



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2026 – 04:55 pm BST

PDB ID : 9RWY / pdb_00009rwy
Title : Crystal structure of bifunctional catalase-phenol oxidase from a marine-derived Cladosporium species complexed with catechol
Authors : Kosinas, C.; Ferousi, C.; Pantelakis, O.I.; Topakas, E.; Dimarogona, M.
Deposited on : 2025-07-10
Resolution : 1.95 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	:	1.8.4, CSD as541be (2020)
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

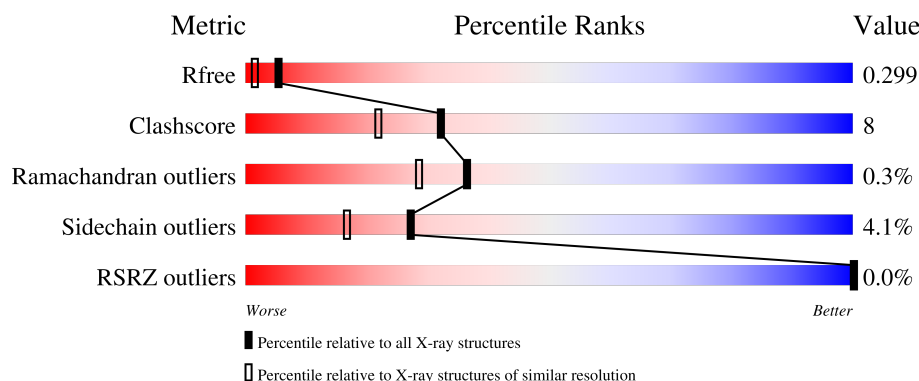
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

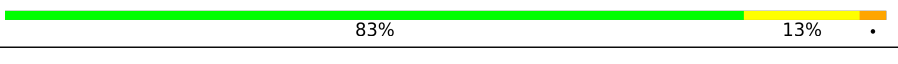
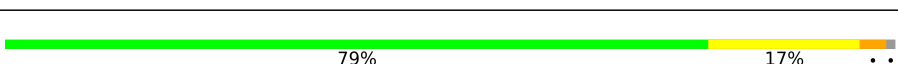
The reported resolution of this entry is 1.95 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	
1	B	509	
1	C	509	
1	D	509	
1	E	509	

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Mol	Chain	Length	Quality of chain
1	F	509	 80% 17% ..
1	G	509	 79% 17% ..
1	H	509	 80% 17% .

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
4	NAG	G	603	-	-	X	-
6	PEG	F	602	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called catalase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4088	2571	721	787	9			
1	B	507	Total	C	N	O	S	0	2	0
			4104	2581	724	790	9			
1	D	505	Total	C	N	O	S	0	1	0
			4084	2569	723	783	9			
1	C	507	Total	C	N	O	S	0	2	0
			4104	2583	726	786	9			
1	E	502	Total	C	N	O	S	0	3	0
			4084	2570	722	783	9			
1	F	504	Total	C	N	O	S	0	1	0
			4076	2566	720	781	9			
1	G	498	Total	C	N	O	S	0	1	0
			4039	2541	712	777	9			
1	H	507	Total	C	N	O	S	0	3	0
			4115	2589	730	787	9			

There are 16 discrepancies between the modelled and reference sequences:

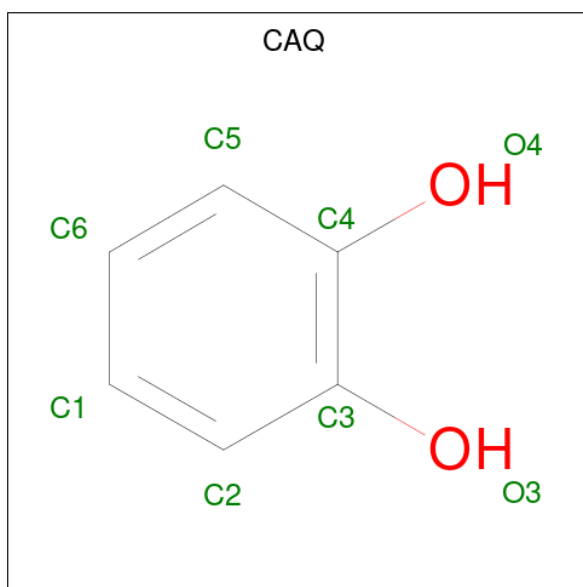
Chain	Residue	Modelled	Actual	Comment	Reference
A	508	ALA	-	expression tag	UNP A0AB34KRF0
A	509	LEU	-	expression tag	UNP A0AB34KRF0
B	508	ALA	-	expression tag	UNP A0AB34KRF0
B	509	LEU	-	expression tag	UNP A0AB34KRF0
D	508	ALA	-	expression tag	UNP A0AB34KRF0
D	509	LEU	-	expression tag	UNP A0AB34KRF0
C	508	ALA	-	expression tag	UNP A0AB34KRF0
C	509	LEU	-	expression tag	UNP A0AB34KRF0
E	508	ALA	-	expression tag	UNP A0AB34KRF0
E	509	LEU	-	expression tag	UNP A0AB34KRF0
F	508	ALA	-	expression tag	UNP A0AB34KRF0
F	509	LEU	-	expression tag	UNP A0AB34KRF0
G	508	ALA	-	expression tag	UNP A0AB34KRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	LEU	-	expression tag	UNP A0AB34KRF0
H	508	ALA	-	expression tag	UNP A0AB34KRF0
H	509	LEU	-	expression tag	UNP A0AB34KRF0

- Molecule 2 is CATECHOL (CCD ID: CAQ) (formula: $C_6H_6O_2$) (labeled as "Ligand of Interest" by depositor).



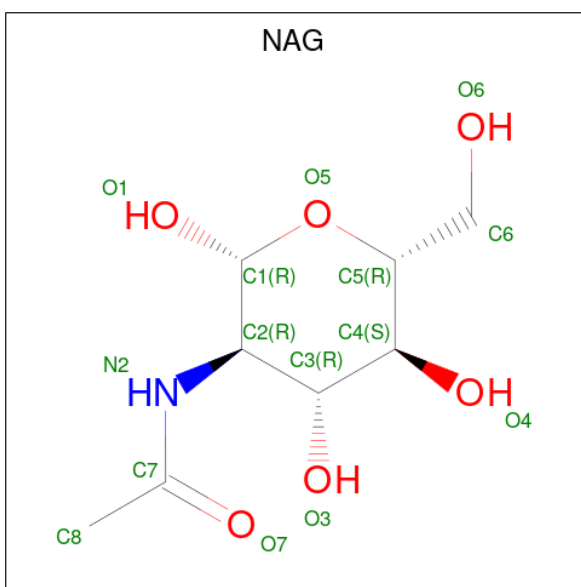
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		

- 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	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



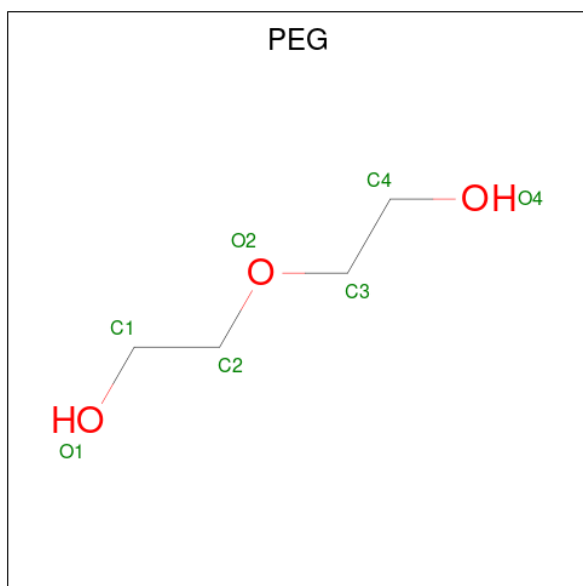
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			7	4	3		
6	F	1	Total	C	O	0	0
			7	4	3		

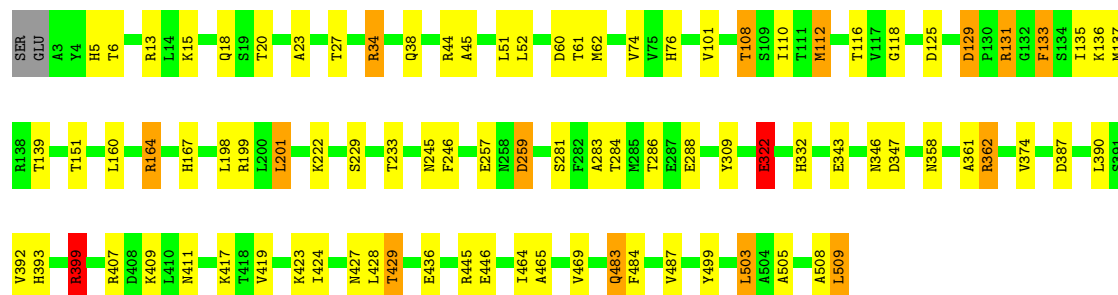
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	250	Total 252	O 252	0	2
7	B	258	Total 264	O 264	0	6
7	D	211	Total 213	O 213	0	2
7	C	225	Total 226	O 226	0	1
7	E	345	Total 348	O 348	0	3
7	F	324	Total 327	O 327	0	3
7	G	319	Total 321	O 321	0	2
7	H	305	Total 307	O 307	0	2



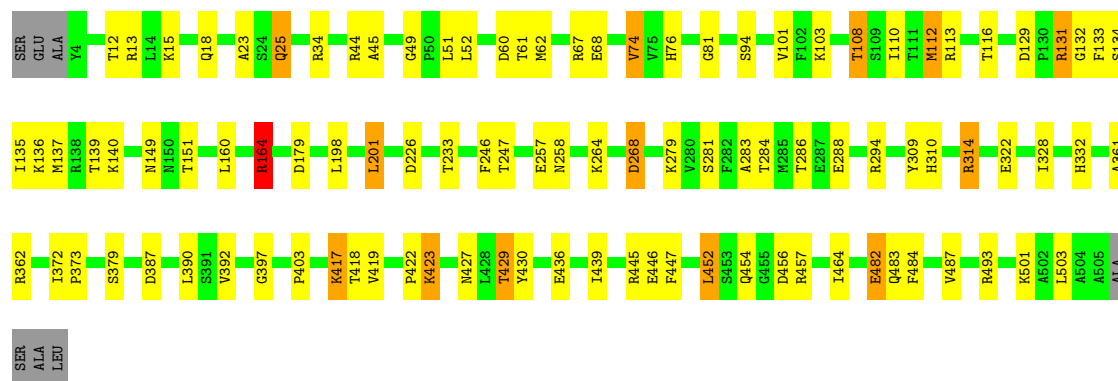
- Molecule 1: catalase

Chain C: 82% 15%



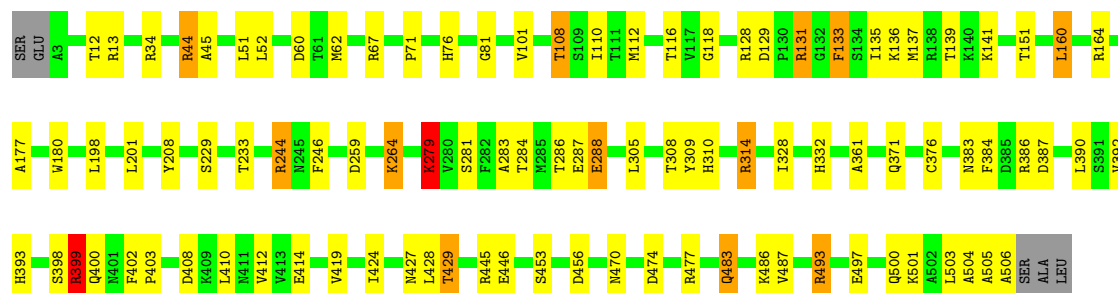
- Molecule 1: catalase

Chain E: 79% 17%



- Molecule 1: catalase

Chain F: 80% 17%



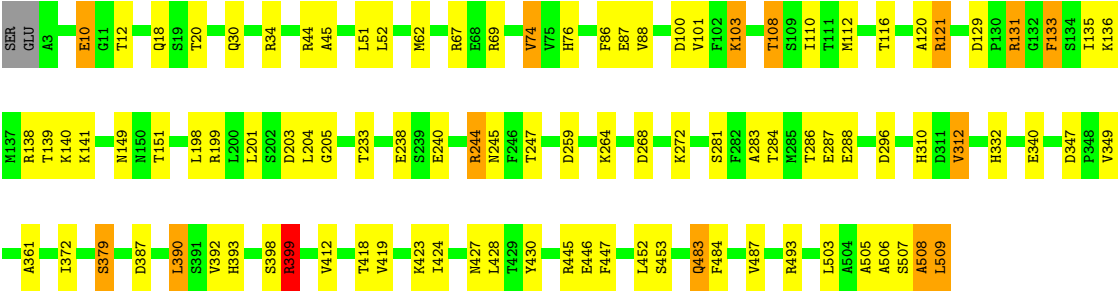
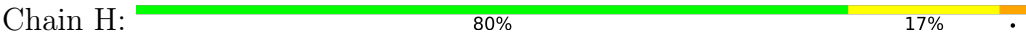
- Molecule 1: catalase

Chain G: 79% 17%





● Molecule 1: catalase



4 Data and refinement statistics

Property	Value
Space group	P 1
Cell constants a, b, c, α , β , γ	91.87Å 92.08Å 168.81Å 83.00° 77.94° 60.10°
Resolution (Å)	79.93 – 1.95 79.93 – 1.95
% Data completeness (in resolution range)	90.5 (79.93-1.95) 89.1 (79.93-1.95)
R_{merge}	0.13
R_{sym}	(Not available)
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.95Å)
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105), REFMAC 5.8.0430 (refmacat 0.4.105)
R, R_{free}	0.256 , 0.295 0.261 , 0.299
R_{free} test set	15664 reflections (4.58%)
Wilson B-factor (Å ²)	30.5
Anisotropy	0.414
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.7
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$
Estimated twinning fraction	0.034 for -h,-h+k,-l
F_o, F_c correlation	0.94
Total number of atoms	35420
Average B, all atoms (Å ²)	37.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.63% 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: NAG, PEG, HEM, CAQ, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/4197	1.16	15/5700 (0.3%)
1	B	0.70	2/4213 (0.0%)	1.18	21/5722 (0.4%)
1	C	0.67	0/4213	1.15	22/5722 (0.4%)
1	D	0.67	0/4193	1.14	17/5694 (0.3%)
1	E	0.76	1/4193 (0.0%)	1.23	23/5694 (0.4%)
1	F	0.74	0/4185	1.20	21/5683 (0.4%)
1	G	0.73	0/4148	1.21	22/5634 (0.4%)
1	H	0.72	0/4224	1.22	20/5736 (0.3%)
All	All	0.71	3/33566 (0.0%)	1.19	161/45585 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	3
1	D	0	7
1	E	0	5
1	F	0	6
1	G	0	8
1	H	0	7
All	All	0	43

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	457	ARG	NE-CZ	6.24	1.40	1.33
1	B	219	HIS	CE1-NE2	-5.45	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	ARG	NE-CZ	-5.19	1.27	1.33

