



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:48 PM UTC

PDB ID : 3RGS / pdb_00003rgs
Title : Structural and kinetic analysis of the beef liver catalase with the ammonia as a ligand
Authors : Purwar, N.; Schmidt, M.
Deposited on : 2011-04-08
Resolution : 1.99 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

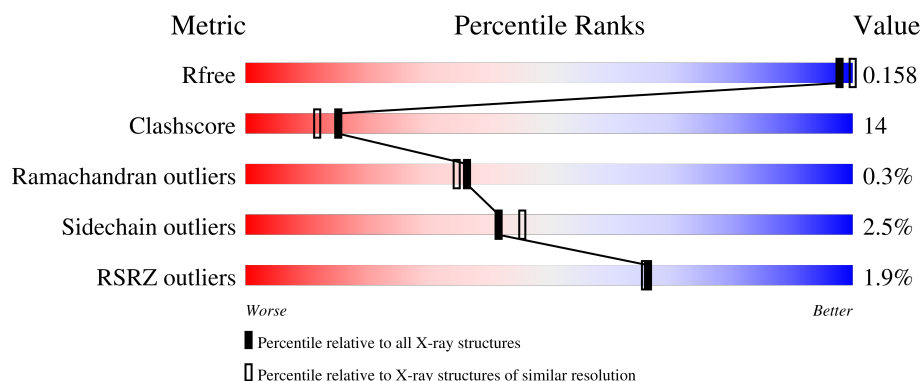
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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.

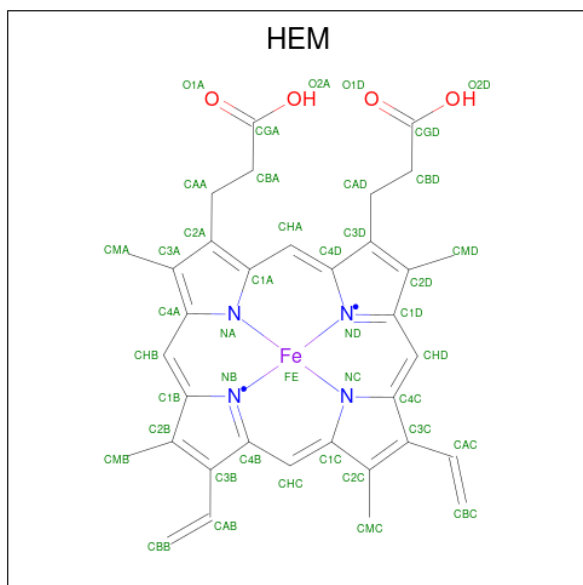
Mol	Chain	Length	Quality of chain
1	A	499	0% 77% 20% .
1	B	499	2% 73% 25% .
1	C	499	2% 75% 23% .
1	D	499	2% 75% 24% .

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 4019	C 2548	N 717	O 738	S 16	0	1	0
1	B	499	Total 4019	C 2548	N 717	O 738	S 16	0	1	0
1	C	499	Total 4019	C 2548	N 717	O 738	S 16	0	1	0
1	D	499	Total 4019	C 2548	N 717	O 738	S 16	0	1	0

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



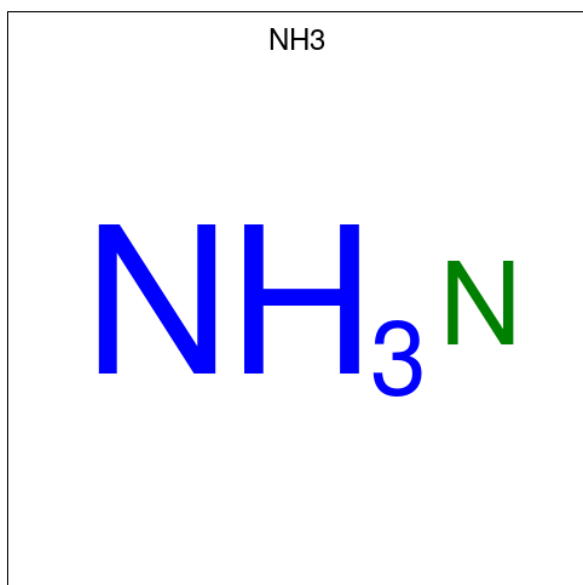
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is AMMONIA (CCD ID: NH3) (formula: H₃N).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	N 1	0	0
3	B	1	Total 1	N 1	0	0
3	C	1	Total 1	N 1	0	0
3	D	1	Total 1	N 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	567	Total 567	O 567	1	0
4	B	577	Total 577	O 577	0	0
4	C	573	Total 573	O 573	1	0

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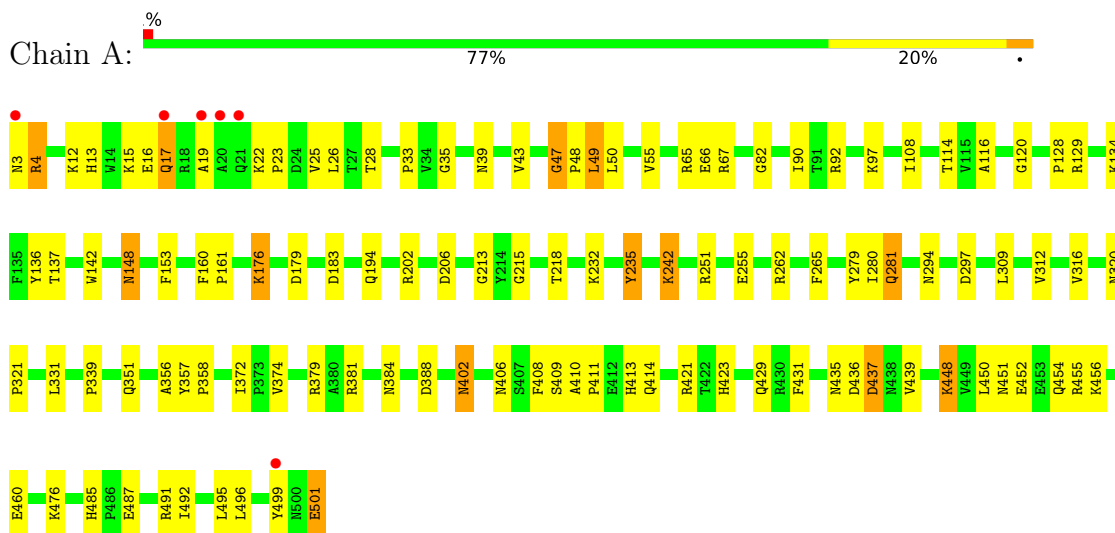
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	549	Total	O	0	0
			549	549		

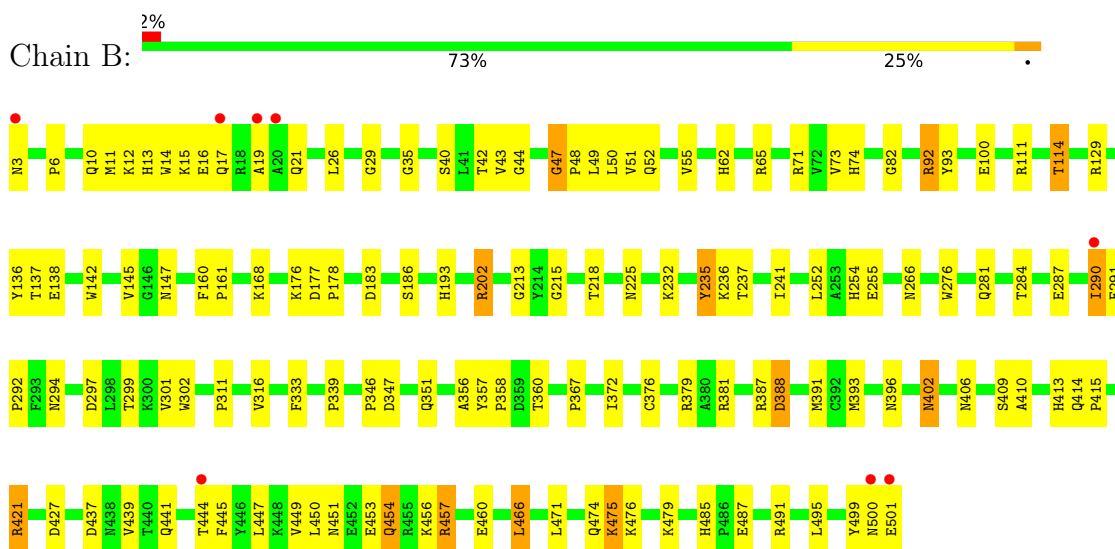
3 Residue-property plots

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

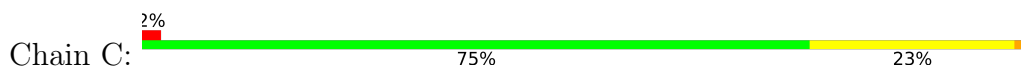
• Molecule 1: Catalase

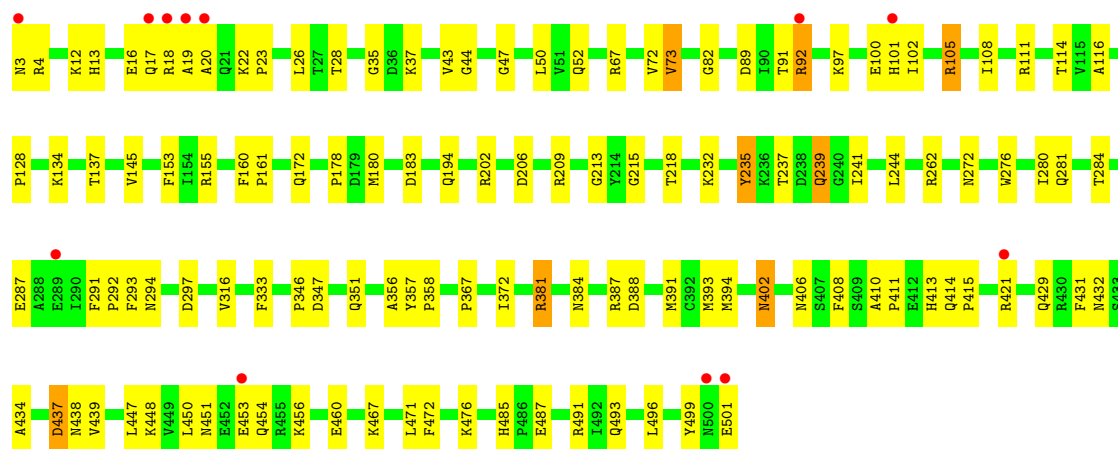


• Molecule 1: Catalase

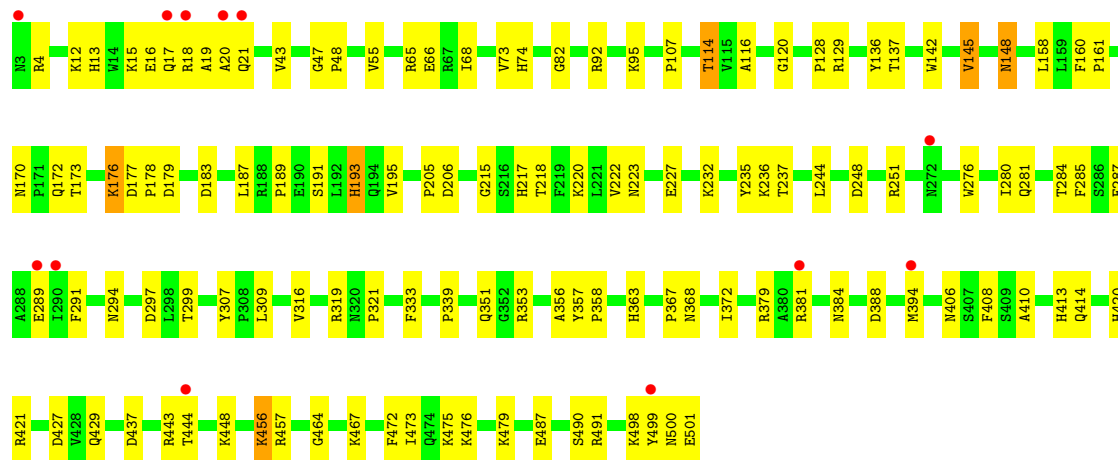
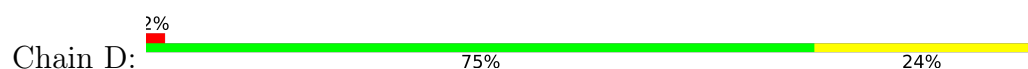


