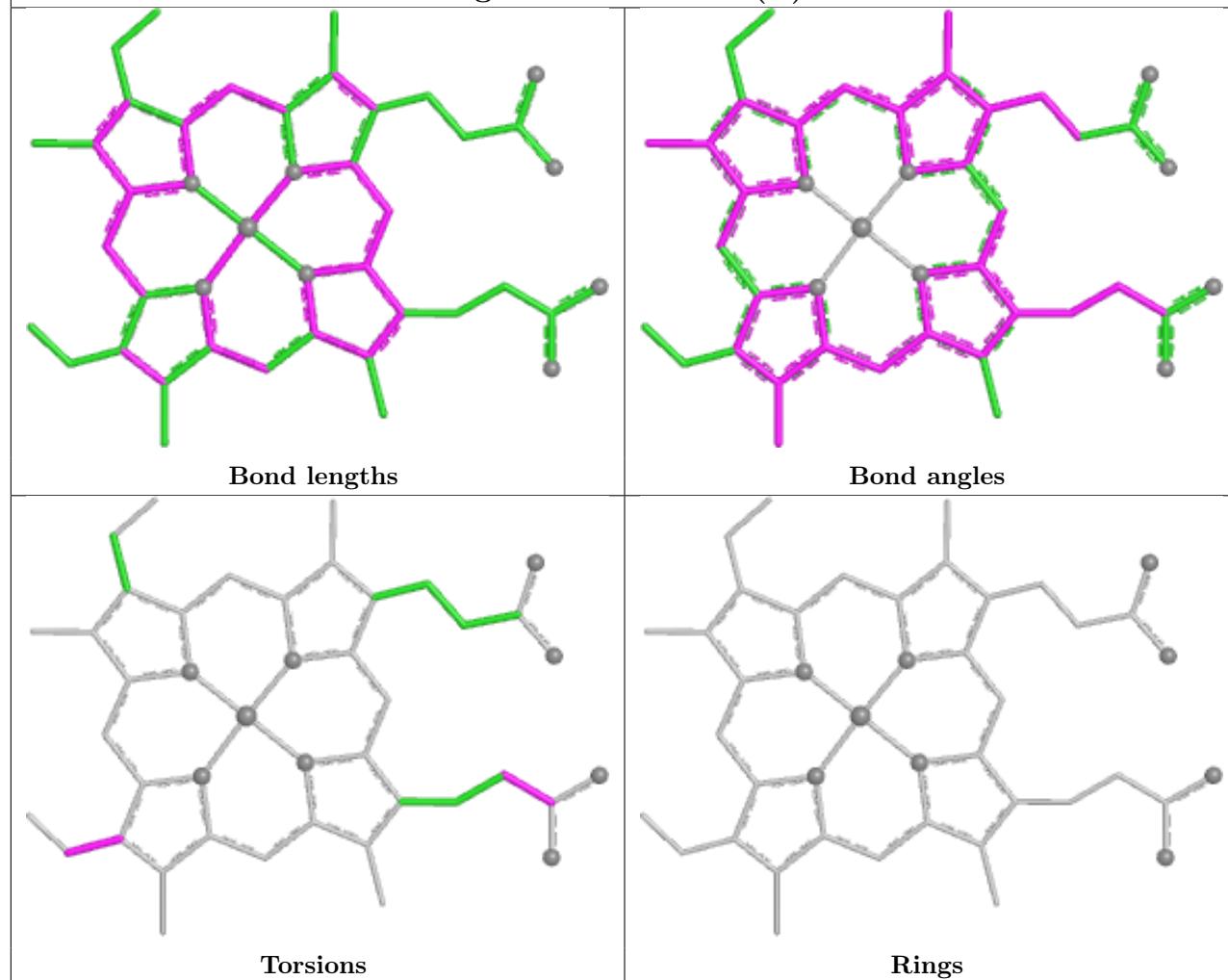
8 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801[A]	HDD	3	0
3	D	802[B]	HEM	9	0
2	D	801[A]	HDD	3	0
2	A	801[A]	HDD	3	0
3	C	802[B]	HEM	15	0
3	A	802[B]	HEM	8	0
3	B	802[B]	HEM	7	0
2	C	801[A]	HDD	2	0