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	131	ARG	CD-NE-CZ	18.01	149.61	124.40
1	G	131	ARG	NE-CZ-NH2	-14.98	105.72	119.20
1	H	131	ARG	NE-CZ-NH2	-14.85	105.83	119.20
1	F	131	ARG	NE-CZ-NH2	-14.81	105.87	119.20
1	E	131	ARG	CD-NE-CZ	14.06	144.09	124.40
1	F	131	ARG	CD-NE-CZ	12.94	142.51	124.40
1	H	131	ARG	NE-CZ-NH1	12.68	134.18	121.50
1	G	131	ARG	CD-NE-CZ	12.38	141.73	124.40
1	E	131	ARG	NE-CZ-NH2	-12.19	108.23	119.20
1	G	131	ARG	NE-CZ-NH1	10.56	132.06	121.50
1	E	164	ARG	NE-CZ-NH1	-10.46	111.04	121.50
1	E	131	ARG	NE-CZ-NH1	9.80	131.30	121.50
1	F	131	ARG	NE-CZ-NH1	9.20	130.70	121.50
1	A	306	ASN	CA-CB-CG	8.82	121.42	112.60
1	F	244	ARG	CA-CB-CG	8.23	130.56	114.10
1	A	131	ARG	NE-CZ-NH2	8.09	126.48	119.20
1	C	322	GLU	CB-CG-CD	-7.97	99.05	112.60
1	H	74	VAL	N-CA-CB	7.87	121.24	110.54
1	B	475	ASP	CA-CB-CG	7.81	120.41	112.60
1	D	131	ARG	NE-CZ-NH2	7.70	126.13	119.20
1	B	131	ARG	NE-CZ-NH2	7.67	126.10	119.20
1	E	164	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	F	308	THR	CA-CB-OG1	-7.42	98.46	109.60
1	C	131	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	B	108	THR	CA-CB-OG1	-7.24	98.74	109.60
1	C	257	GLU	CB-CG-CD	7.22	124.88	112.60
1	G	475	ASP	CA-CB-CG	7.07	119.67	112.60
1	C	362	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	E	108	THR	CA-CB-OG1	-7.00	99.10	109.60
1	B	306	ASN	CA-CB-CG	6.91	119.51	112.60
1	C	362	ARG	CB-CG-CD	6.88	127.13	111.30
1	B	479	THR	CA-CB-OG1	-6.82	99.37	109.60
1	G	108	THR	CA-CB-OG1	-6.79	99.41	109.60
1	C	34	ARG	CG-CD-NE	6.71	126.75	112.00
1	B	308	THR	CA-CB-OG1	-6.70	99.55	109.60
1	H	131	ARG	CG-CD-NE	-6.70	97.25	112.00
1	A	34	ARG	CG-CD-NE	6.66	126.66	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	PHE	N-CA-CB	-6.62	100.85	111.58
1	H	133	PHE	N-CA-CB	-6.50	101.05	111.58
1	E	257	GLU	CB-CG-CD	6.48	123.61	112.60
1	A	60	ASP	CA-CB-CG	6.40	119.00	112.60
1	E	112	MET	CG-SD-CE	6.38	114.94	100.90
1	G	76	HIS	CB-CG-ND1	6.29	132.13	122.70
1	F	399	ARG	CD-NE-CZ	6.26	133.16	124.40
1	C	362	ARG	NE-CZ-NH1	-6.25	115.25	121.50
1	A	483	GLN	N-CA-CB	-6.23	100.95	110.12
1	F	62	MET	CG-SD-CE	6.23	114.60	100.90
1	G	289	GLU	CA-CB-CG	6.22	126.55	114.10
1	G	74	VAL	N-CA-CB	6.14	118.89	110.54
1	D	483	GLN	N-CA-CB	-6.14	101.09	110.12
1	G	133	PHE	N-CA-CB	-6.08	101.73	111.58
1	A	488	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	133	PHE	N-CA-CB	-6.05	101.78	111.58
1	A	131	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	G	483	GLN	N-CA-CB	-6.00	101.30	110.12
1	E	456	ASP	CA-CB-CG	5.99	118.59	112.60
1	H	288	GLU	CB-CG-CD	5.97	122.75	112.60
1	G	286	THR	CA-CB-OG1	-5.95	100.68	109.60
1	G	76	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	D	131	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	H	74	VAL	CB-CA-C	-5.93	104.13	112.14
1	F	279	LYS	CG-CD-CE	5.91	124.90	111.30
1	G	434	GLN	CG-CD-NE2	5.84	125.16	116.40
1	H	10	GLU	CB-CG-CD	-5.83	102.70	112.60
1	F	133	PHE	N-CA-CB	-5.81	102.17	111.58
1	G	74	VAL	CB-CA-C	-5.78	104.34	112.14
1	A	74	VAL	N-CA-CB	5.74	118.35	110.54
1	D	436	GLU	CB-CG-CD	5.72	122.32	112.60
1	H	310	HIS	CB-CG-CD2	-5.72	123.77	131.20
1	C	483	GLN	N-CA-CB	-5.71	101.73	110.12
1	C	133	PHE	N-CA-CB	-5.70	102.35	111.58
1	D	482	GLU	CB-CA-C	-5.66	101.23	110.85
1	C	436	GLU	N-CA-CB	-5.66	102.12	110.49
1	B	310	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	F	259	ASP	CA-CB-CG	5.64	118.24	112.60
1	C	129	ASP	CA-CB-CG	5.63	118.23	112.60
1	F	310	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	G	330	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	B	60	ASP	CA-CB-CG	5.61	118.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	ASP	CA-CB-CG	5.60	118.20	112.60
1	F	483	GLN	N-CA-CB	-5.60	101.89	110.12
1	D	288	GLU	N-CA-CB	5.57	118.15	110.07
1	E	417	LYS	CB-CG-CD	5.56	124.09	111.30
1	E	482[A]	GLU	CB-CG-CD	-5.56	103.15	112.60
1	E	482[B]	GLU	CB-CG-CD	-5.56	103.15	112.60
1	B	131	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	D	347	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	483	GLN	N-CA-CB	-5.50	102.03	110.12
1	E	25	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	B	211	GLN	CB-CA-C	-5.49	98.51	109.99
1	E	268	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	493	ARG	CG-CD-NE	5.46	124.02	112.00
1	G	20	THR	OG1-CB-CG2	5.45	120.21	109.30
1	E	67	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	C	347	ASP	CA-CB-CG	5.44	118.04	112.60
1	E	484	PHE	CA-CB-CG	5.43	119.23	113.80
1	B	253	LYS	CB-CG-CD	5.40	123.73	111.30
1	E	286	THR	CA-CB-OG1	-5.40	101.49	109.60
1	C	436	GLU	CB-CA-C	5.40	119.11	110.09
1	D	211	GLN	CB-CA-C	-5.40	98.71	109.99
1	H	347	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	399	ARG	CD-NE-CZ	5.38	131.93	124.40
1	B	2	GLU	CB-CA-C	5.38	119.06	109.65
1	F	399	ARG	CB-CA-C	-5.38	100.13	109.64
1	B	268	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	456	ASP	CA-CB-CG	5.37	117.97	112.60
1	E	247	THR	CA-CB-OG1	-5.36	101.56	109.60
1	E	60	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	60	ASP	CA-CB-CG	5.33	117.92	112.60
1	G	211	GLN	CB-CA-C	-5.31	98.89	109.99
1	H	238	GLU	CB-CG-CD	-5.31	103.58	112.60
1	G	164	ARG	CG-CD-NE	-5.30	100.33	112.00
1	C	60	ASP	CA-CB-CG	5.29	117.89	112.60
1	G	347	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	399	ARG	CG-CD-NE	-5.28	100.38	112.00
1	D	399	ARG	CG-CD-NE	-5.27	100.41	112.00
1	A	238	GLU	CG-CD-OE2	-5.26	106.29	118.40
1	C	286	THR	CA-CB-OG1	-5.26	101.70	109.60
1	E	423	LYS	CB-CG-CD	5.26	123.41	111.30
1	D	482	GLU	N-CA-CB	5.26	117.94	110.16
1	C	484	PHE	CA-CB-CG	5.26	119.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	484	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	310	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	A	246	PHE	CA-CB-CG	5.24	119.04	113.80
1	D	399	ARG	CB-CA-C	-5.24	100.36	109.64
1	H	286	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	286	THR	CA-CB-OG1	-5.21	101.78	109.60
1	E	179	ASP	CA-CB-CG	5.20	117.80	112.60
1	H	238	GLU	CB-CA-C	-5.20	101.77	110.19
1	F	246	PHE	CA-CB-CG	5.19	118.99	113.80
1	B	129	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	112	MET	CG-SD-CE	5.19	112.32	100.90
1	A	399	ARG	CB-CA-C	-5.18	100.34	109.62
1	H	399	ARG	CB-CA-C	-5.18	100.47	109.64
1	G	20	THR	CA-CB-OG1	-5.17	101.84	109.60
1	E	246	PHE	CA-CB-CG	5.17	118.97	113.80
1	H	259	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	125	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	246	PHE	CA-CB-CG	5.11	118.91	113.80
1	F	60	ASP	CA-CB-CG	5.10	117.70	112.60
1	F	288	GLU	N-CA-CB	5.10	117.46	110.07
1	C	423	LYS	CB-CG-CD	5.09	123.01	111.30
1	H	484	PHE	CA-CB-CG	5.09	118.89	113.80
1	G	246	PHE	CA-CB-CG	5.09	118.89	113.80
1	H	20	THR	N-CA-CB	5.08	118.01	110.49
1	C	259	ASP	CA-CB-CG	5.08	117.68	112.60
1	G	311	ASP	CA-CB-CG	5.07	117.67	112.60
1	H	247	THR	CA-CB-OG1	-5.07	102.00	109.60
1	D	268	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	247	THR	OG1-CB-CG2	5.05	119.40	109.30
1	F	286	THR	CA-CB-OG1	-5.04	102.03	109.60
1	E	310	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	F	12	THR	OG1-CB-CG2	-5.04	99.21	109.30
1	F	399	ARG	CG-CD-NE	-5.04	100.90	112.00
1	H	483	GLN	N-CA-CB	-5.04	102.70	110.12
1	A	133	PHE	N-CA-CB	-5.04	101.64	111.11
1	B	112	MET	CG-SD-CE	5.04	111.98	100.90
1	A	240	GLU	CB-CG-CD	-5.03	104.04	112.60
1	F	44	ARG	CB-CA-C	-5.03	98.39	109.56
1	B	13	ARG	CB-CG-CD	5.03	122.87	111.30
1	D	482	GLU	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	67	ARG	Sidechain
1	A	69	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	493	ARG	Sidechain
1	B	69	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	164	ARG	Sidechain
1	C	399	ARG	Sidechain
1	D	121	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	362[A]	ARG	Sidechain
1	D	399	ARG	Sidechain
1	D	4	TYR	Peptide
1	D	425	GLU	Peptide
1	D	69	ARG	Sidechain
1	E	131	ARG	Sidechain
1	E	164	ARG	Sidechain
1	E	294	ARG	Sidechain
1	E	314	ARG	Sidechain
1	E	362	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	314	ARG	Sidechain
1	F	34	ARG	Sidechain
1	F	399	ARG	Sidechain
1	F	493	ARG	Sidechain
1	F	67	ARG	Sidechain
1	G	121	ARG	Sidechain
1	G	131	ARG	Sidechain
1	G	138	ARG	Sidechain
1	G	244	ARG	Sidechain
1	G	314	ARG	Sidechain
1	G	34	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	493	ARG	Sidechain
1	H	131	ARG	Sidechain
1	H	138	ARG	Sidechain
1	H	141	LYS	Mainchain
1	H	244	ARG	Sidechain
1	H	399	ARG	Sidechain
1	H	67	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	69	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4088	0	3859	71	0
1	B	4104	0	3874	68	0
1	C	4104	0	3881	77	0
1	D	4084	0	3857	62	0
1	E	4084	0	3855	83	0
1	F	4076	0	3852	84	0
1	G	4039	0	3801	74	0
1	H	4115	0	3893	65	0
2	A	8	0	5	2	0
3	A	43	0	30	6	0
3	B	43	0	30	4	0
3	C	43	0	30	2	0
3	D	43	0	30	1	0
3	E	43	0	30	7	0
3	F	43	0	30	3	0
3	G	43	0	30	6	0
3	H	43	0	30	3	0
4	A	14	0	13	5	0
4	B	14	0	13	6	0
4	C	14	0	13	2	0
4	D	14	0	13	3	0
4	G	28	0	26	9	0
4	H	14	0	13	3	0
5	A	4	0	6	1	0
6	E	7	0	10	0	0
6	F	7	0	10	17	0
7	A	252	0	0	11	0
7	B	264	0	0	13	0
7	C	226	0	0	12	1
7	D	213	0	0	11	1
7	E	348	0	0	15	0
7	F	327	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	321	0	0	24	0
7	H	307	0	0	16	0
All	All	35420	0	31234	517	1

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 8.