• Molecule 1: Catalase





• Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.48Å 140.72Å 229.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.38 – 1.99 57.38 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.4 (57.38-1.99) 92.5 (57.38-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 1.98Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.161 , 0.198 0.159 , 0.158	Depositor DCC
R_{free} test set	8629 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18518	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: NH3, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/4149	0.92	21/5637 (0.4%)
1	B	0.36	0/4149	0.94	18/5637 (0.3%)
1	C	0.35	0/4149	0.91	14/5637 (0.2%)
1	D	0.34	0/4149	0.91	19/5637 (0.3%)
All	All	0.35	0/16596	0.92	72/22548 (0.3%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	VAL	N-CA-C	10.01	120.53	112.12
1	B	356	ALA	N-CA-C	8.66	120.72	111.28
1	C	356	ALA	N-CA-C	8.31	121.39	111.33
1	D	356	ALA	N-CA-C	8.19	120.93	111.11
1	A	215	GLY	N-CA-C	-7.91	104.85	114.66
1	A	356	ALA	N-CA-C	7.80	120.47	111.11
1	D	388	ASP	N-CA-C	7.61	119.27	108.00
1	C	215	GLY	N-CA-C	-7.25	105.67	114.66
1	D	55	VAL	N-CA-C	-7.22	103.42	110.72
1	B	215	GLY	N-CA-C	-7.15	105.80	114.66
1	C	388	ASP	N-CA-C	7.01	118.37	108.00
1	B	388	ASP	N-CA-C	7.00	118.37	108.00
1	A	388	ASP	N-CA-C	6.94	118.27	108.00
1	B	372	ILE	N-CA-C	-6.89	102.19	108.95
1	D	215	GLY	N-CA-C	-6.84	106.17	114.66
1	D	183	ASP	N-CA-C	-6.71	103.90	111.14
1	B	47	GLY	CA-C-N	6.63	126.61	119.78
1	B	47	GLY	C-N-CA	6.63	126.61	119.78
1	C	281	GLN	N-CA-C	-6.60	98.96	109.59
1	A	176	LYS	N-CA-C	-6.44	101.59	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	GLN	N-CA-C	-6.31	99.92	109.95
1	A	281	GLN	N-CA-C	-6.10	99.77	109.59
1	C	128	PRO	N-CA-C	-6.07	102.73	111.22
1	A	55	VAL	N-CA-C	-5.88	104.59	111.00
1	A	372	ILE	N-CA-C	-5.81	103.26	108.95
1	B	55	VAL	N-CA-C	-5.78	104.88	110.72
1	C	372	ILE	N-CA-C	-5.70	103.36	108.95
1	C	28	THR	N-CA-C	-5.70	103.18	110.53
1	D	291	PHE	CA-C-N	5.69	125.37	119.56
1	D	291	PHE	C-N-CA	5.69	125.37	119.56
1	A	19	ALA	CB-CA-C	-5.69	110.03	116.63
1	D	19	ALA	CB-CA-C	-5.66	110.07	116.63
1	D	372	ILE	N-CA-C	-5.64	103.42	108.95
1	B	19	ALA	CB-CA-C	-5.63	110.07	116.54
1	A	47	GLY	CA-C-N	5.61	125.92	119.92
1	A	47	GLY	C-N-CA	5.61	125.92	119.92
1	A	128	PRO	N-CA-C	-5.59	103.39	111.22
1	B	114	THR	N-CA-C	-5.56	101.21	109.94
1	C	439	VAL	N-CA-C	5.55	120.88	109.34
1	D	116	ALA	N-CA-C	5.53	118.49	111.69
1	D	145	VAL	N-CA-C	5.49	112.09	106.21
1	D	307	TYR	CA-C-N	5.49	125.41	119.76
1	D	307	TYR	C-N-CA	5.49	125.41	119.76
1	A	114	THR	N-CA-C	-5.48	101.37	109.86
1	C	44	GLY	CA-C-N	5.47	125.12	119.05
1	C	44	GLY	C-N-CA	5.47	125.12	119.05
1	D	218	THR	N-CA-C	-5.43	100.45	109.46
1	C	218	THR	N-CA-C	-5.41	101.16	109.76
1	C	114	THR	N-CA-C	-5.39	101.66	109.31
1	B	183	ASP	N-CA-C	-5.35	105.53	111.36
1	C	116	ALA	N-CA-C	5.33	118.25	111.69
1	D	128	PRO	N-CA-C	-5.32	103.77	111.22
1	A	28	THR	N-CA-C	-5.31	103.02	110.35
1	B	44	GLY	CA-C-N	5.29	125.61	119.47
1	B	44	GLY	C-N-CA	5.29	125.61	119.47
1	D	176	LYS	N-CA-C	-5.28	102.58	110.23
1	D	281	GLN	N-CA-C	-5.28	101.10	109.59
1	D	114	THR	N-CA-C	-5.26	101.67	109.94
1	A	439	VAL	N-CA-C	5.25	120.25	109.34
1	B	409	SER	N-CA-C	5.24	118.94	112.24
1	C	183	ASP	N-CA-C	-5.21	105.52	111.14
1	A	408	PHE	N-CA-C	5.19	118.92	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	THR	N-CA-C	-5.17	100.88	109.46
1	A	116	ALA	N-CA-C	5.16	118.04	111.69
1	A	452	GLU	N-CA-C	5.16	116.59	111.07
1	A	183	ASP	N-CA-C	-5.16	105.74	111.36
1	A	409	SER	N-CA-C	5.11	118.82	112.58
1	A	218	THR	N-CA-C	-5.07	101.05	109.46
1	D	68	ILE	N-CA-C	-5.06	102.38	108.45
1	A	67	ARG	N-CA-C	5.04	118.44	109.96
1	B	176	LYS	N-CA-C	-5.03	102.94	110.23
1	B	100	GLU	N-CA-C	5.00	119.62	111.37

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	103	0
1	B	4019	0	3847	119	0
1	C	4019	0	3847	124	0
1	D	4019	0	3847	114	0
2	A	43	0	30	0	0
2	B	43	0	30	5	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	567	0	0	36	0
4	B	577	0	0	35	0
4	C	573	0	0	43	0
4	D	549	0	0	43	0
All	All	18518	0	15508	431	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 14.