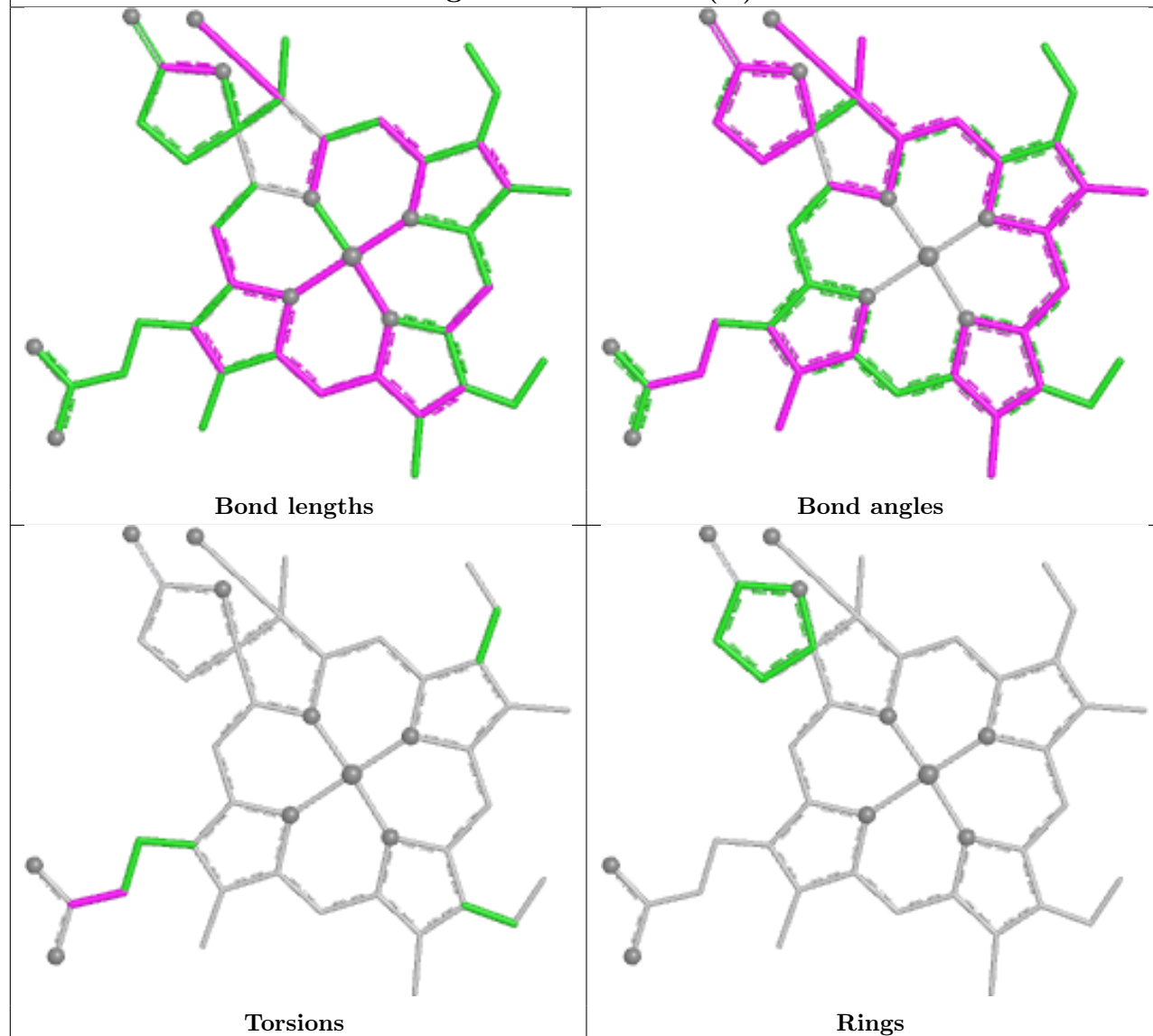
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

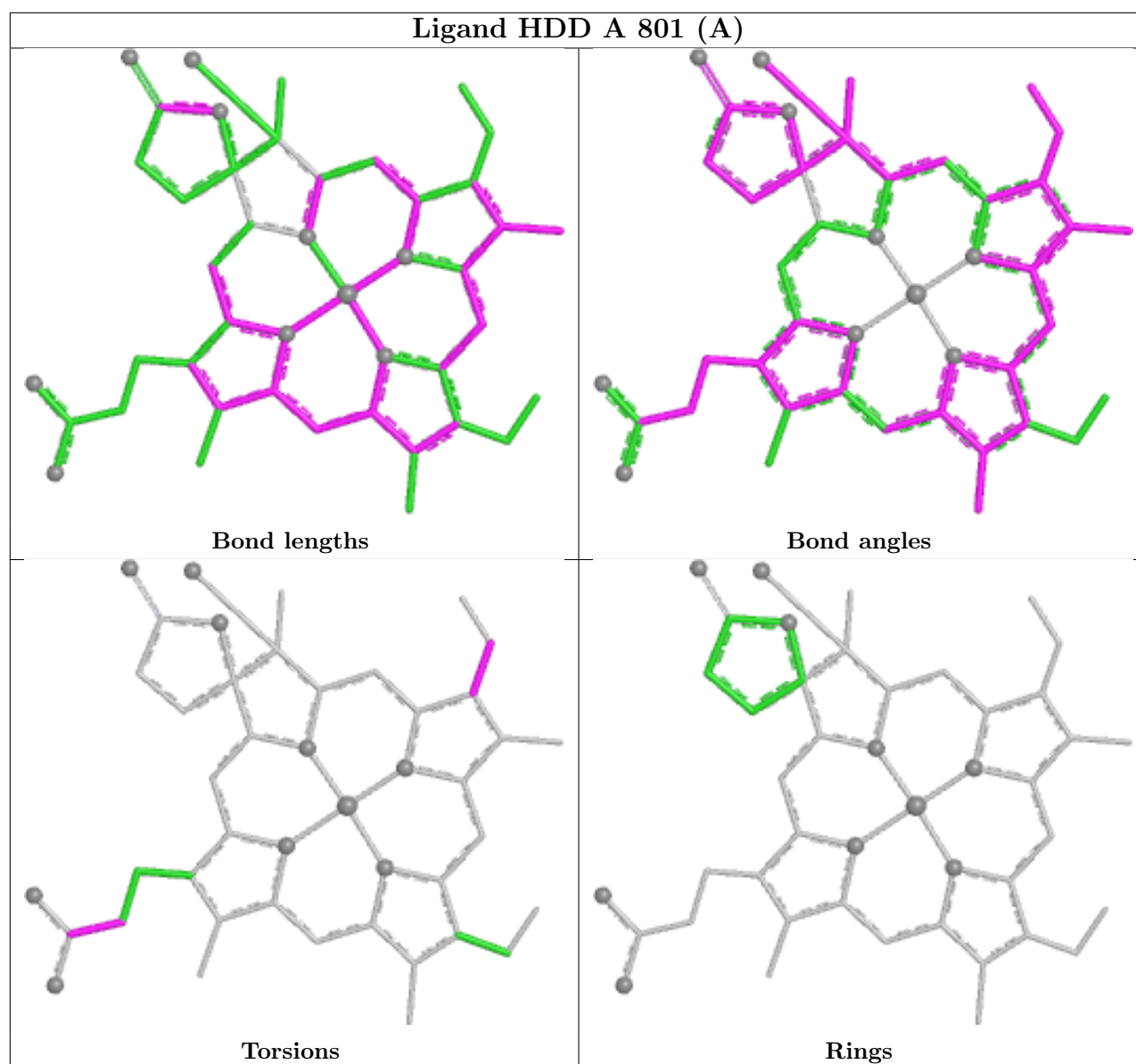


Ligand HEM D 802 (B)

