



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:57 PM UTC

PDB ID : 3RGP / pdb_00003rgp
Title : Structural and Kinetic Analysis of the Beef liver Catalase complexed with Nitric Oxide
Authors : Purwar, N.; Schmidt, M.
Deposited on : 2011-04-08
Resolution : 1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

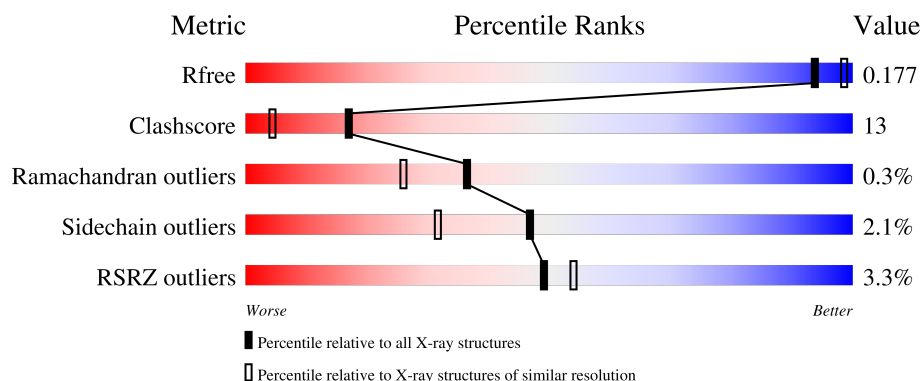
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	499	2% 74% 24% .
1	B	499	4% 72% 25% .
1	C	499	3% 75% 23% .
1	D	499	4% 78% 20% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18276 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	499	Total	C	N	O	S	0	1	0
			4019	2548	717	738	16			
1	B	499	Total	C	N	O	S	0	1	0
			4019	2548	717	738	16			
1	C	499	Total	C	N	O	S	0	1	0
			4019	2548	717	738	16			
1	D	499	Total	C	N	O	S	0	1	0
			4019	2548	717	738	16			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



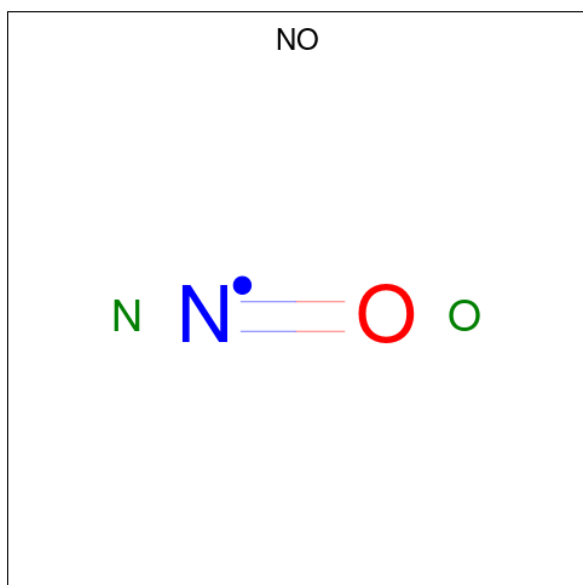
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is NITRIC OXIDE (CCD ID: NO) (formula: NO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O		
			2	1	1		
3	B	1	Total	N	O		
			2	1	1		
3	C	1	Total	N	O		
			2	1	1		
3	D	1	Total	N	O		
			2	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	516	Total	O		
			516	516		
4	B	481	Total	O		
			481	481		
4	C	504	Total	O		
			504	504		

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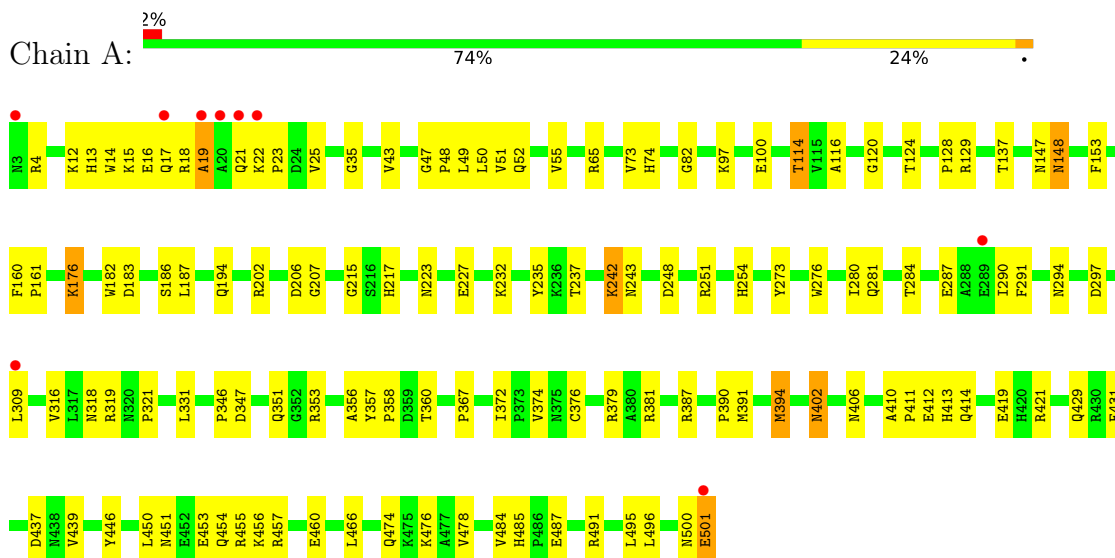
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	519	Total	O	0	0
			519	519		

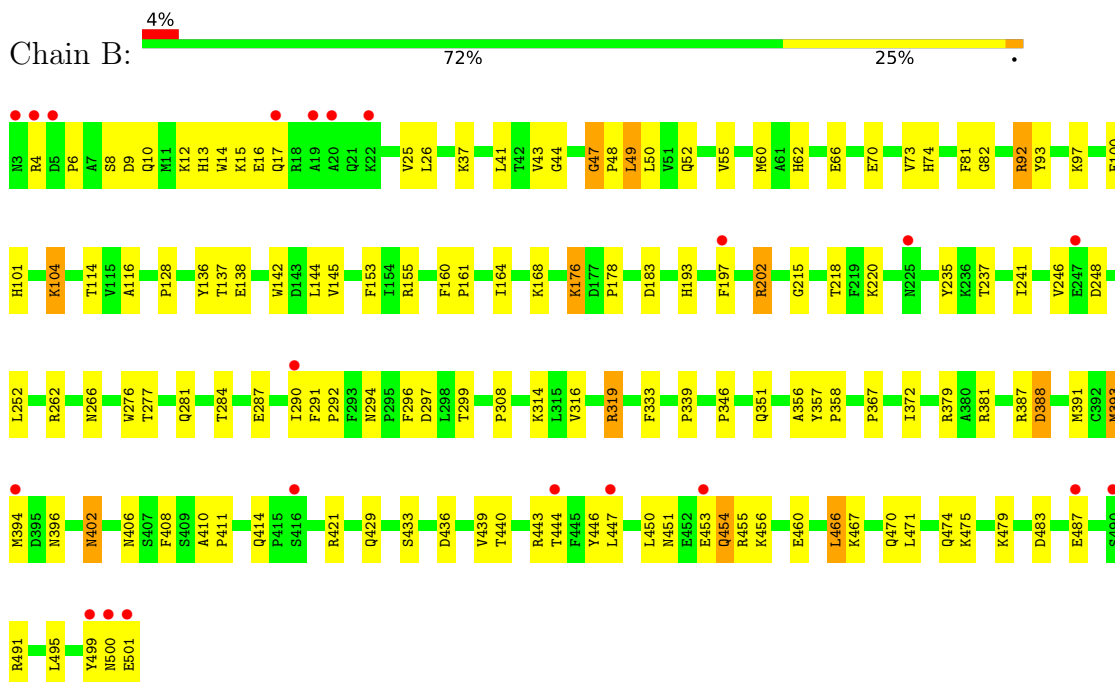
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