All (431) 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:91:THR:HB	4:C:2034:HOH:O	1.16	1.27
1:C:450:LEU:HA	1:C:454:GLN:HE21	1.14	1.13
1:A:242:LYS:HE2	4:A:885:HOH:O	1.56	1.04
1:D:421:ARG:HD3	4:D:1588:HOH:O	1.58	1.03
1:D:475:LYS:HB3	4:D:1715:HOH:O	1.63	0.97
1:B:202:ARG:HH21	1:B:241:ILE:HD13	1.27	0.96
1:B:255:GLU:HB2	4:B:695:HOH:O	1.63	0.96
1:C:92:ARG:HD2	4:C:1374:HOH:O	1.67	0.95
1:C:92:ARG:HG3	4:C:1146:HOH:O	1.65	0.94
1:D:476:LYS:HB3	4:D:2014:HOH:O	1.68	0.93
1:C:111:ARG:HG2	4:C:2159:HOH:O	1.69	0.92
1:B:62:HIS:HE1	1:D:368:ASN:HD21	1.16	0.92
1:B:301:VAL:H	1:B:441:GLN:HE22	1.19	0.90
1:C:491:ARG:HD2	4:C:2170:HOH:O	1.74	0.86
1:C:12:LYS:HE3	4:C:520:HOH:O	1.77	0.83
1:D:456:LYS:HE2	4:D:1069:HOH:O	1.77	0.83
1:C:450:LEU:HA	1:C:454:GLN:NE2	1.94	0.82
1:B:475:LYS:NZ	1:B:475:LYS:HB3	1.93	0.82
4:A:541:HOH:O	1:C:52:GLN:HG3	1.79	0.81
1:C:72:VAL:HG13	1:C:73:VAL:HG23	1.60	0.80
1:D:476:LYS:HD3	4:D:1404:HOH:O	1.80	0.80
1:A:176:LYS:HD3	4:A:1563:HOH:O	1.82	0.79
1:C:451:ASN:OD1	1:C:454:GLN:HG2	1.82	0.79
1:C:178:PRO:HG2	4:C:2261:HOH:O	1.82	0.79
1:C:393:MET:HB3	4:C:513:HOH:O	1.84	0.77
1:C:105:ARG:NH1	4:C:1377:HOH:O	2.17	0.76
1:B:62:HIS:HE1	1:D:368:ASN:ND2	1.82	0.76
1:C:487:GLU:HG2	4:C:2170:HOH:O	1.86	0.76
1:A:202:ARG:NH1	4:A:1813:HOH:O	2.19	0.75
1:B:17:GLN:HG3	4:B:1380:HOH:O	1.86	0.75
1:C:155:ARG:HH22	1:C:438:ASN:HD21	1.31	0.75
1:D:248:ASP:HA	1:D:251:ARG:HH12	1.53	0.74
1:D:176:LYS:NZ	4:D:508:HOH:O	2.19	0.74
1:C:476:LYS:NZ	1:C:476:LYS:HB3	2.02	0.74
1:B:62:HIS:HD2	4:B:1812:HOH:O	1.71	0.74
1:C:453:GLU:HG2	4:C:1821:HOH:O	1.89	0.73
1:D:284:THR:OG1	1:D:287:GLU:HG3	1.88	0.73
1:B:290:ILE:HD13	1:B:290:ILE:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ASP:N	4:A:645:HOH:O	2.22	0.72
1:D:236:LYS:HE3	4:D:1850:HOH:O	1.88	0.72
1:D:444:THR:HG22	4:D:1335:HOH:O	1.87	0.72
1:A:120:GLY:N	4:D:2262:HOH:O	2.03	0.72
1:B:202:ARG:HH21	1:B:241:ILE:CD1	2.01	0.71
1:C:451:ASN:ND2	4:C:1821:HOH:O	2.23	0.71
1:C:450:LEU:CA	1:C:454:GLN:HE21	1.98	0.71
1:A:451:ASN:H	1:A:454:GLN:HE21	1.37	0.70
1:C:241:ILE:HD11	4:C:1408:HOH:O	1.90	0.70
1:A:436:ASP:C	4:A:645:HOH:O	2.34	0.70
1:C:471:LEU:HD13	4:C:666:HOH:O	1.91	0.70
1:D:490:SER:HA	4:D:2128:HOH:O	1.92	0.70
1:B:500:ASN:CG	4:B:1424:HOH:O	2.34	0.69
1:A:33:PRO:HG3	4:C:1854:HOH:O	1.90	0.69
1:D:476:LYS:CD	4:D:1404:HOH:O	2.40	0.69
1:B:255:GLU:HG2	4:B:887:HOH:O	1.92	0.69
1:C:241:ILE:HD13	4:C:2163:HOH:O	1.92	0.69
1:A:4:ARG:HD2	4:A:1009:HOH:O	1.92	0.68
1:D:473:ILE:HA	1:D:476:LYS:HE2	1.75	0.68
1:C:487:GLU:O	1:C:491:ARG:HG3	1.94	0.67
1:C:421:ARG:HG2	4:C:1066:HOH:O	1.94	0.67
1:C:12:LYS:O	1:C:16:GLU:HG3	1.94	0.67
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.61	0.66
1:B:43:VAL:CG1	1:B:48:PRO:HD2	2.26	0.66
1:D:444:THR:HG21	4:D:1269:HOH:O	1.95	0.66
1:C:448:LYS:HE2	4:C:1632:HOH:O	1.94	0.66
1:D:251:ARG:NE	4:D:1072:HOH:O	2.22	0.66
1:C:239:GLN:CG	4:C:1814:HOH:O	2.44	0.65
1:D:12:LYS:O	1:D:16:GLU:HG3	1.95	0.65
1:B:284:THR:OG1	1:B:287:GLU:HG3	1.97	0.65
1:A:456:LYS:O	1:A:460:GLU:HG3	1.97	0.65
1:D:319:ARG:NH1	4:D:623:HOH:O	2.26	0.64
1:D:251:ARG:NH2	4:D:1072:HOH:O	2.29	0.64
1:B:376[C]:CYS:SG	4:B:1862:HOH:O	2.55	0.64
1:B:475:LYS:HB3	1:B:475:LYS:HZ3	1.62	0.64
1:C:499:TYR:C	1:C:501:GLU:H	2.05	0.64
1:D:448:LYS:HD2	4:D:1923:HOH:O	1.96	0.64
1:D:248:ASP:HA	1:D:251:ARG:NH1	2.12	0.64
1:C:155:ARG:HH12	1:C:438:ASN:HD22	1.43	0.64
1:A:13:HIS:HD2	4:A:646:HOH:O	1.80	0.64
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ALA:N	4:C:1838:HOH:O	2.31	0.63
1:D:251:ARG:NH1	1:D:251:ARG:HB3	2.12	0.63
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.28	0.63
1:B:12:LYS:O	1:B:16:GLU:HG2	1.99	0.63
1:D:223:ASN:HD21	1:D:227:GLU:HB2	1.64	0.63
1:B:147:ASN:ND2	2:B:1:HEM:HAC	2.13	0.63
1:B:450:LEU:HB3	1:B:454:GLN:HG3	1.79	0.63
1:B:379:ARG:HH21	1:B:379:ARG:HG3	1.64	0.63
2:B:1:HEM:HBA1	4:B:789:HOH:O	1.98	0.63
1:C:13:HIS:O	1:C:17:GLN:HG2	1.98	0.63
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.64	0.62
1:A:3:ASN:CG	4:A:1613:HOH:O	2.41	0.62
1:A:485:HIS:HD2	1:A:487:GLU:HB3	1.64	0.62
1:B:92:ARG:HG3	4:B:627:HOH:O	1.99	0.62
1:D:499:TYR:C	1:D:501:GLU:H	2.06	0.62
1:A:421:ARG:HG2	4:A:2140:HOH:O	1.99	0.62
1:B:71:ARG:HD3	4:B:754:HOH:O	2.00	0.62
1:B:414:GLN:NE2	4:B:1487:HOH:O	2.33	0.62
1:C:262:ARG:NH1	4:C:613:HOH:O	2.12	0.62
1:C:476:LYS:CD	4:D:2033:HOH:O	2.48	0.61
1:C:294:ASN:HB3	1:C:297:ASP:HB2	1.83	0.61
1:A:202:ARG:NH2	4:A:2205:HOH:O	2.31	0.61
1:A:476:LYS:HE3	4:A:529:HOH:O	2.00	0.61
1:A:435:ASN:C	4:A:645:HOH:O	2.44	0.61
1:B:10:GLN:HE21	1:C:172:GLN:HE21	1.48	0.61
1:C:291:PHE:CD1	1:C:292:PRO:HD2	2.35	0.61
1:B:236:LYS:NZ	4:B:984:HOH:O	2.35	0.60
1:C:476:LYS:HD2	4:D:2033:HOH:O	2.01	0.60
1:A:351:GLN:HG3	4:A:757:HOH:O	2.01	0.60
1:A:436:ASP:N	4:A:645:HOH:O	2.35	0.60
1:C:414:GLN:CD	4:C:2045:HOH:O	2.44	0.60
2:B:1:HEM:HAD2	4:B:754:HOH:O	2.01	0.60
1:B:13:HIS:HD2	4:B:671:HOH:O	1.84	0.60
1:B:178:PRO:HG2	4:B:842:HOH:O	2.02	0.60
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.66	0.60
1:D:170:ASN:HD22	1:D:173:THR:H	1.49	0.59
1:B:111:ARG:NH2	4:B:754:HOH:O	2.35	0.59
1:D:18:ARG:CD	4:D:813:HOH:O	2.50	0.59
1:B:6:PRO:HG2	1:B:266:ASN:OD1	2.02	0.59
1:C:284:THR:OG1	1:C:287:GLU:HG3	2.03	0.59
1:B:491:ARG:O	1:B:495:LEU:HD23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2256:HOH:O	1:D:363:HIS:HD2	1.86	0.58
1:C:239:GLN:CD	4:C:1814:HOH:O	2.46	0.58
1:A:251:ARG:NH1	1:A:251:ARG:HB3	2.18	0.58
1:C:487:GLU:OE1	4:C:568:HOH:O	2.16	0.58
1:A:3:ASN:HA	4:A:1213:HOH:O	2.03	0.58
1:B:147:ASN:CG	2:B:1:HEM:HAC	2.28	0.58
1:A:448:LYS:HE2	4:A:950:HOH:O	2.04	0.58
1:C:202:ARG:NH1	4:C:1966:HOH:O	2.35	0.58
1:C:202:ARG:HD3	4:C:1966:HOH:O	2.03	0.58
1:B:475:LYS:HB3	1:B:475:LYS:HZ2	1.69	0.57
1:B:487:GLU:O	1:B:491:ARG:HG3	2.03	0.57
1:B:62:HIS:CE1	1:D:368:ASN:HD21	2.08	0.57
1:A:50:LEU:HD23	1:B:50:LEU:HD13	1.87	0.57
1:C:19:ALA:O	1:C:20:ALA:HB3	2.04	0.57
1:C:239:GLN:HB3	4:C:1814:HOH:O	2.04	0.57
1:D:406:ASN:HD21	1:D:410:ALA:HB3	1.68	0.57
1:B:414:GLN:CD	4:B:1487:HOH:O	2.47	0.57
1:C:476:LYS:HB3	1:C:476:LYS:HZ2	1.70	0.56
1:D:18:ARG:HD2	4:D:813:HOH:O	2.05	0.56
1:B:138:GLU:HG2	4:B:1464:HOH:O	2.05	0.56
1:B:43:VAL:O	1:B:43:VAL:HG13	2.05	0.56
1:B:3:ASN:HB2	4:B:1555:HOH:O	2.04	0.56
1:B:15:LYS:HD3	1:D:408:PHE:HA	1.89	0.55
1:B:202:ARG:HG2	1:B:202:ARG:NH1	2.22	0.55
1:B:447:LEU:HD11	1:B:485:HIS:HD2	1.71	0.55
1:B:451:ASN:H	1:B:454:GLN:CG	2.20	0.55
1:C:394:MET:N	4:C:513:HOH:O	2.10	0.55
