



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:45 AM UTC

PDB ID : 3ZJ4 / pdb_00003zj4
Title : Neurospora Crassa Catalase-3 expressed in E. coli, triclinic form.
Authors : Zarate-Romero, A.; Rudino-Pinera, E.
Deposited on : 2013-01-17
Resolution : 3.10 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

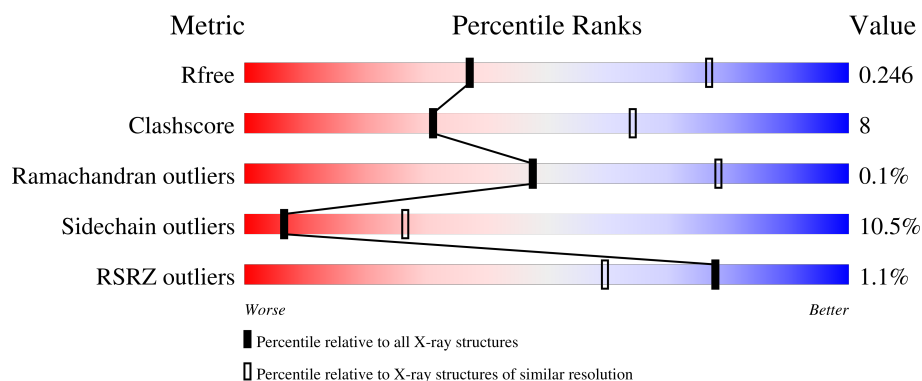
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	746	% 66% 22% • 9%
1	B	746	2% 66% 22% • 9%
1	C	746	% 68% 21% • 9%
1	D	746	% 68% 20% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21505 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	0	0
			5331	3376	940	1009	6			
1	B	681	Total	C	N	O	S	0	0	0
			5340	3381	941	1012	6			
1	C	680	Total	C	N	O	S	0	0	0
			5331	3376	940	1009	6			
1	D	680	Total	C	N	O	S	0	0	0
			5331	3376	940	1009	6			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP Q9C169
A	-25	ASN	-	expression tag	UNP Q9C169
A	-24	HIS	-	expression tag	UNP Q9C169
A	-23	LYS	-	expression tag	UNP Q9C169
A	-22	VAL	-	expression tag	UNP Q9C169
A	-21	HIS	-	expression tag	UNP Q9C169
A	-20	HIS	-	expression tag	UNP Q9C169
A	-19	HIS	-	expression tag	UNP Q9C169
A	-18	HIS	-	expression tag	UNP Q9C169
A	-17	HIS	-	expression tag	UNP Q9C169
A	-16	HIS	-	expression tag	UNP Q9C169
A	-15	ILE	-	expression tag	UNP Q9C169
A	-14	GLU	-	expression tag	UNP Q9C169
A	-13	GLY	-	expression tag	UNP Q9C169
A	-12	ARG	-	expression tag	UNP Q9C169
A	-11	HIS	-	expression tag	UNP Q9C169
A	-10	MET	-	expression tag	UNP Q9C169
A	-9	GLU	-	expression tag	UNP Q9C169
A	-8	LEU	-	expression tag	UNP Q9C169
A	-7	GLY	-	expression tag	UNP Q9C169
A	-6	THR	-	expression tag	UNP Q9C169

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP Q9C169
A	-4	GLU	-	expression tag	UNP Q9C169
A	-3	GLY	-	expression tag	UNP Q9C169
A	-2	SER	-	expression tag	UNP Q9C169
A	-1	GLU	-	expression tag	UNP Q9C169
A	0	PHE	-	expression tag	UNP Q9C169
B	-26	MET	-	expression tag	UNP Q9C169
B	-25	ASN	-	expression tag	UNP Q9C169
B	-24	HIS	-	expression tag	UNP Q9C169
B	-23	LYS	-	expression tag	UNP Q9C169
B	-22	VAL	-	expression tag	UNP Q9C169
B	-21	HIS	-	expression tag	UNP Q9C169
B	-20	HIS	-	expression tag	UNP Q9C169
B	-19	HIS	-	expression tag	UNP Q9C169
B	-18	HIS	-	expression tag	UNP Q9C169
B	-17	HIS	-	expression tag	UNP Q9C169
B	-16	HIS	-	expression tag	UNP Q9C169
B	-15	ILE	-	expression tag	UNP Q9C169
B	-14	GLU	-	expression tag	UNP Q9C169
B	-13	GLY	-	expression tag	UNP Q9C169
B	-12	ARG	-	expression tag	UNP Q9C169
B	-11	HIS	-	expression tag	UNP Q9C169
B	-10	MET	-	expression tag	UNP Q9C169
B	-9	GLU	-	expression tag	UNP Q9C169
B	-8	LEU	-	expression tag	UNP Q9C169
B	-7	GLY	-	expression tag	UNP Q9C169
B	-6	THR	-	expression tag	UNP Q9C169
B	-5	LEU	-	expression tag	UNP Q9C169
B	-4	GLU	-	expression tag	UNP Q9C169
B	-3	GLY	-	expression tag	UNP Q9C169
B	-2	SER	-	expression tag	UNP Q9C169
B	-1	GLU	-	expression tag	UNP Q9C169
B	0	PHE	-	expression tag	UNP Q9C169
C	-26	MET	-	expression tag	UNP Q9C169
C	-25	ASN	-	expression tag	UNP Q9C169
C	-24	HIS	-	expression tag	UNP Q9C169
C	-23	LYS	-	expression tag	UNP Q9C169
C	-22	VAL	-	expression tag	UNP Q9C169
C	-21	HIS	-	expression tag	UNP Q9C169
C	-20	HIS	-	expression tag	UNP Q9C169
C	-19	HIS	-	expression tag	UNP Q9C169
C	-18	HIS	-	expression tag	UNP Q9C169

Continued on next page...

Continued from previous page...