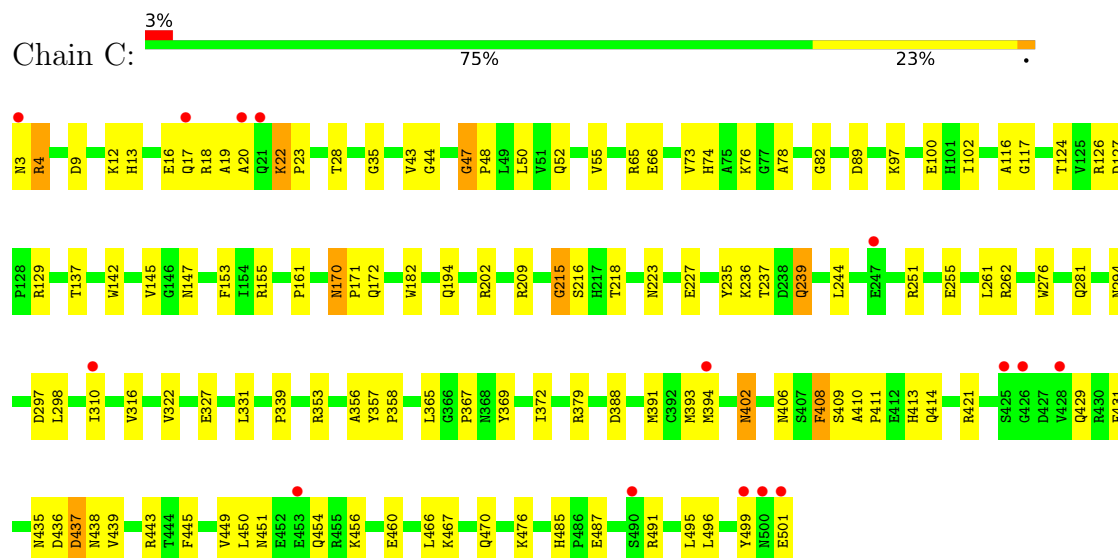
• Molecule 1: Catalase



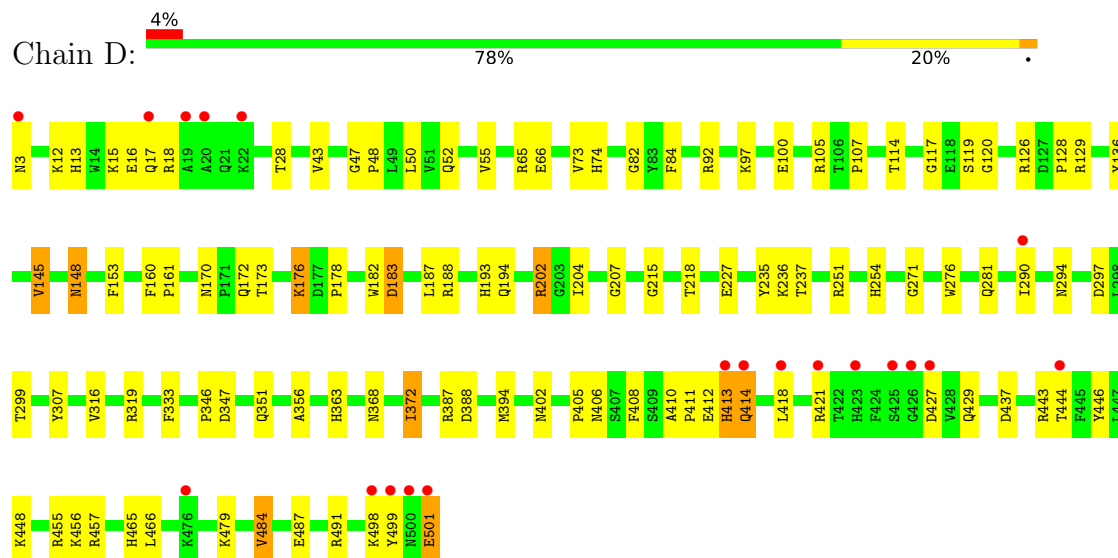
• Molecule 1: Catalase



• Molecule 1: Catalase



• Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.11Å 139.94Å 228.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.30 – 1.88 40.30 – 1.88	Depositor EDS
% Data completeness (in resolution range)	92.0 (40.30-1.88) 92.1 (40.30-1.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.214 0.179 , 0.177	Depositor DCC
R_{free} test set	10359 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18276	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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, NO

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	0.38	0/4149	0.92	16/5637 (0.3%)
1	B	0.36	0/4149	0.92	19/5637 (0.3%)
1	C	0.38	0/4149	0.92	22/5637 (0.4%)
1	D	0.37	0/4149	0.93	20/5637 (0.4%)
All	All	0.37	0/16596	0.92	77/22548 (0.3%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ALA	N-CA-C	8.20	120.95	111.11
1	B	356	ALA	N-CA-C	8.05	121.07	111.33
1	A	372	ILE	N-CA-C	-8.02	101.09	108.95
1	D	356	ALA	N-CA-C	7.96	120.67	111.11
1	C	356	ALA	N-CA-C	7.74	120.70	111.33
1	B	436	ASP	N-CA-C	-7.37	101.34	110.41
1	C	215	GLY	N-CA-C	-7.36	105.54	114.66
1	D	215	GLY	N-CA-C	-7.26	105.66	114.66
1	A	215	GLY	N-CA-C	-7.24	105.68	114.66
1	B	215	GLY	N-CA-C	-7.21	105.72	114.66
1	D	388	ASP	N-CA-C	7.18	118.62	108.00
1	C	388	ASP	N-CA-C	6.57	117.72	108.00
1	C	47	GLY	CA-C-N	6.49	126.40	119.85
1	C	47	GLY	C-N-CA	6.49	126.40	119.85
1	A	55	VAL	N-CA-C	-6.46	104.19	110.72
1	D	281	GLN	N-CA-C	-6.36	99.35	109.59
1	D	28	THR	N-CA-C	-6.26	102.46	110.53
1	D	128	PRO	N-CA-C	-6.25	102.47	111.22
1	D	55	VAL	N-CA-C	-6.22	104.68	110.53
1	D	372	ILE	N-CA-C	-6.21	102.87	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ASP	N-CA-C	-6.14	104.50	111.14
1	D	183	ASP	N-CA-C	-6.04	104.61	111.14
1	C	170	ASN	CA-C-N	5.96	126.38	119.47
1	C	170	ASN	C-N-CA	5.96	126.38	119.47
1	C	281	GLN	N-CA-C	-5.94	100.03	109.59
1	D	484	VAL	N-CA-C	-5.91	105.09	110.82
1	B	47	GLY	CA-C-N	5.85	126.18	119.92
1	B	47	GLY	C-N-CA	5.85	126.18	119.92
1	A	281	GLN	N-CA-C	-5.84	100.19	109.59
1	B	116	ALA	N-CA-C	5.84	118.87	111.69
1	B	176	LYS	N-CA-C	-5.84	101.77	110.23
1	D	307	TYR	CA-C-N	5.80	125.73	119.76
1	D	307	TYR	C-N-CA	5.80	125.73	119.76
1	B	372	ILE	N-CA-C	-5.79	103.27	108.95
1	D	117	GLY	N-CA-C	5.71	118.49	111.93
1	B	55	VAL	N-CA-C	-5.69	104.97	110.72
1	A	128	PRO	N-CA-C	-5.66	103.29	111.22
1	C	372	ILE	N-CA-C	-5.64	103.42	108.95
1	B	439	VAL	N-CA-C	5.62	121.04	109.34
1	C	322	VAL	N-CA-C	-5.54	107.04	111.81
1	C	408	PHE	N-CA-C	5.54	119.61	112.41
1	D	218	THR	N-CA-C	-5.49	101.03	109.76
1	A	114	THR	N-CA-C	-5.46	101.39	109.86
1	C	117	GLY	N-CA-C	5.45	118.19	111.93
1	B	183	ASP	N-CA-C	-5.45	105.26	111.14
1	C	124	THR	N-CA-C	5.42	118.22	110.68
1	C	28	THR	N-CA-C	-5.41	102.89	110.35
1	D	114	THR	N-CA-C	-5.39	101.48	109.94
1	D	119	SER	N-CA-C	5.38	118.64	111.75
1	C	394	MET	CB-CA-C	-5.35	109.43	115.79
1	A	484	VAL	N-CA-C	-5.33	105.64	110.82
1	B	388	ASP	N-CA-C	5.33	117.98	109.02
1	D	176	LYS	N-CA-C	-5.33	103.11	110.35
1	C	55	VAL	N-CA-C	-5.33	105.34	110.72
1	C	439	VAL	N-CA-C	5.30	120.36	109.34
1	B	218	THR	N-CA-C	-5.30	100.67	109.46
1	B	153	PHE	N-CA-C	5.30	117.97	111.82
1	A	439	VAL	N-CA-C	5.27	120.29	109.34
1	C	116	ALA	N-CA-C	5.24	118.14	111.69
1	D	188	ARG	CA-C-N	5.24	124.90	119.56
1	D	188	ARG	C-N-CA	5.24	124.90	119.56
1	B	44	GLY	CA-C-N	5.24	124.86	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	GLY	C-N-CA	5.24	124.86	119.05
1	A	176	LYS	N-CA-C	-5.23	102.65	110.23
1	D	145	VAL	N-CA-C	5.19	111.76	106.21
1	B	440	THR	N-CA-C	5.15	117.29	111.11
1	B	128	PRO	N-CA-C	-5.13	104.04	111.22
1	B	281	GLN	N-CA-C	-5.10	101.38	109.59
1	C	44	GLY	CA-C-N	5.09	125.12	119.32
1	C	44	GLY	C-N-CA	5.09	125.12	119.32
1	A	116	ALA	N-CA-C	5.07	117.92	111.69
1	C	409	SER	N-CA-C	5.05	118.74	112.58
1	A	291	PHE	CA-C-N	5.04	124.71	119.56
1	A	291	PHE	C-N-CA	5.04	124.71	119.56
1	C	218	THR	N-CA-C	-5.04	101.09	109.46
1	A	394	MET	CB-CA-C	-5.03	110.76	116.54
1	A	124	THR	N-CA-C	5.02	117.66	110.68

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	4019	0	3847	102	0
1	B	4019	0	3847	129	0
1	C	4019	0	3847	110	0
1	D	4019	0	3847	100	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	516	0	0	23	0
4	B	481	0	0	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	504	0	0	34	1
4	D	519	0	0	32	0
All	All	18276	0	15508	403	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 13.