1:A:12:LYS:O	1:A:16:GLU:HG3	2.05	0.55
1:A:251:ARG:HB3	1:A:251:ARG:HH11	1.72	0.55
1:B:447:LEU:HD11	1:B:485:HIS:CD2	2.41	0.55
1:C:97:LYS:O	1:C:100:GLU:HB2	2.07	0.55
1:A:381:ARG:HG2	1:A:381:ARG:NH1	2.22	0.55
1:C:92:ARG:CD	4:C:1374:HOH:O	2.39	0.55
1:D:429:GLN:NE2	4:D:1949:HOH:O	2.40	0.54
1:B:456:LYS:O	1:B:460:GLU:HG3	2.06	0.54
1:D:251:ARG:CZ	4:D:1072:HOH:O	2.55	0.54
1:D:107:PRO:HG2	1:D:136:TYR:HB2	1.88	0.54
1:C:155:ARG:HH12	1:C:438:ASN:ND2	2.05	0.54
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.90	0.54
1:C:393:MET:CB	4:C:513:HOH:O	2.49	0.54
1:D:251:ARG:NH1	4:D:1437:HOH:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.43	0.54
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.72	0.54
1:B:92:ARG:HD2	1:B:93:TYR:CE2	2.42	0.53
1:C:485:HIS:CE1	1:C:487:GLU:HB2	2.43	0.53
1:B:136:TYR:O	1:B:379:ARG:HG3	2.08	0.53
1:C:447:LEU:HD11	1:C:485:HIS:CD2	2.42	0.53
1:A:402:ASN:C	1:A:402:ASN:HD22	2.17	0.53
1:C:393:MET:CA	4:C:513:HOH:O	2.55	0.53
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.73	0.53
1:C:50:LEU:HD22	1:D:48:PRO:HB2	1.90	0.53
1:D:18:ARG:HD3	1:D:21:GLN:HB2	1.90	0.53
1:C:402:ASN:C	1:C:402:ASN:HD22	2.17	0.53
1:D:170:ASN:ND2	1:D:172:GLN:H	2.07	0.53
1:A:49:LEU:HD13	1:B:51:VAL:HG21	1.90	0.53
1:A:492:ILE:O	1:A:496:LEU:HD13	2.09	0.53
1:B:402:ASN:C	1:B:402:ASN:HD22	2.17	0.52
1:B:444:THR:HG21	4:B:1528:HOH:O	2.09	0.52
1:D:379:ARG:NE	4:D:957:HOH:O	2.32	0.52
1:D:18:ARG:NH2	4:D:974:HOH:O	2.42	0.52
1:A:66:GLU:HG2	1:C:387:ARG:O	2.10	0.52
1:A:451:ASN:H	1:A:454:GLN:NE2	2.06	0.52
1:A:176:LYS:HG3	4:A:2135:HOH:O	2.08	0.52
1:D:498:LYS:HD3	1:D:498:LYS:C	2.35	0.52
1:A:476:LYS:CE	4:A:529:HOH:O	2.56	0.52
1:D:18:ARG:CD	1:D:21:GLN:HB2	2.39	0.52
1:A:43:VAL:O	1:A:43:VAL:HG13	2.09	0.51
1:B:360:THR:HG21	2:B:1:HEM:HBA1	1.92	0.51
1:B:52:GLN:HB2	4:D:505:HOH:O	2.08	0.51
1:C:451:ASN:H	1:C:454:GLN:CG	2.23	0.51
4:A:1376:HOH:O	1:D:321:PRO:HG2	2.09	0.51
1:B:387:ARG:O	1:D:66:GLU:HG2	2.10	0.51
1:D:487:GLU:O	1:D:491:ARG:HG3	2.11	0.51
1:A:153:PHE:CE1	1:A:194:GLN:HG3	2.44	0.51
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.08	0.51
1:B:291:PHE:CD1	1:B:292:PRO:HD2	2.46	0.51
1:D:251:ARG:HB3	1:D:251:ARG:HH11	1.75	0.51
1:A:429:GLN:HG2	1:A:431:PHE:CZ	2.46	0.51
1:B:255:GLU:OE2	4:B:887:HOH:O	2.19	0.51
1:C:92:ARG:NH1	4:C:920:HOH:O	2.43	0.50
1:D:223:ASN:ND2	1:D:227:GLU:HB2	2.24	0.50
1:A:414:GLN:O	1:C:35:GLY:HA2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:TYR:C	1:A:501:GLU:H	2.18	0.50
1:B:479:LYS:HE2	4:B:2012:HOH:O	2.11	0.50
1:C:432:ASN:ND2	1:C:434:ALA:H	2.10	0.50
1:D:20:ALA:HB3	4:D:1043:HOH:O	2.11	0.50
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.94	0.50
1:D:443:ARG:NE	4:D:1925:HOH:O	2.37	0.50
1:B:351:GLN:HG3	4:B:604:HOH:O	2.12	0.50
1:A:17:GLN:HG3	4:A:2026:HOH:O	2.11	0.50
1:B:3:ASN:N	4:B:1555:HOH:O	2.44	0.50
1:B:43:VAL:O	1:B:47:GLY:HA3	2.12	0.50
1:C:22:LYS:HD3	1:C:23:PRO:N	2.26	0.50
1:C:421:ARG:HH21	1:D:429:GLN:HE22	1.59	0.50
1:A:213:GLY:HA3	1:A:235:TYR:CE2	2.46	0.49
1:A:262:ARG:NH2	4:A:1017:HOH:O	2.19	0.49
1:D:443:ARG:HD2	4:D:1925:HOH:O	2.11	0.49
1:D:457:ARG:HG2	4:D:929:HOH:O	2.11	0.49
1:A:455:ARG:NH2	4:A:895:HOH:O	2.34	0.49
1:A:460:GLU:HA	1:A:495:LEU:HD13	1.93	0.49
1:D:294:ASN:HB3	1:D:297:ASP:HB2	1.94	0.49
1:C:450:LEU:HB3	1:C:454:GLN:HG3	1.94	0.49
1:B:254:HIS:HD2	4:B:2051:HOH:O	1.94	0.49
1:A:451:ASN:O	1:A:455:ARG:HG3	2.12	0.49
1:A:460:GLU:HA	4:A:2180:HOH:O	2.11	0.49
1:D:381:ARG:HH11	1:D:381:ARG:HG2	1.78	0.49
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.93	0.49
1:B:357:TYR:HA	4:B:789:HOH:O	2.13	0.49
1:B:21:GLN:NE2	4:B:2253:HOH:O	2.30	0.49
1:C:456:LYS:O	1:C:460:GLU:HG3	2.12	0.49
1:C:499:TYR:C	1:C:501:GLU:N	2.69	0.49
1:D:136:TYR:O	1:D:379:ARG:HG3	2.13	0.49
1:C:3:ASN:N	1:C:3:ASN:HD22	2.11	0.48
4:A:2226:HOH:O	1:B:421:ARG:CD	2.62	0.48
1:C:16:GLU:C	1:C:18:ARG:H	2.22	0.48
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.96	0.48
1:B:26:LEU:HD13	1:D:384:ASN:HA	1.94	0.48
1:B:213:GLY:HA3	1:B:235:TYR:CE2	2.49	0.48
1:A:25:VAL:HG13	1:C:414:GLN:HG2	1.93	0.48
1:C:92:ARG:H	1:C:92:ARG:HD3	1.77	0.48
1:D:427:ASP:HB2	1:D:429:GLN:HE21	1.77	0.48
1:A:129:ARG:H	1:A:148:ASN:ND2	2.11	0.48
1:A:487:GLU:HG2	1:A:491:ARG:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:GLU:CB	4:C:2029:HOH:O	2.60	0.48
1:D:476:LYS:HD2	4:D:1539:HOH:O	2.13	0.48
1:A:414:GLN:HG3	4:A:1815:HOH:O	2.14	0.48
1:B:160:PHE:HB3	1:B:161:PRO:HD3	1.95	0.48
1:C:239:GLN:CB	4:C:1814:HOH:O	2.62	0.48
1:D:394:MET:HB2	4:D:821:HOH:O	2.14	0.48
1:B:391:MET:HE3	1:B:393:MET:CE	2.44	0.48
1:C:391:MET:HE3	1:C:393:MET:CE	2.44	0.48
1:D:178:PRO:HG2	4:D:556:HOH:O	2.14	0.48
1:D:13:HIS:O	1:D:17:GLN:HG3	2.14	0.47
1:A:48:PRO:HB2	1:B:50:LEU:HD12	1.96	0.47
1:A:294:ASN:HB3	1:A:297:ASP:HB2	1.96	0.47
1:D:15:LYS:O	1:D:18:ARG:HB3	2.13	0.47
1:A:43:VAL:O	1:A:47:GLY:HA3	2.14	0.47
1:A:92:ARG:NH2	4:A:1078:HOH:O	2.45	0.47
1:D:129:ARG:HG3	1:D:205:PRO:HG3	1.96	0.47
1:A:148:ASN:N	1:A:148:ASN:HD22	2.12	0.47
1:D:421:ARG:HH11	1:D:421:ARG:HB3	1.80	0.47
1:D:499:TYR:C	1:D:501:GLU:N	2.73	0.47
1:A:82:GLY:HA3	1:A:316:VAL:O	2.15	0.47
1:A:148:ASN:HD22	1:A:148:ASN:H	1.62	0.47
1:B:168:LYS:HE3	1:C:67:ARG:HH21	1.79	0.47
1:C:485:HIS:HE1	4:C:568:HOH:O	1.98	0.47
1:D:73:VAL:O	1:D:74:HIS:HB2	2.14	0.47
1:D:251:ARG:HH11	1:D:251:ARG:CB	2.28	0.47
1:D:357:TYR:HB2	1:D:358:PRO:HD3	1.95	0.47
1:D:92:ARG:HD3	4:D:2040:HOH:O	2.15	0.47
1:D:475:LYS:HD3	4:D:1486:HOH:O	2.14	0.47
4:A:2226:HOH:O	1:B:421:ARG:CB	2.63	0.47
1:B:499:TYR:C	1:B:501:GLU:H	2.22	0.47
1:B:367:PRO:HG3	1:D:65:ARG:HD3	1.97	0.47
1:C:293:PHE:HE2	1:C:437:ASP:OD1	1.98	0.47
1:C:476:LYS:HB3	1:C:476:LYS:HZ3	1.77	0.47
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.97	0.46
1:C:209:ARG:O	1:C:239:GLN:HG2	2.16	0.46
1:B:445:PHE:HA	1:B:449:VAL:CG2	2.45	0.46
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.45	0.46
1:A:384:ASN:HA	1:C:26:LEU:HD13	1.98	0.46
1:D:351:GLN:HG3	4:D:1070:HOH:O	2.15	0.46
1:A:22:LYS:HD2	1:A:23:PRO:HD2	1.98	0.46
1:A:136:TYR:O	1:A:379:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:HIS:HA	1:B:114:THR:O	2.16	0.46
1:B:388:ASP:H	1:B:396:ASN:HD21	1.61	0.46
1:C:241:ILE:N	1:C:241:ILE:HD12	2.31	0.46
1:A:202:ARG:HG3	1:A:202:ARG:HH11	1.80	0.46
1:D:17:GLN:HB2	4:D:1331:HOH:O	2.16	0.46
1:B:381:ARG:HG2	1:B:381:ARG:NH1	2.29	0.46
1:A:202:ARG:NH1	1:A:202:ARG:HG3	2.31	0.46
1:D:443:ARG:CD	4:D:1925:HOH:O	2.64	0.46
1:A:142:TRP:HB2	1:A:339:PRO:HD3	1.96	0.45