All (517) 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:H:245:ASN:HD22	4:H:602:NAG:C1	1.02	1.65
1:G:245:ASN:HD22	4:G:602:NAG:C1	1.12	1.61
1:B:245:ASN:HD22	4:B:602:NAG:C1	1.08	1.60
1:A:245:ASN:HD22	4:A:603:NAG:C1	1.01	1.59
1:C:245:ASN:HD22	4:C:602:NAG:C1	0.99	1.58
1:D:245:ASN:HD22	4:D:602:NAG:C1	1.32	1.42
1:C:245:ASN:ND2	4:C:602:NAG:C1	1.78	1.41
1:H:245:ASN:ND2	4:H:602:NAG:C1	1.79	1.40
1:G:245:ASN:ND2	4:G:602:NAG:C1	1.81	1.37
1:A:245:ASN:ND2	4:A:603:NAG:C1	1.86	1.34
1:B:245:ASN:ND2	4:B:602:NAG:C1	1.94	1.28
1:C:20:THR:HG22	1:C:322:GLU:OE2	1.50	1.12
1:D:245:ASN:ND2	4:D:602:NAG:C1	2.18	1.05
1:F:410:LEU:HB2	6:F:602:PEG:O4	1.57	1.04
4:G:603:NAG:H81	7:G:884:HOH:O	1.63	0.97
1:B:506:ALA:O	1:B:507:SER:C	2.03	0.95
1:A:275:TYR:O	5:A:604:EDO:H12	1.68	0.93
1:H:268:ASP:HB3	7:H:951:HOH:O	1.70	0.92
3:G:601:HEM:HMB1	3:G:601:HEM:HBB2	1.54	0.89
1:F:410:LEU:HB2	6:F:602:PEG:HO4	1.34	0.88
1:A:107:LYS:HB3	7:A:797:HOH:O	1.72	0.88
1:B:436:GLU:OE2	1:B:439:ILE:HG21	1.72	0.88
2:A:601:CAQ:H6	1:C:259:ASP:OD2	1.75	0.86
1:G:288:GLU:HG3	7:G:862:HOH:O	1.74	0.85
1:A:112:MET:HE2	1:A:135:ILE:HD12	1.56	0.85
1:E:493[A]:ARG:HE	1:E:493[A]:ARG:HA	1.41	0.85
1:E:13:ARG:CZ	1:F:13:ARG:HD2	2.07	0.85
3:A:602:HEM:HMB2	3:A:602:HEM:HBB2	1.59	0.84
1:G:427:ASN:OD1	4:G:603:NAG:C1	2.27	0.83
1:B:287:GLU:OE1	7:B:702:HOH:O	1.97	0.81
1:G:31:GLN:HG2	7:H:841:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:ARG:HH22	6:F:602:PEG:C1	1.93	0.80
1:D:112:MET:HE3	1:D:135:ILE:CD1	2.11	0.80
1:A:112:MET:HE2	1:A:135:ILE:CD1	2.12	0.79
1:G:416:PRO:HG3	7:G:955:HOH:O	1.81	0.78
7:D:707:HOH:O	1:C:390:LEU:HD11	1.85	0.77
1:G:108:THR:HG22	7:G:991:HOH:O	1.84	0.77
1:F:180:TRP:HD1	7:F:900:HOH:O	1.67	0.77
1:E:493[A]:ARG:HA	1:E:493[A]:ARG:NE	1.96	0.75
1:C:20:THR:CG2	1:C:322:GLU:OE2	2.32	0.74
1:E:288:GLU:HG3	7:E:917:HOH:O	1.86	0.74
3:A:602:HEM:HBC2	3:A:602:HEM:CMC	2.18	0.74
3:A:602:HEM:HBC2	3:A:602:HEM:HMC2	1.70	0.73
1:D:112:MET:HE3	1:D:135:ILE:HD12	1.68	0.73
1:D:31:GLN:OE1	1:D:60:ASP:HB3	1.88	0.73
1:F:112:MET:HE3	1:F:135:ILE:CD1	2.18	0.72
1:H:296:ASP:OD2	7:H:701[A]:HOH:O	2.07	0.72
1:F:400:GLN:HB2	6:F:602:PEG:H31	1.70	0.72
1:E:482[B]:GLU:HG2	7:E:887:HOH:O	1.89	0.72
1:H:112:MET:HE3	1:H:135:ILE:CD1	2.19	0.71
1:A:430:TYR:HB3	1:C:38:GLN:OE1	1.91	0.71
1:B:157:ARG:NH1	7:B:705:HOH:O	2.23	0.71
1:B:112:MET:HE3	1:B:135:ILE:CD1	2.21	0.70
3:B:601:HEM:HMB1	3:B:601:HEM:HBB2	1.74	0.70
1:F:410:LEU:CB	6:F:602:PEG:O4	2.38	0.70
1:E:258:ASN:HB2	7:E:945:HOH:O	1.90	0.70
3:C:601:HEM:HBB2	3:C:601:HEM:HMB2	1.74	0.70
1:A:112:MET:CE	1:A:135:ILE:HD12	2.22	0.69
1:A:504:ALA:O	1:A:507:SER:N	2.25	0.69
1:H:30:GLN:HB3	7:H:883:HOH:O	1.92	0.69
7:E:873:HOH:O	1:F:412:VAL:HA	1.92	0.68
1:E:149:ASN:ND2	3:E:601:HEM:HAC	2.07	0.68
1:E:13:ARG:NE	1:F:13:ARG:CD	2.57	0.68
1:F:112:MET:HE3	1:F:135:ILE:HD12	1.75	0.67
1:F:371:GLN:O	1:F:393:HIS:HE1	1.78	0.67
1:G:112:MET:HE3	1:G:135:ILE:CD1	2.25	0.67
1:B:101:VAL:HG23	1:B:108:THR:HG21	1.77	0.66
3:G:601:HEM:NC	7:G:703:HOH:O	2.23	0.66
1:F:470:ASN:HB3	7:F:900:HOH:O	1.94	0.66
1:B:399:ARG:HD2	7:B:775:HOH:O	1.96	0.66
1:E:101:VAL:HG23	1:E:108:THR:HG21	1.78	0.66
1:D:469:VAL:HG22	1:D:503:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:MET:HE3	1:C:135:ILE:CD1	2.25	0.66
1:F:112:MET:CE	1:F:133:PHE:CE1	2.78	0.65
1:E:112:MET:CE	1:E:133:PHE:CE1	2.80	0.65
1:F:386:ARG:HH22	6:F:602:PEG:H11	1.60	0.65
1:G:427:ASN:CG	4:G:603:NAG:C1	2.70	0.65
1:B:112:MET:HE3	1:B:135:ILE:HD12	1.77	0.64
1:A:482:GLU:CD	7:A:701:HOH:O	2.40	0.64
1:E:12:THR:HG22	1:F:393:HIS:CE1	2.32	0.64
1:H:112:MET:HE3	1:H:135:ILE:HD12	1.79	0.64
1:H:112:MET:CE	1:H:133:PHE:CE1	2.79	0.64
1:C:409:LYS:HE2	7:C:866:HOH:O	1.96	0.64
1:B:112:MET:CE	1:B:133:PHE:CE1	2.80	0.64
7:B:726:HOH:O	1:D:170:LYS:HD3	1.98	0.64
1:E:149:ASN:CG	3:E:601:HEM:HAC	2.23	0.64
1:D:112:MET:CE	1:D:133:PHE:CE1	2.81	0.64
1:E:226:ASP:HA	1:E:418:THR:CG2	2.27	0.64
1:F:160:LEU:HD23	1:H:62:MET:HE2	1.80	0.64
1:G:112:MET:CE	1:G:133:PHE:CE1	2.80	0.63
1:F:386:ARG:HH22	6:F:602:PEG:H12	1.60	0.63
1:C:445:ARG:HD3	1:C:487:VAL:O	1.98	0.63
1:C:469:VAL:HG22	1:C:503:LEU:HD13	1.80	0.63
1:G:101:VAL:HG23	1:G:108:THR:HG21	1.80	0.63
1:B:430:TYR:HB3	1:D:38:GLN:OE1	1.97	0.63
1:C:112:MET:CE	1:C:133:PHE:CE1	2.82	0.63
1:E:226:ASP:HA	1:E:418:THR:HG22	1.80	0.63
1:A:219:HIS:CE1	1:A:353:ARG:HH11	2.17	0.63
1:D:399:ARG:NH2	1:C:18:GLN:O	2.32	0.63
1:C:112:MET:HE3	1:C:135:ILE:HD12	1.80	0.63
1:F:383:ASN:O	6:F:602:PEG:H12	1.99	0.63
1:G:112:MET:HE3	1:G:135:ILE:HD12	1.81	0.63
1:H:445:ARG:HD3	1:H:487:VAL:O	1.99	0.62
1:D:445:ARG:HD3	1:D:487:VAL:O	1.98	0.62
1:E:390:LEU:HB2	1:F:390:LEU:HD12	1.81	0.62
1:A:466:GLY:C	7:A:755:HOH:O	2.42	0.62
1:B:219:HIS:HD2	1:B:347:ASP:OD2	1.82	0.62
1:B:219:HIS:CE1	1:B:353:ARG:HH11	2.18	0.62
1:C:164:ARG:HH12	1:C:167:HIS:CE1	2.17	0.62
1:A:445:ARG:HD3	1:A:487:VAL:O	2.00	0.61
1:B:445:ARG:HD3	1:B:487:VAL:O	1.99	0.61
1:G:445:ARG:HD3	1:G:487:VAL:O	1.99	0.61
1:F:445:ARG:HD3	1:F:487:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:GLN:NE2	7:G:712:HOH:O	2.32	0.61
1:E:112:MET:HE3	1:E:135:ILE:CD1	2.30	0.61
1:F:101:VAL:HG23	1:F:108:THR:HG21	1.81	0.61
1:F:493:ARG:HG2	1:F:497:GLU:OE1	2.01	0.61
1:F:208:TYR:CD2	1:F:244:ARG:HD3	2.36	0.61
1:C:101:VAL:HG23	1:C:108:THR:HG21	1.83	0.61
1:A:493:ARG:NE	1:A:497:GLU:OE1	2.31	0.60
1:D:392:VAL:HG21	1:C:392:VAL:HG21	1.84	0.60
1:E:445:ARG:HD3	1:E:487:VAL:O	2.01	0.60
1:G:393:HIS:CE1	1:H:12:THR:HB	2.37	0.60
1:C:417:LYS:HE2	7:C:723:HOH:O	2.01	0.60
1:D:18:GLN:O	1:C:399:ARG:NH2	2.35	0.59
1:C:417:LYS:CE	7:C:723:HOH:O	2.49	0.59
1:H:101:VAL:HG23	1:H:108:THR:HG21	1.84	0.59
1:G:399:ARG:NH2	1:H:18:GLN:O	2.35	0.59
1:A:18:GLN:O	1:B:399:ARG:NH2	2.35	0.59
1:E:18:GLN:O	1:F:399:ARG:NH2	2.36	0.59
1:A:8:LEU:HD22	1:B:374:VAL:HA	1.85	0.59
1:E:112:MET:HE3	1:E:135:ILE:HD12	1.85	0.59
1:D:112:MET:HE3	1:D:135:ILE:HD11	1.85	0.58
3:A:602:HEM:HBB2	3:A:602:HEM:CMB	2.32	0.58
1:A:219:HIS:HD2	1:A:347:ASP:OD2	1.86	0.58
1:B:384:PHE:HB2	1:C:164:ARG:NE	2.18	0.58
1:C:62:MET:HE3	1:C:62:MET:HA	1.86	0.58
3:A:602:HEM:HMC2	3:A:602:HEM:CBC	2.34	0.58
1:F:118:GLY:HA3	7:F:877:HOH:O	2.04	0.58
1:A:240:GLU:OE2	1:A:279:LYS:HE2	2.05	0.57
1:F:128:ARG:HG2	7:F:845:HOH:O	2.05	0.57
1:F:412:VAL:CG2	7:F:892:HOH:O	2.53	0.57
1:C:509:LEU:HD13	1:C:509:LEU:O	2.05	0.57
1:F:180:TRP:CD1	7:F:900:HOH:O	2.48	0.57
1:G:427:ASN:O	1:G:429:THR:HG22	2.05	0.57
1:A:240:GLU:OE2	1:A:279:LYS:CE	2.53	0.57
1:D:101:VAL:HG23	1:D:108:THR:HG21	1.85	0.56
1:F:112:MET:CE	1:F:133:PHE:HE1	2.17	0.56
1:F:384:PHE:CE1	6:F:602:PEG:H21	2.39	0.56
1:H:112:MET:CE	1:H:133:PHE:HE1	2.17	0.56
1:D:112:MET:CE	1:D:133:PHE:HE1	2.19	0.56
1:F:208:TYR:CD2	1:F:244:ARG:CD	2.89	0.56
1:B:112:MET:CE	1:B:133:PHE:HE1	2.18	0.56
1:G:149:ASN:ND2	3:G:601:HEM:HAC	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ARG:CZ	1:F:13:ARG:CD	2.82	0.56
1:D:364:ARG:NE	3:D:601:HEM:O1A	2.39	0.55
1:G:390:LEU:HD23	1:H:372:ILE:HD11	1.87	0.55
1:B:364:ARG:NE	3:B:601:HEM:O1A	2.38	0.55
1:E:15:LYS:HE3	1:F:376:CYS:SG	2.45	0.55
1:H:86:PHE:CZ	1:H:88:VAL:HG22	2.41	0.55
1:A:66:ASN:HA	1:C:74[B]:VAL:HG21	1.88	0.55
1:B:435:ILE:HG21	1:E:454:GLN:HG2	1.88	0.55
1:F:399:ARG:HD2	6:F:602:PEG:O1	2.07	0.55
1:A:505:ALA:C	1:A:507:SER:N	2.65	0.54
1:C:15:LYS:NZ	7:C:721:HOH:O	2.40	0.54
1:E:112:MET:CE	1:E:133:PHE:HE1	2.20	0.54
1:F:264[B]:LYS:HE2	7:F:736:HOH:O	2.07	0.54
1:H:112:MET:HE3	1:H:135:ILE:HD11	1.90	0.54
1:G:112:MET:CE	1:G:133:PHE:HE1	2.20	0.54
1:B:219:HIS:HE1	1:B:353:ARG:HH11	1.56	0.54
1:E:13:ARG:NE	1:F:13:ARG:HD2	2.22	0.54
1:G:415:LYS:NZ	1:G:421:GLU:OE2	2.40	0.54
1:A:160:LEU:HD11	1:C:61:THR:HG21	1.89	0.54
1:A:203:ASP:HB2	7:A:766:HOH:O	2.07	0.54
1:E:392:VAL:HG21	1:F:392:VAL:HG21	1.90	0.54
1:C:427:ASN:O	1:C:429:THR:HG22	2.07	0.54
1:G:236:LYS:NZ	1:G:238:GLU:OE2	2.33	0.53
1:A:160:LEU:HD11	1:C:61:THR:CG2	2.38	0.53
1:A:392:VAL:HG21	1:B:392:VAL:HG21	1.91	0.53
1:A:219:HIS:HE1	1:A:353:ARG:HH11	1.54	0.53
1:E:76:HIS:CE1	3:E:601:HEM:C2D	2.97	0.53
1:B:60:ASP:O	1:B:64:THR:OG1	2.21	0.53
1:E:74[A]:VAL:HG13	7:G:865:HOH:O	2.07	0.53
3:C:601:HEM:HBB2	3:C:601:HEM:CMB	2.37	0.53
1:G:76:HIS:HE1	7:G:913:HOH:O	1.90	0.53
1:A:427:ASN:O	1:A:429:THR:HG22	2.09	0.53
1:D:473:ASN:ND2	7:D:705:HOH:O	2.30	0.53
1:A:189:GLN:HG2	7:D:775:HOH:O	2.08	0.52
1:A:245:ASN:ND2	4:A:603:NAG:C2	2.67	0.52
1:C:417:LYS:NZ	7:C:723:HOH:O	2.41	0.52
1:F:414:GLU:CD	7:F:724:HOH:O	2.51	0.52
1:F:279:LYS:HB3	7:F:903:HOH:O	2.08	0.52
1:E:427:ASN:O	1:E:429:THR:HG22	2.09	0.52
1:A:504:ALA:O	1:A:507:SER:CA	2.58	0.52
1:D:413:VAL:HB	7:D:744:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:ASP:OD2	1:H:140:LYS:HE3	2.10	0.52
1:E:13:ARG:NE	1:F:13:ARG:HD3	2.23	0.52
1:B:306:ASN:ND2	7:B:707:HOH:O	2.38	0.52
1:B:15:LYS:HA	7:B:779[A]:HOH:O	2.08	0.51
1:D:410:LEU:HB2	1:C:23:ALA:HB1	1.92	0.51
1:F:386:ARG:NH2	6:F:602:PEG:H11	2.25	0.51
1:E:430:TYR:CE2	1:H:419:VAL:HG13	2.45	0.51
1:A:160:LEU:HD11	1:C:61:THR:HB	1.92	0.51
1:G:378:PHE:CD2	1:H:10:GLU:OE2	2.63	0.51
1:D:390:LEU:HB2	1:C:390:LEU:HD13	1.92	0.51
1:C:164:ARG:HA	1:C:164:ARG:HH11	1.75	0.51
1:C:44:ARG:HG2	1:C:51:LEU:HD23	1.92	0.51
1:G:13:ARG:NH1	7:G:716:HOH:O	2.33	0.51
1:A:332:HIS:CD2	1:A:361:ALA:HB2	2.45	0.50
1:E:23:ALA:HB1	6:F:602:PEG:O4	2.11	0.50
1:F:44:ARG:HG2	1:F:51:LEU:HD23	1.92	0.50
1:G:332:HIS:CD2	1:G:361:ALA:HB2	2.46	0.50
1:G:457:ARG:HD2	7:G:846:HOH:O	2.12	0.50
1:C:332:HIS:CD2	1:C:361:ALA:HB2	2.46	0.50
3:F:601:HEM:HBC2	3:F:601:HEM:HMC2	1.94	0.50
1:C:112:MET:CE	1:C:133:PHE:HE1	2.24	0.50
1:G:18:GLN:O	1:H:399:ARG:NH2	2.44	0.50
1:H:332:HIS:CD2	1:H:361:ALA:HB2	2.47	0.50
1:D:332:HIS:CD2	1:D:361:ALA:HB2	2.47	0.50
1:E:264:LYS:HE2	1:E:268:ASP:OD2	2.12	0.50
1:E:427:ASN:O	1:E:429:THR:CG2	2.60	0.50
1:H:149:ASN:CG	3:H:601:HEM:HAC	2.37	0.50
1:D:62:MET:HE3	1:D:62:MET:HA	1.92	0.50
1:E:25:GLN:HG2	7:E:713:HOH:O	2.11	0.50
1:F:279:LYS:CD	7:F:903:HOH:O	2.60	0.50
1:F:400:GLN:O	6:F:602:PEG:C3	2.60	0.50
1:A:169:GLN:C	7:A:740:HOH:O	2.54	0.49
1:F:177:ALA:HB3	1:H:264:LYS:HE2	1.93	0.49
1:A:13:ARG:HD2	1:B:13:ARG:CZ	2.41	0.49
1:B:383:ASN:HB2	7:B:713:HOH:O	2.11	0.49
1:E:332:HIS:CD2	1:E:361:ALA:HB2	2.46	0.49
1:F:110:ILE:HA	1:F:136:LYS:O	2.12	0.49
1:H:507:SER:C	1:H:509:LEU:H	2.21	0.49
1:F:279:LYS:HD3	7:F:903:HOH:O	2.11	0.49
1:H:199[B]:ARG:NH2	7:H:717:HOH:O	2.38	0.49
2:A:601:CAQ:C6	1:C:259:ASP:OD2	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:THR:HB	1:C:393:HIS:CE1	2.47	0.49
1:F:332:HIS:CD2	1:F:361:ALA:HB2	2.48	0.49
1:F:408:ASP:O	6:F:602:PEG:H41	2.12	0.49
1:H:349:VAL:HG13	3:H:601:HEM:HBB1	1.95	0.49
1:E:430:TYR:CE2	1:H:419:VAL:CG1	2.96	0.49
1:C:427:ASN:O	1:C:429:THR:CG2	2.61	0.49
1:E:423:LYS:NZ	7:E:705:HOH:O	2.31	0.49
1:F:112:MET:HE3	1:F:135:ILE:HD11	1.92	0.49
1:G:423:LYS:HG3	1:G:424:ILE:N	2.28	0.49
1:G:427:ASN:CG	4:G:603:NAG:O5	2.56	0.49
1:B:110:ILE:HA	1:B:136:LYS:O	2.13	0.48
1:D:110:ILE:HA	1:D:136:LYS:O	2.13	0.48
1:F:445:ARG:HD2	7:F:915:HOH:O	2.13	0.48
1:G:112:MET:HE3	1:G:135:ILE:HD11	1.95	0.48
1:G:378:PHE:CE2	1:H:10:GLU:OE2	2.66	0.48
1:F:279:LYS:HE2	1:F:314:ARG:HG2	1.95	0.48
1:A:44:ARG:HG2	1:A:51:LEU:HD23	1.95	0.48
1:B:332:HIS:CD2	1:B:361:ALA:HB2	2.48	0.48
1:G:16:GLU:OE2	7:G:701:HOH:O	2.20	0.48
1:C:110:ILE:HA	1:C:136:LYS:O	2.12	0.48
1:A:427:ASN:O	1:A:429:THR:CG2	2.61	0.48
1:G:427:ASN:O	1:G:429:THR:CG2	2.61	0.48
1:B:112:MET:HE3	1:B:135:ILE:HD11	1.95	0.48
1:C:118:GLY:HA3	7:C:845:HOH:O	2.14	0.48
1:E:397:GLY:HA2	7:E:871:HOH:O	2.13	0.48
1:H:244:ARG:HD2	7:H:881:HOH:O	2.13	0.48
1:E:134:SER:OG	3:E:601:HEM:HBD2	2.14	0.48
1:A:112:MET:HE2	1:A:135:ILE:HD11	1.95	0.48
1:E:62:MET:HE3	1:E:62:MET:HA	1.96	0.48
3:G:601:HEM:HBB2	3:G:601:HEM:CMB	2.34	0.48
1:H:264:LYS:NZ	7:H:708:HOH:O	2.32	0.48
1:D:121:ARG:HD3	7:D:828:HOH:O	2.12	0.48
1:E:110:ILE:HA	1:E:136:LYS:O	2.13	0.48
1:F:427:ASN:O	1:F:429:THR:CG2	2.62	0.48
1:F:428:LEU:HD13	1:G:422:PRO:HD2	1.95	0.48
7:D:870:HOH:O	1:C:343:GLU:HG2	2.13	0.47
1:H:203:ASP:HA	7:H:753:HOH:O	2.14	0.47
1:F:419:VAL:CG1	1:G:430:TYR:CE2	2.98	0.47
1:A:234:ARG:HD3	7:A:898:HOH:O	2.13	0.47
1:B:435:ILE:CG2	1:E:454:GLN:HG2	2.44	0.47
1:D:501:LYS:NZ	7:D:719:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:HG13	1:D:430:TYR:CZ	2.50	0.47
1:D:13:ARG:NE	1:C:13:ARG:HD3	2.29	0.47
1:C:112:MET:HE3	1:C:135:ILE:HD11	1.96	0.47
1:G:242:GLY:HA3	7:G:904:HOH:O	2.14	0.47
1:H:88:VAL:HG13	1:H:312:VAL:HG13	1.97	0.47
1:A:6:THR:HG21	1:B:109:SER:OG	2.15	0.47
1:A:110:ILE:HA	1:A:136:LYS:O	2.14	0.47
1:E:12:THR:CG2	1:F:393:HIS:CE1	2.97	0.47
1:H:45:ALA:HB2	1:H:52:LEU:HD21	1.97	0.47
1:E:68:GLU:OE2	1:G:167:HIS:NE2	2.44	0.47
1:H:110:ILE:HA	1:H:136:LYS:O	2.14	0.47
1:A:482:GLU:OE2	7:A:701:HOH:O	2.19	0.47
1:B:62:MET:HE3	1:B:62:MET:HA	1.96	0.47
1:B:245:ASN:ND2	4:B:602:NAG:O5	2.43	0.47
1:G:110:ILE:HA	1:G:136:LYS:O	2.15	0.47
1:G:169:GLN:HB3	7:G:765:HOH:O	2.15	0.47
1:A:351:GLN:HG3	7:A:792:HOH:O	2.14	0.47
1:D:427:ASN:O	1:D:429:THR:CG2	2.62	0.47
1:G:94:SER:HB2	1:G:103:LYS:HE2	1.96	0.47
1:A:505:ALA:C	1:A:507:SER:H	2.23	0.46
1:B:297:ILE:HG23	7:B:781:HOH:O	2.15	0.46
7:B:802:HOH:O	1:D:74:VAL:CG1	2.63	0.46
1:A:381:VAL:HB	1:B:15:LYS:HE2	1.96	0.46
1:D:427:ASN:O	1:D:429:THR:HG22	2.15	0.46
1:G:81:GLY:HA3	1:G:328:ILE:HD12	1.97	0.46
1:A:245:ASN:ND2	4:A:603:NAG:O5	2.46	0.46
1:B:233:THR:HA	1:B:283:ALA:O	2.15	0.46
1:E:94:SER:HB2	1:E:103:LYS:HE2	1.98	0.46
1:G:427:ASN:ND2	4:G:603:NAG:H5	2.29	0.46
1:H:505:ALA:O	1:H:508:ALA:HB3	2.15	0.46
1:C:229:SER:OG	7:C:701:HOH:O	2.21	0.46
1:D:493:ARG:NH1	7:D:721:HOH:O	2.49	0.46
1:E:422:PRO:HD2	1:H:428:LEU:HD13	1.97	0.46
1:F:279:LYS:CB	7:F:903:HOH:O	2.63	0.46
1:F:486:LYS:HE3	1:F:486:LYS:HA	1.98	0.46
1:D:222:LYS:HD2	1:D:344:PRO:O	2.16	0.46
1:C:233:THR:HA	1:C:283:ALA:O	2.16	0.46
1:G:411:ASN:OD1	7:G:702:HOH:O	2.20	0.46
1:E:423:LYS:HD2	1:H:427:ASN:OD1	2.15	0.46
1:G:45:ALA:HB2	1:G:52:LEU:HD21	1.98	0.46
1:A:45:ALA:HB2	1:A:52:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:76:HIS:CE1	7:G:913:HOH:O	2.68	0.46
1:A:233:THR:HA	1:A:283:ALA:O	2.16	0.45
1:A:240:GLU:OE2	1:A:314:ARG:NE	2.43	0.45
1:E:427:ASN:HD22	1:H:423:LYS:HA	1.81	0.45
1:G:309:TYR:HB2	7:G:715:HOH:O	2.15	0.45
7:A:874:HOH:O	1:B:390:LEU:HD11	2.16	0.45
1:F:229:SER:HA	7:F:882:HOH:O	2.16	0.45
1:B:456:ASP:CG	4:B:602:NAG:H83	2.41	0.45
1:F:504:ALA:C	1:F:506:ALA:H	2.24	0.45
1:H:340:GLU:HG3	1:H:418:THR:OG1	2.16	0.45
1:B:493:ARG:HH21	1:B:493:ARG:HB3	1.80	0.45
1:E:61:THR:HB	1:G:160:LEU:HD11	1.99	0.45
1:F:427:ASN:O	1:F:429:THR:HG22	2.16	0.45
1:H:103:LYS:HA	1:H:103:LYS:HE2	1.99	0.45
1:H:120:ALA:O	1:H:121[B]:ARG:C	2.59	0.45
1:A:385:ASP:HA	7:A:826:HOH:O	2.16	0.45
1:B:437:GLY:HA2	1:E:454:GLN:OE1	2.17	0.45
1:B:446:GLU:OE2	1:B:451:GLN:NE2	2.45	0.45
1:D:245:ASN:HD22	4:D:602:NAG:C2	2.17	0.45
1:H:268:ASP:CB	7:H:951:HOH:O	2.43	0.45
1:H:507:SER:C	7:H:758:HOH:O	2.60	0.45
1:E:164:ARG:HH11	1:E:164:ARG:HD2	1.44	0.45
1:E:436:GLU:HB2	7:E:897:HOH:O	2.15	0.45
1:G:193:ALA:HB2	7:G:790:HOH:O	2.17	0.45
1:F:400:GLN:HB2	6:F:602:PEG:C3	2.44	0.45
1:B:160:LEU:HD11	1:D:61:THR:HB	1.99	0.45
1:F:403:PRO:HA	7:F:824:HOH:O	2.16	0.45
1:B:384:PHE:CB	1:C:164:ARG:NE	2.80	0.45
1:F:287:GLU:HG3	7:F:854:HOH:O	2.15	0.45
3:G:601:HEM:HMB1	3:G:601:HEM:CBB	2.34	0.45
3:F:601:HEM:CMB	3:F:601:HEM:HBB2	2.47	0.44
1:B:69:ARG:NH2	7:B:726:HOH:O	2.49	0.44
1:B:281:SER:HB3	1:B:309:TYR:HB3	1.99	0.44
1:D:11:GLY:HA2	7:D:706:HOH:O	2.16	0.44
1:C:281:SER:HB3	1:C:309:TYR:HB3	1.99	0.44
1:E:281:SER:HB3	1:E:309:TYR:HB3	1.99	0.44
1:F:383:ASN:O	6:F:602:PEG:C1	2.65	0.44
1:H:44:ARG:HG2	1:H:51:LEU:HD23	1.99	0.44
1:G:279:LYS:HE2	1:G:314:ARG:HG2	1.99	0.44
1:D:45:ALA:HB2	1:D:52:LEU:HD21	1.98	0.44
1:D:465:ALA:HB1	1:D:499:TYR:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ILE:HG22	1:F:137:MET:HG2	1.99	0.44
1:H:233:THR:HA	1:H:283:ALA:O	2.18	0.44
1:D:390:LEU:CB	1:C:390:LEU:HD13	2.46	0.44
1:E:61:THR:CG2	1:G:164:ARG:NH2	2.81	0.44
1:G:446:GLU:OE2	1:G:451:GLN:NE2	2.44	0.44
1:B:456:ASP:OD2	4:B:602:NAG:H83	2.18	0.44
7:G:792:HOH:O	1:H:412:VAL:HA	2.17	0.44
1:E:113:ARG:HD3	3:E:601:HEM:O1D	2.17	0.44
1:E:279:LYS:HE2	1:E:314:ARG:HG2	2.00	0.44
7:G:852:HOH:O	1:H:390:LEU:HD11	2.17	0.44
1:G:233:THR:HA	1:G:283:ALA:O	2.17	0.44
1:D:110:ILE:HG22	1:D:137:MET:HG2	2.00	0.44
1:D:233:THR:HA	1:D:283:ALA:O	2.17	0.44
1:G:379:SER:HB2	7:G:746:HOH:O	2.17	0.44
1:H:493:ARG:HD2	7:H:966:HOH:O	2.17	0.44
1:D:26:LEU:O	1:C:411:ASN:HB2	2.17	0.43
1:D:411:ASN:O	1:C:27:THR:HA	2.17	0.43
1:E:45:ALA:HB2	1:E:52:LEU:HD21	2.00	0.43
1:A:110:ILE:HG22	1:A:137:MET:HG2	1.99	0.43
1:B:427:ASN:O	1:B:429:THR:CG2	2.65	0.43
1:D:201:LEU:HD22	1:D:464:ILE:HA	1.99	0.43
1:E:233:THR:HA	1:E:283:ALA:O	2.17	0.43
1:D:164:ARG:HH21	1:D:164:ARG:CG	2.30	0.43
3:B:601:HEM:HMB3	1:D:62:MET:HE1	2.00	0.43
1:E:419:VAL:CG1	1:H:430:TYR:CE1	3.01	0.43
1:F:233:THR:HA	1:F:283:ALA:O	2.18	0.43
1:B:45:ALA:HB2	1:B:52:LEU:HD21	2.00	0.43
1:C:505:ALA:O	1:C:508:ALA:HB3	2.19	0.43
1:F:45:ALA:HB2	1:F:52:LEU:HD21	1.99	0.43
1:F:279:LYS:CG	7:F:903:HOH:O	2.67	0.43
1:H:205:GLY:HA2	7:H:712:HOH:O	2.18	0.43
1:B:74[A]:VAL:HG11	1:D:66:ASN:HA	2.01	0.43
7:G:847:HOH:O	1:H:393:HIS:HE1	2.00	0.43
1:H:240:GLU:HG2	7:H:976:HOH:O	2.19	0.43
1:E:279:LYS:HG3	7:E:730:HOH:O	2.19	0.43
1:D:305:LEU:HD23	1:D:305:LEU:HA	1.91	0.43
1:C:201:LEU:HD22	1:C:464:ILE:HA	2.00	0.43
1:C:222:LYS:HD2	7:C:739:HOH:O	2.18	0.43
1:D:109:SER:OG	1:C:6:THR:HG21	2.19	0.43
1:E:112:MET:HE2	1:E:133:PHE:CE1	2.54	0.43
1:B:167:HIS:CD2	7:D:789:HOH:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:SER:HB3	1:D:309:TYR:HB3	2.01	0.43
1:E:110:ILE:HG22	1:E:137:MET:HG2	2.01	0.43
1:E:140:LYS:HB2	7:E:715:HOH:O	2.19	0.43
1:E:322:GLU:O	1:F:398:SER:HB3	2.18	0.43
1:A:167:HIS:HB3	1:D:401:ASN:OD1	2.18	0.42
1:A:310:HIS:CE1	7:A:773:HOH:O	2.72	0.42
1:C:346:ASN:N	7:C:731:HOH:O	2.48	0.42
1:G:392:VAL:HG21	1:H:392:VAL:HG21	2.01	0.42
1:C:199[B]:ARG:NH1	7:C:735:HOH:O	2.52	0.42
1:G:30:GLN:HB3	7:G:870:HOH:O	2.20	0.42
1:A:134:SER:OG	3:A:602:HEM:HBD2	2.20	0.42
1:A:160:LEU:HD11	1:C:61:THR:CB	2.49	0.42
1:C:45:ALA:HB2	1:C:52:LEU:HD21	2.01	0.42
1:E:44:ARG:HG2	1:E:51:LEU:HD23	2.00	0.42
1:F:281:SER:HB3	1:F:309:TYR:HB3	2.01	0.42
1:D:319:GLN:OE1	1:C:5:HIS:HA	2.20	0.42
1:D:410:LEU:HD12	1:C:23:ALA:O	2.18	0.42
1:G:12:THR:HB	1:H:393:HIS:CE1	2.54	0.42
1:E:390:LEU:CB	1:F:390:LEU:HD12	2.47	0.42
1:F:410:LEU:N	6:F:602:PEG:O4	2.52	0.42
1:H:204:LEU:HD21	4:H:602:NAG:C8	2.50	0.42
1:H:379:SER:HB2	7:H:754:HOH:O	2.18	0.42
1:C:399:ARG:HD2	7:C:769:HOH:O	2.18	0.42
1:A:245:ASN:HB2	4:A:603:NAG:C1	2.49	0.42
1:A:376:CYS:SG	1:B:15:LYS:HD2	2.60	0.42
1:B:411:ASN:HA	7:B:763:HOH:O	2.19	0.42
1:E:447:PHE:CZ	1:E:452:LEU:HD11	2.55	0.42
1:C:160:LEU:HD12	1:C:160:LEU:HA	1.87	0.42
1:H:506:ALA:O	1:H:509:LEU:HD13	2.19	0.42
1:D:112:MET:CE	1:D:135:ILE:CD1	2.90	0.42
1:E:51:LEU:H	1:G:351:GLN:HE21	1.66	0.42
1:E:149:ASN:ND2	3:E:601:HEM:CAC	2.80	0.42
1:G:149:ASN:ND2	3:G:601:HEM:CAC	2.82	0.42
1:G:427:ASN:HD21	4:G:603:NAG:H5	1.84	0.42
1:A:402:PHE:HB2	1:A:403:PRO:HD2	2.01	0.42
1:C:110:ILE:HG22	1:C:137:MET:HG2	2.02	0.42
1:E:201:LEU:HD22	1:E:464:ILE:HA	2.02	0.42
1:F:371:GLN:O	1:F:393:HIS:CE1	2.65	0.42
1:A:446:GLU:OE2	1:A:451:GLN:NE2	2.43	0.41
1:E:112:MET:CE	1:E:135:ILE:CD1	2.98	0.41
1:E:132:GLY:HA3	3:E:601:HEM:HMD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:SER:HB2	7:E:703:HOH:O	2.19	0.41
1:G:67:ARG:NE	7:G:747:HOH:O	2.53	0.41
1:A:281:SER:HB3	1:A:309:TYR:HB3	2.02	0.41
1:D:44:ARG:HG2	1:D:51:LEU:HD23	2.00	0.41
1:D:447:PHE:CZ	1:D:452:LEU:HD11	2.55	0.41
7:E:849:HOH:O	1:G:74:VAL:HG13	2.20	0.41
1:F:164:ARG:N	1:F:164:ARG:HD2	2.35	0.41
1:H:423:LYS:N	7:H:735:HOH:O	2.52	0.41
1:B:364:ARG:HD2	7:B:739:HOH:O	2.19	0.41
1:E:76:HIS:HA	1:E:116:THR:O	2.20	0.41
1:B:31[B]:GLN:H	1:B:31[B]:GLN:CD	2.28	0.41
1:F:305:LEU:HD23	1:F:305:LEU:HA	1.92	0.41
1:G:345:SER:HB2	7:G:752:HOH:O	2.20	0.41
1:A:61:THR:HB	1:C:160:LEU:HD11	2.01	0.41
1:A:76:HIS:HA	1:A:116:THR:O	2.20	0.41
1:B:245:ASN:HB2	4:B:602:NAG:C1	2.50	0.41
1:B:422:PRO:HD2	1:C:428:LEU:HD13	2.03	0.41
1:E:372:ILE:O	1:E:373:PRO:C	2.64	0.41
1:G:427:ASN:ND2	4:G:603:NAG:C5	2.84	0.41
1:E:61:THR:CG2	1:G:164:ARG:HH22	2.34	0.41
1:F:128:ARG:CG	7:F:845:HOH:O	2.64	0.41
1:F:402:PHE:HB2	1:F:403:PRO:HD2	2.03	0.41
1:G:44:ARG:HG2	1:G:51:LEU:HD23	2.03	0.41
1:A:13:ARG:CD	1:B:13:ARG:CZ	2.98	0.41
1:B:402:PHE:HB2	1:B:403:PRO:HD2	2.02	0.41
1:B:415:LYS:NZ	1:B:421:GLU:OE2	2.42	0.41
1:D:359:ASP:HA	1:D:362[B]:ARG:CZ	2.51	0.41
1:C:112:MET:HG2	1:C:135:ILE:HD12	2.03	0.41
1:C:465:ALA:HB1	1:C:499:TYR:HA	2.02	0.41
1:F:141:LYS:NZ	7:F:749[A]:HOH:O	2.54	0.41
1:B:201:LEU:HD22	1:B:464:ILE:HA	2.02	0.41
1:E:417:LYS:HE2	7:E:772:HOH:O	2.19	0.41
1:G:322:GLU:O	1:H:398:SER:HB3	2.21	0.41
1:H:447:PHE:CZ	1:H:452:LEU:HD11	2.55	0.41
3:B:601:HEM:HBB2	3:B:601:HEM:CMB	2.47	0.41
1:D:76:HIS:HA	1:D:116:THR:O	2.20	0.41
1:D:115:SER:O	1:D:131:ARG:HA	2.21	0.41
1:C:76:HIS:HA	1:C:116:THR:O	2.20	0.41
1:E:74[A]:VAL:HG11	1:G:65:PHE:O	2.21	0.41
1:G:277:ALA:HA	1:G:315:MET:O	2.21	0.41
1:G:281:SER:HB3	1:G:309:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:MET:HE3	1:H:133:PHE:HE1	1.84	0.41
1:C:509:LEU:C	1:C:509:LEU:HD22	2.45	0.41
1:E:439:ILE:HG22	7:E:867:HOH:O	2.21	0.41
1:F:81:GLY:HA3	1:F:328:ILE:HD12	2.02	0.41
1:G:112:MET:CE	1:G:135:ILE:CD1	2.98	0.41
1:A:40:GLN:HE21	1:C:164:ARG:HG3	1.85	0.40
1:C:62:MET:HE3	1:C:62:MET:CA	2.51	0.40
1:E:403:PRO:HA	7:E:892:HOH:O	2.21	0.40
1:A:504:ALA:C	1:A:507:SER:H	2.23	0.40
1:E:81:GLY:HA3	1:E:328:ILE:HD12	2.02	0.40
1:F:477:ARG:HD2	7:F:702:HOH:O	2.21	0.40
1:G:164:ARG:HH21	1:G:164:ARG:HD2	1.72	0.40
1:H:121[B]:ARG:NH2	7:H:740:HOH:O	2.54	0.40
1:A:26:LEU:O	1:B:411:ASN:HB2	2.21	0.40
1:A:54:GLN:HE22	1:C:428:LEU:HD11	1.85	0.40
1:A:115:SER:O	1:A:131:ARG:HA	2.21	0.40
1:B:430:TYR:CE2	1:C:419:VAL:CG1	3.04	0.40
1:E:45:ALA:O	1:E:49:GLY:HA3	2.21	0.40
1:E:160:LEU:HD12	1:E:160:LEU:HA	1.83	0.40
3:F:601:HEM:HBB2	3:F:601:HEM:HMB2	2.02	0.40
1:B:385:ASP:O	7:B:703:HOH:O	2.22	0.40
1:D:8:LEU:HD22	1:C:374:VAL:HA	2.03	0.40
1:C:358:ASN:O	1:C:362:ARG:HG3	2.22	0.40
1:G:76:HIS:HA	1:G:116:THR:O	2.21	0.40
1:H:349:VAL:HG13	3:H:601:HEM:CBB	2.52	0.40
1:A:20:THR:HG22	1:A:322:GLU:OE2	2.20	0.40
1:A:370:GLN:HE22	1:B:31[A]:GLN:HB3	1.86	0.40
1:A:488:ASP:OD1	1:A:490:ALA:HB3	2.22	0.40
1:B:112:MET:CE	1:B:135:ILE:CD1	2.97	0.40
1:B:160:LEU:HD12	1:B:160:LEU:HA	1.93	0.40
1:D:14:LEU:HA	7:D:708:HOH:O	2.20	0.40
1:C:407:ARG:HB3	7:C:745:HOH:O	2.20	0.40
1:F:76:HIS:HA	1:F:116:THR:O	2.21	0.40
1:F:419:VAL:HG13	1:G:430:TYR:CE2	2.57	0.40
1:H:76:HIS:HA	1:H:116:THR:O	2.21	0.40