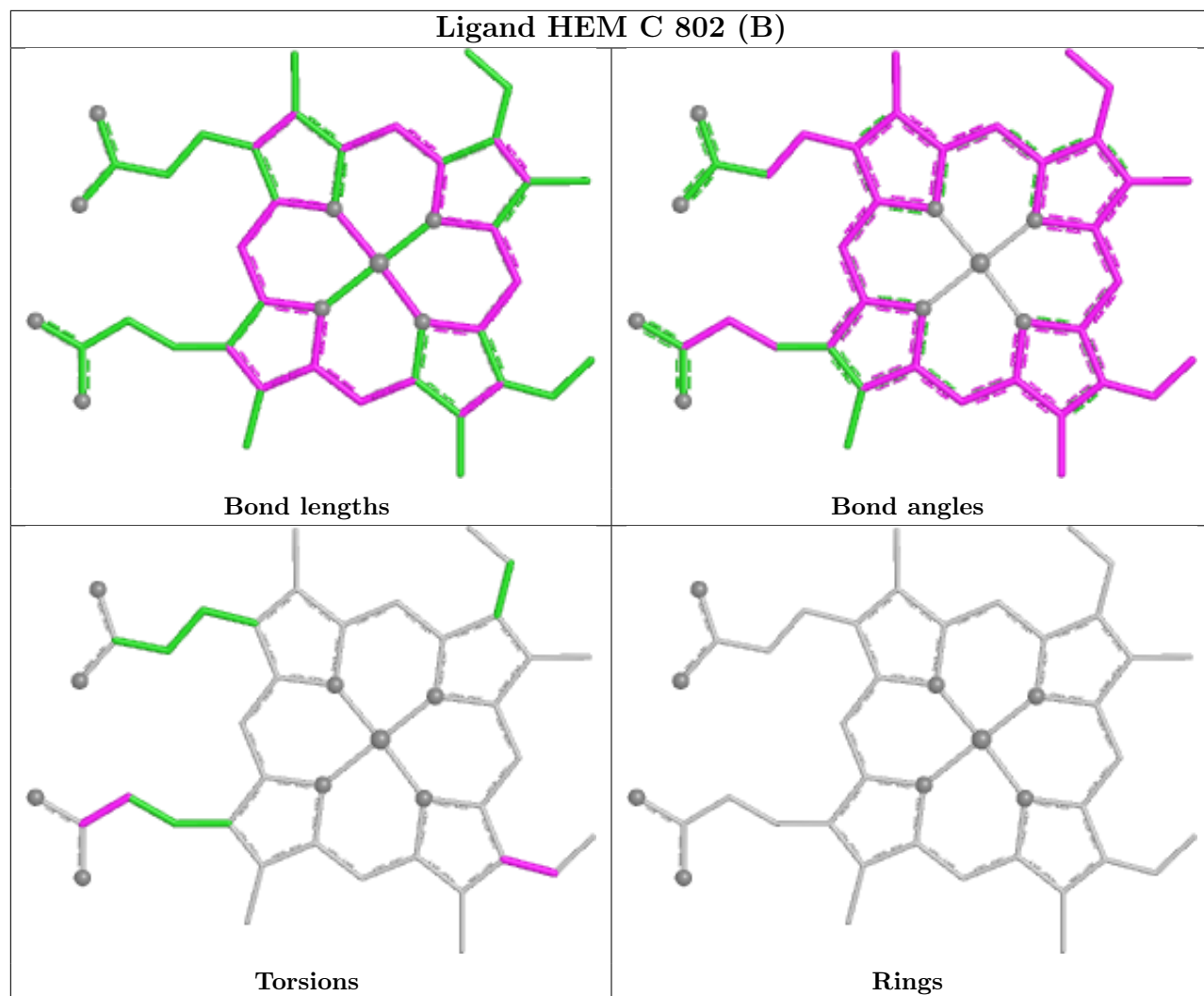


Ligand HDD D 801 (A)