1:B:17:GLN:CG	4:B:1380:HOH:O	2.56	0.45
1:B:476:LYS:NZ	4:B:1767:HOH:O	2.40	0.45
1:D:464:GLY:O	1:D:467:LYS:HE2	2.16	0.45
1:A:26:LEU:HD13	1:C:384:ASN:HA	1.98	0.45
1:A:429:GLN:HG2	1:A:431:PHE:CE2	2.51	0.45
1:D:193:HIS:HD2	1:D:299:THR:O	1.99	0.45
1:C:89:ASP:N	1:C:102:ILE:HD11	2.31	0.45
1:D:475:LYS:NZ	4:D:1715:HOH:O	2.46	0.45
1:B:65:ARG:HD3	1:D:367:PRO:HG3	1.97	0.45
1:C:111:ARG:C	4:C:2159:HOH:O	2.59	0.45
1:A:262:ARG:NE	4:A:1017:HOH:O	2.47	0.45
1:C:17:GLN:HG3	4:C:1596:HOH:O	2.15	0.45
1:B:82:GLY:HA3	1:B:316:VAL:O	2.17	0.45
1:D:18:ARG:HG2	4:D:813:HOH:O	2.16	0.45
1:D:220:LYS:NZ	1:D:420:HIS:HD2	2.15	0.45
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.47	0.45
1:B:346:PRO:O	1:B:347:ASP:C	2.60	0.45
1:C:429:GLN:HG2	1:C:431:PHE:CZ	2.52	0.45
1:A:35:GLY:HA2	1:C:414:GLN:O	2.16	0.45
1:A:206:ASP:CB	1:A:242:LYS:HD2	2.47	0.45
1:B:311:PRO:HG3	4:B:1534:HOH:O	2.17	0.45
1:C:476:LYS:HG3	4:C:1337:HOH:O	2.17	0.45
1:D:236:LYS:HD2	4:D:1876:HOH:O	2.16	0.45
1:A:232:LYS:HB2	1:A:281:GLN:HB2	1.99	0.44
1:A:321:PRO:HG2	4:D:611:HOH:O	2.16	0.44
1:B:225:ASN:ND2	4:B:1218:HOH:O	2.50	0.44
1:B:454:GLN:HE21	1:B:454:GLN:HB3	1.59	0.44
1:D:82:GLY:HA3	1:D:316:VAL:O	2.17	0.44
1:D:129:ARG:H	1:D:148:ASN:ND2	2.15	0.44
1:B:29:GLY:HA3	4:B:566:HOH:O	2.17	0.44
1:B:402:ASN:C	1:B:402:ASN:ND2	2.75	0.44
1:D:498:LYS:HD3	1:D:498:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HE2	1:B:302:TRP:CE2	2.52	0.44
1:B:35:GLY:HA2	1:D:414:GLN:O	2.17	0.44
1:A:39:ASN:C	1:D:158:LEU:HD12	2.42	0.44
1:A:402:ASN:C	1:A:402:ASN:ND2	2.76	0.44
1:A:414:GLN:HB2	4:A:1815:HOH:O	2.17	0.44
1:C:237:THR:HA	1:C:276:TRP:CD1	2.53	0.44
1:C:493:GLN:NE2	4:C:1499:HOH:O	2.13	0.44
1:D:95:LYS:HG2	1:D:222:VAL:O	2.18	0.44
1:D:187:LEU:C	1:D:189:PRO:HD3	2.42	0.44
1:A:15:LYS:HD2	1:C:408:PHE:HA	1.98	0.44
4:A:2226:HOH:O	1:B:421:ARG:HD2	2.18	0.44
1:B:466:LEU:HD22	1:B:474:GLN:HG2	2.00	0.44
1:C:43:VAL:O	1:C:47:GLY:HA3	2.18	0.44
1:D:148:ASN:N	1:D:148:ASN:HD22	2.14	0.44
1:A:17:GLN:CG	4:A:2026:HOH:O	2.66	0.43
1:A:65:ARG:HD3	1:C:367:PRO:HG3	1.99	0.43
1:B:42:THR:HA	1:B:50:LEU:CD2	2.48	0.43
1:C:108:ILE:HA	1:C:134:LYS:O	2.18	0.43
1:C:153:PHE:CE1	1:C:194:GLN:HG3	2.53	0.43
1:D:217:HIS:CD2	1:D:353:ARG:HH11	2.36	0.43
1:A:232:LYS:O	1:A:280:ILE:HA	2.17	0.43
1:A:414:GLN:CG	4:A:1815:HOH:O	2.65	0.43
1:D:472:PHE:O	1:D:476:LYS:HG3	2.17	0.43
1:A:206:ASP:HB2	1:A:242:LYS:HD2	1.98	0.43
1:B:479:LYS:HG3	4:B:2012:HOH:O	2.16	0.43
1:D:232:LYS:O	1:D:280:ILE:HA	2.19	0.43
1:A:450:LEU:HA	1:A:454:GLN:NE2	2.33	0.43
1:B:193:HIS:HD2	1:B:299:THR:O	2.00	0.43
1:B:357:TYR:HB2	1:B:358:PRO:HD3	2.00	0.43
1:A:108:ILE:HA	1:A:134:LYS:O	2.19	0.43
1:A:265:PHE:HA	1:A:320:ASN:HD21	1.83	0.43
1:B:73:VAL:O	1:B:74:HIS:HB2	2.18	0.43
1:B:453:GLU:HG2	1:B:457:ARG:NH1	2.33	0.43
1:C:206:ASP:HA	1:C:244:LEU:HG	2.01	0.43
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.54	0.43
1:C:232:LYS:O	1:C:280:ILE:HA	2.17	0.43
1:A:331:LEU:HD13	1:A:374:VAL:CG2	2.49	0.43
1:B:40:SER:HB3	1:B:49:LEU:CD1	2.48	0.43
1:C:453:GLU:HB2	4:C:2029:HOH:O	2.19	0.43
1:D:479:LYS:HD3	1:D:479:LYS:C	2.44	0.43
1:A:487:GLU:HG2	1:A:491:ARG:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:ARG:HB3	1:D:421:ARG:NH1	2.32	0.43
1:A:90:ILE:HG21	1:A:312:VAL:HG22	2.00	0.43
1:B:50:LEU:HD22	1:B:50:LEU:N	2.34	0.43
1:B:237:THR:HA	1:B:276:TRP:CD1	2.54	0.43
1:C:346:PRO:O	1:C:347:ASP:C	2.62	0.43
1:B:74:HIS:HB3	4:B:754:HOH:O	2.19	0.42
1:B:138:GLU:CG	4:B:1464:HOH:O	2.66	0.42
1:C:17:GLN:CD	4:C:1596:HOH:O	2.62	0.42
1:D:145:VAL:HG22	1:D:333:PHE:HB3	2.02	0.42
1:C:145:VAL:HG22	1:C:333:PHE:HB3	2.00	0.42
1:D:148:ASN:HD22	1:D:148:ASN:H	1.66	0.42
1:D:206:ASP:HA	1:D:244:LEU:HG	2.01	0.42
1:B:11:MET:HE2	1:C:180:MET:HG3	2.01	0.42
1:B:16:GLU:HG2	1:B:16:GLU:H	1.69	0.42
1:D:120:GLY:N	4:D:2262:HOH:O	1.99	0.42
1:A:279:TYR:HB2	1:A:309:LEU:HD12	2.01	0.42
1:A:423:HIS:HB2	1:B:427:ASP:OD1	2.19	0.42
4:B:639:HOH:O	1:C:351:GLN:HG3	2.19	0.42
1:C:499:TYR:O	1:C:501:GLU:HG3	2.20	0.42
1:D:43:VAL:O	1:D:47:GLY:HA3	2.20	0.42
1:A:487:GLU:CG	1:A:491:ARG:HD2	2.50	0.42
1:B:14:TRP:O	1:B:17:GLN:HG2	2.20	0.42
1:C:357:TYR:HB2	1:C:358:PRO:HD3	2.00	0.42
1:C:410:ALA:HB1	1:C:411:PRO:HD2	2.00	0.42
1:A:251:ARG:O	1:A:255:GLU:HG3	2.20	0.42
1:C:472:PHE:O	1:C:476:LYS:HG3	2.20	0.42
1:C:82:GLY:HA3	1:C:316:VAL:O	2.20	0.42
1:C:26:LEU:HD21	1:C:37:LYS:HD3	2.01	0.42
1:D:74:HIS:HA	1:D:114:THR:O	2.20	0.42
1:D:177:ASP:OD1	1:D:179:ASP:HB2	2.20	0.41
1:B:43:VAL:HG12	1:B:48:PRO:HD2	2.02	0.41
1:D:142:TRP:HB2	1:D:339:PRO:HD3	2.01	0.41
1:A:179:ASP:CG	1:D:4:ARG:HH22	2.27	0.41
1:C:160:PHE:HB3	1:C:161:PRO:HD3	2.02	0.41
1:C:467:LYS:HD2	1:C:499:TYR:CD1	2.55	0.41
1:D:473:ILE:HA	1:D:476:LYS:CE	2.47	0.41
1:A:213:GLY:HA3	1:A:235:TYR:CD2	2.54	0.41
1:D:499:TYR:O	1:D:501:GLU:HG3	2.20	0.41
1:A:97:LYS:NZ	4:A:937:HOH:O	2.53	0.41
1:B:177:ASP:HA	1:B:178:PRO:HD2	1.94	0.41
1:C:410:ALA:HB1	1:C:411:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:SER:O	1:D:195:VAL:HG23	2.20	0.41
1:D:476:LYS:HE3	1:D:476:LYS:HB2	1.84	0.41
1:A:3:ASN:OD1	4:A:1213:HOH:O	2.22	0.41
1:A:251:ARG:HH11	1:A:251:ARG:CB	2.34	0.41
1:C:272:ASN:ND2	4:C:946:HOH:O	2.44	0.41
1:A:49:LEU:HB2	1:D:351:GLN:HB3	2.01	0.41
1:B:142:TRP:HB2	1:B:339:PRO:HD3	2.03	0.41
1:B:186:SER:HB2	1:B:476:LYS:HG3	2.02	0.41
1:B:491:ARG:O	1:B:495:LEU:CD2	2.68	0.41
1:D:237:THR:HA	1:D:276:TRP:CD1	2.55	0.41
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.85	0.41
1:D:170:ASN:HD22	1:D:172:GLN:H	1.69	0.41
1:C:3:ASN:N	1:C:3:ASN:ND2	2.69	0.40
1:A:3:ASN:CA	4:A:1213:HOH:O	2.66	0.40
1:C:91:THR:HG22	1:C:91:THR:O	2.21	0.40
1:C:381:ARG:HB2	1:C:381:ARG:HH11	1.85	0.40
1:C:402:ASN:C	1:C:402:ASN:ND2	2.77	0.40
1:A:4:ARG:HH22	1:D:179:ASP:CG	2.29	0.40
1:B:414:GLN:HA	1:B:415:PRO:HD2	1.89	0.40
1:B:421:ARG:HG2	1:B:421:ARG:HH11	1.85	0.40
1:B:471:LEU:HD21	1:B:500:ASN:ND2	2.36	0.40
1:C:100:GLU:HG2	1:C:101:HIS:CE1	2.57	0.40
1:C:414:GLN:HA	1:C:415:PRO:HD2	1.93	0.40
1:D:285:PHE:O	1:D:289:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	499/499 (100%)	476 (95%)	22 (4%)	1 (0%)	43 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	499/499 (100%)	477 (96%)	21 (4%)	1 (0%)	43	42
1	C	499/499 (100%)	475 (95%)	23 (5%)	1 (0%)	43	42
1	D	499/499 (100%)	479 (96%)	18 (4%)	2 (0%)	30	27
All	All	1996/1996 (100%)	1907 (96%)	84 (4%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	ASP
1	C	437	ASP
1	B	437	ASP
1	D	437	ASP
1	D	500	ASN