All (1) 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)
7:D:899:HOH:O	7:C:890:HOH:O[1_455]	2.00	0.20

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	505/509 (99%)	487 (96%)	16 (3%)	2 (0%)	30	21
1	B	507/509 (100%)	490 (97%)	16 (3%)	1 (0%)	43	36
1	C	507/509 (100%)	487 (96%)	19 (4%)	1 (0%)	43	36
1	D	504/509 (99%)	486 (96%)	17 (3%)	1 (0%)	43	36
1	E	503/509 (99%)	484 (96%)	18 (4%)	1 (0%)	43	36
1	F	503/509 (99%)	485 (96%)	16 (3%)	2 (0%)	30	21
1	G	497/509 (98%)	478 (96%)	17 (3%)	2 (0%)	30	21
1	H	508/509 (100%)	487 (96%)	17 (3%)	4 (1%)	16	8
All	All	4034/4072 (99%)	3884 (96%)	136 (3%)	14 (0%)	36	28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	4	TYR
1	H	121[A]	ARG
1	H	121[B]	ARG
1	A	506	ALA
1	F	505	ALA
1	H	508	ALA
1	A	387	ASP
1	C	387	ASP
1	F	387	ASP
1	H	387	ASP
1	D	387	ASP
1	G	387	ASP
1	B	387	ASP
1	E	387	ASP

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	429/430 (100%)	409 (95%)	20 (5%)	23	12
1	B	431/430 (100%)	414 (96%)	17 (4%)	28	18
1	C	430/430 (100%)	414 (96%)	16 (4%)	30	20
1	D	428/430 (100%)	411 (96%)	17 (4%)	28	17
1	E	429/430 (100%)	414 (96%)	15 (4%)	32	22
1	F	427/430 (99%)	405 (95%)	22 (5%)	21	9
1	G	425/430 (99%)	412 (97%)	13 (3%)	35	26
1	H	431/430 (100%)	408 (95%)	23 (5%)	20	9
All	All	3430/3440 (100%)	3287 (96%)	143 (4%)	27	16

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	THR
1	A	129	ASP
1	A	134	SER
1	A	139	THR
1	A	151	THR
1	A	198	LEU
1	A	201	LEU
1	A	264	LYS
1	A	272	LYS
1	A	284	THR
1	A	429	THR
1	A	436	GLU
1	A	446	GLU
1	A	453	SER
1	A	475	ASP
1	A	483	GLN
1	A	493	ARG
1	A	501	LYS
1	A	503	LEU

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Mol	Chain	Res	Type
1	A	507	SER
1	B	2	GLU
1	B	64	THR
1	B	129	ASP
1	B	139	THR
1	B	151	THR
1	B	198	LEU
1	B	201	LEU
1	B	244	ARG
1	B	284	THR
1	B	287	GLU
1	B	306	ASN
1	B	429	THR
1	B	446	GLU
1	B	483	GLN
1	B	493	ARG
1	B	501	LYS
1	B	503	LEU
1	D	4	TYR
1	D	34	ARG
1	D	108	THR
1	D	129	ASP
1	D	139	THR
1	D	151	THR
1	D	164	ARG
1	D	198	LEU
1	D	201	LEU
1	D	264	LYS
1	D	284	THR
1	D	288	GLU
1	D	390	LEU
1	D	429	THR
1	D	446	GLU
1	D	483	GLN
1	D	503	LEU
1	C	34	ARG
1	C	108	THR
1	C	129	ASP
1	C	139	THR
1	C	151	THR
1	C	198	LEU
1	C	201	LEU

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Mol	Chain	Res	Type
1	C	284	THR
1	C	288	GLU
1	C	322	GLU
1	C	424	ILE
1	C	429	THR
1	C	446	GLU
1	C	483	GLN
1	C	503	LEU
1	C	509	LEU
1	E	34	ARG
1	E	74[A]	VAL
1	E	74[B]	VAL
1	E	129	ASP
1	E	139	THR
1	E	151	THR
1	E	198	LEU
1	E	201	LEU
1	E	284	THR
1	E	429	THR
1	E	446	GLU
1	E	452	LEU
1	E	483	GLN
1	E	501	LYS
1	E	503	LEU
1	F	71	PRO
1	F	108	THR
1	F	129	ASP
1	F	139	THR
1	F	151	THR
1	F	160	LEU
1	F	198	LEU
1	F	201	LEU
1	F	264[A]	LYS
1	F	264[B]	LYS
1	F	279	LYS
1	F	284	THR
1	F	288	GLU
1	F	424	ILE
1	F	429	THR
1	F	446	GLU
1	F	453	SER
1	F	474	ASP

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Mol	Chain	Res	Type
1	F	483	GLN
1	F	500	GLN
1	F	501	LYS
1	F	503	LEU
1	G	74	VAL
1	G	129	ASP
1	G	139	THR
1	G	151	THR
1	G	164	ARG
1	G	198	LEU
1	G	201	LEU
1	G	284	THR
1	G	288	GLU
1	G	417	LYS
1	G	429	THR
1	G	446	GLU
1	G	483	GLN
1	H	34	ARG
1	H	74	VAL
1	H	87	GLU
1	H	103	LYS
1	H	108	THR
1	H	129	ASP
1	H	139	THR
1	H	151	THR
1	H	198	LEU
1	H	201	LEU
1	H	272	LYS
1	H	281	SER
1	H	284	THR
1	H	287	GLU
1	H	312	VAL
1	H	379	SER
1	H	390	LEU
1	H	424	ILE
1	H	446	GLU
1	H	453	SER
1	H	483	GLN
1	H	503	LEU
1	H	509	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	A	219	HIS
1	A	245	ASN
1	A	370	GLN
1	A	427	ASN
1	B	196	GLN
1	B	219	HIS
1	B	245	ASN
1	B	310	HIS
1	B	370	GLN
1	B	411	ASN
1	D	196	GLN
1	D	245	ASN
1	D	370	GLN
1	D	411	ASN
1	C	18	GLN
1	C	31	GLN
1	C	245	ASN
1	C	411	ASN
1	C	427	ASN
1	E	40	GLN
1	E	337	ASN
1	E	427	ASN
1	F	5	HIS
1	F	18	GLN
1	F	196	GLN
1	F	393	HIS
1	G	76	HIS
1	G	245	ASN
1	G	351	GLN
1	H	31	GLN
1	H	54	GLN
1	H	212	HIS
1	H	245	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	E	601	1	50,50,50	2.34	18 (36%)	66,82,82	1.75	14 (21%)
3	HEM	G	601	1	50,50,50	2.50	12 (24%)	66,82,82	1.81	20 (30%)
6	PEG	E	602	-	6,6,6	0.22	0	5,5,5	0.07	0
3	HEM	B	601	1	50,50,50	2.27	12 (24%)	66,82,82	1.81	16 (24%)
4	NAG	G	602	-	14,14,15	0.58	0	17,19,21	1.72	3 (17%)
4	NAG	H	602	-	14,14,15	0.48	0	17,19,21	1.50	3 (17%)
3	HEM	D	601	1	50,50,50	2.72	17 (34%)	66,82,82	1.72	14 (21%)
4	NAG	B	602	-	14,14,15	0.39	0	17,19,21	1.27	3 (17%)
6	PEG	F	602	-	6,6,6	0.37	0	5,5,5	0.30	0
4	NAG	C	602	-	14,14,15	0.52	0	17,19,21	1.56	3 (17%)
3	HEM	H	601	1	50,50,50	2.14	15 (30%)	66,82,82	1.59	14 (21%)
4	NAG	A	603	-	14,14,15	0.53	0	17,19,21	1.48	1 (5%)
4	NAG	G	603	-	14,14,15	0.40	0	17,19,21	1.86	3 (17%)
5	EDO	A	604	-	3,3,3	0.16	0	2,2,2	0.29	0
3	HEM	A	602	1	50,50,50	1.75	14 (28%)	66,82,82	1.34	6 (9%)
3	HEM	C	601	1	50,50,50	2.16	14 (28%)	66,82,82	1.33	7 (10%)
2	CAQ	A	601	-	8,8,8	0.36	0	10,10,10	0.54	0
3	HEM	F	601	1	50,50,50	2.08	13 (26%)	66,82,82	1.40	10 (15%)
4	NAG	D	602	-	14,14,15	0.57	0	17,19,21	1.30	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	E	601	1	-	4/14/54/54	-
3	HEM	G	601	1	-	4/14/54/54	-
6	PEG	E	602	-	-	3/4/4/4	-
3	HEM	B	601	1	-	2/14/54/54	-
4	NAG	G	602	-	-	2/6/23/26	0/1/1/1
4	NAG	H	602	-	-	2/6/23/26	0/1/1/1
3	HEM	D	601	1	-	2/14/54/54	-
4	NAG	B	602	-	-	2/6/23/26	0/1/1/1
6	PEG	F	602	-	-	4/4/4/4	-
4	NAG	C	602	-	-	1/6/23/26	0/1/1/1
3	HEM	H	601	1	-	2/14/54/54	-
4	NAG	A	603	-	-	2/6/23/26	0/1/1/1
4	NAG	G	603	-	-	5/6/23/26	0/1/1/1
5	EDO	A	604	-	-	1/1/1/1	-
3	HEM	A	602	1	-	2/14/54/54	-
3	HEM	C	601	1	-	4/14/54/54	-
2	CAQ	A	601	-	-	-	0/1/1/1
3	HEM	F	601	1	-	4/14/54/54	-
4	NAG	D	602	-	-	2/6/23/26	0/1/1/1