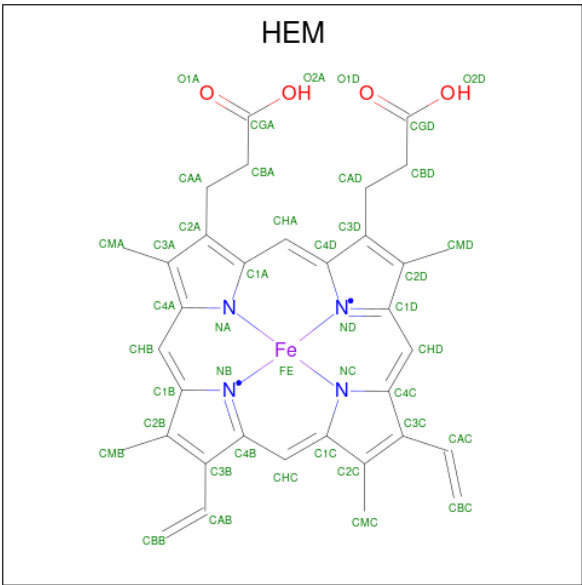
Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	expression tag	UNP Q9C169
C	-16	HIS	-	expression tag	UNP Q9C169
C	-15	ILE	-	expression tag	UNP Q9C169
C	-14	GLU	-	expression tag	UNP Q9C169
C	-13	GLY	-	expression tag	UNP Q9C169
C	-12	ARG	-	expression tag	UNP Q9C169
C	-11	HIS	-	expression tag	UNP Q9C169
C	-10	MET	-	expression tag	UNP Q9C169
C	-9	GLU	-	expression tag	UNP Q9C169
C	-8	LEU	-	expression tag	UNP Q9C169
C	-7	GLY	-	expression tag	UNP Q9C169
C	-6	THR	-	expression tag	UNP Q9C169
C	-5	LEU	-	expression tag	UNP Q9C169
C	-4	GLU	-	expression tag	UNP Q9C169
C	-3	GLY	-	expression tag	UNP Q9C169
C	-2	SER	-	expression tag	UNP Q9C169
C	-1	GLU	-	expression tag	UNP Q9C169
C	0	PHE	-	expression tag	UNP Q9C169
D	-26	MET	-	expression tag	UNP Q9C169
D	-25	ASN	-	expression tag	UNP Q9C169
D	-24	HIS	-	expression tag	UNP Q9C169
D	-23	LYS	-	expression tag	UNP Q9C169
D	-22	VAL	-	expression tag	UNP Q9C169
D	-21	HIS	-	expression tag	UNP Q9C169
D	-20	HIS	-	expression tag	UNP Q9C169
D	-19	HIS	-	expression tag	UNP Q9C169
D	-18	HIS	-	expression tag	UNP Q9C169
D	-17	HIS	-	expression tag	UNP Q9C169
D	-16	HIS	-	expression tag	UNP Q9C169
D	-15	ILE	-	expression tag	UNP Q9C169
D	-14	GLU	-	expression tag	UNP Q9C169
D	-13	GLY	-	expression tag	UNP Q9C169
D	-12	ARG	-	expression tag	UNP Q9C169
D	-11	HIS	-	expression tag	UNP Q9C169
D	-10	MET	-	expression tag	UNP Q9C169
D	-9	GLU	-	expression tag	UNP Q9C169
D	-8	LEU	-	expression tag	UNP Q9C169
D	-7	GLY	-	expression tag	UNP Q9C169
D	-6	THR	-	expression tag	UNP Q9C169
D	-5	LEU	-	expression tag	UNP Q9C169
D	-4	GLU	-	expression tag	UNP Q9C169
D	-3	GLY	-	expression tag	UNP Q9C169

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q9C169
D	-1	GLU	-	expression tag	UNP Q9C169
D	0	PHE	-	expression tag	UNP Q9C169

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

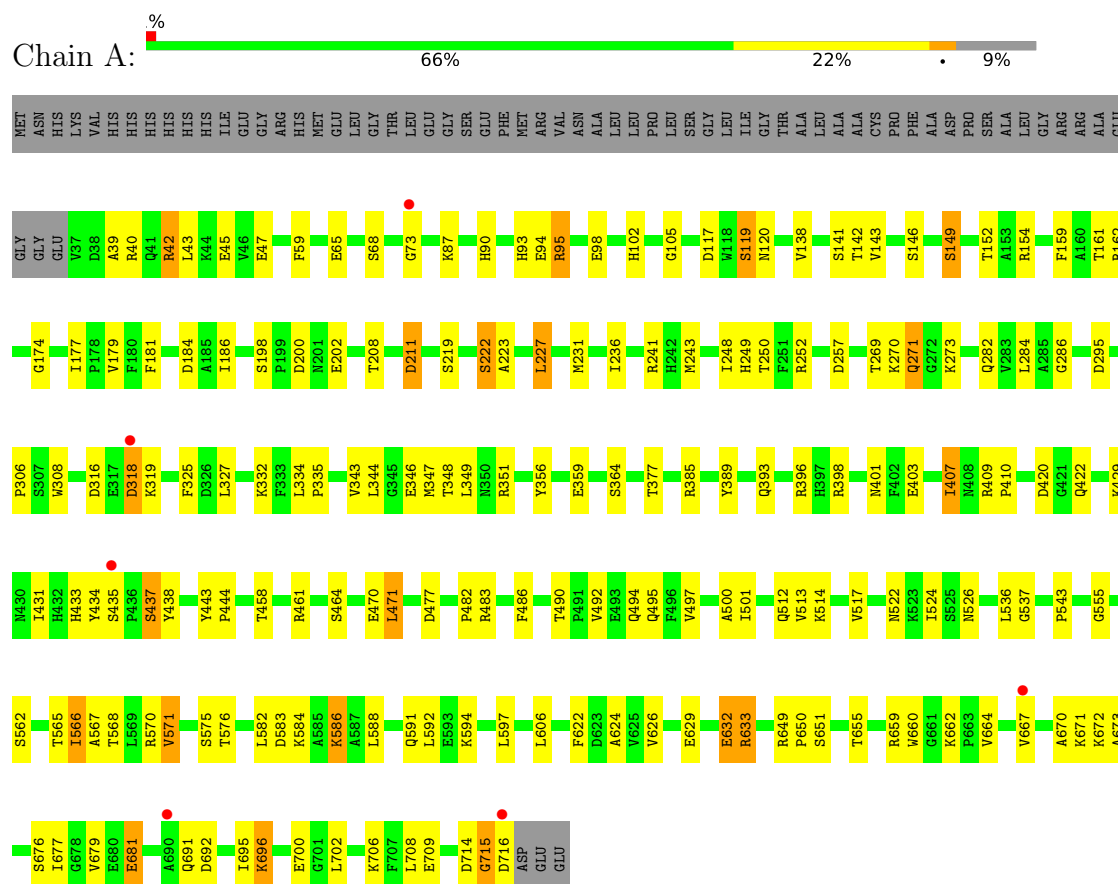


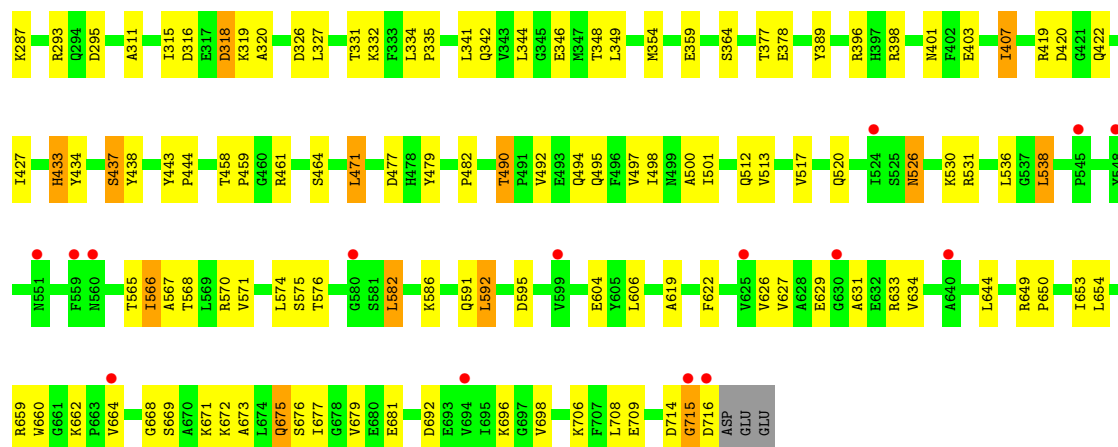
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots

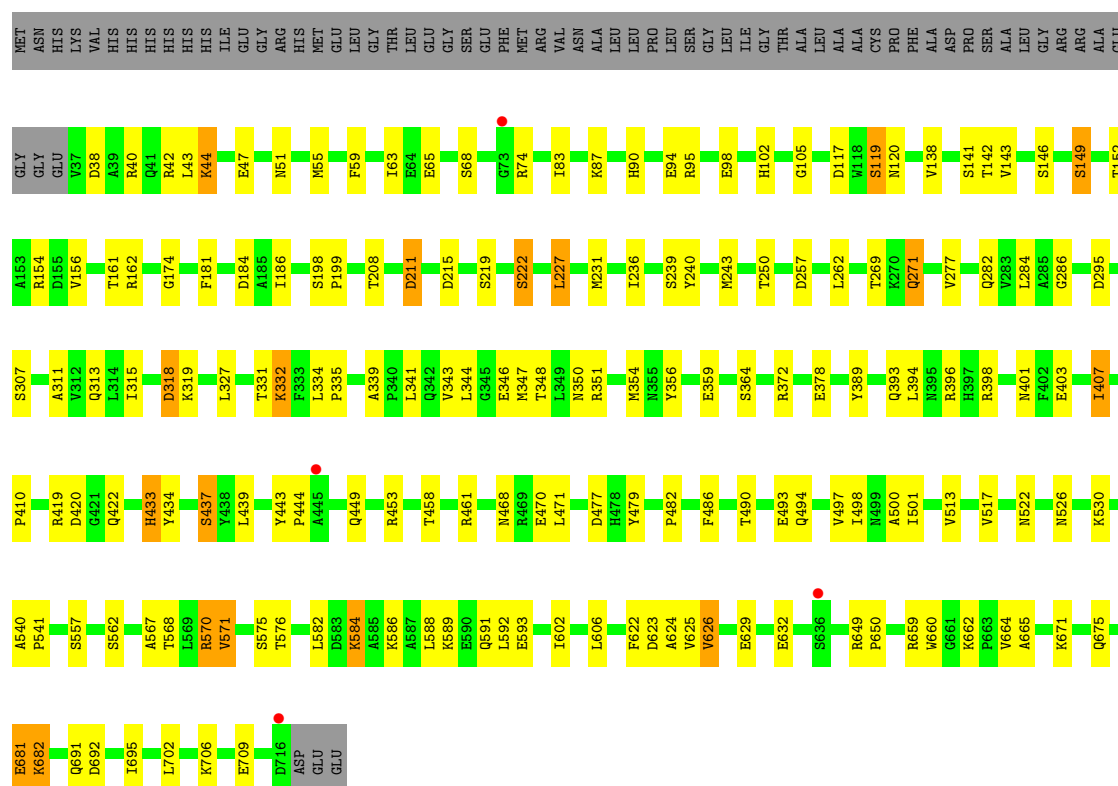
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-3