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%)	422 (98%)	11 (2%)	42	45
1	B	433/431 (100%)	419 (97%)	14 (3%)	34	35
1	C	433/431 (100%)	422 (98%)	11 (2%)	42	45
1	D	433/431 (100%)	426 (98%)	7 (2%)	55	62
All	All	1732/1724 (100%)	1689 (98%)	43 (2%)	42	45

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	17	GLN
1	A	49	LEU
1	A	137	THR
1	A	148	ASN
1	A	235	TYR

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Mol	Chain	Res	Type
1	A	242	LYS
1	A	402	ASN
1	A	413	HIS
1	A	448	LYS
1	A	501	GLU
1	B	92	ARG
1	B	129	ARG
1	B	137	THR
1	B	202	ARG
1	B	235	TYR
1	B	252	LEU
1	B	290	ILE
1	B	402	ASN
1	B	413	HIS
1	B	421	ARG
1	B	454	GLN
1	B	457	ARG
1	B	466	LEU
1	B	475	LYS
1	C	4	ARG
1	C	73	VAL
1	C	92	ARG
1	C	105	ARG
1	C	137	THR
1	C	235	TYR
1	C	239	GLN
1	C	381	ARG
1	C	402	ASN
1	C	413	HIS
1	C	496	LEU
1	D	137	THR
1	D	148	ASN
1	D	193	HIS
1	D	235	TYR
1	D	309	LEU
1	D	413	HIS
1	D	456	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS

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Mol	Chain	Res	Type
1	A	148	ASN
1	A	254	HIS
1	A	320	ASN
1	A	337	ASN
1	A	402	ASN
1	A	454	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	225	ASN
1	B	254	HIS
1	B	272	ASN
1	B	337	ASN
1	B	396	ASN
1	B	402	ASN
1	B	441	GLN
1	B	461	ASN
1	B	500	ASN
1	C	21	GLN
1	C	172	GLN
1	C	254	HIS
1	C	272	ASN
1	C	337	ASN
1	C	386	GLN
1	C	402	ASN
1	C	432	ASN
1	C	438	ASN
1	C	454	GLN
1	C	474	GLN
1	C	480	ASN
1	C	485	HIS
1	D	3	ASN
1	D	52	GLN
1	D	148	ASN
1	D	167	GLN
1	D	170	ASN
1	D	193	HIS
1	D	337	ASN

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Mol	Chain	Res	Type
1	D	363	HIS
1	D	368	ASN
1	D	420	HIS
1	D	429	GLN
1	D	500	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are modelled with single atom - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	B	1	3,1	50,50,50	1.07	4 (8%)	67,82,82	0.85	1 (1%)
2	HEM	A	1	3,1	50,50,50	1.09	4 (8%)	67,82,82	0.88	1 (1%)
2	HEM	C	1	3,1	50,50,50	1.16	4 (8%)	67,82,82	0.90	2 (2%)
2	HEM	D	1	3,1	50,50,50	1.16	4 (8%)	67,82,82	0.91	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	B	1	3,1	-	6/14/54/54	-
2	HEM	A	1	3,1	-	3/14/54/54	-
2	HEM	C	1	3,1	-	2/14/54/54	-
2	HEM	D	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	A	1	HEM	CBC-CAC	3.20	1.45	1.30
2	D	1	HEM	CBC-CAC	3.17	1.45	1.30
2	B	1	HEM	CBB-CAB	3.10	1.45	1.30
2	B	1	HEM	CBC-CAC	3.09	1.45	1.30
2	C	1	HEM	CBB-CAB	2.99	1.44	1.30
2	A	1	HEM	CBB-CAB	2.99	1.44	1.30
2	C	1	HEM	CBC-CAC	2.98	1.44	1.30
2	D	1	HEM	CBB-CAB	2.95	1.44	1.30
2	C	1	HEM	CAB-C3B	-2.76	1.40	1.47
2	A	1	HEM	CAC-C3C	-2.60	1.40	1.47
2	D	1	HEM	CAB-C3B	-2.59	1.40	1.47
2	B	1	HEM	CAC-C3C	-2.56	1.40	1.47
2	B	1	HEM	CAB-C3B	-2.53	1.40	1.47
2	A	1	HEM	CAB-C3B	-2.50	1.40	1.47
2	C	1	HEM	CAC-C3C	-2.49	1.40	1.47
2	D	1	HEM	CAC-C3C	-2.47	1.40	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	HEM	C3B-C4B-NB	3.18	111.75	109.47
2	A	1	HEM	C3B-C4B-NB	2.79	111.47	109.47
2	C	1	HEM	C3B-C4B-NB	2.66	111.38	109.47
2	B	1	HEM	C3B-C4B-NB	2.56	111.31	109.47
2	C	1	HEM	CAD-C3D-C2D	-2.30	123.57	127.87

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	HEM	C2C-C3C-CAC-CBC

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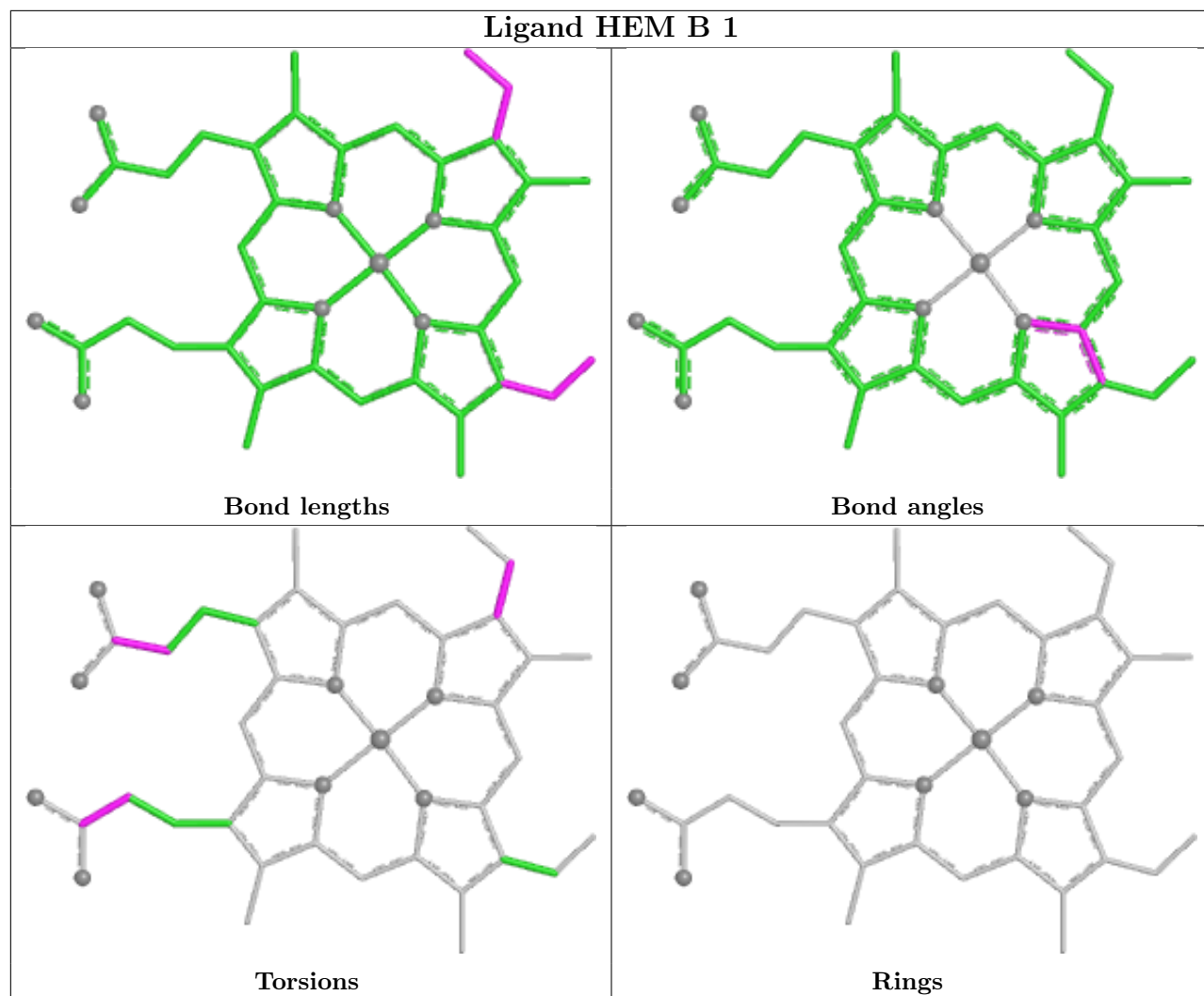
Mol	Chain	Res	Type	Atoms
2	B	1	HEM	C4C-C3C-CAC-CBC
2	A	1	HEM	CAD-CBD-CGD-O2D
2	D	1	HEM	CAD-CBD-CGD-O2D
2	C	1	HEM	CAD-CBD-CGD-O2D
2	A	1	HEM	CAD-CBD-CGD-O1D
2	B	1	HEM	CAD-CBD-CGD-O2D
2	D	1	HEM	CAD-CBD-CGD-O1D
2	C	1	HEM	CAD-CBD-CGD-O1D
2	B	1	HEM	CAD-CBD-CGD-O1D
2	B	1	HEM	CAA-CBA-CGA-O2A
2	A	1	HEM	CAA-CBA-CGA-O2A
2	B	1	HEM	CAA-CBA-CGA-O1A