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	HEM	FE-NC	11.23	2.33	1.95
3	G	601	HEM	FE-NB	9.54	2.24	1.94
3	E	601	HEM	FE-NB	8.53	2.21	1.94
3	B	601	HEM	FE-NC	7.68	2.21	1.95
3	F	601	HEM	FE-NB	7.62	2.18	1.94
3	H	601	HEM	FE-NA	6.90	2.18	1.95
3	E	601	HEM	C1B-NB	-6.65	1.28	1.40
3	D	601	HEM	C1D-C2D	-5.92	1.33	1.44
3	H	601	HEM	FE-NB	5.80	2.12	1.94
3	G	601	HEM	FE-NA	5.75	2.14	1.95
3	G	601	HEM	CHD-C4C	5.56	1.49	1.38
3	B	601	HEM	FE-NA	5.36	2.13	1.95
3	C	601	HEM	C1D-C2D	-5.31	1.34	1.44
3	B	601	HEM	C4D-C3D	-5.02	1.36	1.45
3	F	601	HEM	C1D-C2D	-5.02	1.34	1.44
3	D	601	HEM	C1A-NA	-4.95	1.30	1.39
3	C	601	HEM	FE-NC	4.90	2.11	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	HEM	C1A-NA	-4.81	1.30	1.39
3	C	601	HEM	C4A-NA	-4.80	1.30	1.39
3	G	601	HEM	FE-ND	4.70	2.09	1.94
3	D	601	HEM	C4D-C3D	-4.63	1.37	1.45
3	C	601	HEM	FE-NB	4.61	2.09	1.94
3	D	601	HEM	C3C-C4C	-4.58	1.37	1.46
3	A	602	HEM	C3C-C4C	-4.51	1.38	1.46
3	B	601	HEM	C1C-NC	-4.40	1.31	1.39
3	G	601	HEM	C3C-C4C	-4.38	1.38	1.46
3	A	602	HEM	C1D-C2D	-4.20	1.36	1.44
3	G	601	HEM	C1A-C2A	-4.19	1.36	1.44
3	C	601	HEM	C4D-ND	-4.08	1.33	1.40
3	C	601	HEM	C4D-C3D	-4.06	1.38	1.45
3	E	601	HEM	FE-ND	4.05	2.07	1.94
3	E	601	HEM	C3C-C4C	-4.04	1.38	1.46
3	H	601	HEM	C4D-C3D	-4.00	1.38	1.45
3	C	601	HEM	C3C-C4C	-3.93	1.39	1.46
3	D	601	HEM	FE-ND	-3.89	1.82	1.94
3	C	601	HEM	C1C-C2C	-3.88	1.37	1.45
3	G	601	HEM	C1B-NB	-3.78	1.33	1.40
3	D	601	HEM	C1C-C2C	-3.77	1.37	1.45
3	B	601	HEM	C1D-C2D	-3.68	1.37	1.44
3	G	601	HEM	C4A-NA	-3.67	1.32	1.39
3	A	602	HEM	C1B-NB	-3.66	1.34	1.40
3	D	601	HEM	FE-NB	3.64	2.06	1.94
3	F	601	HEM	FE-NA	3.64	2.07	1.95
3	B	601	HEM	C1B-C2B	-3.54	1.37	1.44
3	F	601	HEM	C4D-C3D	-3.54	1.38	1.45
3	H	601	HEM	C1A-C2A	-3.54	1.37	1.44
3	H	601	HEM	FE-NC	3.53	2.07	1.95
3	D	601	HEM	C4D-ND	-3.47	1.34	1.40
3	H	601	HEM	C3C-C4C	-3.44	1.39	1.46
3	B	601	HEM	C3C-C2C	3.33	1.44	1.37
3	F	601	HEM	C3B-C4B	-3.29	1.38	1.44
3	B	601	HEM	C3C-C4C	-3.27	1.40	1.46
3	C	601	HEM	C1A-C2A	-3.26	1.38	1.44
3	E	601	HEM	C4D-C3D	-3.26	1.39	1.45
3	D	601	HEM	C1B-C2B	-3.23	1.38	1.44
3	F	601	HEM	C3C-C2C	3.16	1.43	1.37
3	F	601	HEM	C3C-C4C	-3.15	1.40	1.46
3	D	601	HEM	C1C-NC	-3.13	1.33	1.39
3	A	602	HEM	C4D-C3D	-3.09	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	HEM	C3B-C2B	3.07	1.43	1.37
3	A	602	HEM	C1B-C2B	-3.02	1.38	1.44
3	D	601	HEM	C1B-NB	-3.01	1.35	1.40
3	C	601	HEM	C4A-C3A	-2.99	1.36	1.43
3	C	601	HEM	C1B-C2B	-2.99	1.38	1.44
3	E	601	HEM	FE-NA	2.98	2.05	1.95
3	E	601	HEM	CHD-C4C	2.97	1.44	1.38
3	H	601	HEM	C1D-C2D	-2.94	1.38	1.44
3	E	601	HEM	C1C-NC	-2.93	1.34	1.39
3	B	601	HEM	C4A-C3A	-2.83	1.36	1.43
3	E	601	HEM	O2A-CGA	-2.82	1.21	1.30
3	E	601	HEM	C1D-C2D	-2.77	1.39	1.44
3	D	601	HEM	O2A-CGA	-2.77	1.21	1.30
3	E	601	HEM	C1A-NA	-2.76	1.34	1.39
3	G	601	HEM	C3B-C4B	-2.76	1.39	1.44
3	E	601	HEM	C4A-NA	-2.75	1.34	1.39
3	F	601	HEM	O2A-CGA	-2.74	1.21	1.30
3	G	601	HEM	C1C-C2C	-2.74	1.39	1.45
3	D	601	HEM	C1A-C2A	-2.74	1.39	1.44
3	C	601	HEM	C3B-C4B	-2.70	1.39	1.44
3	F	601	HEM	CAB-C3B	-2.70	1.40	1.47
3	F	601	HEM	C1B-C2B	-2.69	1.39	1.44
3	G	601	HEM	C4A-C3A	-2.67	1.37	1.43
3	A	602	HEM	C1D-ND	-2.65	1.33	1.38
3	F	601	HEM	FE-ND	2.62	2.03	1.94
3	A	602	HEM	C3B-C4B	-2.62	1.39	1.44
3	H	601	HEM	C3B-C2B	2.58	1.42	1.37
3	H	601	HEM	C3B-C4B	-2.57	1.39	1.44
3	A	602	HEM	C1A-NA	-2.53	1.34	1.39
3	C	601	HEM	C1B-NB	-2.50	1.36	1.40
3	A	602	HEM	C1C-NC	-2.49	1.34	1.39
3	A	602	HEM	CHD-C1D	-2.48	1.33	1.39
3	B	601	HEM	C3B-C4B	-2.42	1.40	1.44
3	H	601	HEM	C4A-C3A	-2.41	1.37	1.43
3	F	601	HEM	C4A-NA	-2.39	1.35	1.39
3	E	601	HEM	C4A-C3A	-2.37	1.37	1.43
3	H	601	HEM	FE-ND	2.28	2.01	1.94
3	E	601	HEM	FE-NC	2.27	2.02	1.95
3	D	601	HEM	C3B-C4B	-2.25	1.40	1.44
3	B	601	HEM	C1C-C2C	-2.21	1.41	1.45
3	H	601	HEM	C1A-NA	-2.20	1.35	1.39
3	E	601	HEM	CHA-C1A	2.20	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	HEM	C1D-ND	-2.19	1.34	1.38
3	G	601	HEM	FE-NC	2.18	2.02	1.95
3	A	602	HEM	CHA-C4D	-2.16	1.34	1.38
3	H	601	HEM	CHC-C4B	2.16	1.44	1.39
3	H	601	HEM	C1B-NB	-2.16	1.36	1.40
3	A	602	HEM	FE-NC	2.13	2.02	1.95
3	A	602	HEM	CHD-C4C	-2.12	1.34	1.38
3	D	601	HEM	C1D-ND	-2.11	1.34	1.38
3	E	601	HEM	C3B-C4B	-2.10	1.40	1.44
3	D	601	HEM	C4A-C3A	-2.08	1.38	1.43
3	A	602	HEM	CAC-C3C	-2.03	1.41	1.47
3	E	601	HEM	C4D-ND	-2.03	1.36	1.40
3	C	601	HEM	C1C-NC	-2.02	1.35	1.39
3	H	601	HEM	C1C-NC	-2.00	1.35	1.39

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	HEM	CHB-C1B-NB	-5.66	117.40	124.37
3	B	601	HEM	CHC-C1C-NC	-5.51	118.47	124.44
3	D	601	HEM	CHD-C1D-ND	5.11	129.97	124.42
3	C	601	HEM	CAA-CBA-CGA	4.96	124.28	113.60
4	A	603	NAG	C2-N2-C7	4.93	129.92	122.90
3	D	601	HEM	C4C-C3C-C2C	-4.67	102.92	106.75
3	B	601	HEM	CAA-CBA-CGA	4.53	123.36	113.60
3	G	601	HEM	CAA-CBA-CGA	4.48	123.25	113.60
3	H	601	HEM	CHD-C4C-NC	-4.37	119.71	124.44
4	G	603	NAG	C2-N2-C7	4.36	129.11	122.90
4	G	603	NAG	C1-C2-N2	4.34	117.91	110.49
4	G	602	NAG	O5-C1-C2	4.34	118.14	111.29
3	F	601	HEM	CHC-C1C-NC	4.22	129.01	124.44
4	H	602	NAG	C2-N2-C7	4.18	128.85	122.90
3	B	601	HEM	O1D-CGD-CBD	-4.16	109.72	123.08
4	C	602	NAG	C1-C2-N2	-4.07	103.54	110.49
3	B	601	HEM	C4C-NC-C1C	4.02	109.29	105.35
3	G	601	HEM	CHB-C1B-NB	-4.00	119.44	124.37
3	G	601	HEM	C3B-C2B-C1B	4.00	109.46	106.49
3	A	602	HEM	O2D-CGD-CBD	3.94	126.70	114.03
3	G	601	HEM	C4A-C3A-C2A	3.93	111.43	106.83
4	B	602	NAG	C1-C2-N2	3.92	117.18	110.49
4	D	602	NAG	C1-C2-N2	-3.87	103.88	110.49
4	G	602	NAG	C2-N2-C7	3.86	128.40	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	C4B-C3B-C2B	-3.86	104.05	107.11
3	D	601	HEM	CHB-C1B-NB	3.82	129.09	124.37
3	F	601	HEM	CHC-C4B-NB	-3.72	120.38	124.42
3	B	601	HEM	C3B-C2B-C1B	3.72	109.24	106.49
3	D	601	HEM	CHC-C1C-NC	-3.61	120.54	124.44
4	G	603	NAG	C1-O5-C5	3.60	117.07	112.19
3	E	601	HEM	C1A-CHA-C4D	3.60	134.88	126.34
3	B	601	HEM	O2D-CGD-CBD	3.57	125.51	114.03
3	E	601	HEM	C1C-CHC-C4B	3.55	133.72	126.06
3	A	602	HEM	O1D-CGD-CBD	-3.47	111.92	123.08
3	C	601	HEM	CBA-CAA-C2A	3.45	122.22	112.63
3	E	601	HEM	C4B-C3B-C2B	-3.43	104.39	107.11
3	F	601	HEM	C1B-NB-C4B	3.38	108.56	105.07
3	H	601	HEM	O1D-CGD-CBD	-3.36	112.28	123.08
3	E	601	HEM	O1D-CGD-CBD	-3.36	112.29	123.08
3	F	601	HEM	CHC-C4B-C3B	3.23	132.08	125.13
3	E	601	HEM	CHD-C1D-ND	-3.21	120.92	124.42
3	H	601	HEM	C4D-ND-C1D	3.20	108.38	105.07
3	G	601	HEM	C4B-C3B-C2B	-3.19	104.58	107.11
3	D	601	HEM	CAA-CBA-CGA	3.17	120.41	113.60
3	E	601	HEM	CHD-C1D-C2D	3.13	129.87	124.98
3	H	601	HEM	C1B-NB-C4B	3.13	108.30	105.07
3	B	601	HEM	CHC-C1C-C2C	3.10	131.98	125.48
3	H	601	HEM	C4C-CHD-C1D	3.08	132.70	126.06
3	D	601	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
3	A	602	HEM	C3B-C2B-C1B	2.99	108.71	106.49
3	D	601	HEM	C3C-C2C-C1C	2.98	109.92	107.08
3	B	601	HEM	C4C-C3C-C2C	-2.97	104.31	106.75
3	H	601	HEM	O2D-CGD-CBD	2.90	123.34	114.03
3	H	601	HEM	C2A-C1A-NA	-2.85	106.97	110.15
3	H	601	HEM	C4A-NA-C1A	2.84	108.13	105.35
3	D	601	HEM	O2A-CGA-CBA	-2.84	104.91	114.03
3	B	601	HEM	CHB-C4A-NA	2.81	129.01	123.85
3	A	602	HEM	CMC-C2C-C1C	2.79	129.63	124.71
3	G	601	HEM	C4A-NA-C1A	2.77	108.06	105.35
3	B	601	HEM	C4C-CHD-C1D	2.75	131.99	126.06
3	G	601	HEM	CMB-C2B-C3B	-2.70	121.69	128.30
3	B	601	HEM	CMB-C2B-C3B	-2.69	121.71	128.30
3	H	601	HEM	CMA-C3A-C2A	2.69	131.42	125.61
3	E	601	HEM	O2D-CGD-CBD	2.68	122.63	114.03
3	H	601	HEM	C4A-CHB-C1B	2.67	132.66	126.34
3	E	601	HEM	CHC-C1C-NC	-2.65	121.58	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	601	HEM	C4A-NA-C1A	2.63	107.92	105.35
4	H	602	NAG	C1-O5-C5	2.62	115.74	112.19
3	E	601	HEM	C4D-ND-C1D	2.57	107.73	105.07
3	B	601	HEM	CMB-C2B-C1B	2.55	128.92	125.04
3	G	601	HEM	CAC-C3C-C4C	-2.55	118.75	124.90
4	C	602	NAG	O5-C1-C2	-2.54	107.28	111.29
3	G	601	HEM	C1C-CHC-C4B	2.52	131.50	126.06
4	C	602	NAG	C1-O5-C5	-2.51	108.80	112.19
3	H	601	HEM	C4A-C3A-C2A	-2.48	103.93	106.83
3	B	601	HEM	CHA-C1A-C2A	2.47	130.75	125.36
3	G	601	HEM	CMB-C2B-C1B	2.47	128.80	125.04
3	C	601	HEM	C1A-C2A-C3A	-2.46	103.02	106.89
3	B	601	HEM	C4A-NA-C1A	2.44	107.74	105.35
3	D	601	HEM	CHC-C1C-C2C	2.43	130.58	125.48
3	F	601	HEM	CHB-C1B-NB	-2.43	121.38	124.37
3	D	601	HEM	CHB-C1B-C2B	-2.39	120.08	126.73
3	E	601	HEM	CAC-C3C-C4C	-2.39	119.13	124.90
3	G	601	HEM	O1A-CGA-CBA	-2.37	115.48	123.08
3	G	601	HEM	C1B-NB-C4B	2.36	107.51	105.07
3	B	601	HEM	CAD-CBD-CGD	-2.31	108.63	113.60
3	H	601	HEM	C3B-C2B-C1B	-2.31	104.77	106.49
3	C	601	HEM	CMD-C2D-C1D	2.30	128.54	125.04
3	D	601	HEM	C4A-C3A-C2A	-2.30	104.14	106.83
3	G	601	HEM	C4C-C3C-C2C	2.29	108.63	106.75
3	E	601	HEM	O2A-CGA-O1A	-2.28	117.61	123.30
3	G	601	HEM	C3C-C2C-C1C	-2.27	104.91	107.08
3	H	601	HEM	CHD-C4C-C3C	2.26	129.12	125.26
3	G	601	HEM	CMC-C2C-C1C	2.25	128.68	124.71
3	G	601	HEM	C1A-CHA-C4D	2.25	131.68	126.34
3	G	601	HEM	C4C-NC-C1C	2.24	107.55	105.35
3	C	601	HEM	CMC-C2C-C1C	2.21	128.61	124.71
3	A	602	HEM	CAD-C3D-C4D	2.20	128.50	124.66
3	E	601	HEM	C4C-C3C-C2C	-2.20	104.95	106.75
4	B	602	NAG	C1-O5-C5	2.19	115.16	112.19
3	D	601	HEM	C4D-ND-C1D	2.18	107.32	105.07
3	E	601	HEM	CAA-C2A-C1A	2.18	129.18	124.89
3	C	601	HEM	CAA-C2A-C1A	2.15	129.12	124.89
4	G	602	NAG	O4-C4-C5	2.15	114.63	109.30
3	C	601	HEM	O1D-CGD-CBD	-2.13	116.23	123.08
3	H	601	HEM	C1A-C2A-C3A	2.12	110.23	106.89
3	F	601	HEM	CHA-C4D-C3D	2.11	129.30	125.33
4	B	602	NAG	O3-C3-C2	-2.11	105.09	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	601	HEM	CHA-C1A-C2A	2.11	129.96	125.36
3	F	601	HEM	C4A-CHB-C1B	2.09	131.29	126.34
3	F	601	HEM	CHC-C1C-C2C	-2.08	121.12	125.48
3	G	601	HEM	CBD-CAD-C3D	2.08	118.39	112.63
3	B	601	HEM	CHA-C1A-NA	-2.07	120.03	123.85
3	D	601	HEM	O1A-CGA-CBA	2.07	129.74	123.08
3	G	601	HEM	CHB-C1B-C2B	2.05	132.43	126.73
3	G	601	HEM	CHA-C4D-ND	-2.03	121.87	124.37
3	F	601	HEM	C4B-C3B-C2B	2.03	108.73	107.11
4	H	602	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	603	NAG	C4-C5-C6-O6
4	G	603	NAG	O5-C5-C6-O6
4	A	603	NAG	C8-C7-N2-C2
4	A	603	NAG	O7-C7-N2-C2
4	B	602	NAG	C8-C7-N2-C2
4	H	602	NAG	C8-C7-N2-C2
4	H	602	NAG	O7-C7-N2-C2
4	G	603	NAG	C1-C2-N2-C7
6	F	602	PEG	O1-C1-C2-O2
4	D	602	NAG	O5-C5-C6-O6
4	B	602	NAG	O7-C7-N2-C2
6	E	602	PEG	O2-C3-C4-O4
6	F	602	PEG	O2-C3-C4-O4
6	F	602	PEG	C1-C2-O2-C3
4	D	602	NAG	C4-C5-C6-O6
4	G	602	NAG	O7-C7-N2-C2
4	G	603	NAG	O7-C7-N2-C2
3	C	601	HEM	C2A-CAA-CBA-CGA
6	E	602	PEG	C4-C3-O2-C2
3	F	601	HEM	CAA-CBA-CGA-O1A
6	F	602	PEG	C4-C3-O2-C2
3	F	601	HEM	CAD-CBD-CGD-O1D
3	G	601	HEM	CAD-CBD-CGD-O1D
3	C	601	HEM	CAD-CBD-CGD-O2D
4	G	602	NAG	C8-C7-N2-C2
3	A	602	HEM	CAD-CBD-CGD-O1D
3	G	601	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
3	E	601	HEM	CAD-CBD-CGD-O2D
3	F	601	HEM	CAD-CBD-CGD-O2D
3	F	601	HEM	CAA-CBA-CGA-O2A
3	E	601	HEM	CAD-CBD-CGD-O1D
3	C	601	HEM	C1A-C2A-CAA-CBA
4	G	603	NAG	C8-C7-N2-C2
3	A	602	HEM	CAD-CBD-CGD-O2D
3	H	601	HEM	CAD-CBD-CGD-O2D
4	C	602	NAG	C8-C7-N2-C2
3	B	601	HEM	CAD-CBD-CGD-O2D
3	C	601	HEM	CAD-CBD-CGD-O1D
3	G	601	HEM	CAA-CBA-CGA-O1A
3	H	601	HEM	CAD-CBD-CGD-O1D
3	E	601	HEM	C4C-C3C-CAC-CBC
3	B	601	HEM	CAD-CBD-CGD-O1D
3	E	601	HEM	CAA-CBA-CGA-O2A
3	G	601	HEM	CAA-CBA-CGA-O2A
6	E	602	PEG	O1-C1-C2-O2
3	D	601	HEM	CAD-CBD-CGD-O1D
3	D	601	HEM	CAD-CBD-CGD-O2D
5	A	604	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 80 short contacts:

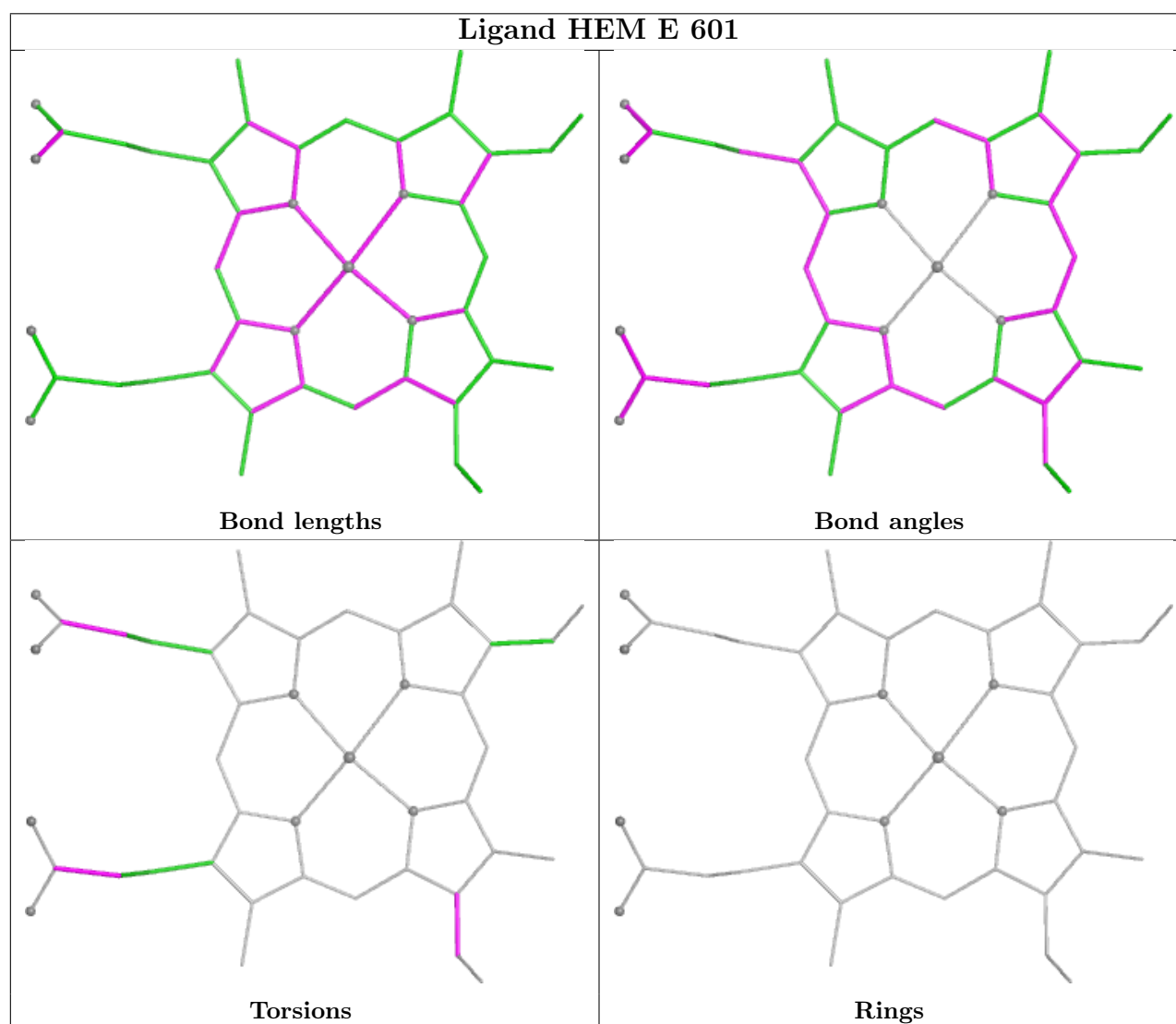
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	HEM	7	0
3	G	601	HEM	6	0
3	B	601	HEM	4	0
4	G	602	NAG	2	0
4	H	602	NAG	3	0
3	D	601	HEM	1	0
4	B	602	NAG	6	0
6	F	602	PEG	17	0
4	C	602	NAG	2	0
3	H	601	HEM	3	0
4	A	603	NAG	5	0
4	G	603	NAG	7	0
5	A	604	EDO	1	0
3	A	602	HEM	6	0
3	C	601	HEM	2	0
2	A	601	CAQ	2	0

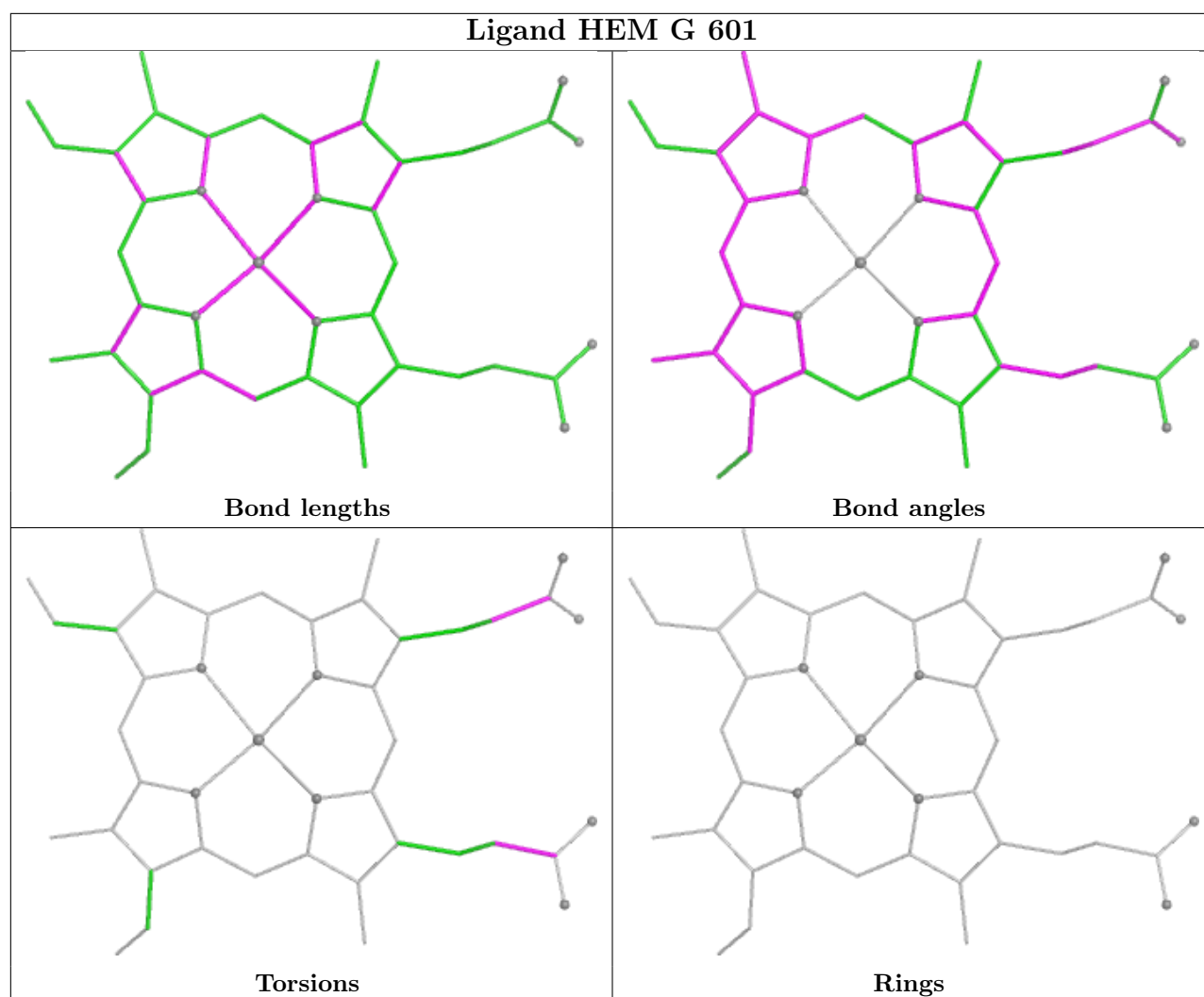
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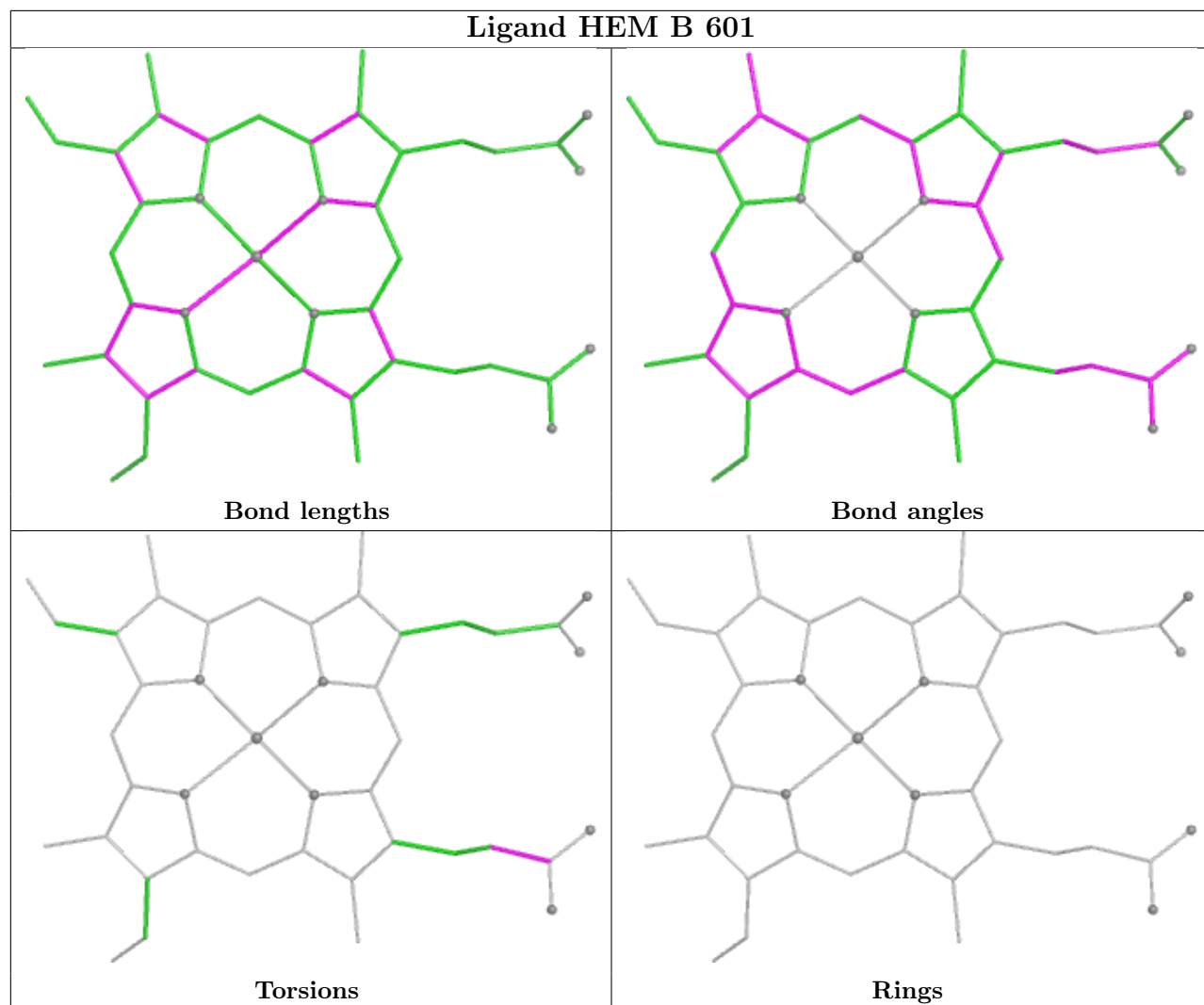
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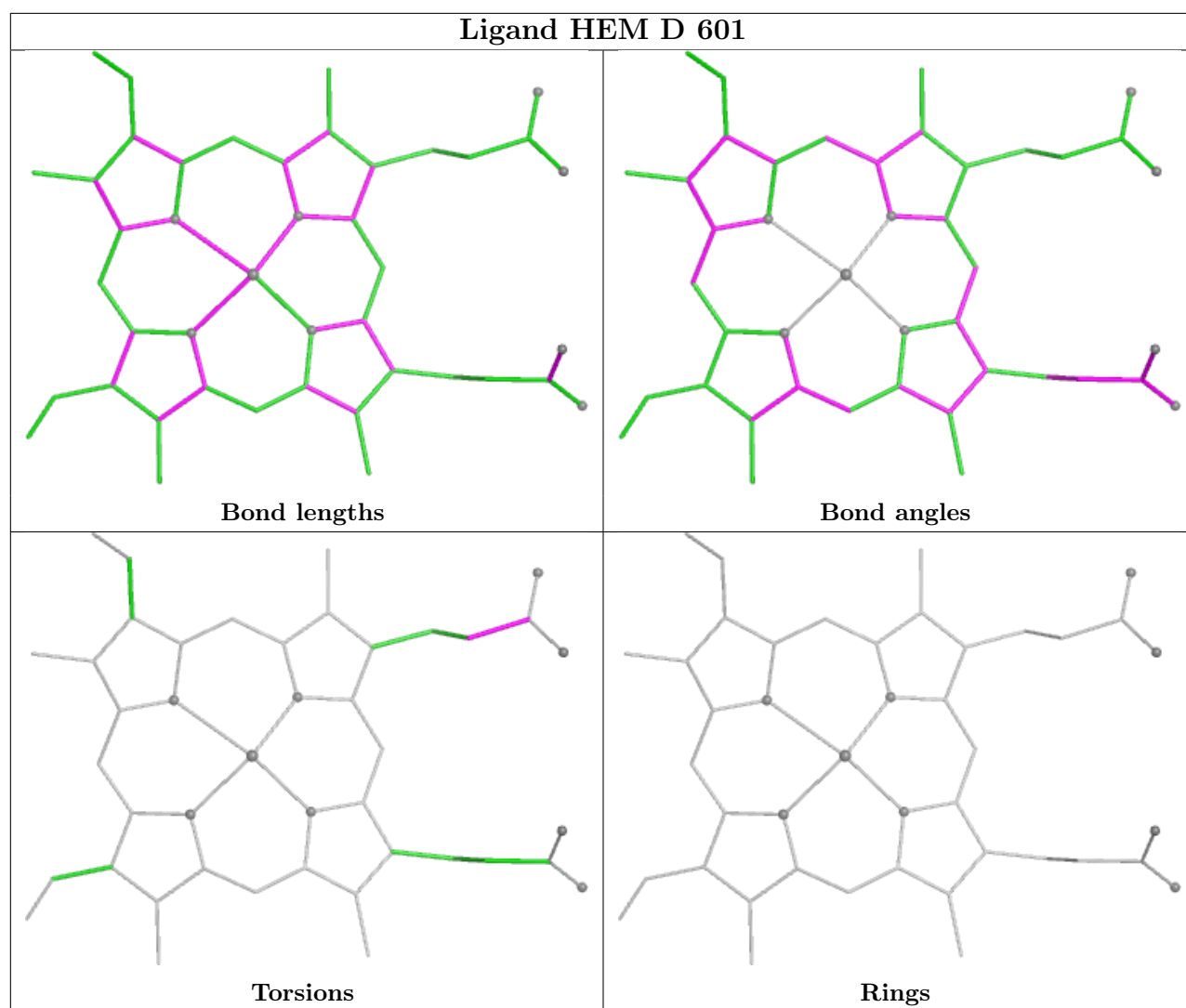
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	HEM	3	0
4	D	602	NAG	3	0