All (403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:LEU:HA	1:C:454:GLN:HE21	1.20	1.03
1:B:197:PHE:HB3	4:B:970:HOH:O	1.65	0.94
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.19	0.91
1:B:351:GLN:HE22	1:D:52:GLN:HE21	1.24	0.84
1:A:456:LYS:HE2	4:A:1802:HOH:O	1.78	0.83
1:D:176:LYS:HG3	4:D:1931:HOH:O	1.77	0.82
4:B:1385:HOH:O	1:D:418:LEU:HD11	1.79	0.81
1:C:236:LYS:HG3	4:C:1294:HOH:O	1.81	0.80
1:B:104:LYS:HE2	4:B:1323:HOH:O	1.79	0.79
1:B:319:ARG:HD3	4:B:572:HOH:O	1.83	0.78
1:B:26:LEU:HD21	1:B:37:LYS:HE3	1.65	0.78
1:C:450:LEU:HA	1:C:454:GLN:NE2	1.96	0.77
1:C:3:ASN:HB3	4:C:1941:HOH:O	1.85	0.77
1:B:37:LYS:HG2	4:B:511:HOH:O	1.84	0.76
1:A:412:GLU:HG3	4:A:1399:HOH:O	1.85	0.76
1:D:92:ARG:HD3	4:D:1616:HOH:O	1.85	0.75
1:B:62:HIS:HE1	1:D:368:ASN:ND2	1.85	0.74
1:A:419:GLU:HG2	4:A:1670:HOH:O	1.87	0.73
1:C:262:ARG:NH1	4:C:986:HOH:O	2.18	0.73
1:C:155:ARG:HH12	1:C:438:ASN:HD22	1.37	0.72
1:A:456:LYS:O	1:A:460:GLU:HG3	1.89	0.72
1:C:261:LEU:HD22	4:C:2016:HOH:O	1.89	0.72
1:D:92:ARG:HG2	4:D:771:HOH:O	1.90	0.71
1:C:379:ARG:HD3	4:C:1292:HOH:O	1.90	0.71
1:B:17:GLN:HG3	4:B:1818:HOH:O	1.90	0.71
1:B:262:ARG:HG3	4:B:595:HOH:O	1.89	0.71
1:A:381:ARG:HD2	4:A:1822:HOH:O	1.90	0.70
1:B:491:ARG:O	1:B:495:LEU:HD23	1.92	0.70
1:C:437:ASP:N	4:C:842:HOH:O	2.24	0.70
1:C:451:ASN:OD1	1:C:454:GLN:HG2	1.91	0.70
1:D:202:ARG:HG3	4:D:741:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2020:HOH:O	1:D:363:HIS:HD2	1.74	0.69
1:A:421:ARG:HD3	1:B:429:GLN:NE2	2.08	0.69
1:C:262:ARG:HD2	4:C:986:HOH:O	1.92	0.69
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.56	0.69
4:A:1744:HOH:O	1:B:421:ARG:HD3	1.93	0.69
1:C:450:LEU:CA	1:C:454:GLN:HE21	2.01	0.68
1:C:476:LYS:NZ	1:C:476:LYS:HB3	2.08	0.68
1:B:202:ARG:HH21	1:B:241:ILE:CD1	2.06	0.68
1:A:50:LEU:HD13	1:B:50:LEU:HD13	1.76	0.68
1:B:62:HIS:HD2	4:B:1354:HOH:O	1.76	0.67
1:B:92:ARG:HD2	1:B:93:TYR:CE2	2.29	0.67
1:B:26:LEU:HD21	1:B:37:LYS:CE	2.24	0.67
1:A:429:GLN:HB3	1:B:421:ARG:HD2	1.77	0.67
1:C:155:ARG:HH22	1:C:438:ASN:HD21	1.40	0.67
1:C:445:PHE:CZ	1:C:450:LEU:HD11	2.29	0.66
1:B:393:MET:HE3	1:D:372:ILE:HA	1.76	0.66
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.30	0.66
1:D:429:GLN:HB2	4:D:1179:HOH:O	1.94	0.66
1:D:487:GLU:O	1:D:491:ARG:HG3	1.96	0.66
1:D:448:LYS:HA	1:D:448:LYS:HE2	1.77	0.65
1:C:262:ARG:CD	4:C:986:HOH:O	2.45	0.65
1:B:466:LEU:HD22	1:B:474:GLN:HG2	1.77	0.65
1:C:485:HIS:CD2	1:C:487:GLU:HB3	2.32	0.65
1:A:491:ARG:O	1:A:495:LEU:HD23	1.97	0.65
1:D:170:ASN:ND2	1:D:172:GLN:H	1.95	0.65
2:B:1:HEM:HBA1	4:B:1360:HOH:O	1.96	0.65
1:C:487:GLU:O	1:C:491:ARG:HG3	1.97	0.65
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.10	0.64
1:D:227:GLU:OE1	4:D:1359:HOH:O	2.14	0.64
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.28	0.64
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.78	0.64
1:D:456:LYS:HE3	4:D:1982:HOH:O	1.96	0.64
1:B:220:LYS:NZ	4:B:544:HOH:O	2.30	0.63
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.28	0.63
1:B:262:ARG:HD2	4:B:638:HOH:O	1.97	0.62
1:A:206:ASP:CB	1:A:242:LYS:HD2	2.28	0.62
1:A:451:ASN:H	1:A:454:GLN:HE21	1.46	0.62
1:B:37:LYS:H	1:D:413:HIS:CE1	2.18	0.62
1:B:450:LEU:HB3	1:B:454:GLN:HG3	1.80	0.62
1:A:421:ARG:NH2	4:A:1747:HOH:O	2.31	0.62
1:C:155:ARG:HH12	1:C:438:ASN:ND2	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:THR:HG21	4:B:1647:HOH:O	1.98	0.61
1:B:456:LYS:O	1:B:460:GLU:HG3	2.00	0.61
1:C:485:HIS:HD2	1:C:487:GLU:HB3	1.66	0.61
1:D:271:GLY:HA2	4:D:1542:HOH:O	1.99	0.61
1:D:479:LYS:HD3	1:D:479:LYS:C	2.26	0.61
1:D:319:ARG:NH1	4:D:626:HOH:O	2.24	0.60
1:A:12:LYS:O	1:A:16:GLU:HG3	2.01	0.60
1:B:308:PRO:HB3	4:B:1877:HOH:O	2.01	0.60
1:C:19:ALA:O	1:C:20:ALA:HB3	2.01	0.60
1:A:186:SER:HB2	1:A:476:LYS:HG2	1.83	0.60
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.66	0.60
1:A:379:ARG:HD3	4:A:1773:HOH:O	2.00	0.59
1:D:3:ASN:HB2	4:D:1274:HOH:O	2.01	0.59
1:B:284:THR:OG1	1:B:287:GLU:HG3	2.03	0.59
1:A:414:GLN:CD	4:A:1146:HOH:O	2.46	0.59
1:B:402:ASN:C	1:B:402:ASN:HD22	2.09	0.59
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.85	0.59
1:A:376[A]:CYS:SG	4:A:1508:HOH:O	2.56	0.58
1:B:101:HIS:O	1:B:104:LYS:HB2	2.03	0.58
1:C:443:ARG:HB2	4:C:1010:HOH:O	2.02	0.58
1:A:351:GLN:HG3	4:A:730:HOH:O	2.03	0.58
1:D:12:LYS:O	1:D:16:GLU:HG3	2.02	0.58
1:A:206:ASP:HB2	1:A:242:LYS:HD2	1.86	0.58
1:B:202:ARG:HH21	1:B:241:ILE:HD13	1.67	0.58
1:B:164:ILE:O	1:B:168:LYS:HG2	2.03	0.58
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.04	0.58
1:C:251:ARG:O	1:C:255:GLU:HG3	2.03	0.57
1:B:499:TYR:C	1:B:501:GLU:H	2.11	0.57
1:B:388:ASP:H	1:B:396:ASN:HD21	1.51	0.57
1:C:435:ASN:C	4:C:842:HOH:O	2.47	0.57
1:C:12:LYS:O	1:C:16:GLU:HG3	2.03	0.57
1:C:435:ASN:HB3	4:C:2012:HOH:O	2.05	0.57
1:D:498:LYS:O	1:D:498:LYS:HD3	2.04	0.57
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.69	0.57
1:C:161:PRO:HG2	4:C:541:HOH:O	2.05	0.57
1:D:498:LYS:O	1:D:501:GLU:HG3	2.05	0.57
1:A:414:GLN:NE2	4:A:1146:HOH:O	2.38	0.56
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.35	0.56
1:C:436:ASP:N	4:C:842:HOH:O	2.39	0.56
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.87	0.56
1:D:15:LYS:O	1:D:18:ARG:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLN:NE2	4:B:1621:HOH:O	2.39	0.56
1:D:251:ARG:NH1	4:D:1783:HOH:O	2.34	0.56
1:A:294:ASN:HB3	1:A:297:ASP:HB2	1.88	0.56
1:D:290:ILE:HG22	1:D:290:ILE:O	2.05	0.56
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.70	0.56
1:A:187:LEU:HD21	4:B:2025:HOH:O	2.05	0.56
1:A:202:ARG:CZ	4:A:1740:HOH:O	2.53	0.56
1:B:487:GLU:O	1:B:491:ARG:HG3	2.06	0.56
1:B:453:GLU:CB	4:B:1364:HOH:O	2.54	0.55
1:C:97:LYS:O	1:C:100:GLU:HB2	2.06	0.55
1:A:248:ASP:HA	1:A:251:ARG:NH1	2.21	0.55
1:A:429:GLN:CB	1:B:421:ARG:HD2	2.35	0.55
1:B:41:LEU:HD12	1:B:50:LEU:HB2	1.89	0.55
1:C:18:ARG:NE	4:C:592:HOH:O	2.25	0.55
1:C:485:HIS:CD2	1:C:487:GLU:H	2.24	0.55
1:A:394:MET:HE3	4:A:1025:HOH:O	2.07	0.55
1:A:453:GLU:CG	1:A:457:ARG:HH12	2.20	0.55
1:B:14:TRP:O	1:B:17:GLN:HG2	2.07	0.55
1:B:414:GLN:NE2	4:B:1972:HOH:O	2.38	0.55
1:A:51:VAL:HG21	1:B:49:LEU:HD13	1.87	0.55
1:D:129:ARG:H	1:D:148:ASN:ND2	2.04	0.55
1:D:170:ASN:HD22	1:D:173:THR:H	1.55	0.55
1:D:444:THR:HG21	4:D:1230:HOH:O	2.06	0.55
1:D:120:GLY:N	4:D:638:HOH:O	2.08	0.54
1:C:89:ASP:HB2	1:C:102:ILE:HD11	1.89	0.54
1:C:456:LYS:O	1:C:460:GLU:HG3	2.07	0.54
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.87	0.54
1:D:465:HIS:CD2	4:D:1276:HOH:O	2.60	0.54
1:B:277:THR:OG1	1:B:314:LYS:HE3	2.07	0.54
1:B:25:VAL:HG13	1:D:414:GLN:HG3	1.89	0.54
1:C:294:ASN:HB3	1:C:297:ASP:HB2	1.89	0.54
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.07	0.54
1:C:153:PHE:CE1	1:C:194:GLN:HG3	2.43	0.54
1:B:319:ARG:HH11	1:B:319:ARG:HB3	1.72	0.54
1:D:82:GLY:HA3	1:D:316:VAL:O	2.08	0.54
1:D:13:HIS:O	1:D:17:GLN:HG3	2.08	0.54
1:D:170:ASN:HD22	1:D:172:GLN:H	1.56	0.53
1:B:136:TYR:O	1:B:379:ARG:HG3	2.08	0.53
1:A:248:ASP:HA	1:A:251:ARG:HH12	1.73	0.53
1:B:475:LYS:NZ	1:B:475:LYS:HB3	2.23	0.53
1:B:262:ARG:NH2	4:B:1356:HOH:O	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:O	1:A:21:GLN:HB3	2.08	0.53
1:C:142:TRP:HB2	1:C:339:PRO:HD3	1.91	0.53
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.91	0.53
1:D:43:VAL:HG13	1:D:43:VAL:O	2.09	0.53
1:D:498:LYS:HD3	1:D:498:LYS:C	2.34	0.52
1:C:236:LYS:CE	4:C:664:HOH:O	2.57	0.52
1:A:487:GLU:O	1:A:491:ARG:HG3	2.08	0.52
1:B:82:GLY:HA3	1:B:316:VAL:O	2.10	0.52
1:B:97:LYS:O	1:B:100:GLU:HB2	2.09	0.52
1:D:427:ASP:HB2	1:D:429:GLN:HE21	1.75	0.52
1:B:92:ARG:HD2	1:B:93:TYR:CZ	2.45	0.52
1:B:138:GLU:H	1:B:138:GLU:CD	2.18	0.52
1:A:17:GLN:NE2	4:A:1631:HOH:O	2.43	0.52
1:A:309:LEU:HD23	4:A:1499:HOH:O	2.09	0.52
1:D:97:LYS:O	1:D:100:GLU:HB2	2.09	0.52
1:A:429:GLN:HG2	1:A:431:PHE:CZ	2.45	0.52
1:C:48:PRO:HB2	1:D:50:LEU:HD22	1.91	0.52
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.91	0.52
1:A:387:ARG:O	1:C:66:GLU:HG2	2.10	0.51
1:D:193:HIS:HE1	4:D:1085:HOH:O	1.93	0.51
1:A:242:LYS:HD3	1:A:243:ASN:N	2.25	0.51
1:B:391:MET:HE3	1:B:393:MET:HE1	1.92	0.51
1:A:43:VAL:O	1:A:43:VAL:HG13	2.10	0.51
1:B:92:ARG:HD2	1:B:93:TYR:CD2	2.43	0.51
1:B:168:LYS:HB3	4:B:610:HOH:O	2.10	0.51
1:B:248:ASP:O	1:B:252:LEU:HD13	2.10	0.51
1:B:52:GLN:HB2	4:D:505:HOH:O	2.10	0.51
1:A:13:HIS:HD2	4:A:578:HOH:O	1.94	0.51
4:A:563:HOH:O	1:C:52:GLN:HG3	2.11	0.51
1:B:176:LYS:NZ	4:B:2022:HOH:O	2.21	0.51
1:C:4:ARG:HD3	1:C:9:ASP:OD1	2.10	0.51
1:B:451:ASN:OD1	1:B:454:GLN:HG2	2.11	0.51
1:A:453:GLU:CD	4:A:2004:HOH:O	2.54	0.50
1:B:467:LYS:HD3	1:B:499:TYR:CG	2.46	0.50
1:C:261:LEU:CD2	4:C:2016:HOH:O	2.50	0.50
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.75	0.50
1:B:13:HIS:HD2	4:B:575:HOH:O	1.93	0.50
1:B:453:GLU:HB2	4:B:1364:HOH:O	2.12	0.50
1:D:394:MET:CE	4:D:1088:HOH:O	2.60	0.50
1:B:74:HIS:HA	1:B:114:THR:O	2.11	0.49
1:D:73:VAL:O	1:D:74:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG13	1:C:414:GLN:HG2	1.93	0.49
1:A:402:ASN:C	1:A:402:ASN:HD22	2.19	0.49
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.94	0.49
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.94	0.49
1:D:148:ASN:H	1:D:148:ASN:HD22	1.59	0.49