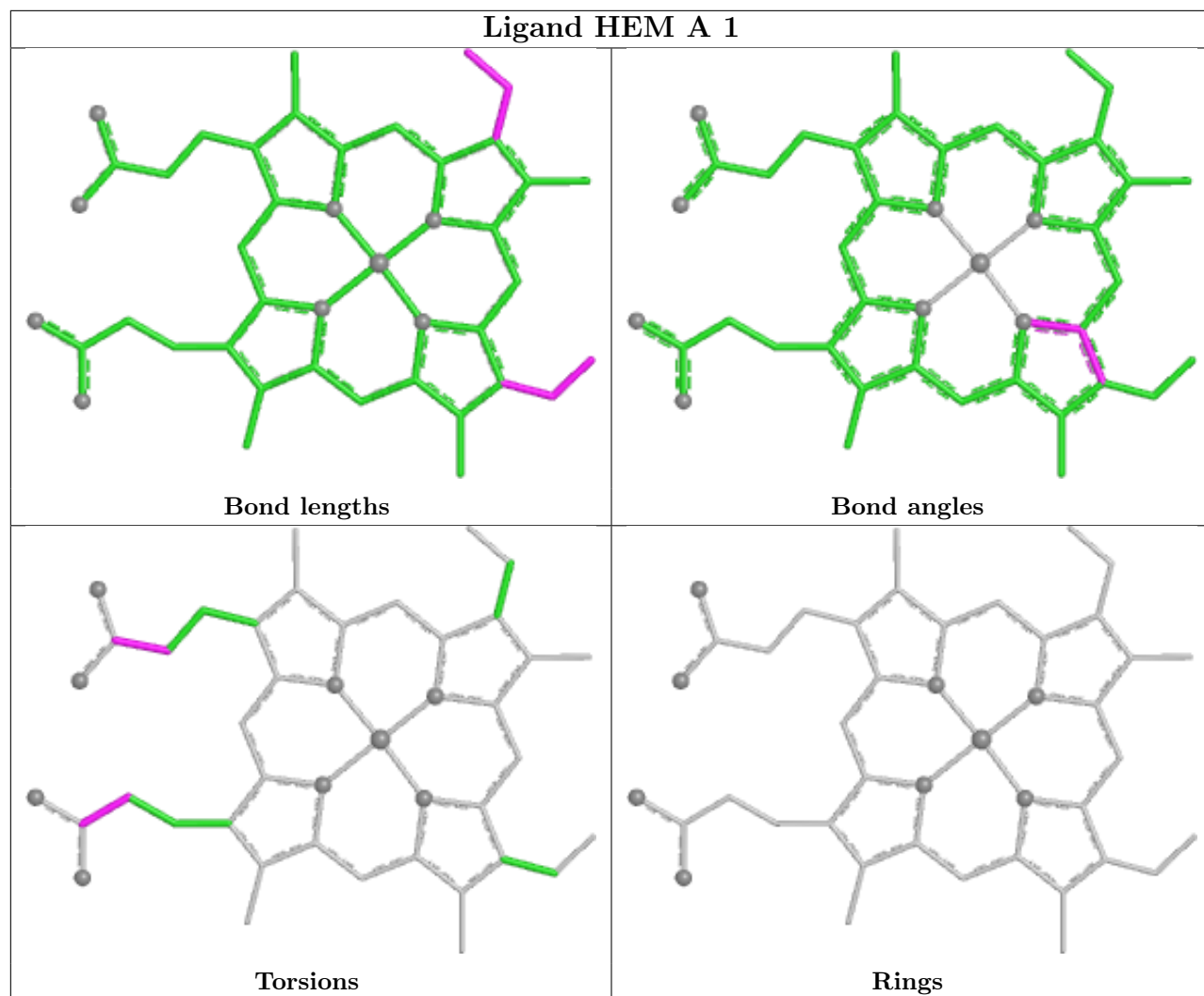
There are no ring outliers.

1 monomer is involved in 5 short contacts:

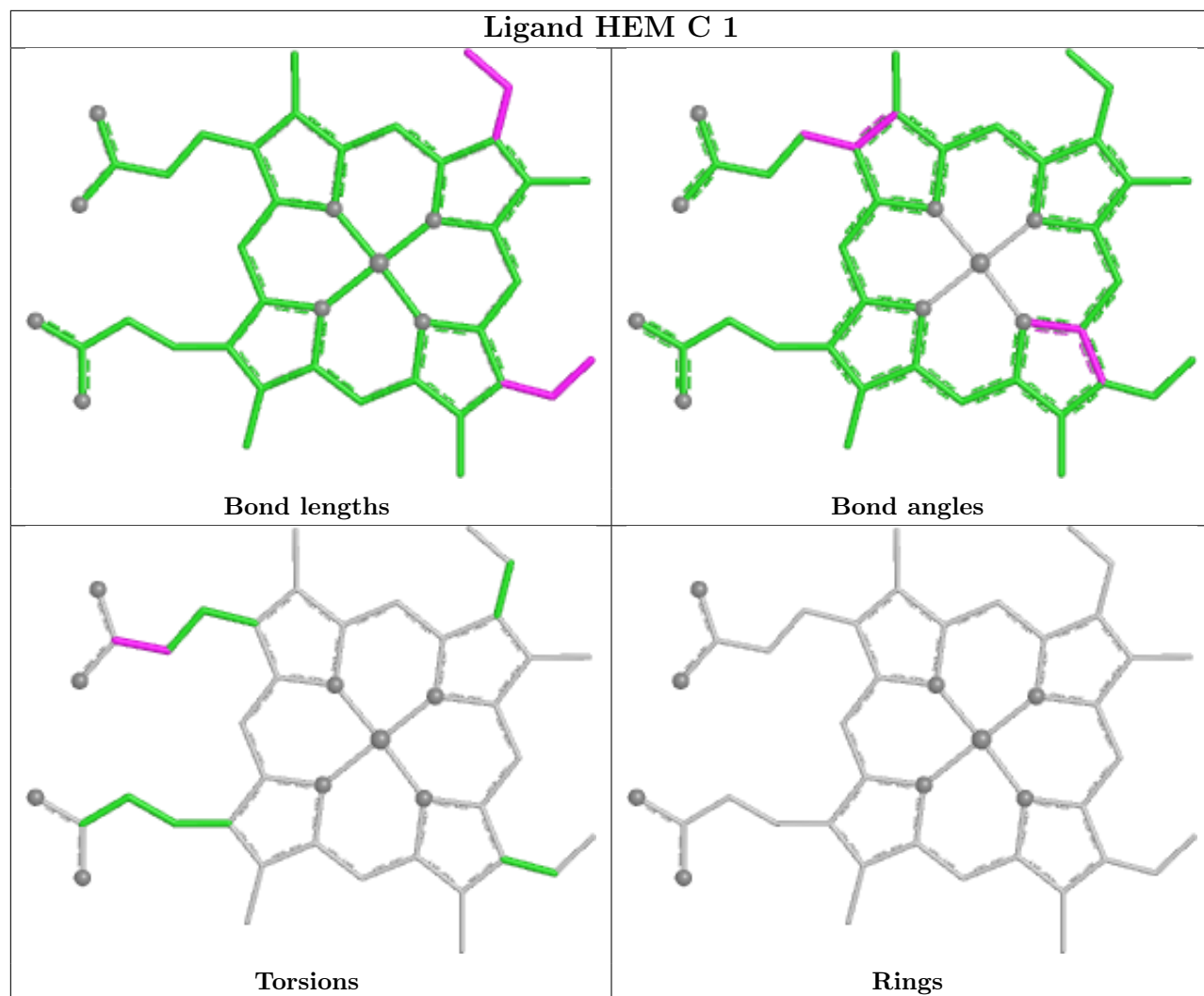
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	HEM	5	0

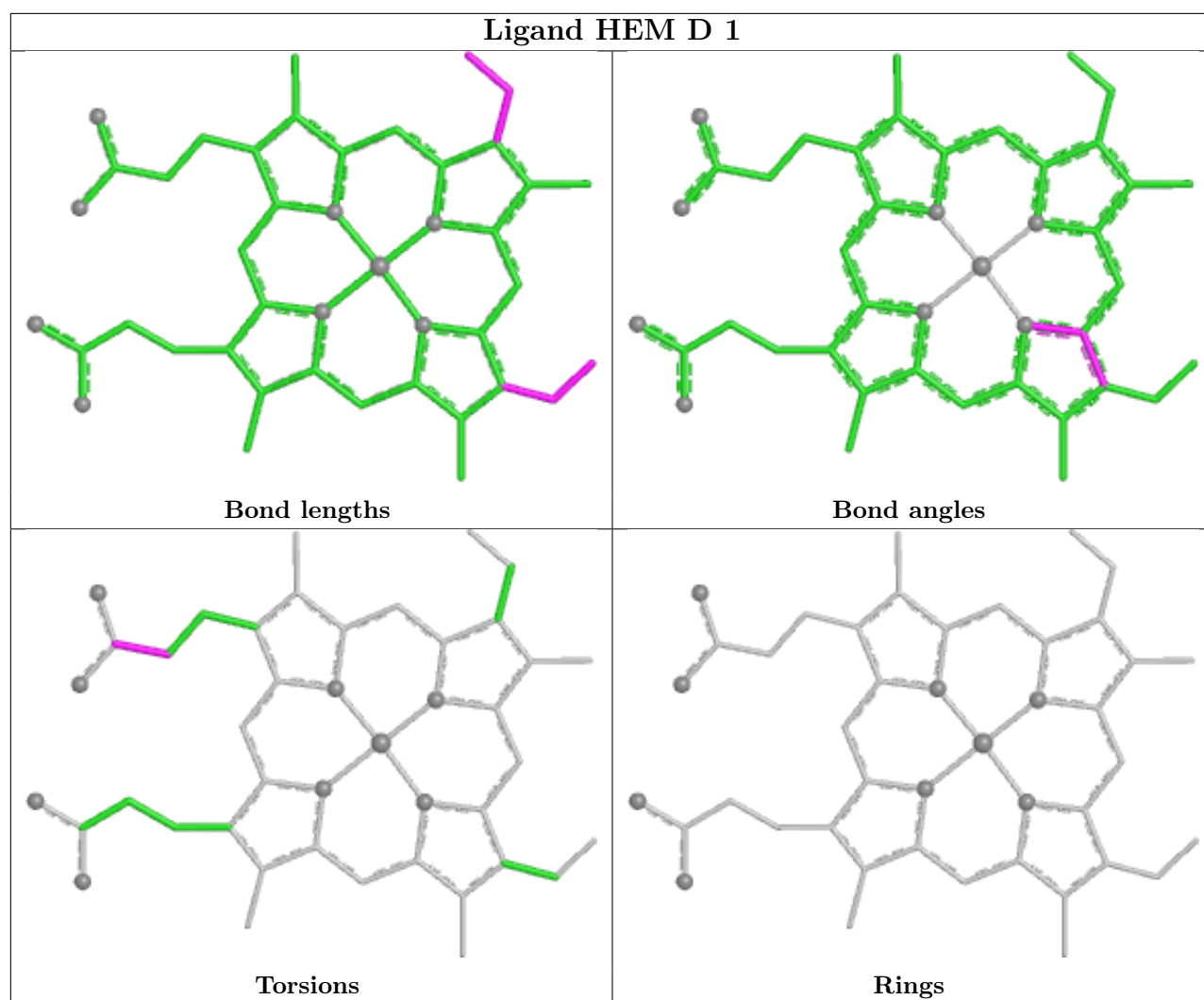
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