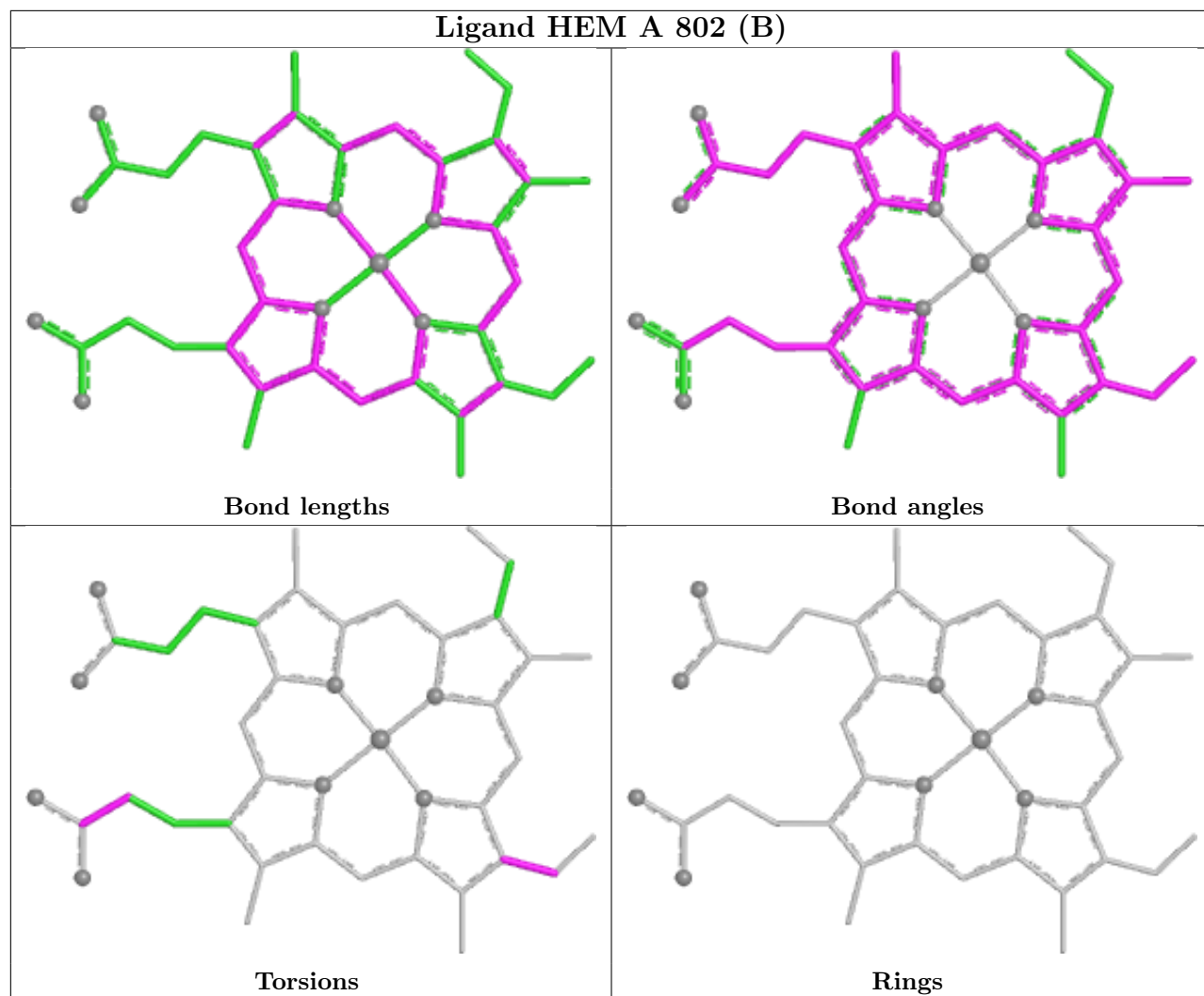




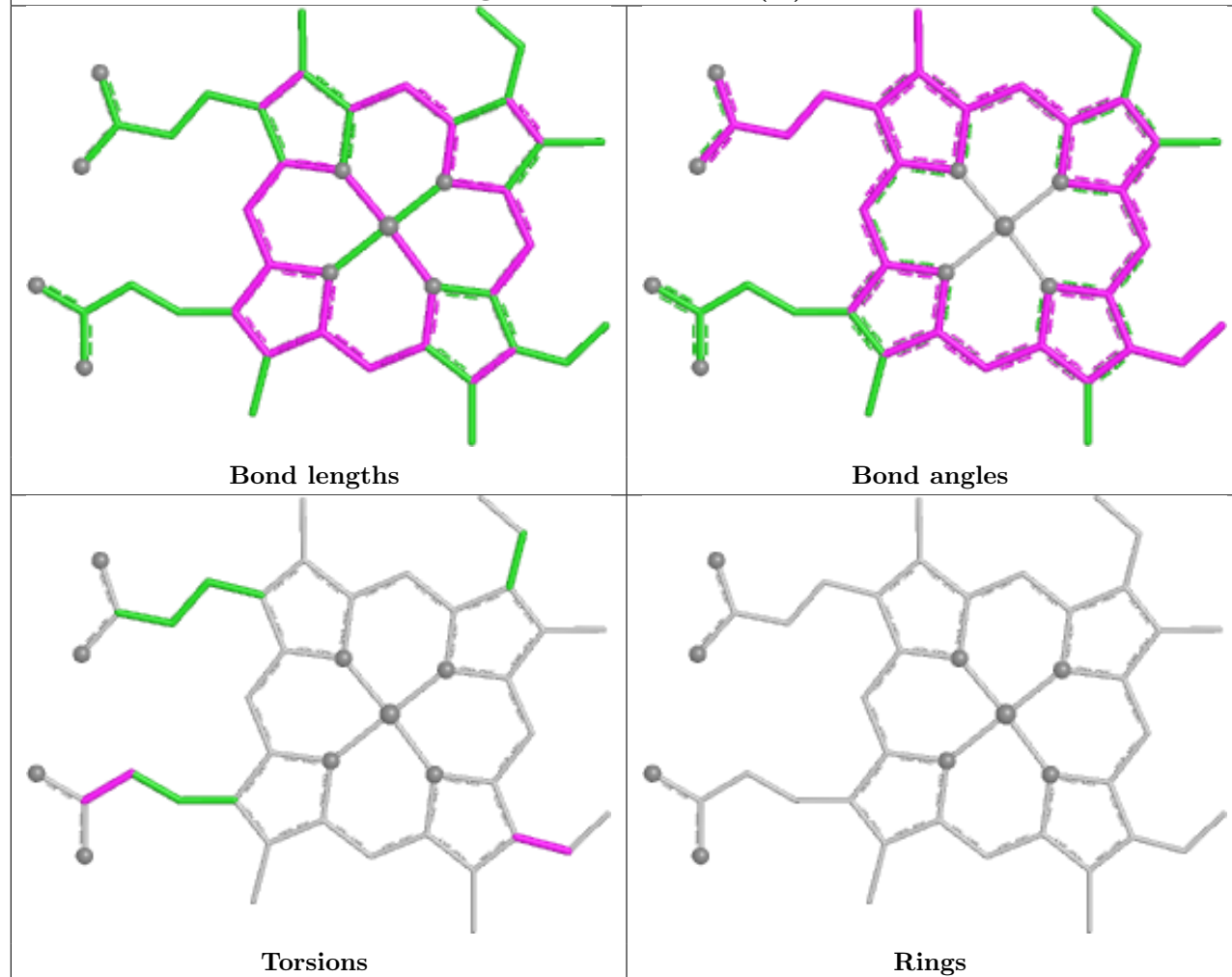
Ligand HEM C 802 (B)