1:B:246:VAL:HG23	4:B:1464:HOH:O	2.12	0.49
1:B:12:LYS:O	1:B:16:GLU:HG2	2.12	0.49
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.48	0.49
1:C:501:GLU:HG2	4:C:1448:HOH:O	2.12	0.49
1:C:209:ARG:O	1:C:239:GLN:HG2	2.12	0.49
1:B:444:THR:HG23	4:B:947:HOH:O	2.12	0.49
1:D:15:LYS:NZ	4:D:717:HOH:O	2.40	0.49
1:A:14:TRP:CH2	1:A:18:ARG:HD2	2.47	0.48
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.95	0.48
1:B:414:GLN:HB2	4:B:1485:HOH:O	2.12	0.48
1:C:379:ARG:NH1	4:C:1292:HOH:O	2.46	0.48
1:D:394:MET:HE2	4:D:1088:HOH:O	2.12	0.48
1:B:10:GLN:HE21	1:C:172:GLN:HE21	1.60	0.48
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.79	0.48
1:B:178:PRO:HG2	4:B:1121:HOH:O	2.13	0.48
1:C:12:LYS:HE2	4:C:1734:HOH:O	2.13	0.48
1:C:476:LYS:HB3	1:C:476:LYS:HZ3	1.78	0.48
1:A:153:PHE:CE1	1:A:194:GLN:HG3	2.49	0.48
1:A:321:PRO:HG2	4:D:748:HOH:O	2.13	0.48
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.95	0.48
1:B:319:ARG:HH11	1:B:319:ARG:CB	2.26	0.48
1:C:171:PRO:HG3	1:D:402:ASN:ND2	2.29	0.48
1:A:360:THR:HG21	2:A:1:HEM:HBA1	1.96	0.48
1:B:155:ARG:HD2	1:B:433:SER:O	2.14	0.48
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.95	0.48
1:C:310:ILE:N	1:C:310:ILE:HD12	2.29	0.48
1:D:351:GLN:HG3	4:D:1634:HOH:O	2.14	0.47
1:B:408:PHE:HA	1:D:15:LYS:HD2	1.96	0.47
1:A:254:HIS:HD2	1:D:254:HIS:CD2	2.32	0.47
1:C:476:LYS:HB3	1:C:476:LYS:HZ2	1.80	0.47
1:C:22:LYS:HD3	1:C:23:PRO:N	2.30	0.47
1:C:499:TYR:O	1:C:501:GLU:HG3	2.14	0.47
1:D:412:GLU:CG	4:D:1168:HOH:O	2.62	0.47
1:A:120:GLY:N	4:D:638:HOH:O	2.19	0.47
1:B:202:ARG:HE	1:B:241:ILE:HD13	1.80	0.47
1:B:454:GLN:HE21	1:B:454:GLN:HB3	1.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:LYS:CG	4:C:1294:HOH:O	2.51	0.47
1:C:402:ASN:C	1:C:402:ASN:HD22	2.22	0.47
1:C:451:ASN:CG	1:C:454:GLN:HG2	2.40	0.47
1:C:202:ARG:NH1	4:C:1098:HOH:O	2.47	0.47
1:B:43:VAL:O	1:B:47:GLY:HA3	2.15	0.47
1:B:367:PRO:HG3	1:D:65:ARG:HD3	1.96	0.47
1:C:78:ALA:CB	1:C:261:LEU:HD13	2.45	0.46
1:B:296:PHE:CD2	1:B:346:PRO:HG2	2.49	0.46
1:B:470:GLN:NE2	4:B:1574:HOH:O	2.32	0.46
1:C:73:VAL:O	1:C:74:HIS:HB2	2.16	0.46
1:B:451:ASN:H	1:B:454:GLN:CG	2.29	0.46
1:D:107:PRO:HG2	1:D:136:TYR:HB2	1.97	0.46
1:D:412:GLU:HB2	4:D:1168:HOH:O	2.15	0.46
1:B:104:LYS:HE3	4:B:1731:HOH:O	2.14	0.46
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.45	0.46
4:B:505:HOH:O	1:D:52:GLN:HB2	2.16	0.46
1:C:357:TYR:HB2	1:C:358:PRO:HD3	1.97	0.46
1:B:402:ASN:C	1:B:402:ASN:ND2	2.72	0.46
1:A:319:ARG:NH1	4:A:671:HOH:O	2.35	0.46
1:A:18:ARG:O	1:A:19:ALA:C	2.58	0.46
1:B:101:HIS:HD2	4:B:1753:HOH:O	1.98	0.46
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.81	0.46
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.81	0.46
1:A:254:HIS:CD2	1:D:254:HIS:HD2	2.34	0.45
1:C:429:GLN:HG2	1:C:431:PHE:CZ	2.51	0.45
1:D:443:ARG:HG3	1:D:484:VAL:O	2.15	0.45
1:A:176:LYS:HG2	4:D:609:HOH:O	2.16	0.45
1:C:215:GLY:O	1:C:216:SER:HB2	2.16	0.45
4:C:1188:HOH:O	1:D:421:ARG:HB3	2.16	0.45
1:A:74:HIS:HA	1:A:114:THR:O	2.16	0.45
1:A:446:TYR:CZ	1:A:455:ARG:HD3	2.51	0.45
1:B:70:GLU:HG2	4:C:650:HOH:O	2.17	0.45
1:D:148:ASN:HD22	1:D:148:ASN:N	2.12	0.45
1:A:97:LYS:O	1:A:100:GLU:HB2	2.17	0.45
1:A:381:ARG:HG2	1:A:381:ARG:NH1	2.30	0.45
1:C:391:MET:HE3	1:C:393:MET:CE	2.46	0.45
1:A:379:ARG:CD	4:A:1773:HOH:O	2.60	0.45
1:B:43:VAL:O	1:B:43:VAL:HG13	2.16	0.45
1:B:104:LYS:CE	4:B:1731:HOH:O	2.64	0.45
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.47	0.45
1:B:237:THR:HA	1:B:276:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.97	0.45
1:C:485:HIS:HE1	4:C:609:HOH:O	1.99	0.45
1:D:43:VAL:CG1	1:D:48:PRO:HD2	2.47	0.45
1:B:92:ARG:HD3	1:B:92:ARG:C	2.42	0.45
1:C:147:ASN:CG	2:C:1:HEM:HAC	2.41	0.45
1:C:445:PHE:HA	1:C:449:VAL:CG2	2.47	0.45
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.35	0.45
1:D:410:ALA:HB1	1:D:411:PRO:HD2	1.99	0.45
1:D:413:HIS:O	1:D:414:GLN:CB	2.64	0.45
1:D:457:ARG:HG2	4:D:580:HOH:O	2.16	0.45
1:D:207:GLY:O	4:D:1075:HOH:O	2.20	0.44
1:A:148:ASN:N	1:A:148:ASN:HD22	2.14	0.44
1:A:391:MET:HE1	1:C:369:TYR:HA	1.98	0.44
1:B:60:MET:HE1	1:C:161:PRO:HD3	1.98	0.44
1:A:35:GLY:HA2	1:C:414:GLN:O	2.18	0.44
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.52	0.44
1:A:148:ASN:HD22	1:A:148:ASN:H	1.65	0.44
1:C:485:HIS:CE1	4:C:609:HOH:O	2.70	0.44
1:A:52:GLN:HB2	4:C:510:HOH:O	2.18	0.44
1:B:499:TYR:C	1:B:501:GLU:N	2.75	0.44
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.33	0.44
1:D:236:LYS:HD2	4:D:1009:HOH:O	2.18	0.44
1:B:193:HIS:HE1	4:B:886:HOH:O	1.99	0.44
1:C:223:ASN:HD21	1:C:227:GLU:HB2	1.83	0.44
1:C:445:PHE:CE2	1:C:450:LEU:HD11	2.52	0.44
1:A:15:LYS:HD2	1:C:408:PHE:HA	1.99	0.44
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.99	0.44
1:C:445:PHE:O	1:C:450:LEU:HD13	2.17	0.44
1:A:290:ILE:HD12	1:A:290:ILE:C	2.43	0.43
1:B:443:ARG:O	1:B:447:LEU:HG	2.17	0.43
1:C:421:ARG:HG2	1:D:429:GLN:HB3	2.00	0.43
1:D:145:VAL:HG22	1:D:333:PHE:HB3	1.99	0.43
1:B:193:HIS:HD2	1:B:299:THR:O	2.01	0.43
1:C:19:ALA:O	1:C:20:ALA:CB	2.65	0.43
1:D:499:TYR:C	1:D:501:GLU:H	2.27	0.43
1:A:43:VAL:O	1:A:47:GLY:HA3	2.18	0.43
1:A:412:GLU:CG	4:A:1399:HOH:O	2.54	0.43
1:B:142:TRP:HB2	1:B:339:PRO:HD3	2.01	0.43
1:B:394:MET:HB2	4:B:1355:HOH:O	2.19	0.43
1:C:78:ALA:HB2	1:C:261:LEU:HD13	2.00	0.43
1:C:436:ASP:C	4:C:842:HOH:O	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:GLN:HG2	4:D:1480:HOH:O	2.18	0.43
1:D:202:ARG:NH2	4:D:602:HOH:O	2.40	0.43
1:A:207:GLY:O	4:A:1394:HOH:O	2.21	0.43
1:C:17:GLN:HG3	4:C:849:HOH:O	2.19	0.43
1:D:413:HIS:O	1:D:414:GLN:HB2	2.18	0.43
1:D:443:ARG:NH1	1:D:484:VAL:O	2.52	0.43
1:B:138:GLU:CD	1:B:138:GLU:N	2.77	0.43
1:C:216:SER:HB3	1:C:298:LEU:HD11	2.01	0.43
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.34	0.43
1:D:346:PRO:O	1:D:347:ASP:C	2.61	0.43
1:A:414:GLN:O	1:C:35:GLY:HA2	2.18	0.43
1:B:81:PHE:HB2	1:B:319:ARG:HD2	2.01	0.42
1:D:182:TRP:CD2	1:D:466:LEU:HD13	2.54	0.42
1:B:4:ARG:NH1	1:B:8:SER:C	2.77	0.42
1:A:237:THR:HA	1:A:276:TRP:CD1	2.54	0.42
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.18	0.42
1:B:471:LEU:HD21	1:B:500:ASN:ND2	2.35	0.42
1:C:410:ALA:HB1	1:C:411:PRO:HD2	2.00	0.42
1:C:451:ASN:H	1:C:454:GLN:CG	2.33	0.42
1:D:84:PHE:O	1:D:105:ARG:HA	2.20	0.42
1:D:412:GLU:O	1:D:413:HIS:O	2.36	0.42
1:A:82:GLY:HA3	1:A:316:VAL:O	2.19	0.42
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.49	0.42
1:A:331:LEU:HD13	1:A:374:VAL:CG2	2.49	0.42
1:A:487:GLU:CG	1:A:491:ARG:HD2	2.49	0.42
1:B:66:GLU:HG2	1:D:387:ARG:O	2.20	0.42
1:A:290:ILE:HD12	4:A:1927:HOH:O	2.20	0.42
1:A:500:ASN:O	1:A:501:GLU:HB2	2.18	0.42
1:D:193:HIS:HD2	1:D:299:THR:O	2.03	0.42
1:C:126:ARG:O	1:C:127:ASP:HB2	2.19	0.42
1:D:413:HIS:O	1:D:414:GLN:HG2	2.20	0.42
1:D:479:LYS:HD3	1:D:479:LYS:O	2.20	0.42
1:A:65:ARG:HD3	1:C:367:PRO:HG3	2.02	0.41
1:C:170:ASN:HA	1:C:171:PRO:HD3	1.87	0.41
1:C:460:GLU:HA	1:C:495:LEU:HD13	2.02	0.41
1:D:487:GLU:HB2	4:D:1556:HOH:O	2.20	0.41
1:A:232:LYS:O	1:A:280:ILE:HA	2.20	0.41
1:B:4:ARG:NH1	1:B:9:ASP:OD1	2.54	0.41
1:B:50:LEU:HD22	1:B:50:LEU:N	2.35	0.41
1:C:476:LYS:HD3	4:C:971:HOH:O	2.19	0.41
4:C:1681:HOH:O	1:D:405:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PRO:HG2	4:D:798:HOH:O	2.20	0.41
1:A:273:TYR:CD1	1:A:318:ASN:HA	2.56	0.41
1:B:4:ARG:NH2	1:C:470:GLN:HG3	2.35	0.41
1:C:223:ASN:ND2	1:C:227:GLU:HB2	2.35	0.41
1:C:251:ARG:HD3	4:C:1934:HOH:O	2.20	0.41
1:D:237:THR:HA	1:D:276:TRP:CD1	2.56	0.41
1:A:391:MET:HE3	1:C:365:LEU:O	2.21	0.41
1:A:22:LYS:HG3	1:A:23:PRO:HD2	2.03	0.41
1:A:129:ARG:H	1:A:148:ASN:ND2	2.18	0.41
1:A:346:PRO:O	1:A:347:ASP:C	2.64	0.41
1:A:453:GLU:CG	1:A:457:ARG:NH1	2.84	0.41
1:B:15:LYS:HD2	1:D:408:PHE:HA	2.01	0.41
1:B:25:VAL:HG13	1:D:414:GLN:CG	2.50	0.41
1:C:13:HIS:O	1:C:17:GLN:HG2	2.20	0.41
1:C:153:PHE:CZ	1:C:194:GLN:HG3	2.56	0.41
1:C:182:TRP:CD2	1:C:466:LEU:HD13	2.55	0.41
1:C:237:THR:HA	1:C:276:TRP:CD1	2.55	0.41
1:C:327:GLU:O	1:C:331:LEU:HG	2.21	0.41
1:D:153:PHE:CE2	1:D:194:GLN:HG3	2.56	0.41
1:D:446:TYR:CZ	1:D:455:ARG:HD2	2.56	0.41
1:B:379:ARG:NE	4:B:531:HOH:O	2.40	0.41
1:D:126:ARG:HA	1:D:204:ILE:HG12	2.03	0.41
1:D:410:ALA:HB1	1:D:411:PRO:CD	2.50	0.41
1:A:73:VAL:O	1:A:74:HIS:HB2	2.19	0.40
1:A:402:ASN:C	1:A:402:ASN:ND2	2.76	0.40
1:B:73:VAL:O	1:B:74:HIS:HB2	2.21	0.40
1:B:387:ARG:O	1:D:66:GLU:HG2	2.21	0.40
1:C:82:GLY:HA3	1:C:316:VAL:O	2.21	0.40
1:B:314:LYS:NZ	4:B:1796:HOH:O	2.44	0.40
1:B:479:LYS:HE2	1:B:483:ASP:OD1	2.21	0.40
1:D:43:VAL:O	1:D:47:GLY:HA3	2.21	0.40
1:D:183:ASP:O	1:D:187:LEU:HG	2.21	0.40
1:A:147:ASN:ND2	2:A:1:HEM:CAC	2.84	0.40
1:A:390:PRO:HB3	4:C:805:HOH:O	2.20	0.40
1:B:62:HIS:CE1	1:D:368:ASN:ND2	2.76	0.40
1:B:290:ILE:HD12	1:B:290:ILE:HA	1.94	0.40
1:B:446:TYR:CZ	1:B:455:ARG:HD2	2.56	0.40
1:A:182:TRP:CD2	1:A:466:LEU:HD13	2.56	0.40
1:A:474:GLN:O	1:A:478:VAL:HG23	2.22	0.40
1:B:144:LEU:HD13	1:B:144:LEU:C	2.45	0.40
1:C:3:ASN:CB	4:C:1941:HOH:O	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:O	1:C:47:GLY:HA3	2.22	0.40
1:C:145:VAL:HB	1:C:353:ARG:HH22	1.86	0.40
1:C:402:ASN:C	1:C:402:ASN:ND2	2.79	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)
4:C:666:HOH:O	4:C:774:HOH:O[3_555]	2.07	0.13