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	499/499 (100%)	-0.32	6 (1%) 76 76	7, 15, 29, 55	1 (0%)
1	B	499/499 (100%)	-0.27	8 (1%) 70 70	7, 15, 30, 57	1 (0%)
1	C	499/499 (100%)	-0.28	12 (2%) 59 59	7, 14, 31, 61	1 (0%)
1	D	499/499 (100%)	-0.19	12 (2%) 59 59	7, 16, 32, 58	1 (0%)
All	All	1996/1996 (100%)	-0.27	38 (1%) 66 66	7, 15, 31, 61	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	ILE	4.4
1	A	20	ALA	4.1
1	D	17	GLN	3.9
1	B	17	GLN	3.8
1	C	19	ALA	3.6
1	B	19	ALA	3.6
1	D	3	ASN	3.5
1	B	500	ASN	3.4
1	C	17	GLN	3.4
1	C	92	ARG	3.2
1	C	18	ARG	3.2
1	A	3	ASN	3.1
1	C	3	ASN	3.0
1	D	18	ARG	3.0
1	D	272	ASN	2.8
1	D	499	TYR	2.7
1	D	20	ALA	2.7
1	B	501	GLU	2.6
1	B	3	ASN	2.6
1	A	499	TYR	2.6
1	B	444	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	444	THR	2.5
1	C	500	ASN	2.5
1	C	421	ARG	2.5
1	A	17	GLN	2.5
1	A	21	GLN	2.4
1	B	20	ALA	2.4
1	A	19	ALA	2.3
1	C	20	ALA	2.3
1	D	394	MET	2.3
1	D	289	GLU	2.3
1	C	101	HIS	2.3
1	C	453	GLU	2.2
1	C	501	GLU	2.1
1	D	290	ILE	2.1
1	D	21	GLN	2.1
1	D	381	ARG	2.0
1	C	289	GLU	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($\text{\AA}^2$)	Q<0.9
3	NH3	B	502	1/1	0.97	0.08	13,13,13,13	0
3	NH3	C	502	1/1	0.97	0.09	13,13,13,13	1
3	NH3	D	502	1/1	0.97	0.10	13,13,13,13	0
2	HEM	D	1	43/43	0.99	0.05	10,13,15,16	0
3	NH3	A	502	1/1	0.99	0.05	11,11,11,11	1
2	HEM	A	1	43/43	0.99	0.05	7,10,15,17	0

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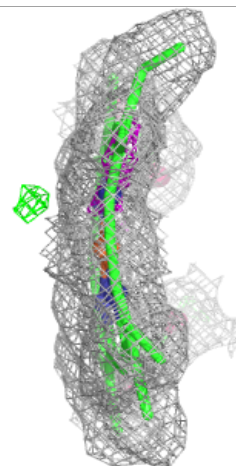
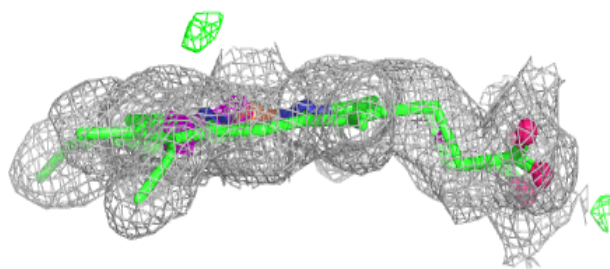
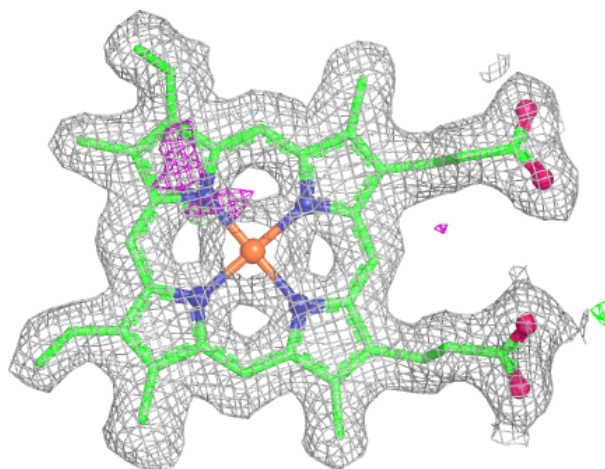
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	1	43/43	0.99	0.04	6,11,15,17	0
2	HEM	C	1	43/43	0.99	0.05	8,11,14,15	0

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.

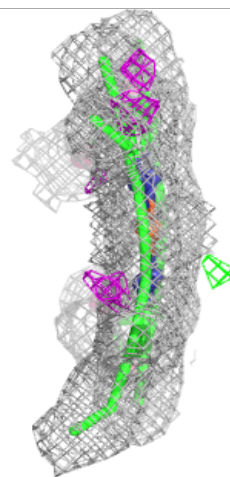
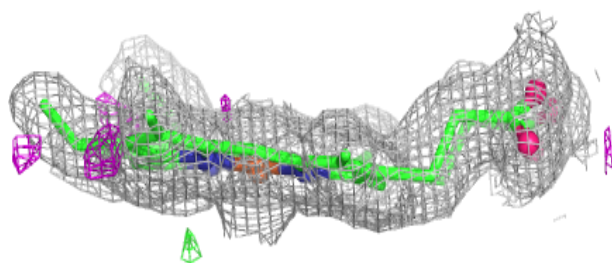
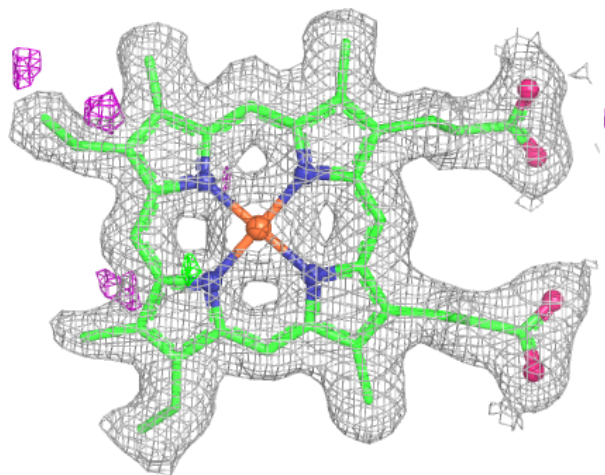
Electron density around HEM D 1:

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



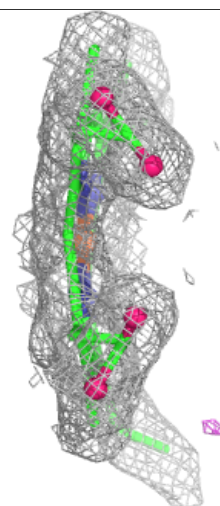
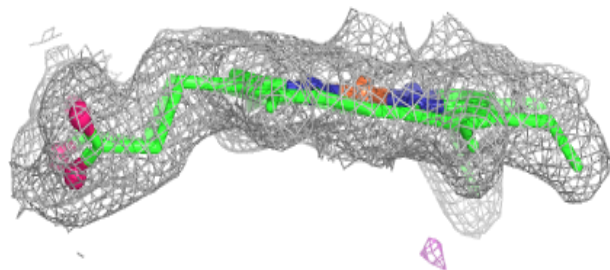
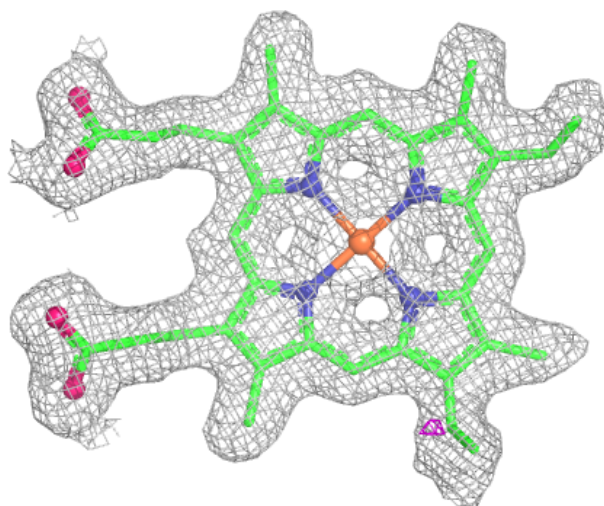
Electron density around HEM A 1:

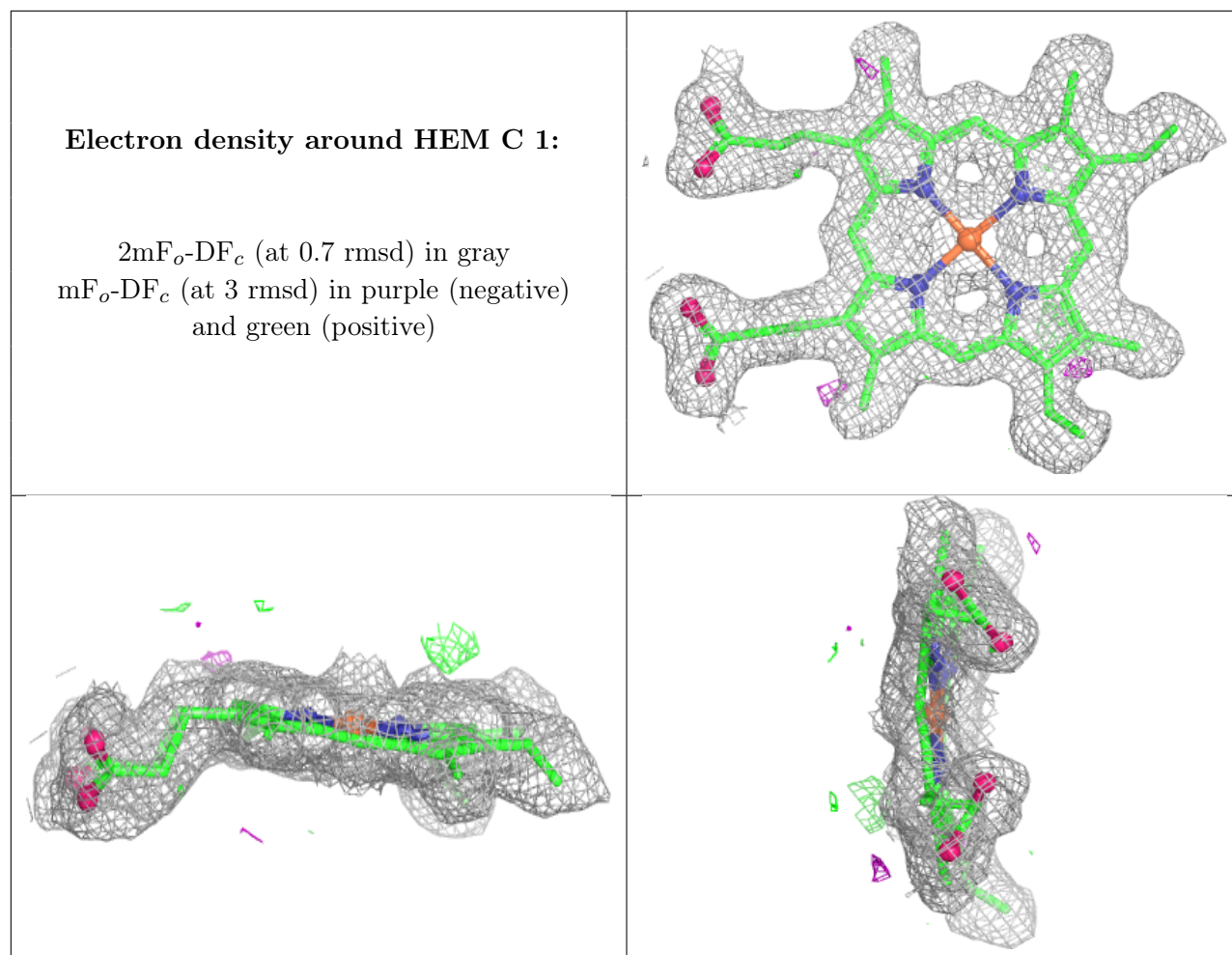
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.