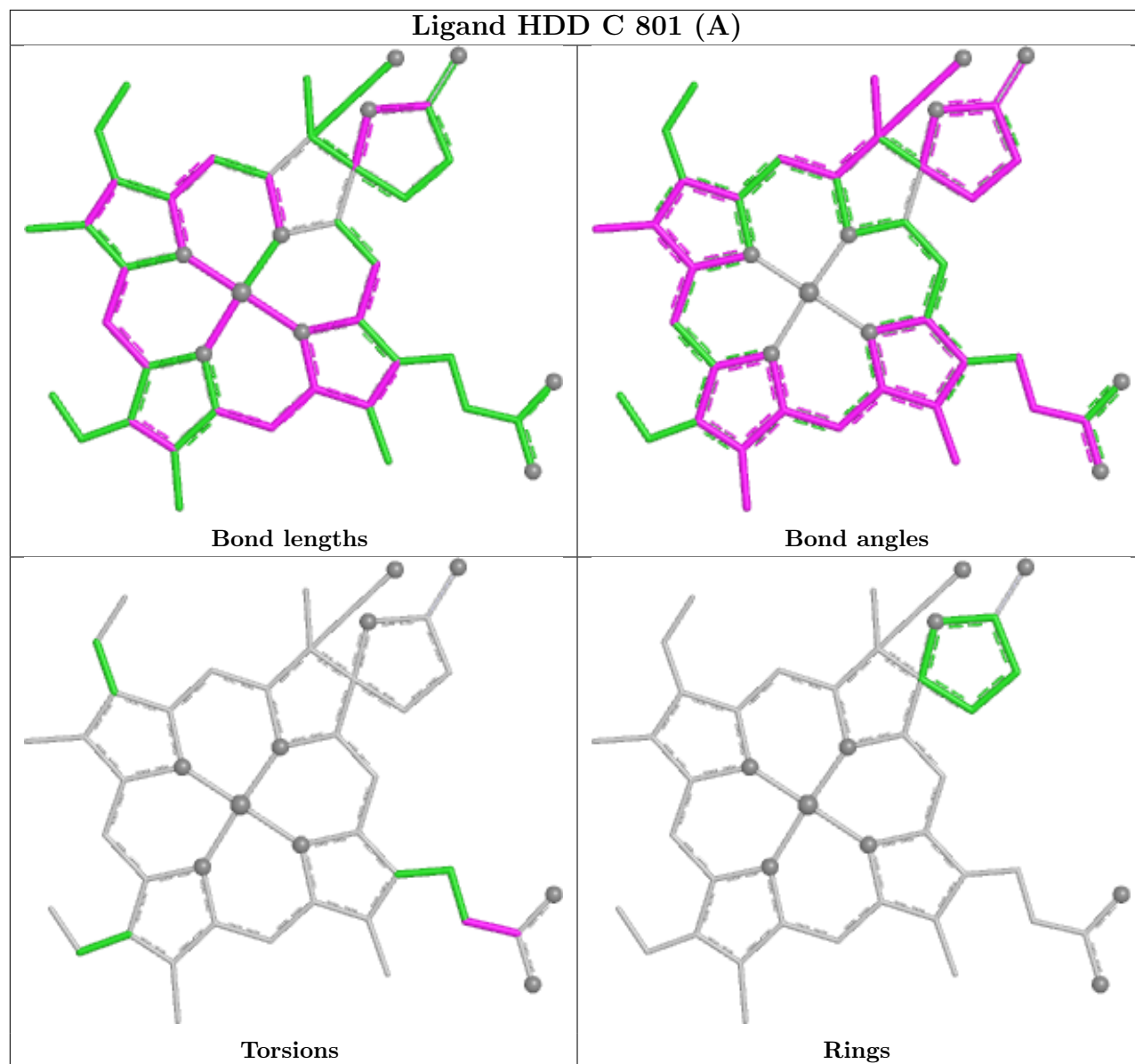


Ligand HEM A 802 (B)



Ligand HEM B 802 (B)





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	725/753 (96%)	-0.60	5 (0%) 84 86	4, 11, 29, 60	4 (0%)
1	B	725/753 (96%)	-0.46	5 (0%) 84 86	5, 13, 36, 56	1 (0%)
1	C	725/753 (96%)	-0.49	6 (0%) 82 85	5, 12, 34, 56	3 (0%)
1	D	725/753 (96%)	-0.60	3 (0%) 88 90	4, 11, 28, 58	3 (0%)
All	All	2900/3012 (96%)	-0.54	19 (0%) 84 86	4, 11, 33, 60	11 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	3.7
1	A	711	ALA	3.4
1	A	710	ILE	3.2
1	C	725	ASP	3.2
1	A	712	ASP	3.0
1	B	726	GLY	2.8
1	C	595	ASP	2.8
1	B	583	LYS	2.6
1	A	713	GLN	2.6
1	C	596	GLY	2.4
1	D	595	ASP	2.4
1	B	568	ASP	2.3
1	D	28	SER	2.2
1	C	724	ALA	2.1
1	A	725	ASP	2.1
1	D	749	ASP	2.1
1	B	611	VAL	2.0
1	B	725	ASP	2.0
1	C	750	LYS	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	OCS	B	669	9/10	0.93	0.09	25,27,36,37	0
1	OCS	C	669	9/10	0.93	0.09	25,28,36,40	0
1	OCS	D	669	9/10	0.94	0.09	18,21,28,33	0
1	OCS	A	669	9/10	0.95	0.08	15,19,27,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