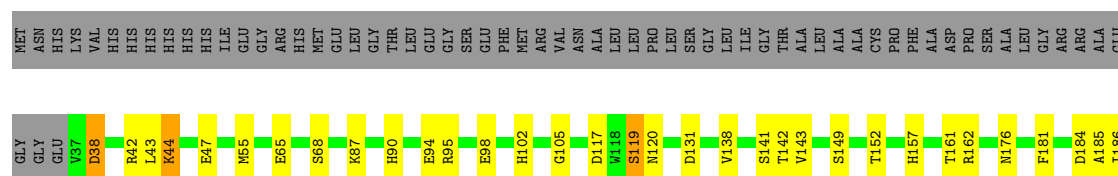


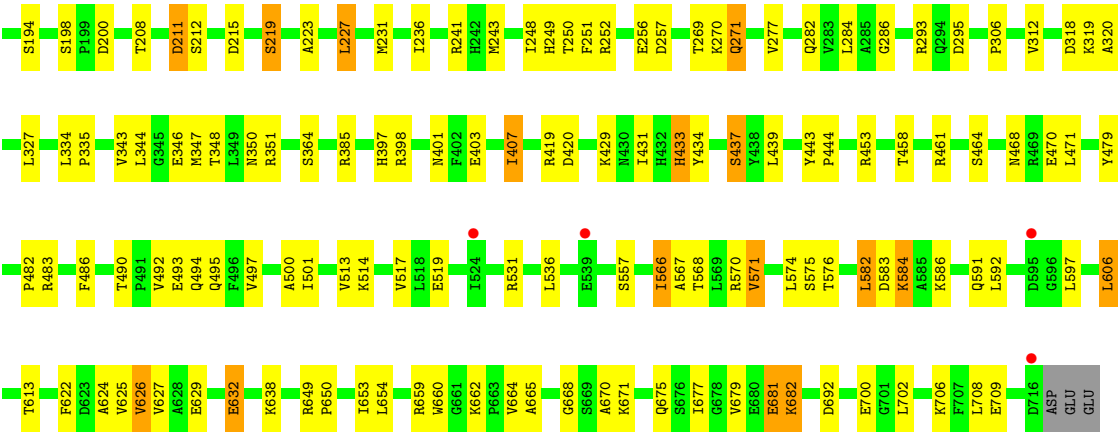


• Molecule 1: CATALASE-3



• Molecule 1: CATALASE-3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.44Å 88.21Å 104.40Å 82.08° 82.48° 62.33°	Depositor
Resolution (Å)	29.40 – 3.10 29.40 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.40-3.10) 98.7 (29.40-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.11Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.197 , 0.245 0.200 , 0.246	Depositor DCC
R_{free} test set	2451 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	21505	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.30	0/5464	0.76	2/7412 (0.0%)
1	B	0.30	0/5473	0.75	0/7424
1	C	0.29	0/5464	0.74	0/7412
1	D	0.29	0/5464	0.75	0/7412
All	All	0.29	0/21865	0.75	2/29660 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	SER	CA-C-N	-7.06	111.02	119.84
1	A	435	SER	C-N-CA	-7.06	111.02	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5331	0	5150	100	0
1	B	5340	0	5156	103	0
1	C	5331	0	5150	90	1
1	D	5331	0	5151	87	1
2	A	43	0	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	7	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
All	All	21505	0	20727	344	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 (344) 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:622:PHE:O	1:C:662:LYS:NZ	2.15	0.79
1:A:584:LYS:HD3	1:A:629:GLU:HB3	1.65	0.77
1:D:622:PHE:O	1:D:662:LYS:NZ	2.18	0.73
1:A:186:ILE:O	1:D:87:LYS:NZ	2.22	0.71
1:A:332:LYS:NZ	1:A:477:ASP:O	2.22	0.71
1:A:73:GLY:H	1:D:468:ASN:HD21	1.39	0.70
1:A:248:ILE:HD12	2:A:4000:HEM:HMB1	1.73	0.69
1:A:622:PHE:O	1:A:662:LYS:NZ	2.20	0.69
1:B:420:ASP:HB2	1:D:94:GLU:HG2	1.75	0.69
1:B:87:LYS:NZ	1:C:186:ILE:O	2.25	0.69
1:B:671:LYS:O	1:B:675:GLN:NE2	2.26	0.68
1:B:248:ILE:HD12	2:B:4000:HEM:HMB1	1.76	0.68
1:A:458:THR:HB	1:A:461:ARG:HG3	1.77	0.67
1:A:117:ASP:OD1	1:A:119:SER:OG	2.12	0.67
1:D:248:ILE:HD12	2:D:4000:HEM:HMB1	1.77	0.67
1:A:94:GLU:HG2	1:C:420:ASP:HB2	1.76	0.66
1:B:458:THR:HB	1:B:461:ARG:HG3	1.78	0.66
1:D:38:ASP:OD2	1:D:44:LYS:NZ	2.21	0.66
1:D:486:PHE:O	1:D:494:GLN:NE2	2.28	0.65
1:D:624:ALA:HB2	1:D:702:LEU:HD21	1.79	0.65
1:A:434:TYR:CE2	1:A:437:SER:HB2	2.32	0.64
1:C:117:ASP:OD1	1:C:119:SER:OG	2.15	0.64
1:A:567:ALA:O	1:A:568:THR:OG1	2.15	0.64
1:A:571:VAL:HG13	1:A:624:ALA:HB3	1.79	0.64
1:D:571:VAL:HG13	1:D:624:ALA:HB3	1.80	0.64
1:C:181:PHE:O	1:C:222:SER:OG	2.15	0.63
1:D:458:THR:HB	1:D:461:ARG:HG3	1.81	0.62
1:C:419:ARG:HG3	1:C:433:HIS:HD2	1.64	0.62
1:B:354:MET:SD	1:D:429:LYS:HG2	2.39	0.62
1:B:94:GLU:HG2	1:D:420:ASP:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ARG:HG3	1:D:433:HIS:HD2	1.65	0.61
1:A:39:ALA:O	1:A:42:ARG:NH1	2.34	0.60
1:B:673:ALA:O	1:B:676:SER:OG	2.17	0.60
1:D:495:GLN:OE1	1:D:531:ARG:NH2	2.28	0.60
1:C:458:THR:HB	1:C:461:ARG:HG3	1.82	0.60
1:A:420:ASP:HB2	1:C:94:GLU:HG2	1.84	0.60
1:B:90:HIS:NE2	1:D:401:ASN:OD1	2.33	0.60
1:C:262:LEU:HB2	1:C:315:ILE:HB	1.83	0.60
1:C:584:LYS:HD2	1:C:629:GLU:HB3	1.83	0.60
1:D:584:LYS:HD2	1:D:629:GLU:HB3	1.84	0.60
1:D:117:ASP:OD1	1:D:119:SER:OG	2.20	0.60
1:C:269:THR:OG1	1:C:271:GLN:NE2	2.35	0.60
1:C:567:ALA:O	1:C:568:THR:OG1	2.18	0.60
1:C:346:GLU:OE2	1:C:348:THR:OG1	2.20	0.60
1:D:138:VAL:HG22	1:D:161:THR:HG23	1.83	0.59
1:B:49:ASP:HB2	1:D:429:LYS:HE3	1.83	0.59
2:C:4000:HEM:HMB2	2:C:4000:HEM:HBB2	1.84	0.59
1:B:186:ILE:O	1:C:87:LYS:NZ	2.28	0.59
1:B:318:ASP:OD1	1:B:318:ASP:N	2.26	0.59
2:D:4000:HEM:HMB1	2:D:4000:HEM:HBB2	1.84	0.59
1:B:117:ASP:OD1	1:B:119:SER:OG	2.21	0.59
1:C:318:ASP:OD1	1:C:318:ASP:N	2.35	0.59
1:B:419:ARG:HG3	1:B:433:HIS:HD2	1.67	0.59
1:B:567:ALA:O	1:B:568:THR:OG1	2.17	0.58
1:A:401:ASN:OD1	1:C:90:HIS:NE2	2.33	0.58
1:D:256:GLU:OE2	1:D:453:ARG:NH1	2.36	0.58
1:A:162:ARG:NH2	1:A:364:SER:O	2.36	0.58
1:B:434:TYR:CE2	1:B:437:SER:HB2	2.38	0.58
1:A:346:GLU:OE2	1:A:348:THR:OG1	2.22	0.57
1:B:39:ALA:O	1:B:42:ARG:NH1	2.37	0.57
1:A:90:HIS:NE2	1:C:401:ASN:OD1	2.35	0.57
1:D:567:ALA:O	1:D:568:THR:OG1	2.19	0.57
1:A:40:ARG:NH2	1:A:47:GLU:OE2	2.38	0.56
1:B:574:LEU:HD12	1:B:627:VAL:HG22	1.87	0.56