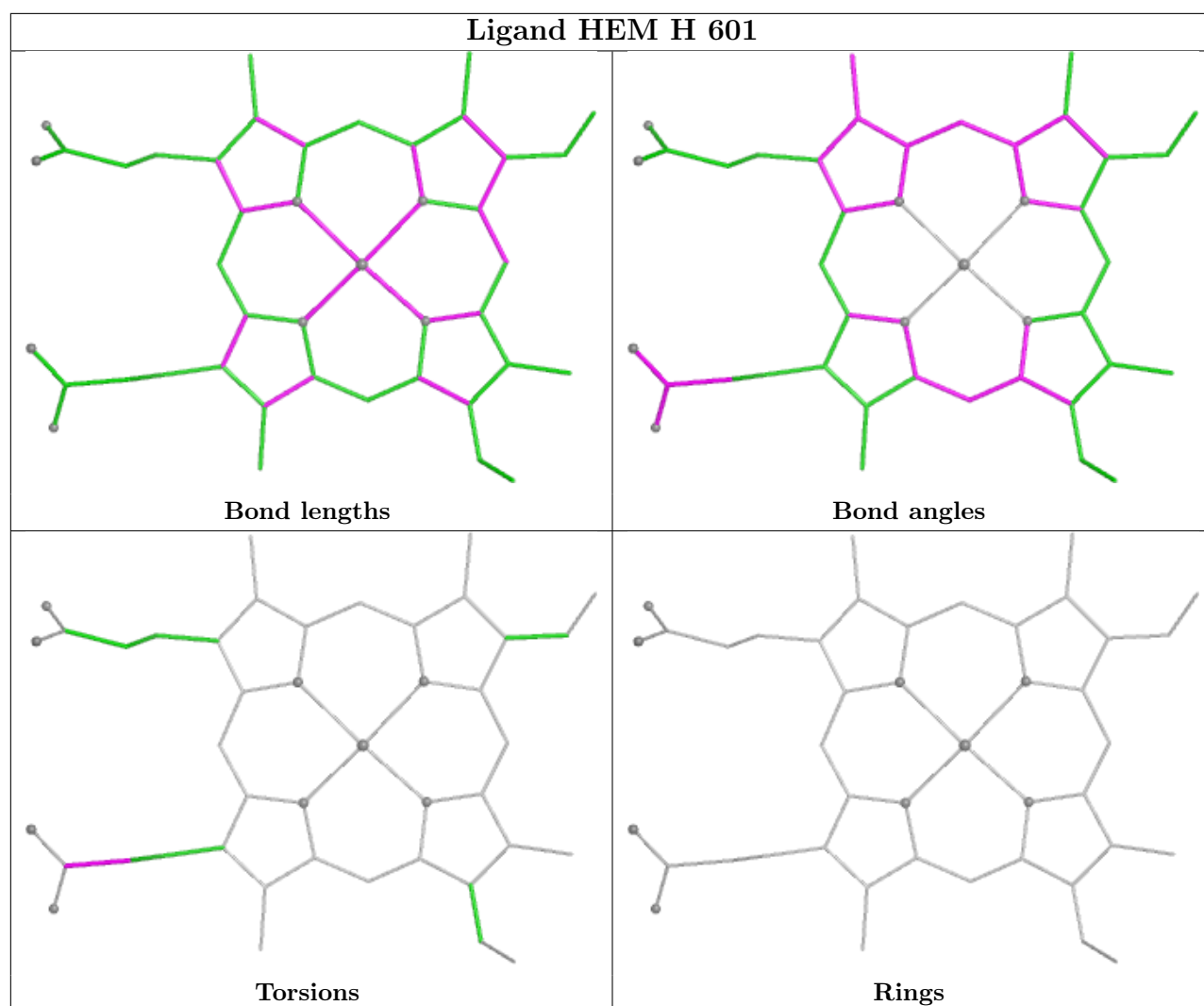
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

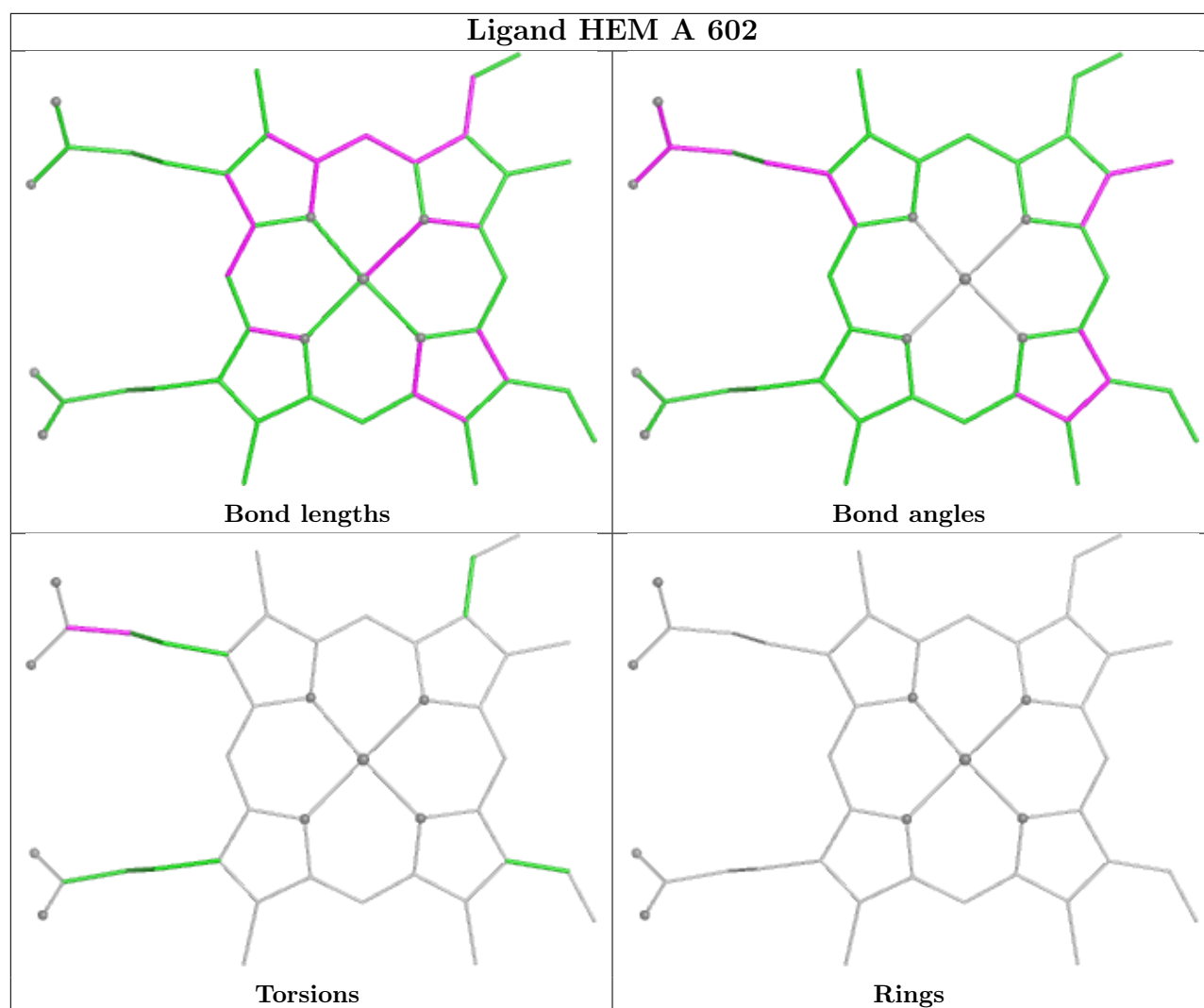


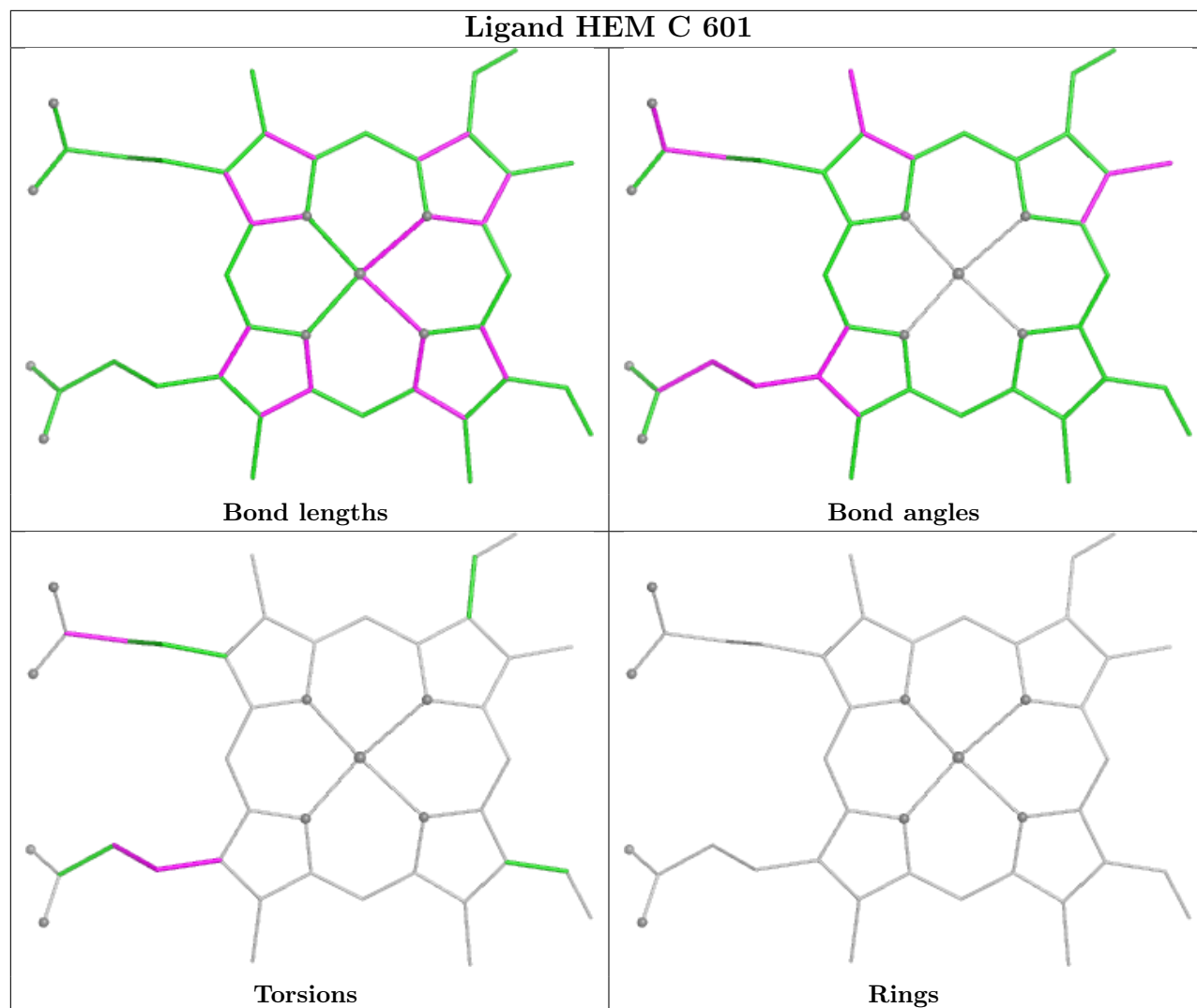


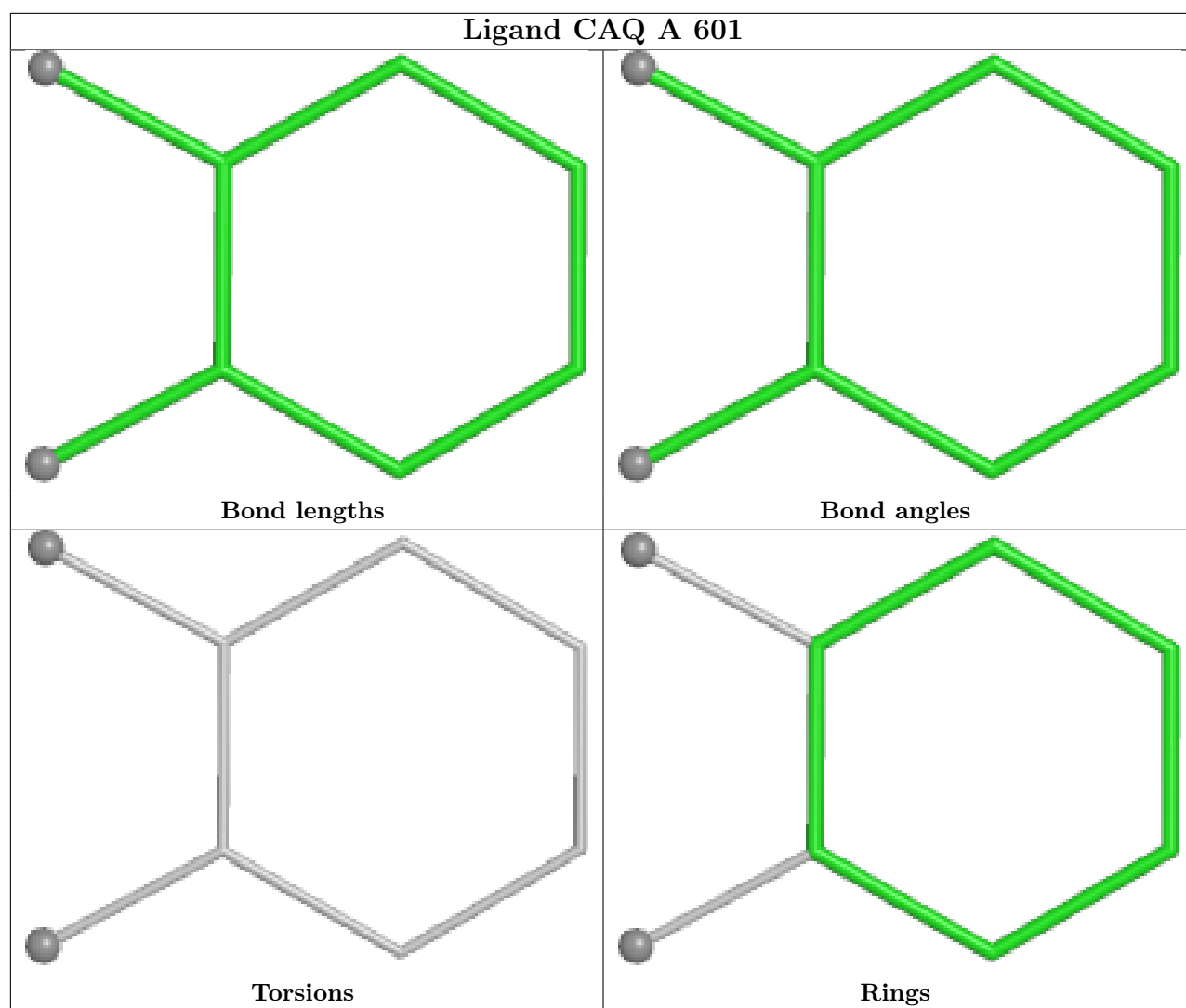


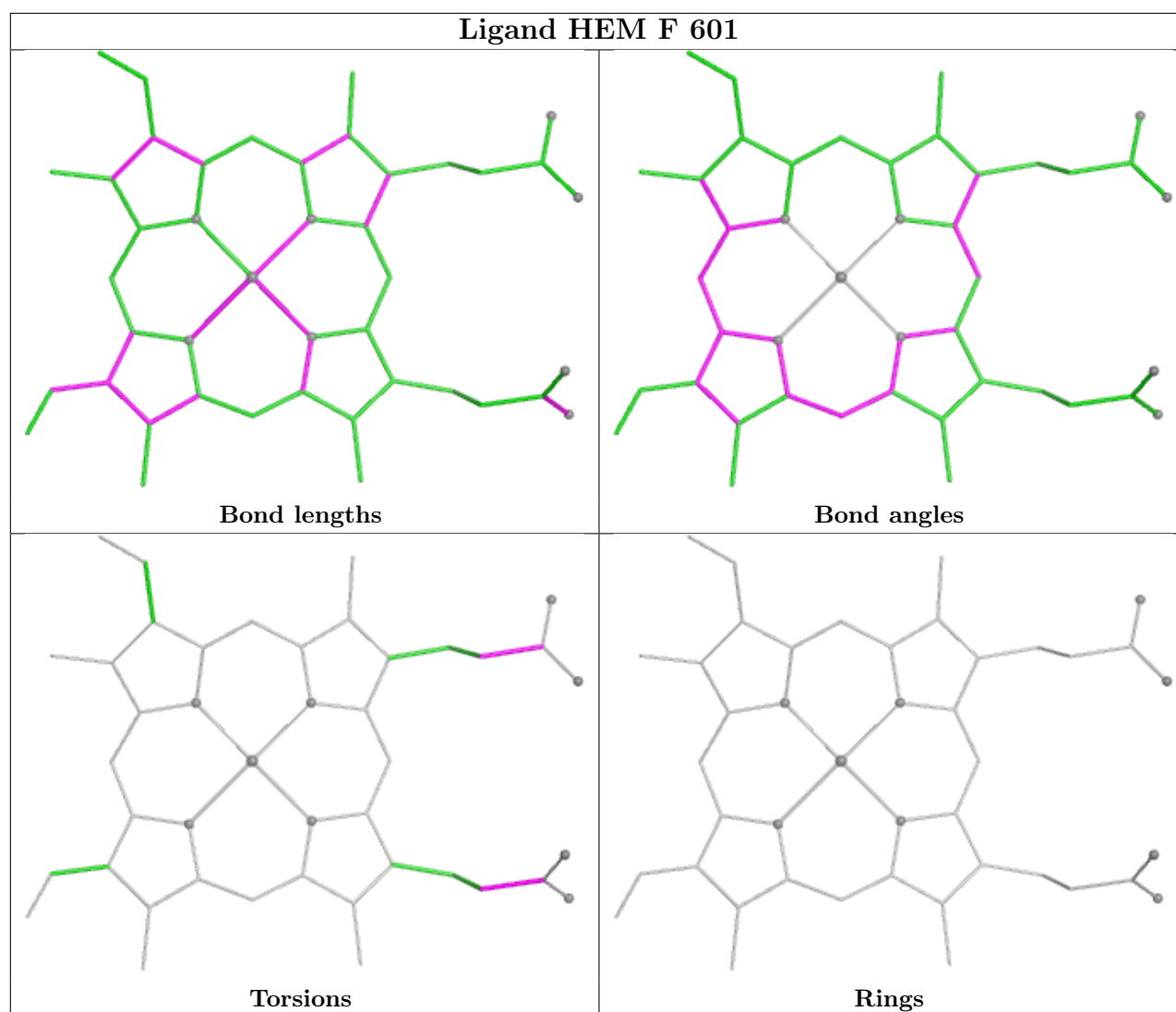












5.7 Other polymers [i](#)

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 [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	507/509 (99%)	-1.09	1 (0%) 91 92	22, 36, 58, 105	0
1	B	507/509 (99%)	-1.09	0 100 100	12, 38, 55, 79	2 (0%)
1	C	507/509 (99%)	-1.03	0 100 100	12, 40, 62, 82	2 (0%)
1	D	505/509 (99%)	-1.02	0 100 100	14, 41, 63, 86	1 (0%)
1	E	502/509 (98%)	-1.11	0 100 100	12, 32, 45, 65	3 (0%)
1	F	504/509 (99%)	-1.08	0 100 100	15, 34, 50, 87	1 (0%)
1	G	498/509 (97%)	-1.13	0 100 100	22, 34, 49, 74	1 (0%)
1	H	507/509 (99%)	-1.07	0 100 100	12, 35, 52, 85	3 (0%)
All	All	4037/4072 (99%)	-1.08	1 (0%) 100 100	12, 36, 57, 105	13 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