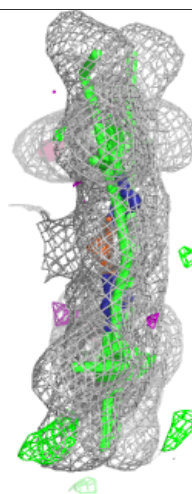
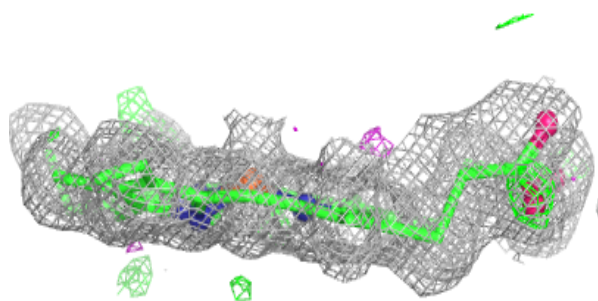
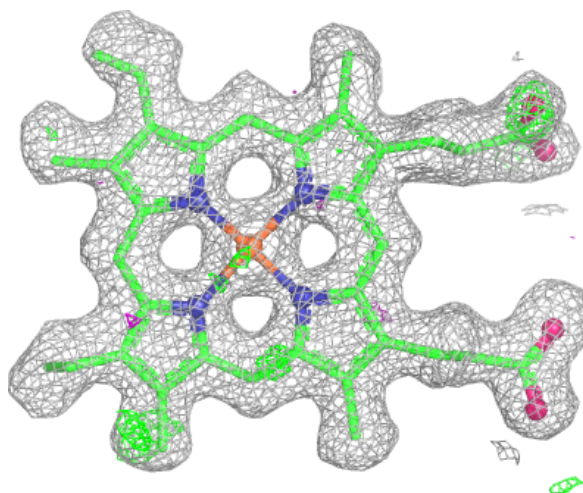
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HEM	A	802[B]	43/43	0.97	0.06	3,4,5,5	43
3	HEM	B	802[B]	43/43	0.97	0.07	4,5,6,6	43
3	HEM	C	802[B]	43/43	0.98	0.06	3,5,5,5	43
3	HEM	D	802[B]	43/43	0.98	0.06	3,4,5,5	43
2	HDD	A	801[A]	44/44	0.99	0.05	4,6,9,11	44
2	HDD	B	801[A]	44/44	0.99	0.05	5,6,10,13	44
2	HDD	C	801[A]	44/44	0.99	0.05	5,6,9,11	44
2	HDD	D	801[A]	44/44	0.99	0.05	4,5,10,12	44

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.

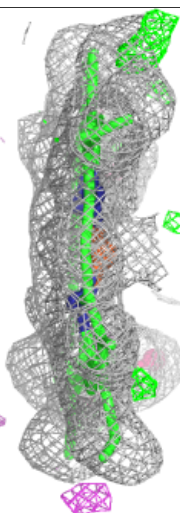
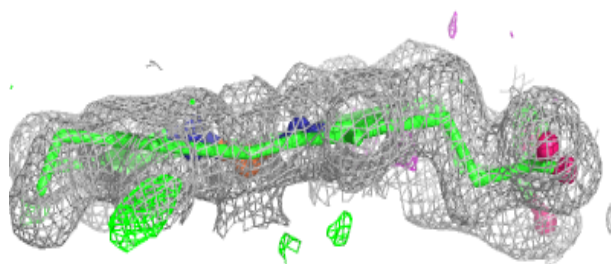
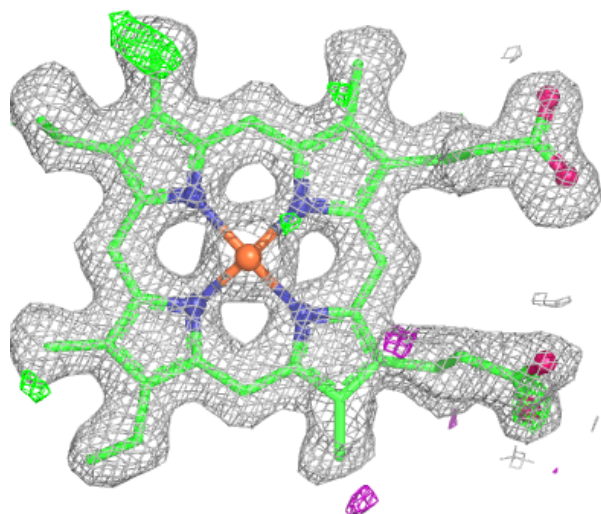
Electron density around HEM A 802 (B):

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



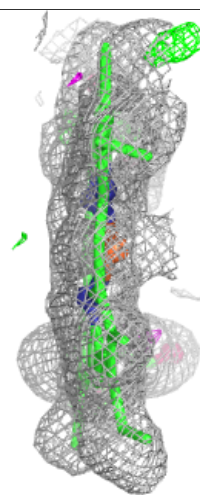
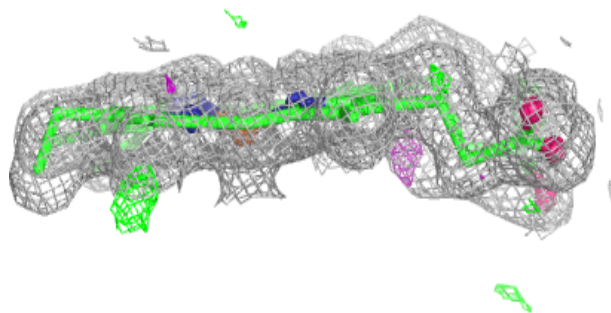
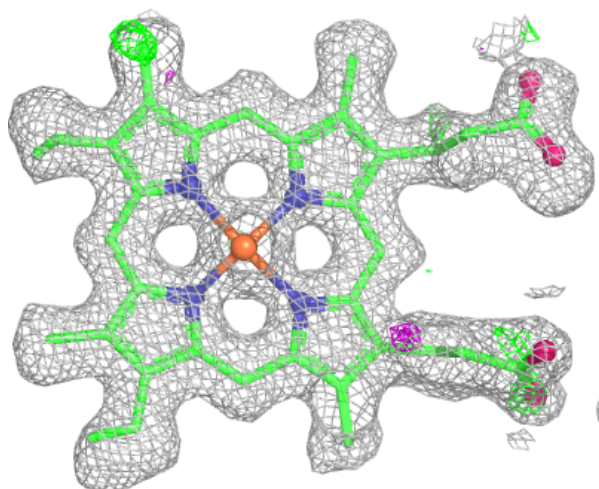
Electron density around HEM B 802 (B):