1:D:312:VAL:HG22	1:D:344:LEU:HD11	1.86	0.56
1:D:492:VAL:HG11	1:D:708:LEU:HB3	1.86	0.56
1:A:87:LYS:NZ	1:D:186:ILE:O	2.30	0.56
2:A:4000:HEM:HMB1	2:A:4000:HEM:HBB2	1.88	0.56
1:D:250:THR:OG1	1:D:327:LEU:O	2.21	0.56
1:B:181:PHE:O	1:B:222:SER:OG	2.24	0.55
1:C:102:HIS:CE1	1:C:143:VAL:HG22	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PHE:HB2	1:A:332:LYS:HG3	1.87	0.55
1:B:575:SER:OG	1:B:576:THR:N	2.39	0.55
1:B:185:ALA:HB1	2:B:4000:HEM:HBC2	1.88	0.55
2:B:4000:HEM:HMB1	2:B:4000:HEM:HBB2	1.89	0.55
1:A:73:GLY:H	1:D:468:ASN:ND2	2.05	0.55
1:D:102:HIS:CE1	1:D:143:VAL:HG22	2.42	0.54
1:A:660:TRP:O	1:A:706:LYS:HE3	2.07	0.54
1:B:40:ARG:NH2	1:B:47:GLU:OE2	2.40	0.54
1:B:162:ARG:NH2	1:B:364:SER:O	2.39	0.54
2:A:4000:HEM:HMC1	2:A:4000:HEM:HBC2	1.89	0.54
1:D:181:PHE:HD1	1:D:223:ALA:HB1	1.73	0.54
1:A:526:ASN:OD1	1:A:543:PRO:HG3	2.08	0.54
1:A:575:SER:OG	1:A:576:THR:N	2.41	0.53
1:B:38:ASP:OD2	1:B:44:LYS:NZ	2.26	0.53
1:B:102:HIS:HA	1:B:142:THR:O	2.08	0.53
1:D:102:HIS:HA	1:D:142:THR:O	2.07	0.53
1:D:583:ASP:HA	1:D:586:LYS:HD3	1.89	0.53
2:C:4000:HEM:HMC1	2:C:4000:HEM:HBC2	1.91	0.53
1:A:715:GLY:O	1:A:716:ASP:HB3	2.09	0.53
1:B:495:GLN:OE1	1:B:531:ARG:NH2	2.29	0.53
1:A:102:HIS:CE1	1:A:143:VAL:HG22	2.44	0.53
1:A:273:LYS:NZ	1:A:555:GLY:O	2.42	0.53
1:A:316:ASP:HB3	1:A:318:ASP:OD1	2.08	0.53
1:C:378:GLU:OE2	1:C:461:ARG:NH1	2.35	0.53
1:D:269:THR:OG1	1:D:271:GLN:NE2	2.42	0.52
1:C:102:HIS:HA	1:C:142:THR:O	2.09	0.52
1:B:181:PHE:HD2	1:B:223:ALA:HB1	1.74	0.52
1:C:146:SER:O	1:C:149:SER:OG	2.27	0.52
1:D:334:LEU:HD12	1:D:335:PRO:HD2	1.92	0.52
1:A:318:ASP:OD1	1:A:318:ASP:N	2.20	0.52
2:D:4000:HEM:HBC2	2:D:4000:HEM:HMC1	1.91	0.52
1:A:269:THR:OG1	1:A:271:GLN:NE2	2.42	0.52
1:A:594:LYS:N	1:A:594:LYS:HD2	2.25	0.52
1:D:241:ARG:HD2	1:D:306:PRO:HB3	1.92	0.51
1:B:211:ASP:OD1	1:B:211:ASP:N	2.43	0.51
1:A:102:HIS:HA	1:A:142:THR:O	2.11	0.51
1:C:359:GLU:HB3	1:C:407:ILE:HD13	1.93	0.51
1:C:571:VAL:HG13	1:C:624:ALA:HB3	1.92	0.51
1:A:146:SER:O	1:A:149:SER:OG	2.29	0.51
1:D:211:ASP:OD1	1:D:211:ASP:N	2.43	0.51
1:A:211:ASP:N	1:A:211:ASP:OD1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASP:N	1:C:211:ASP:OD1	2.43	0.51
1:D:434:TYR:CE2	1:D:437:SER:HB2	2.46	0.51
1:D:566:ILE:HG13	1:D:597:LEU:HD21	1.93	0.50
1:C:632:GLU:CD	1:C:632:GLU:H	2.19	0.50
1:B:269:THR:OG1	1:B:271:GLN:NE2	2.44	0.50
1:B:331:THR:O	1:B:332:LYS:HD3	2.11	0.50
1:C:40:ARG:NH2	1:C:47:GLU:OE2	2.43	0.50
1:D:626:VAL:HB	1:D:665:ALA:HB3	1.93	0.50
1:A:673:ALA:O	1:A:676:SER:OG	2.19	0.50
1:B:252:ARG:CZ	1:B:461:ARG:HD3	2.41	0.50
1:B:566:ILE:HD13	1:B:566:ILE:H	1.77	0.50
2:B:4000:HEM:HBC2	2:B:4000:HEM:HMC1	1.93	0.50
1:C:38:ASP:OD2	1:C:44:LYS:NZ	2.33	0.50
1:A:250:THR:OG1	1:A:327:LEU:O	2.24	0.49
1:C:105:GLY:O	1:C:356:TYR:OH	2.30	0.49
1:B:715:GLY:O	1:B:716:ASP:HB3	2.11	0.49
1:C:162:ARG:NH2	1:C:364:SER:O	2.43	0.49
1:C:174:GLY:HA2	2:C:4000:HEM:HMB1	1.94	0.49
1:C:250:THR:OG1	1:C:327:LEU:O	2.18	0.49
1:B:326:ASP:CG	1:C:74:ARG:HE	2.20	0.49
1:A:691:GLN:O	1:A:695:ILE:HG13	2.13	0.49
1:D:574:LEU:HD12	1:D:627:VAL:HG22	1.95	0.49
1:A:138:VAL:HG22	1:A:161:THR:HG23	1.94	0.48
1:B:105:GLY:O	1:B:293:ARG:NH2	2.47	0.48
1:C:434:TYR:CE2	1:C:437:SER:HB2	2.47	0.48
1:D:493:GLU:OE1	1:D:557:SER:OG	2.27	0.48
1:D:443:TYR:HA	1:D:444:PRO:C	2.38	0.48
1:A:566:ILE:HG13	1:A:597:LEU:HD21	1.94	0.48
1:A:514:LYS:HB3	1:A:536:LEU:HD13	1.95	0.48
1:B:622:PHE:O	1:B:662:LYS:NZ	2.33	0.48
1:A:181:PHE:O	1:A:222:SER:OG	2.31	0.48
1:D:194:SER:O	1:D:212:SER:OG	2.28	0.48
1:A:588:LEU:HD13	1:A:691:GLN:HG3	1.94	0.48
1:B:146:SER:O	1:B:149:SER:OG	2.32	0.48
1:B:262:LEU:HB2	1:B:315:ILE:HB	1.96	0.48
1:A:513:VAL:O	1:A:517:VAL:HG23	2.14	0.47
1:D:575:SER:OG	1:D:576:THR:N	2.47	0.47
1:A:624:ALA:HB2	1:A:702:LEU:HD21	1.96	0.47
1:B:224:LEU:HD11	1:B:520:GLN:HB3	1.97	0.47
1:D:252:ARG:NH1	1:D:461:ARG:HD3	2.30	0.47
1:B:359:GLU:HB3	1:B:407:ILE:HD13	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:TYR:O	1:A:393:GLN:HG2	2.14	0.47
1:B:536:LEU:HB3	1:B:538:LEU:HD12	1.97	0.47
1:B:677:ILE:HG13	1:B:679:VAL:HG23	1.96	0.47
1:D:668:GLY:O	1:D:671:LYS:HG3	2.14	0.47
1:A:252:ARG:NH1	1:A:377:THR:HA	2.29	0.46