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	499/499 (100%)	477 (96%)	20 (4%)	2 (0%)	30	18
1	B	499/499 (100%)	481 (96%)	18 (4%)	0	100	100
1	C	499/499 (100%)	478 (96%)	20 (4%)	1 (0%)	43	34
1	D	499/499 (100%)	472 (95%)	24 (5%)	3 (1%)	21	10
All	All	1996/1996 (100%)	1908 (96%)	82 (4%)	6 (0%)	36	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ASP
1	D	413	HIS
1	D	414	GLN
1	A	19	ALA
1	C	437	ASP
1	D	437	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	433/431 (100%)	423 (98%)	10 (2%)	44	29
1	B	433/431 (100%)	422 (98%)	11 (2%)	42	26
1	C	433/431 (100%)	421 (97%)	12 (3%)	38	22
1	D	433/431 (100%)	429 (99%)	4 (1%)	70	63
All	All	1732/1724 (100%)	1695 (98%)	37 (2%)	47	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	49	LEU
1	A	137	THR
1	A	148	ASN
1	A	235	TYR
1	A	242	LYS
1	A	402	ASN
1	A	413	HIS
1	A	496	LEU
1	A	501	GLU
1	B	49	LEU
1	B	92	ARG
1	B	104	LYS
1	B	137	THR
1	B	202	ARG
1	B	235	TYR
1	B	319	ARG
1	B	393	MET
1	B	402	ASN
1	B	454	GLN
1	B	466	LEU
1	C	4	ARG
1	C	22	LYS
1	C	76	LYS