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



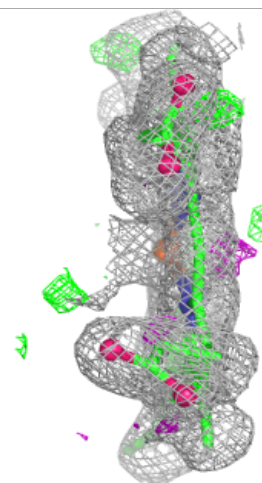
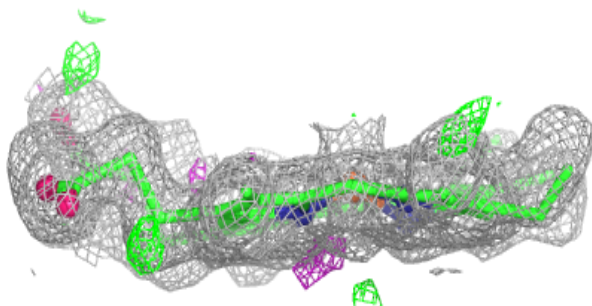
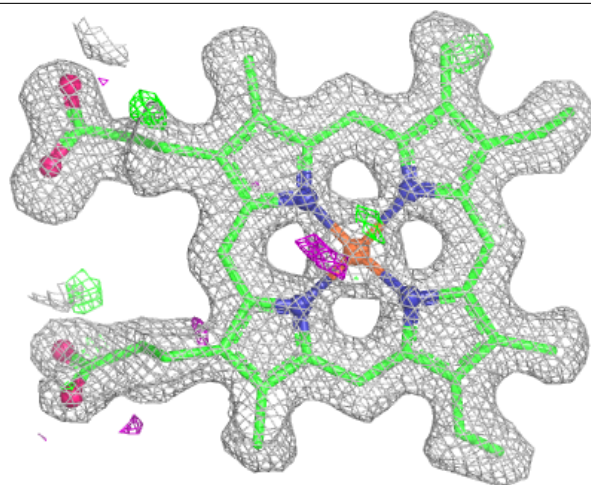
Electron density around HEM C 802 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



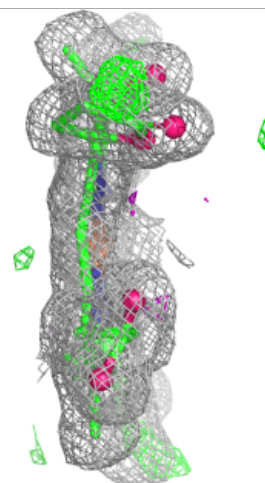
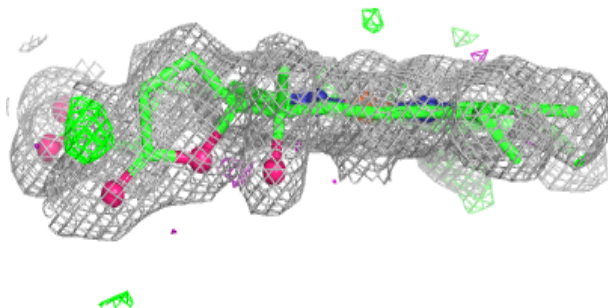
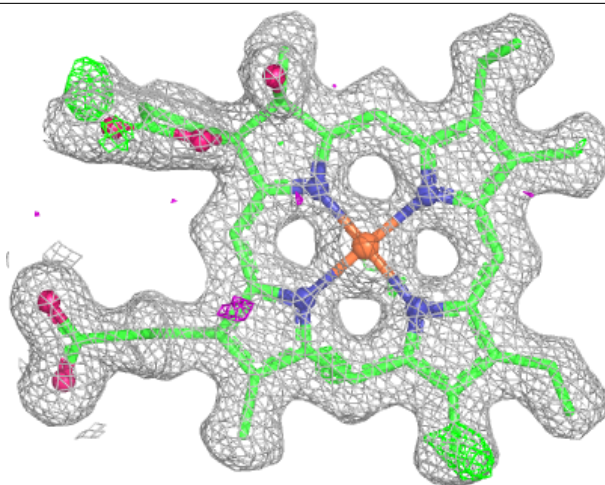
Electron density around HEM D 802 (B):