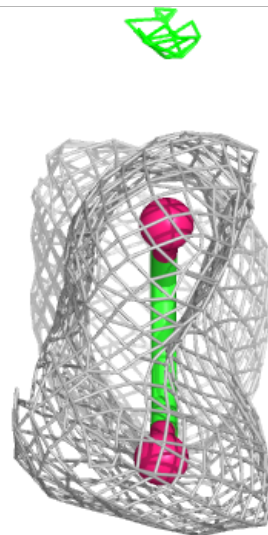
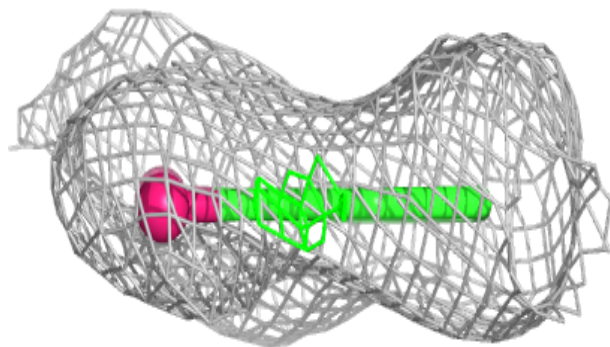
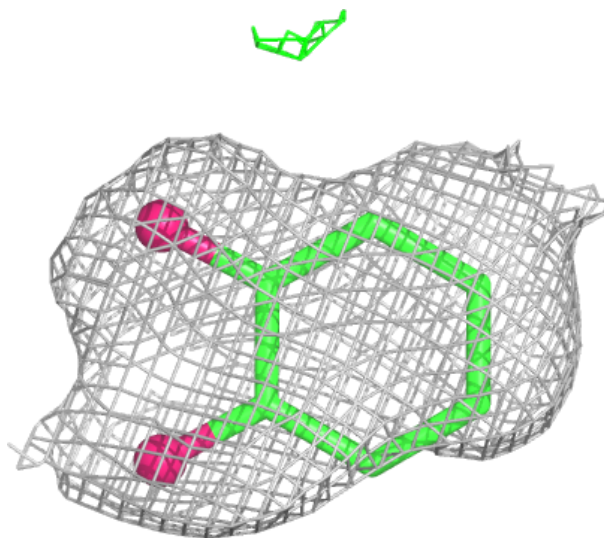
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CAQ	A	601	8/8	0.98	0.06	41,46,52,56	0
4	NAG	H	602	14/15	0.98	0.04	30,39,41,42	0
5	EDO	A	604	4/4	0.98	0.05	45,45,48,51	0
3	HEM	E	601	43/43	0.99	0.03	15,24,28,32	0
3	HEM	F	601	43/43	0.99	0.03	20,24,31,36	0
3	HEM	H	601	43/43	0.99	0.03	20,23,29,32	0
4	NAG	A	603	14/15	0.99	0.03	27,31,34,35	0
4	NAG	B	602	14/15	0.99	0.03	39,44,46,52	0
4	NAG	D	602	14/15	0.99	0.03	36,37,44,44	0
4	NAG	C	602	14/15	0.99	0.04	38,45,53,54	0
4	NAG	G	602	14/15	0.99	0.03	33,37,41,42	0
4	NAG	G	603	14/15	0.99	0.03	46,50,53,53	0
3	HEM	D	601	43/43	0.99	0.03	26,33,37,40	0
3	HEM	C	601	43/43	0.99	0.03	20,29,33,35	0
6	PEG	E	602	7/7	0.99	0.03	39,41,48,49	0
6	PEG	F	602	7/7	0.99	0.06	29,32,40,47	0
3	HEM	G	601	43/43	1.00	0.03	20,24,27,29	0
3	HEM	A	602	43/43	1.00	0.03	21,26,33,35	0
3	HEM	B	601	43/43	1.00	0.03	23,27,33,41	0

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

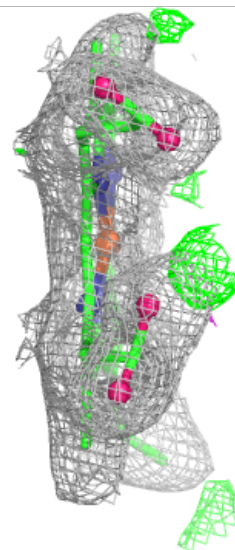
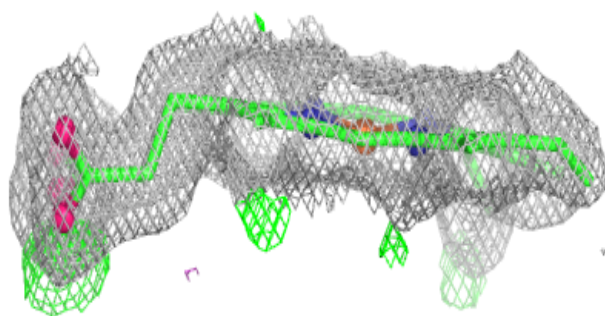
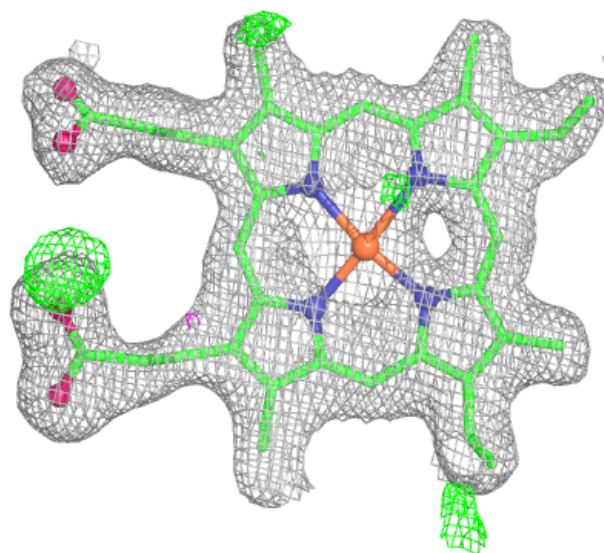
Electron density around CAQ A 601:

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



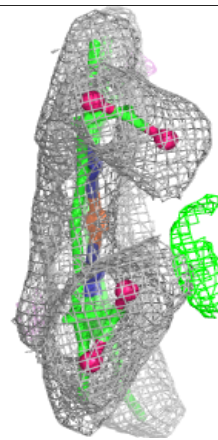
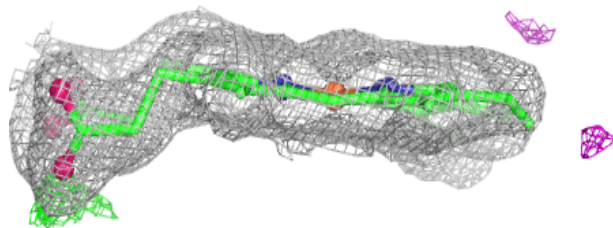
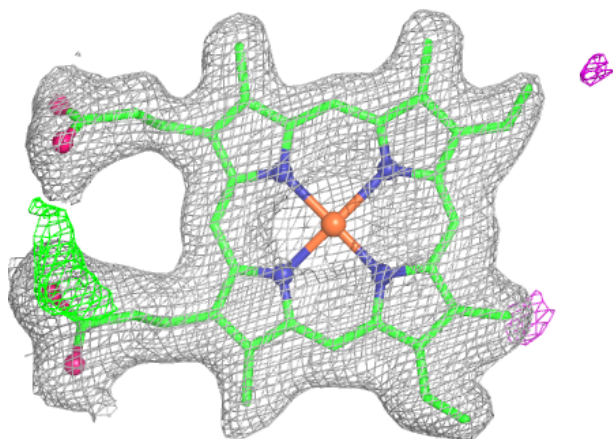
Electron density around HEM E 601:

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



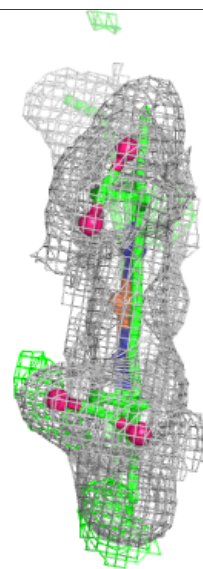
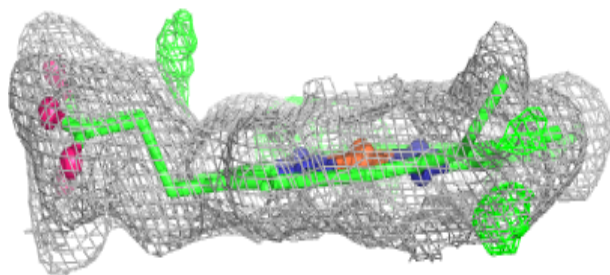
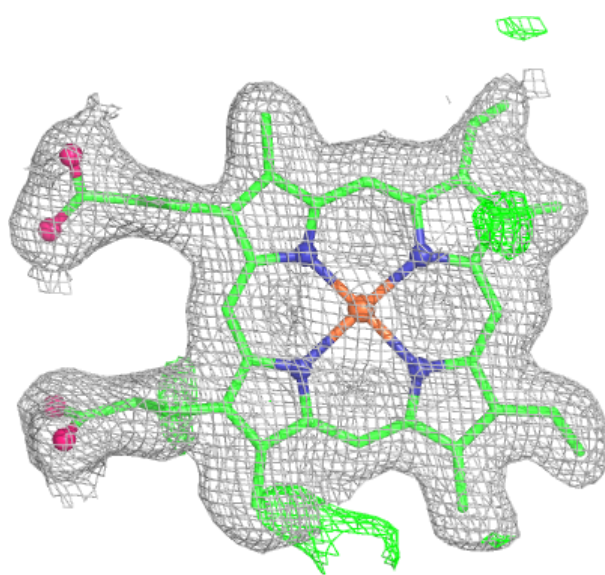
Electron density around HEM F 601:

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



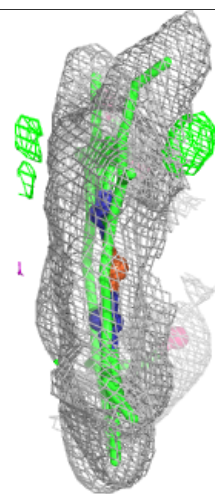
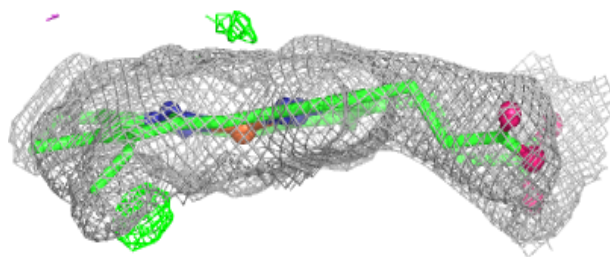
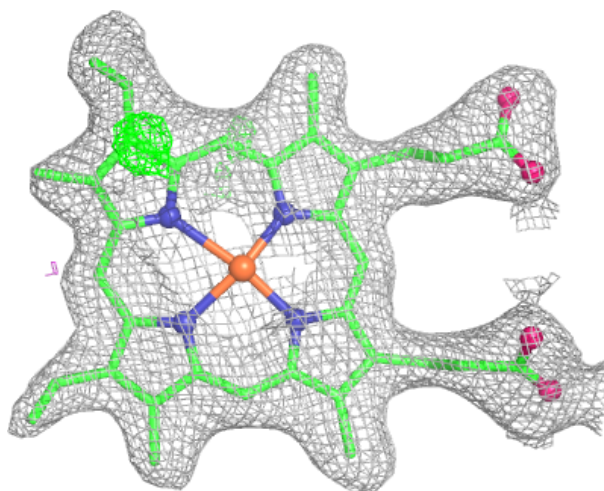
Electron density around HEM H 601:

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



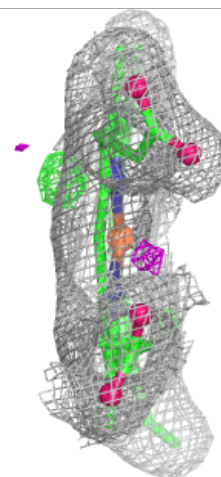
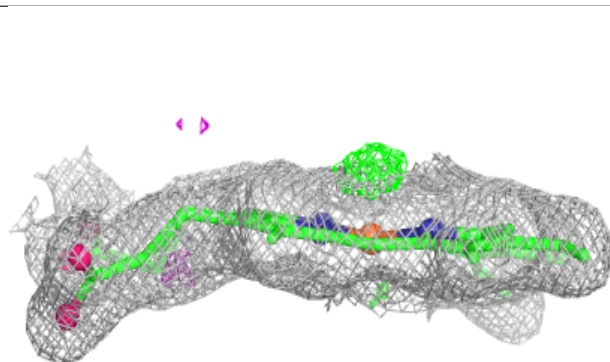
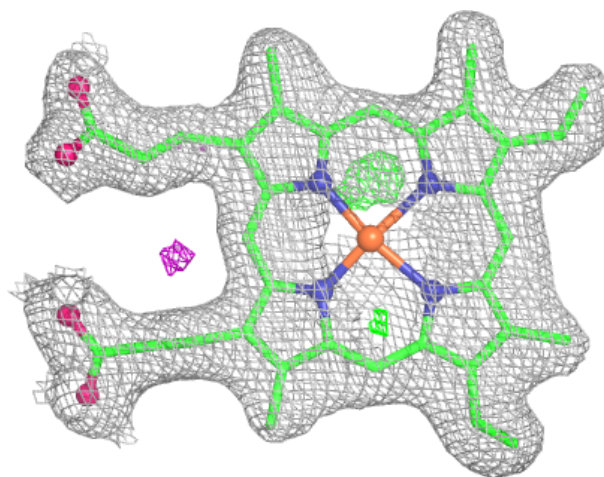
Electron density around HEM D 601:

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



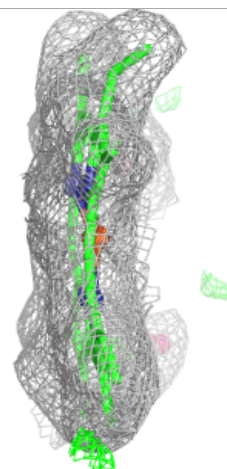
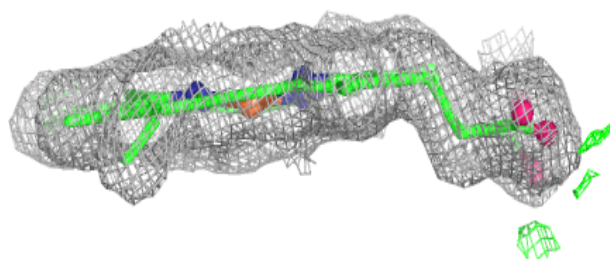
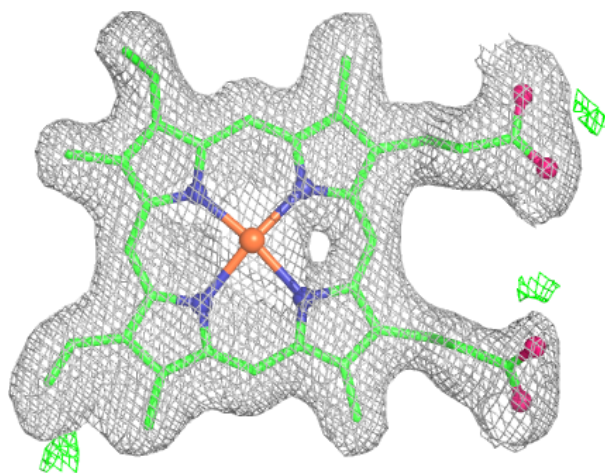
Electron density around HEM C 601:

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



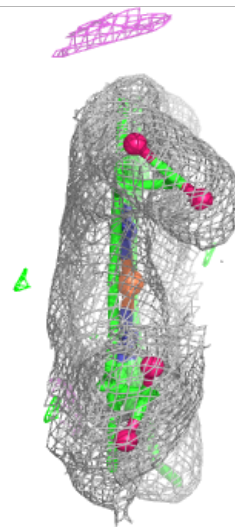
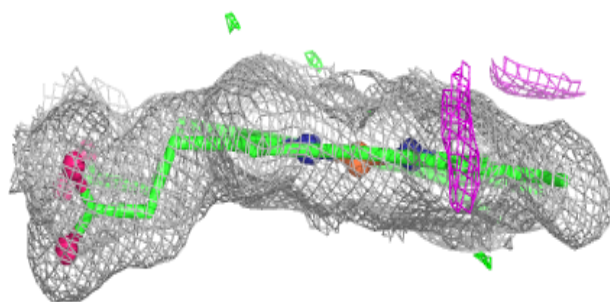
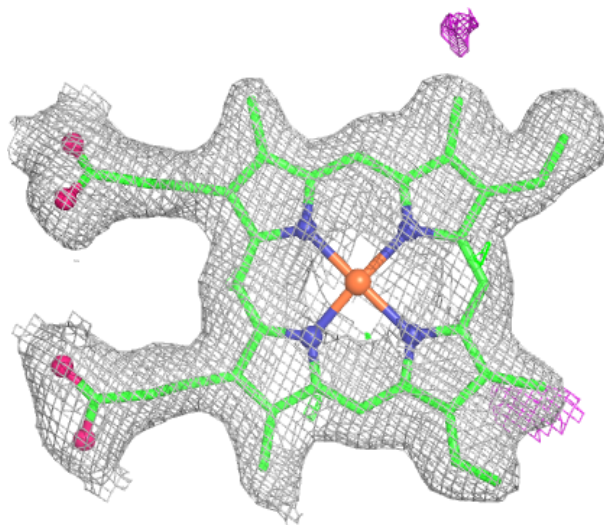
Electron density around HEM G 601:

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



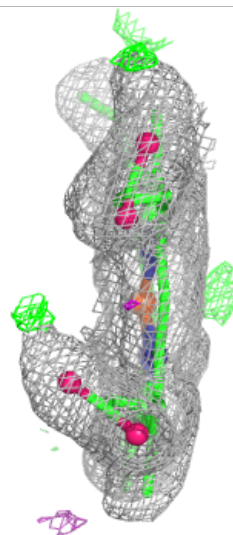
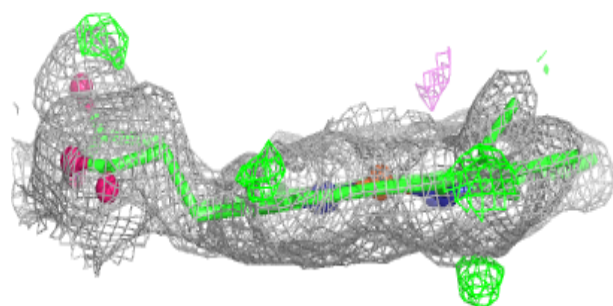
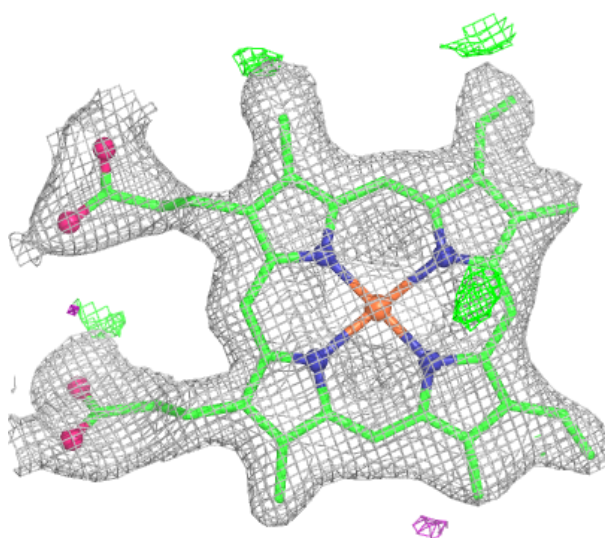
Electron density around HEM A 602:

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



Electron density around HEM B 601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.