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Mol	Chain	Res	Type
1	C	129	ARG
1	C	137	THR
1	C	235	TYR
1	C	239	GLN
1	C	244	LEU
1	C	402	ASN
1	C	413	HIS
1	C	467	LYS
1	C	496	LEU
1	D	148	ASN
1	D	202	ARG
1	D	235	TYR
1	D	501	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	21	GLN
1	A	148	ASN
1	A	167	GLN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	402	ASN
1	A	420	HIS
1	A	454	GLN
1	A	470	GLN
1	A	485	HIS
1	B	13	HIS
1	B	17	GLN
1	B	62	HIS
1	B	167	GLN
1	B	193	HIS
1	B	210	HIS
1	B	272	ASN
1	B	337	ASN
1	B	386	GLN
1	B	396	ASN
1	B	402	ASN
1	B	414	GLN
1	B	429	GLN

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Mol	Chain	Res	Type
1	B	470	GLN
1	C	3	ASN
1	C	21	GLN
1	C	172	GLN
1	C	243	ASN
1	C	272	ASN
1	C	304	HIS
1	C	337	ASN
1	C	386	GLN
1	C	402	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	474	GLN
1	C	480	ASN
1	C	485	HIS
1	C	493	GLN
1	D	3	ASN
1	D	21	GLN
1	D	52	GLN
1	D	148	ASN
1	D	170	ASN
1	D	193	HIS
1	D	210	HIS
1	D	243	ASN
1	D	254	HIS
1	D	304	HIS
1	D	337	ASN
1	D	363	HIS
1	D	368	ASN
1	D	386	GLN
1	D	413	HIS
1	D	420	HIS
1	D	429	GLN
1	D	435	ASN
1	D	470	GLN
1	D	500	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NO	A	502	2	0,1,1	-	-	-		
2	HEM	C	1	3,1	50,50,50	1.18	4 (8%)	67,82,82	0.91	1 (1%)
2	HEM	A	1	3,1	50,50,50	1.10	4 (8%)	67,82,82	0.91	3 (4%)
3	NO	C	502	2	0,1,1	-	-	-		
2	HEM	D	1	3,1	50,50,50	1.14	4 (8%)	67,82,82	0.97	3 (4%)
3	NO	D	502	2	0,1,1	-	-	-		
3	NO	B	502	2	0,1,1	-	-	-		
2	HEM	B	1	3,1	50,50,50	1.15	4 (8%)	67,82,82	0.93	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	1	3,1	-	2/14/54/54	-
2	HEM	C	1	3,1	-	2/14/54/54	-
2	HEM	B	1	3,1	-	2/14/54/54	-
2	HEM	A	1	3,1	-	2/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	HEM	CBC-CAC	3.24	1.45	1.30
2	C	1	HEM	CBC-CAC	3.21	1.45	1.30
2	D	1	HEM	CBC-CAC	3.19	1.45	1.30
2	B	1	HEM	CBB-CAB	3.03	1.44	1.30
2	A	1	HEM	CBC-CAC	3.01	1.44	1.30
2	C	1	HEM	CBB-CAB	2.97	1.44	1.30
2	D	1	HEM	CBB-CAB	2.96	1.44	1.30
2	A	1	HEM	CBB-CAB	2.93	1.44	1.30
2	A	1	HEM	CAB-C3B	-2.83	1.39	1.47
2	B	1	HEM	CAB-C3B	-2.72	1.40	1.47
2	D	1	HEM	CAB-C3B	-2.72	1.40	1.47
2	C	1	HEM	CAC-C3C	-2.48	1.40	1.47
2	D	1	HEM	CAC-C3C	-2.41	1.41	1.47
2	A	1	HEM	CAC-C3C	-2.41	1.41	1.47
2	B	1	HEM	CAC-C3C	-2.35	1.41	1.47
2	C	1	HEM	CAB-C3B	-2.27	1.41	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	HEM	C3B-C4B-NB	3.24	111.80	109.47
2	B	1	HEM	C3B-C4B-NB	2.83	111.50	109.47
2	D	1	HEM	C3B-C4B-NB	2.58	111.32	109.47
2	A	1	HEM	C2D-C1D-ND	2.52	112.81	109.90
2	A	1	HEM	C3B-C4B-NB	2.38	111.18	109.47
2	D	1	HEM	CAD-C3D-C4D	2.35	128.79	124.70
2	A	1	HEM	C1D-C2D-C3D	-2.23	104.64	106.98
2	D	1	HEM	CAD-C3D-C2D	-2.23	123.70	127.87

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	HEM	CAD-CBD-CGD-O2D
2	B	1	HEM	CAD-CBD-CGD-O2D
2	A	1	HEM	CAD-CBD-CGD-O2D
2	D	1	HEM	CAD-CBD-CGD-O2D
2	A	1	HEM	CAD-CBD-CGD-O1D
2	B	1	HEM	CAD-CBD-CGD-O1D
2	C	1	HEM	CAD-CBD-CGD-O1D
2	D	1	HEM	CAD-CBD-CGD-O1D

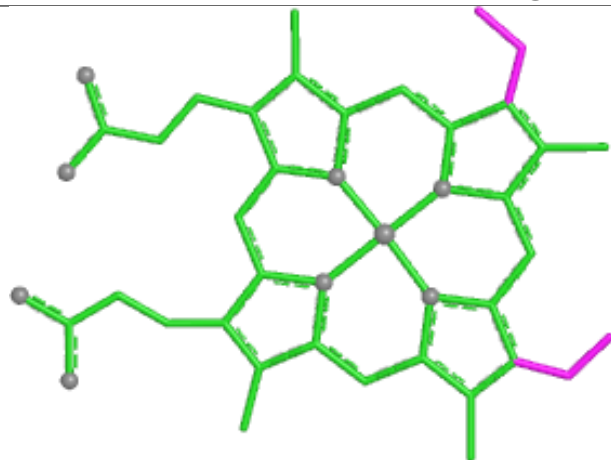
There are no ring outliers.

3 monomers are involved in 4 short contacts:

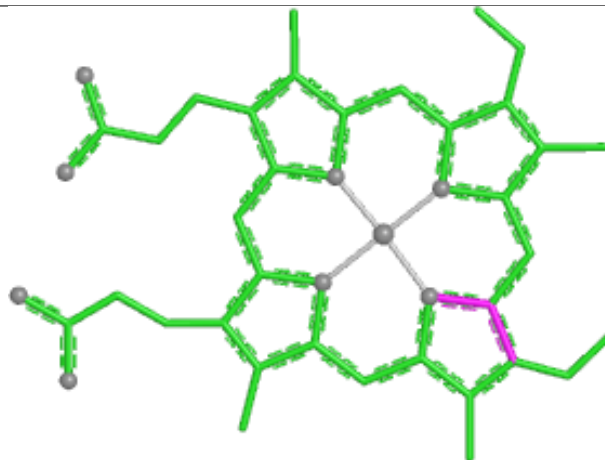
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	HEM	1	0
2	A	1	HEM	2	0
2	B	1	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