1:B:311:ALA:HB1	1:B:341:LEU:HB3	1.97	0.46
1:C:602:ILE:HD11	1:C:622:PHE:CE2	2.49	0.46
1:D:231:MET:HB3	1:D:500:ALA:HB3	1.97	0.46
1:A:359:GLU:HB3	1:A:407:ILE:HD13	1.96	0.46
1:C:522:ASN:OD1	1:C:526:ASN:ND2	2.43	0.46
1:C:660:TRP:O	1:C:706:LYS:HE3	2.15	0.46
1:A:334:LEU:HD12	1:A:335:PRO:HD2	1.96	0.46
1:A:443:TYR:HA	1:A:444:PRO:C	2.40	0.46
1:A:681:GLU:H	1:A:681:GLU:HG3	1.46	0.46
1:C:443:TYR:HA	1:C:444:PRO:C	2.39	0.46
1:D:249:HIS:HB2	1:D:251:PHE:CE1	2.50	0.46
1:D:681:GLU:H	1:D:681:GLU:HG3	1.42	0.46
1:A:482:PRO:HB2	1:A:524:ILE:HD13	1.97	0.46
1:B:389:TYR:OH	2:B:4000:HEM:NA	2.49	0.46
1:B:320:ALA:HA	1:B:327:LEU:HD12	1.98	0.46
1:C:626:VAL:HB	1:C:665:ALA:HB3	1.97	0.46
1:B:443:TYR:HA	1:B:444:PRO:C	2.41	0.46
1:C:240:TYR:HA	1:C:243:MET:HE2	1.97	0.46
1:C:389:TYR:O	1:C:393:GLN:HG2	2.16	0.46
1:C:513:VAL:O	1:C:517:VAL:HG23	2.16	0.46
1:D:227:LEU:O	1:D:231:MET:HG2	2.16	0.46
1:C:439:LEU:HD12	1:D:215:ASP:OD2	2.16	0.46
1:D:185:ALA:HB1	2:D:4000:HEM:HBC2	1.96	0.46
1:C:493:GLU:OE1	1:C:557:SER:OG	2.30	0.46
1:D:320:ALA:HA	1:D:327:LEU:HD12	1.98	0.46
1:B:139:ARG:HD3	2:B:4000:HEM:O2A	2.17	0.45
1:B:401:ASN:OD1	1:D:90:HIS:NE2	2.45	0.45
1:C:575:SER:OG	1:C:576:THR:N	2.45	0.45
1:A:537:GLY:HA3	1:D:606:LEU:O	2.17	0.45
1:B:250:THR:OG1	1:B:327:LEU:O	2.19	0.45
1:D:677:ILE:HG13	1:D:679:VAL:HG23	1.99	0.45
1:B:200:ASP:OD1	1:B:200:ASP:N	2.46	0.45
1:C:486:PHE:O	1:C:494:GLN:NE2	2.42	0.45
1:C:497:VAL:O	1:C:501:ILE:HG13	2.16	0.45
1:D:514:LYS:HB3	1:D:536:LEU:HD13	1.98	0.45
1:D:660:TRP:O	1:D:706:LYS:HE3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:VAL:O	1:B:517:VAL:HG23	2.16	0.45
1:D:682:LYS:HA	1:D:682:LYS:HD3	1.67	0.45
1:C:570:ARG:O	1:C:623:ASP:N	2.46	0.45
1:A:422:GLN:NE2	1:C:396:ARG:O	2.49	0.45
1:B:316:ASP:HB3	1:B:318:ASP:OD1	2.17	0.45
1:B:396:ARG:NH2	2:B:4000:HEM:O1D	2.48	0.45
1:B:227:LEU:O	1:B:231:MET:HG2	2.16	0.45
1:A:95:ARG:HA	1:A:95:ARG:HD3	1.64	0.45
1:A:522:ASN:OD1	1:A:526:ASN:ND2	2.48	0.45
1:B:334:LEU:HD12	1:B:335:PRO:HD2	1.98	0.45
1:B:479:TYR:C	1:B:482:PRO:HD2	2.42	0.45
1:C:453:ARG:HE	1:C:453:ARG:HB3	1.70	0.45
1:B:184:ASP:OD1	1:C:68:SER:OG	2.35	0.45
1:D:215:ASP:O	1:D:219:SER:OG	2.24	0.45
1:A:431:ILE:HA	1:B:199:PRO:HG2	1.98	0.44
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.99	0.44
1:A:152:THR:HG21	1:A:284:LEU:HD23	1.98	0.44
1:A:497:VAL:O	1:A:501:ILE:HG13	2.16	0.44
1:C:588:LEU:HD13	1:C:691:GLN:HG3	1.99	0.44
1:D:497:VAL:O	1:D:501:ILE:HG13	2.18	0.44
1:A:231:MET:HB3	1:A:500:ALA:HB3	2.00	0.44
1:A:583:ASP:HA	1:A:586:LYS:HD3	1.99	0.44
1:B:190:ASP:OD2	1:C:87:LYS:NZ	2.45	0.44
1:B:346:GLU:OE2	1:B:348:THR:OG1	2.36	0.44
1:B:619:ALA:O	1:B:662:LYS:NZ	2.50	0.44
1:B:497:VAL:O	1:B:501:ILE:HG13	2.17	0.44
1:B:582:LEU:HD12	1:B:582:LEU:HA	1.87	0.44
1:A:159:PHE:N	1:A:174:GLY:O	2.42	0.44
1:A:200:ASP:OD1	1:A:200:ASP:N	2.45	0.44
1:B:95:ARG:HA	1:B:95:ARG:HD3	1.71	0.44
1:C:372:ARG:HH12	1:C:449:GLN:HA	1.82	0.44
1:B:490:THR:O	1:B:494:GLN:HG3	2.17	0.44
1:A:396:ARG:O	1:C:422:GLN:NE2	2.50	0.44
1:A:632:GLU:HG2	1:A:672:LYS:HB3	1.99	0.44
1:B:231:MET:HB3	1:B:500:ALA:HB3	2.00	0.44
1:A:181:PHE:HD1	1:A:223:ALA:HB1	1.82	0.43
1:B:631:ALA:O	1:B:634:VAL:HG22	2.18	0.43
1:C:199:PRO:HG2	1:D:431:ILE:HA	1.99	0.43
1:C:227:LEU:O	1:C:231:MET:HG2	2.18	0.43
1:D:649:ARG:HB3	1:D:650:PRO:HD3	1.99	0.43
1:B:231:MET:HB2	1:B:497:VAL:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:NH1	1:A:461:ARG:HD3	2.33	0.43
1:A:651:SER:O	1:A:655:THR:OG1	2.33	0.43
1:D:152:THR:HG21	1:D:284:LEU:HD23	1.99	0.43
1:D:162:ARG:NH2	1:D:364:SER:O	2.47	0.43
1:D:654:LEU:HD12	1:D:654:LEU:HA	1.90	0.43
1:A:492:VAL:HG21	1:A:708:LEU:HB3	1.99	0.43
1:B:649:ARG:O	1:B:653:ILE:HG13	2.19	0.43
1:B:592:LEU:HD12	1:B:592:LEU:HA	1.87	0.43
1:A:73:GLY:N	1:D:468:ASN:HD21	2.13	0.43
1:B:72:GLY:O	1:C:468:ASN:ND2	2.46	0.43
1:B:332:LYS:NZ	1:B:477:ASP:O	2.37	0.43
1:B:660:TRP:O	1:B:706:LYS:HE3	2.19	0.43
1:D:632:GLU:CG	1:D:670:ALA:HA	2.49	0.43
1:B:492:VAL:HG21	1:B:708:LEU:HB3	2.00	0.43
1:D:249:HIS:HE2	1:D:385:ARG:HH11	1.67	0.43
1:D:346:GLU:OE2	1:D:348:THR:OG1	2.36	0.43
1:D:649:ARG:O	1:D:653:ILE:HG13	2.18	0.43
1:A:677:ILE:HG13	1:A:679:VAL:HG23	2.01	0.43