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



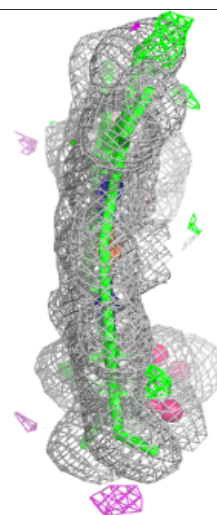
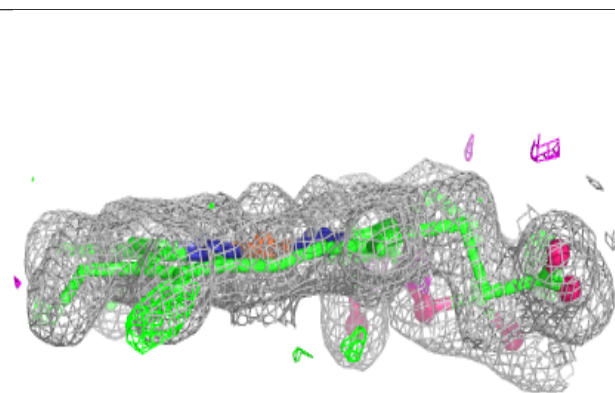
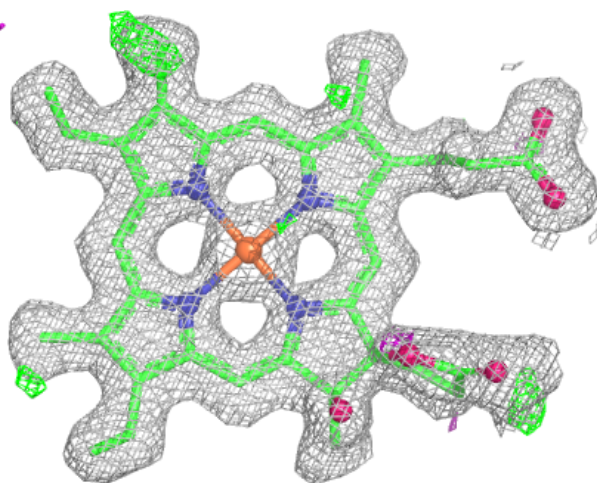
Electron density around HDD A 801 (A):

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



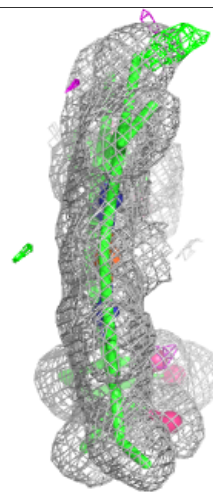
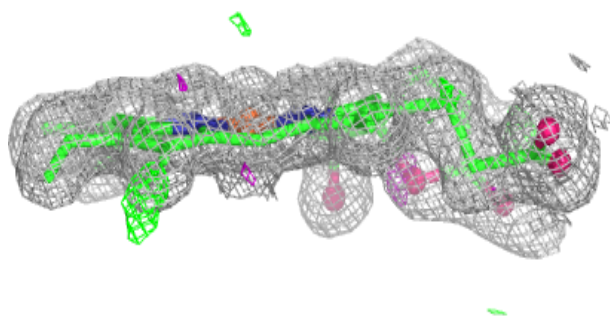
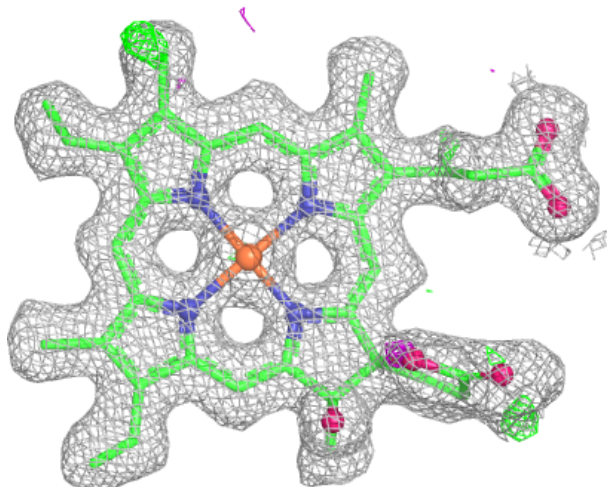
Electron density around HDD B 801 (A):

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



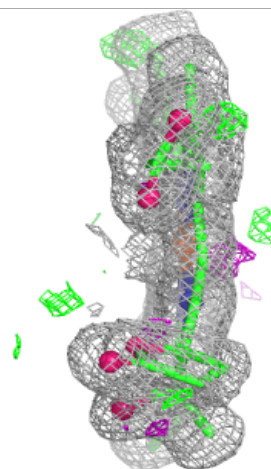
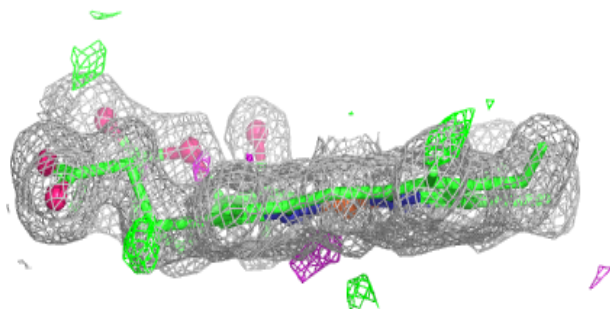
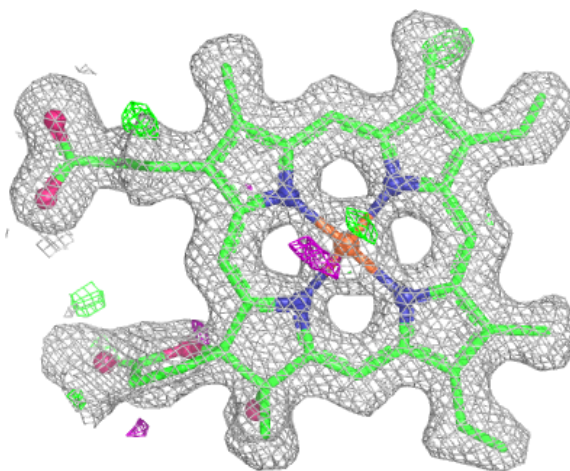
Electron density around HDD C 801 (A):

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.