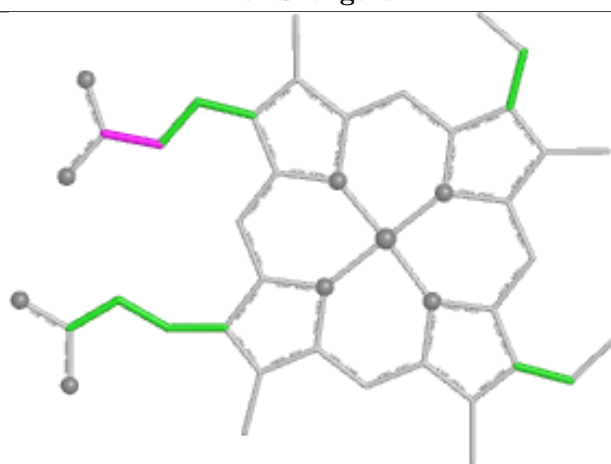
Ligand HEM C 1



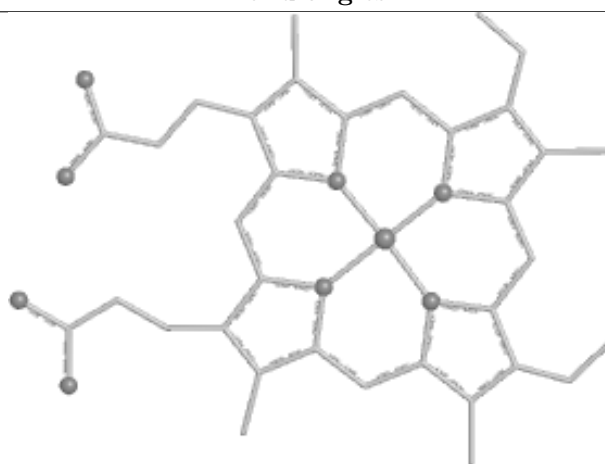
Bond lengths



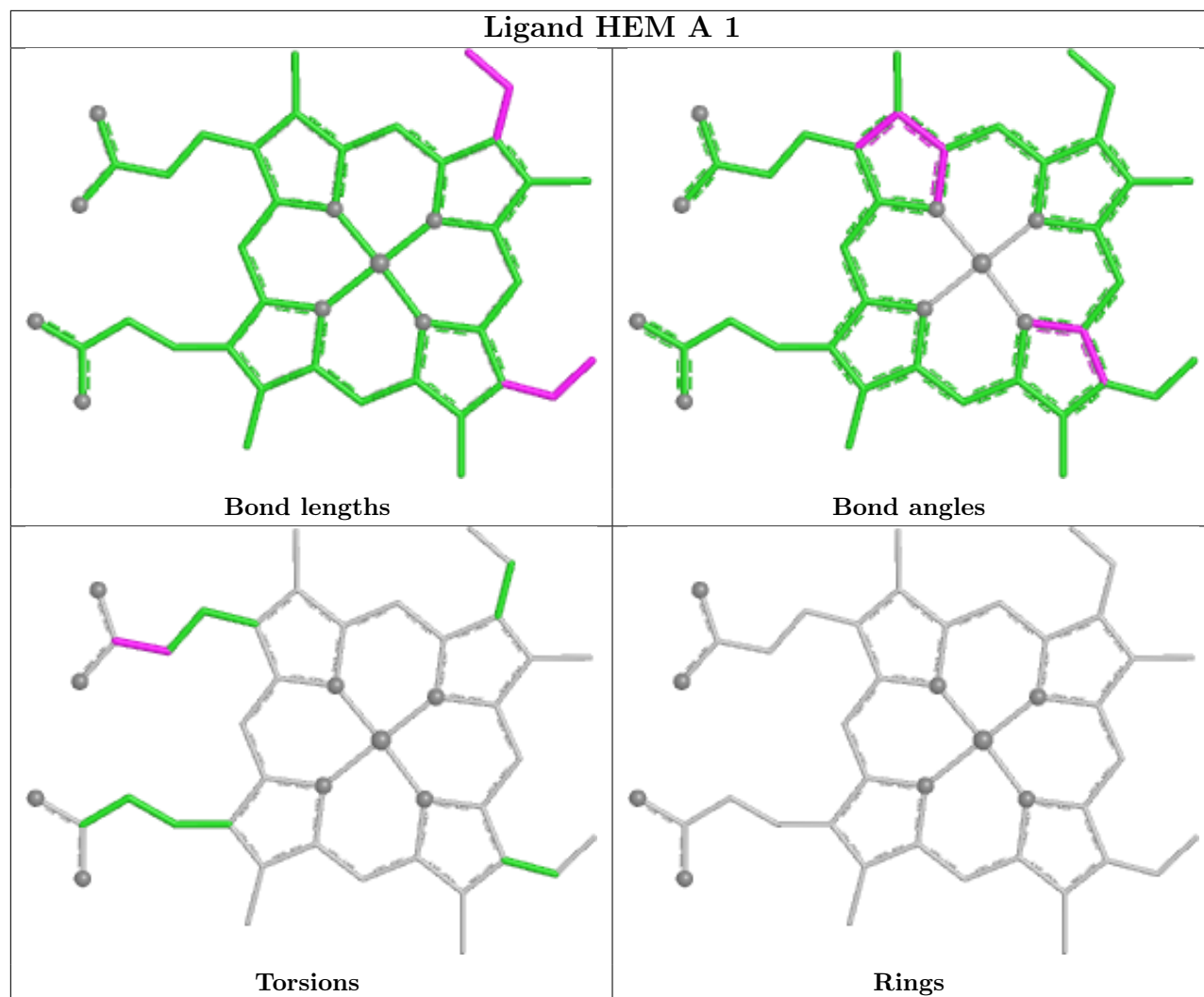
Bond angles



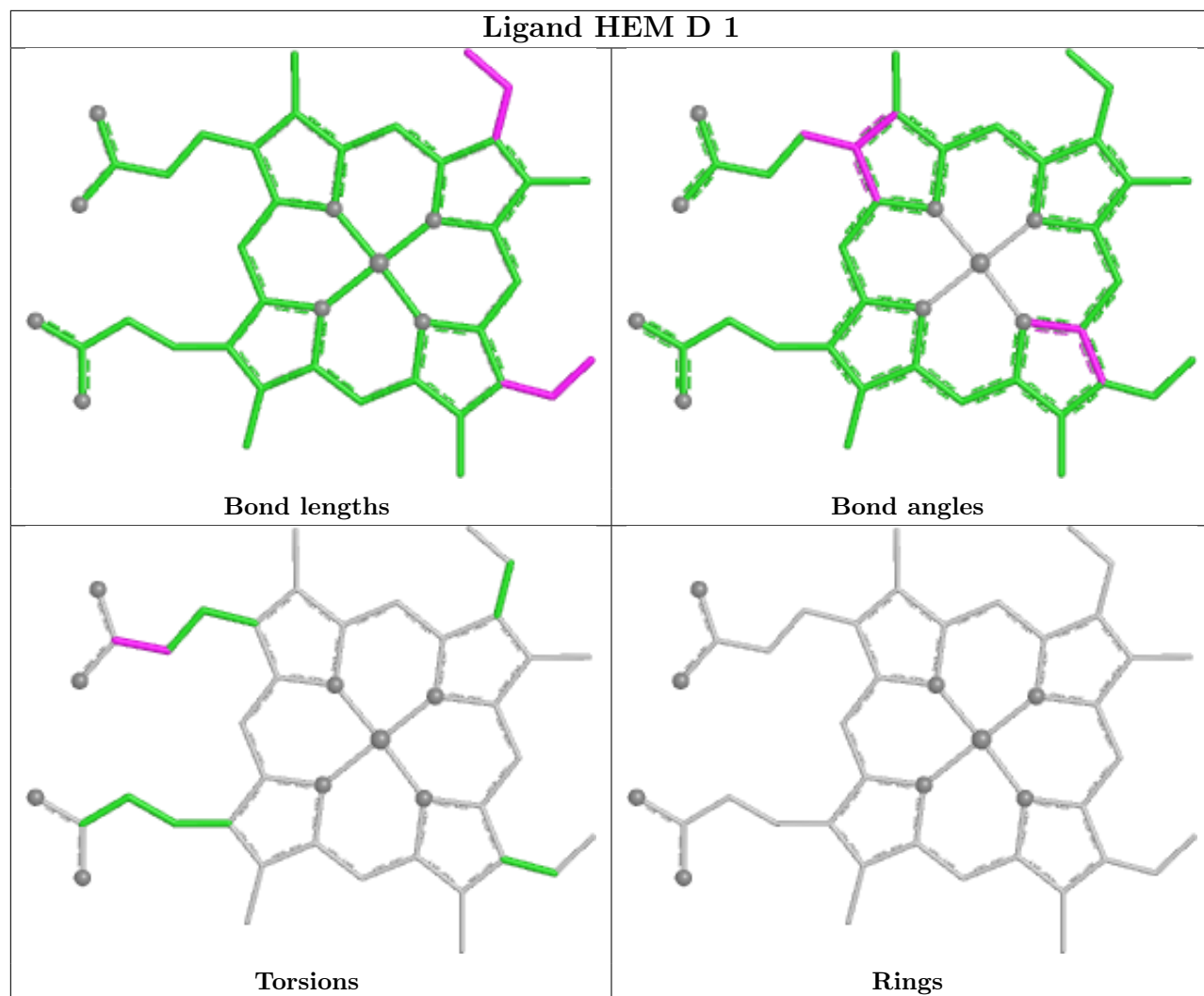
Torsions

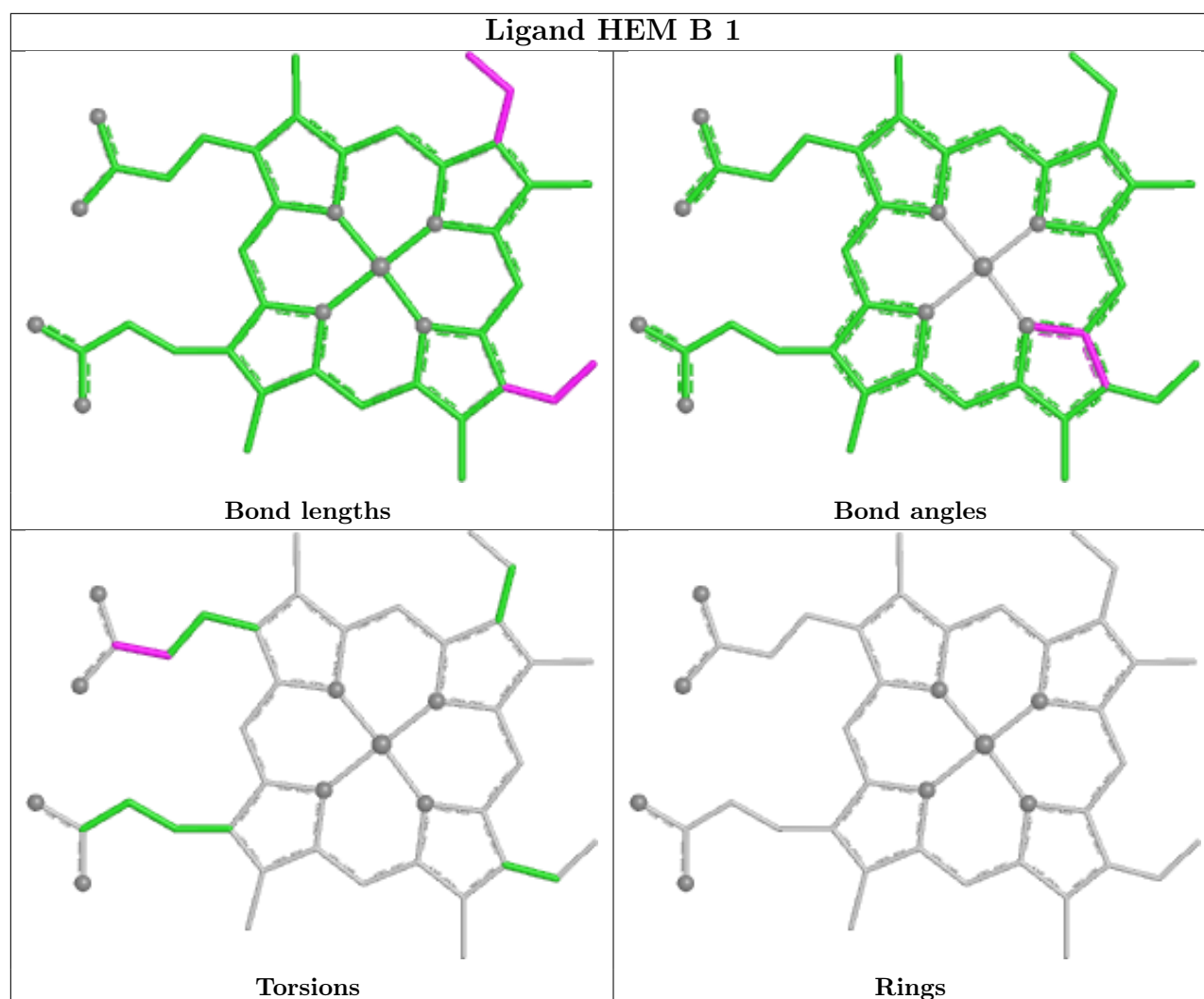


Rings



Ligand HEM D 1





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	499/499 (100%)	-0.24	9 (1%) 67 73	12, 18, 32, 55	1 (0%)
1	B	499/499 (100%)	0.01	21 (4%) 40 44	12, 21, 37, 61	1 (0%)
1	C	499/499 (100%)	-0.07	15 (3%) 52 57	11, 20, 38, 62	1 (0%)
1	D	499/499 (100%)	-0.16	20 (4%) 42 45	12, 19, 35, 63	1 (0%)
All	All	1996/1996 (100%)	-0.12	65 (3%) 49 54	11, 20, 36, 63	4 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	19	ALA	5.8
1	B	17	GLN	5.5
1	C	394	MET	5.1
1	A	3	ASN	4.8
1	B	20	ALA	4.7
1	D	426	GLY	4.6
1	A	19	ALA	4.4
1	C	20	ALA	4.4
1	C	17	GLN	4.4
1	D	501	GLU	4.1
1	D	413	HIS	4.0
1	D	3	ASN	3.8
1	B	3	ASN	3.8
1	B	416	SER	3.7
1	C	426	GLY	3.6
1	D	20	ALA	3.5
1	B	447	LEU	3.4
1	D	17	GLN	3.4
1	B	19	ALA	3.3
1	D	499	TYR	3.2
1	D	444	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	247	GLU	3.2
1	B	197	PHE	3.1
1	B	501	GLU	3.1
1	D	22	LYS	3.0
1	D	498	LYS	3.0
1	B	490	SER	2.9
1	B	4	ARG	2.9
1	A	21	GLN	2.9
1	A	501	GLU	2.8
1	B	444	THR	2.8
1	C	21	GLN	2.7
1	A	17	GLN	2.7
1	D	425	SER	2.7
1	D	421	ARG	2.6
1	B	290	ILE	2.6
1	C	501	GLU	2.5
1	C	3	ASN	2.5
1	D	423	HIS	2.4
1	B	499	TYR	2.4
1	B	5	ASP	2.3
1	C	499	TYR	2.3
1	B	500	ASN	2.3
1	B	22	LYS	2.3
1	B	394	MET	2.3
1	A	289	GLU	2.3
1	B	487	GLU	2.3
1	C	453	GLU	2.3
1	B	247	GLU	2.2
1	B	453	GLU	2.2
1	C	425	SER	2.2
1	D	290	ILE	2.2
1	C	428	VAL	2.2
1	A	309	LEU	2.2