1:B:654:LEU:HD12	1:B:654:LEU:HA	1.88	0.43
1:B:102:HIS:CE1	1:B:143:VAL:HG22	2.54	0.42
1:C:624:ALA:HB2	1:C:702:LEU:HD21	2.01	0.42
1:C:332:LYS:NZ	1:C:477:ASP:O	2.34	0.42
1:D:513:VAL:O	1:D:517:VAL:HG23	2.19	0.42
1:A:282:GLN:O	1:D:286:GLY:HA3	2.19	0.42
1:C:334:LEU:HD12	1:C:335:PRO:HD2	2.01	0.42
1:C:530:LYS:HA	1:C:540:ALA:HB2	2.00	0.42
1:A:59:PHE:C	1:C:410:PRO:HG3	2.44	0.42
1:A:495:GLN:HE22	1:A:714:ASP:CG	2.26	0.42
1:C:350:ASN:O	1:C:351:ARG:HD2	2.20	0.42
1:D:606:LEU:HD13	1:D:613:THR:HG23	2.01	0.42
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.83	0.42
1:A:696:LYS:C	1:A:696:LYS:HD3	2.44	0.42
1:B:649:ARG:HB3	1:B:650:PRO:HD3	2.01	0.42
1:C:63:ILE:HB	1:C:83:ILE:HD13	2.00	0.42
1:C:313:GLN:NE2	1:C:339:ALA:O	2.52	0.42
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.78	0.42
1:B:531:ARG:HG2	1:B:714:ASP:OD2	2.20	0.42
1:A:184:ASP:OD1	1:D:68:SER:OG	2.36	0.42
1:A:667:VAL:N	1:A:670:ALA:HB3	2.35	0.42
1:B:629:GLU:OE2	1:B:668:GLY:HA3	2.20	0.42
1:C:540:ALA:HA	1:C:541:PRO:HD3	1.96	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ASP:OD1	1:D:200:ASP:N	2.42	0.42
1:A:512:GLN:HG2	1:B:438:TYR:CZ	2.54	0.42
1:B:177:ILE:HD13	1:B:229:TRP:HB3	2.00	0.42
1:C:649:ARG:HB3	1:C:650:PRO:HD3	2.02	0.42
1:A:594:LYS:HD2	1:A:594:LYS:H	1.84	0.42
1:B:427:ILE:O	1:D:47:GLU:HA	2.20	0.42
1:B:526:ASN:ND2	1:B:530:LYS:HG3	2.34	0.42
1:C:513:VAL:HG21	1:D:439:LEU:HD11	2.02	0.42
1:C:691:GLN:O	1:C:695:ILE:HG13	2.20	0.42
1:B:143:VAL:HG23	1:B:156:VAL:O	2.20	0.41
1:B:407:ILE:O	1:B:407:ILE:HG13	2.20	0.41
1:D:157:HIS:HB2	1:D:176:ASN:CG	2.45	0.41
1:B:282:GLN:O	1:C:286:GLY:HA3	2.20	0.41
1:C:584:LYS:HB2	1:C:584:LYS:HE2	1.75	0.41
1:A:429:LYS:HG2	1:C:354:MET:SD	2.60	0.41
1:A:438:TYR:CZ	1:B:512:GLN:HG2	2.56	0.41
1:B:286:GLY:HA3	1:C:282:GLN:O	2.20	0.41
1:C:494:GLN:O	1:C:498:ILE:HG13	2.21	0.41
1:C:681:GLU:H	1:C:681:GLU:HG3	1.46	0.41
1:C:682:LYS:HD3	1:C:682:LYS:HA	1.79	0.41
1:A:252:ARG:CZ	1:A:461:ARG:HD3	2.51	0.41
1:A:407:ILE:O	1:A:407:ILE:HG13	2.20	0.41
1:D:453:ARG:HE	1:D:453:ARG:HB3	1.67	0.41
1:A:68:SER:OG	1:D:184:ASP:OD1	2.34	0.41
1:A:177:ILE:HG22	1:A:179:VAL:H	1.84	0.41
1:A:227:LEU:O	1:A:231:MET:HG2	2.20	0.41
1:A:409:ARG:HA	1:A:410:PRO:HD3	1.93	0.41
1:A:649:ARG:HB3	1:A:650:PRO:HD3	2.02	0.41
1:B:252:ARG:NH1	1:B:461:ARG:HD3	2.35	0.41
1:C:152:THR:HG21	1:C:284:LEU:HD23	2.02	0.41
1:C:311:ALA:HB1	1:C:341:LEU:HB3	2.03	0.41
1:A:105:GLY:O	1:A:356:TYR:OH	2.32	0.41
1:A:576:THR:HG21	1:A:633:ARG:HD2	2.02	0.41
1:A:667:VAL:H	1:A:670:ALA:HB3	1.86	0.41
1:B:498:ILE:HG21	1:B:531:ARG:HB3	2.02	0.41
1:C:231:MET:HB3	1:C:500:ALA:HB3	2.03	0.41
1:C:479:TYR:C	1:C:482:PRO:HD2	2.45	0.41
1:A:241:ARG:HA	1:A:308:TRP:CZ2	2.55	0.41
1:B:458:THR:HA	1:B:459:PRO:HD3	1.87	0.41
1:C:215:ASP:CG	1:D:439:LEU:HD13	2.45	0.41
1:C:318:ASP:OD2	1:C:319:LYS:NZ	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLY:HA3	1:D:282:GLN:O	2.20	0.41
1:B:68:SER:OG	1:C:184:ASP:OD1	2.34	0.41
1:B:252:ARG:NH1	1:B:377:THR:HA	2.35	0.41
1:C:143:VAL:HG23	1:C:156:VAL:O	2.21	0.41
1:B:283:VAL:O	1:B:287:LYS:HG2	2.21	0.41
1:B:422:GLN:NE2	1:D:397:HIS:HA	2.36	0.41
1:C:138:VAL:HG22	1:C:161:THR:HG23	2.02	0.41
1:D:350:ASN:O	1:D:351:ARG:HD2	2.21	0.41
1:D:407:ILE:HG13	1:D:407:ILE:O	2.20	0.41
1:B:40:ARG:NH1	1:B:359:GLU:OE2	2.54	0.41
1:C:331:THR:O	1:C:332:LYS:HD2	2.21	0.40
1:C:589:LYS:O	1:C:593:GLU:HG3	2.21	0.40
1:D:105:GLY:O	1:D:293:ARG:NH2	2.54	0.40
1:D:479:TYR:C	1:D:482:PRO:HD2	2.46	0.40
1:A:93:HIS:CE1	1:C:394:LEU:HD13	2.56	0.40
1:A:410:PRO:HG3	1:C:59:PHE:C	2.46	0.40
1:A:696:LYS:HD3	1:A:696:LYS:O	2.21	0.40
1:B:63:ILE:HB	1:B:83:ILE:HD13	2.03	0.40
1:B:110:GLY:HA3	1:B:349:LEU:HD23	2.03	0.40
1:B:492:VAL:HG11	1:B:708:LEU:HB3	2.03	0.40
1:A:306:PRO:HD2	1:A:349:LEU:O	2.21	0.40
1:B:378:GLU:OE2	1:B:461:ARG:NH1	2.44	0.40
1:B:604:GLU:HB3	1:B:644:LEU:HD12	2.04	0.40
1:A:249:HIS:CD2	1:A:385:ARG:HH11	2.39	0.40
1:A:486:PHE:CZ	1:A:494:GLN:HB3	2.56	0.40
1:D:582:LEU:HD12	1:D:582:LEU:HA	1.80	0.40
1:C:407:ILE:O	1:C:407:ILE:HG13	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)
1:C:51:ASN:ND2	1:D:131:ASP:OD2[1_655]	2.08	0.12