1	A	20	ALA	2.2
1	D	476	LYS	2.2
1	C	500	ASN	2.1
1	B	225	ASN	2.1
1	A	22	LYS	2.1
1	D	500	ASN	2.1
1	C	310	ILE	2.1
1	D	427	ASP	2.1
1	C	490	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	418	LEU	2.0
1	D	414	GLN	2.0

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](#)

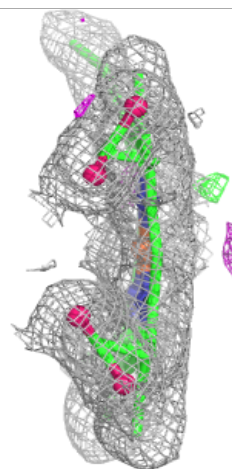
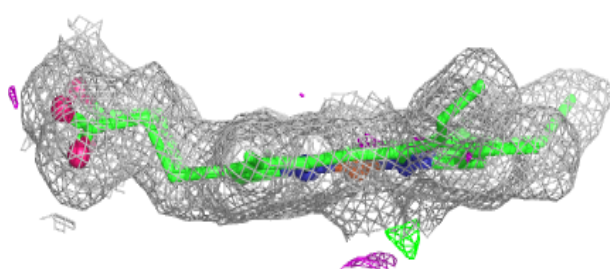
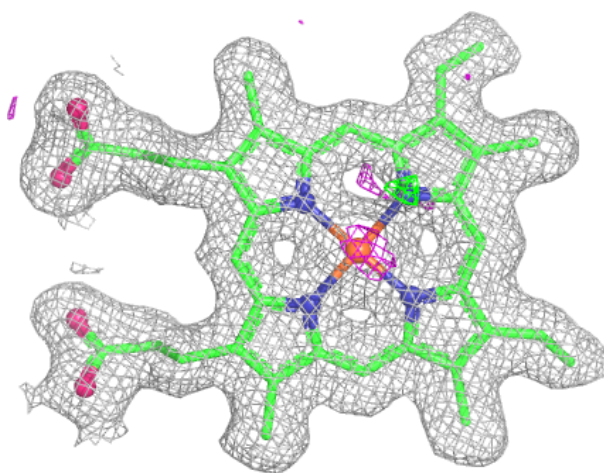
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NO	C	502	2/2	0.93	0.26	27,27,27,31	0
3	NO	B	502	2/2	0.95	0.19	27,27,27,30	0
3	NO	A	502	2/2	0.98	0.15	25,25,25,26	0
2	HEM	B	1	43/43	0.98	0.06	13,17,22,24	0
2	HEM	D	1	43/43	0.98	0.06	12,16,20,23	0
3	NO	D	502	2/2	0.98	0.16	22,22,22,26	0
2	HEM	C	1	43/43	0.99	0.05	14,16,21,23	0
2	HEM	A	1	43/43	0.99	0.05	10,13,18,19	0

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

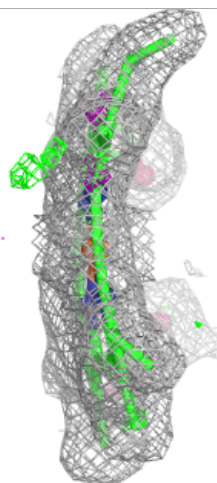
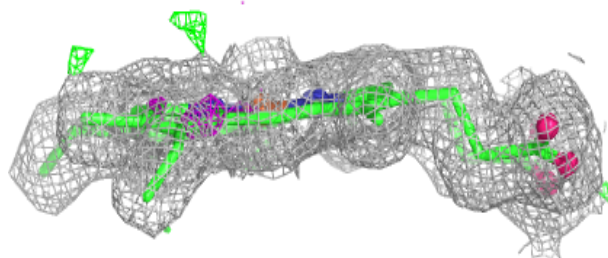
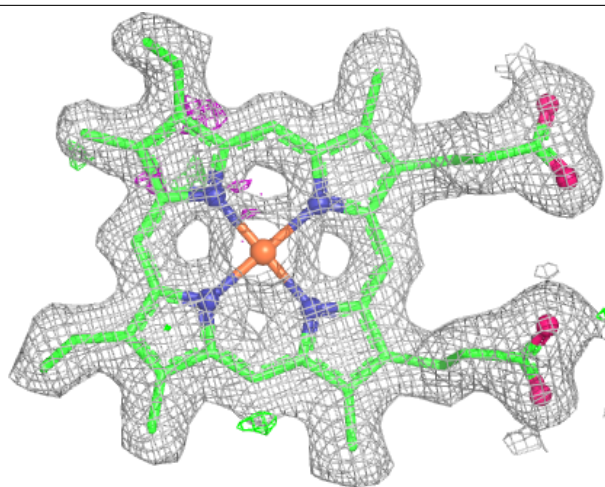
Electron density around HEM B 1:

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



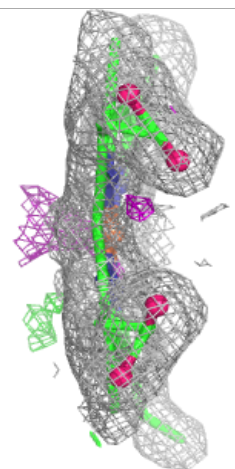
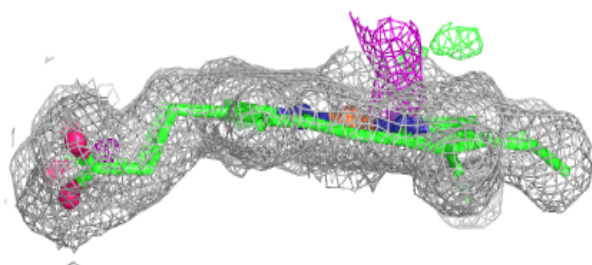
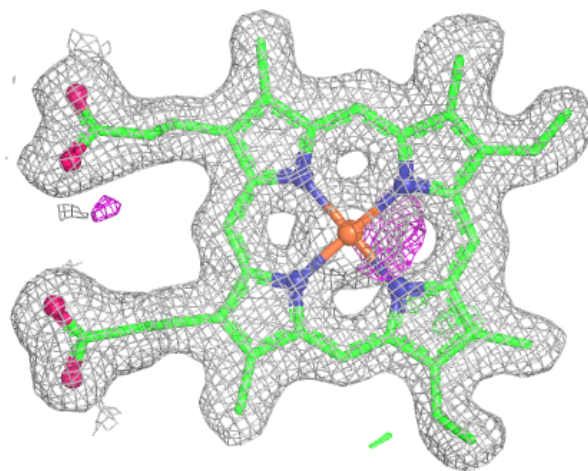
Electron density around HEM D 1:

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



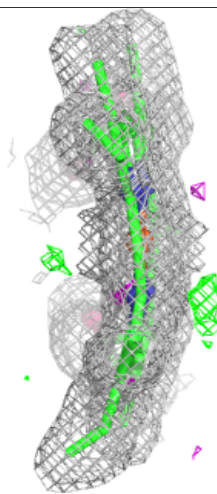
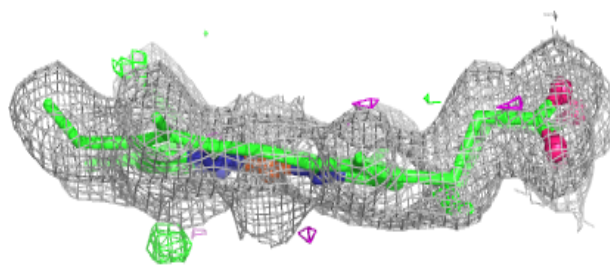
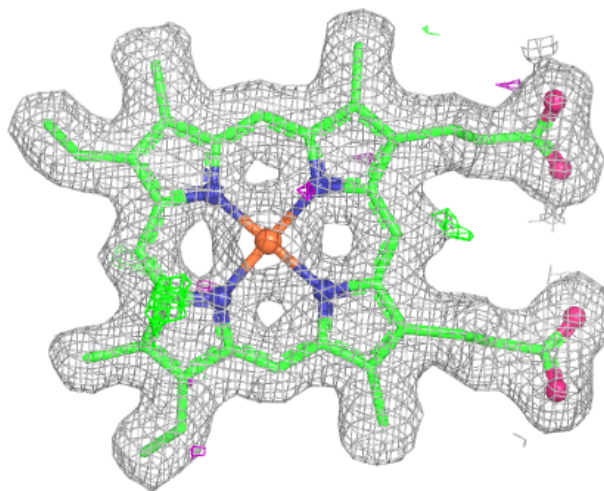
Electron density around HEM C 1:

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



Electron density around HEM A 1:

$2mF_o-DF_c$ (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.