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	678/746 (91%)	653 (96%)	24 (4%)	1 (0%)	48	78
1	B	679/746 (91%)	655 (96%)	22 (3%)	2 (0%)	36	67
1	C	678/746 (91%)	658 (97%)	20 (3%)	0	100	100
1	D	678/746 (91%)	657 (97%)	20 (3%)	1 (0%)	48	78
All	All	2713/2984 (91%)	2623 (97%)	86 (3%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	38	ASP
1	A	715	GLY
1	B	38	ASP
1	B	715	GLY

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	558/609 (92%)	497 (89%)	61 (11%)	6	24
1	B	559/609 (92%)	500 (89%)	59 (11%)	6	26
1	C	558/609 (92%)	501 (90%)	57 (10%)	7	28
1	D	558/609 (92%)	500 (90%)	58 (10%)	7	27
All	All	2233/2436 (92%)	1998 (90%)	235 (10%)	6	26

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	43	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	45	GLU
1	A	65	GLU
1	A	95	ARG
1	A	98	GLU
1	A	119	SER
1	A	120	ASN
1	A	141	SER
1	A	149	SER
1	A	154	ARG
1	A	198	SER
1	A	202	GLU
1	A	208	THR
1	A	211	ASP
1	A	219	SER
1	A	222	SER
1	A	227	LEU
1	A	236	ILE
1	A	243	MET
1	A	257	ASP
1	A	270	LYS
1	A	271	GLN
1	A	295	ASP
1	A	318	ASP
1	A	319	LYS
1	A	343	VAL
1	A	344	LEU
1	A	347	MET
1	A	351	ARG
1	A	398	ARG
1	A	403	GLU
1	A	407	ILE
1	A	433	HIS
1	A	437	SER
1	A	464	SER
1	A	470	GLU
1	A	471	LEU
1	A	483	ARG
1	A	490	THR
1	A	562	SER
1	A	565	THR
1	A	566	ILE
1	A	570	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	571	VAL
1	A	582	LEU
1	A	586	LYS
1	A	591	GLN
1	A	592	LEU
1	A	606	LEU
1	A	626	VAL
1	A	632	GLU
1	A	633	ARG
1	A	659	ARG
1	A	664	VAL
1	A	671	LYS
1	A	681	GLU
1	A	692	ASP
1	A	696	LYS
1	A	700	GLU
1	A	709	GLU
1	B	42	ARG
1	B	43	LEU
1	B	55	MET
1	B	65	GLU
1	B	95	ARG
1	B	98	GLU
1	B	119	SER
1	B	141	SER
1	B	149	SER
1	B	154	ARG
1	B	198	SER
1	B	208	THR
1	B	211	ASP
1	B	219	SER
1	B	222	SER
1	B	226	THR
1	B	227	LEU
1	B	236	ILE
1	B	239	SER
1	B	243	MET
1	B	257	ASP
1	B	271	GLN
1	B	295	ASP
1	B	318	ASP
1	B	319	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	342	GLN
1	B	344	LEU
1	B	398	ARG
1	B	403	GLU
1	B	407	ILE
1	B	433	HIS
1	B	437	SER
1	B	464	SER
1	B	471	LEU
1	B	490	THR
1	B	526	ASN
1	B	538	LEU
1	B	565	THR
1	B	566	ILE
1	B	570	ARG
1	B	571	VAL
1	B	582	LEU
1	B	586	LYS
1	B	591	GLN
1	B	592	LEU
1	B	595	ASP
1	B	606	LEU
1	B	626	VAL
1	B	633	ARG
1	B	659	ARG
1	B	664	VAL
1	B	669	SER
1	B	672	LYS
1	B	675	GLN
1	B	681	GLU
1	B	692	ASP
1	B	696	LYS
1	B	698	VAL
1	B	709	GLU
1	C	42	ARG
1	C	43	LEU
1	C	44	LYS
1	C	55	MET
1	C	65	GLU
1	C	95	ARG
1	C	98	GLU
1	C	119	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	120	ASN
1	C	141	SER
1	C	149	SER
1	C	154	ARG
1	C	198	SER
1	C	208	THR
1	C	211	ASP
1	C	219	SER
1	C	222	SER
1	C	227	LEU
1	C	236	ILE
1	C	239	SER
1	C	257	ASP
1	C	271	GLN
1	C	277	VAL
1	C	295	ASP
1	C	307	SER
1	C	318	ASP
1	C	332	LYS
1	C	343	VAL
1	C	344	LEU
1	C	347	MET
1	C	398	ARG
1	C	403	GLU
1	C	407	ILE
1	C	433	HIS
1	C	437	SER
1	C	470	GLU
1	C	471	LEU
1	C	490	THR
1	C	562	SER
1	C	570	ARG
1	C	571	VAL
1	C	582	LEU
1	C	584	LYS
1	C	586	LYS
1	C	591	GLN
1	C	592	LEU
1	C	606	LEU
1	C	625	VAL
1	C	626	VAL
1	C	659	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	664	VAL
1	C	671	LYS
1	C	675	GLN
1	C	681	GLU
1	C	682	LYS
1	C	692	ASP
1	C	709	GLU
1	D	42	ARG
1	D	43	LEU
1	D	44	LYS
1	D	55	MET
1	D	65	GLU
1	D	95	ARG
1	D	98	GLU
1	D	119	SER
1	D	120	ASN
1	D	141	SER
1	D	149	SER
1	D	198	SER
1	D	208	THR
1	D	211	ASP
1	D	219	SER
1	D	227	LEU
1	D	236	ILE
1	D	243	MET
1	D	257	ASP
1	D	270	LYS
1	D	271	GLN
1	D	277	VAL
1	D	295	ASP
1	D	318	ASP
1	D	319	LYS
1	D	343	VAL
1	D	347	MET
1	D	398	ARG
1	D	403	GLU
1	D	407	ILE
1	D	433	HIS
1	D	437	SER
1	D	464	SER
1	D	470	GLU
1	D	471	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	483	ARG
1	D	490	THR
1	D	519	GLU
1	D	566	ILE
1	D	570	ARG
1	D	571	VAL
1	D	582	LEU
1	D	584	LYS
1	D	591	GLN
1	D	592	LEU
1	D	606	LEU
1	D	625	VAL
1	D	626	VAL
1	D	632	GLU
1	D	638	LYS
1	D	659	ARG
1	D	664	VAL
1	D	675	GLN
1	D	681	GLU
1	D	682	LYS
1	D	692	ASP
1	D	700	GLU
1	D	709	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	446	GLN
1	A	520	GLN
1	A	675	GLN
1	B	175	ASN
1	B	183	GLN
1	B	220	GLN
1	B	415	HIS
1	B	428	HIS
1	B	446	GLN
1	B	522	ASN
1	B	675	GLN
1	C	175	ASN
1	C	313	GLN
1	C	342	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	415	HIS
1	C	428	HIS
1	D	102	HIS
1	D	133	GLN
1	D	175	ASN
1	D	446	GLN
1	D	468	ASN
1	D	478	HIS

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	4000	1	50,50,50	1.91	8 (16%)	67,82,82	1.35	7 (10%)
2	HEM	A	4000	1	50,50,50	1.87	10 (20%)	67,82,82	1.33	6 (8%)
2	HEM	B	4000	1	50,50,50	1.89	8 (16%)	67,82,82	1.34	7 (10%)
2	HEM	D	4000	1	50,50,50	1.85	8 (16%)	67,82,82	1.33	6 (8%)

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	C	4000	1	-	2/14/54/54	-
2	HEM	A	4000	1	-	4/14/54/54	-
2	HEM	B	4000	1	-	2/14/54/54	-
2	HEM	D	4000	1	-	1/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4000	HEM	C3D-C2D	7.98	1.54	1.36
2	A	4000	HEM	C3D-C2D	7.92	1.53	1.36
2	D	4000	HEM	C3D-C2D	7.91	1.53	1.36
2	B	4000	HEM	C3D-C2D	7.89	1.53	1.36
2	C	4000	HEM	FE-ND	4.71	2.09	1.94
2	B	4000	HEM	FE-ND	4.70	2.09	1.94
2	A	4000	HEM	FE-ND	4.59	2.09	1.94
2	D	4000	HEM	FE-ND	4.15	2.07	1.94
2	D	4000	HEM	FE-NB	3.89	2.06	1.94
2	B	4000	HEM	FE-NC	3.73	2.07	1.95
2	A	4000	HEM	FE-NB	3.68	2.06	1.94
2	C	4000	HEM	FE-NA	3.67	2.07	1.95
2	B	4000	HEM	FE-NB	3.63	2.06	1.94
2	C	4000	HEM	FE-NB	3.55	2.05	1.94
2	A	4000	HEM	FE-NC	3.24	2.05	1.95
2	C	4000	HEM	FE-NC	3.24	2.05	1.95
2	D	4000	HEM	FE-NA	3.23	2.05	1.95
2	C	4000	HEM	CAC-C3C	3.17	1.55	1.47
2	A	4000	HEM	CAC-C3C	3.13	1.55	1.47
2	C	4000	HEM	CAB-C3B	3.11	1.55	1.47
2	B	4000	HEM	CAC-C3C	3.11	1.55	1.47
2	D	4000	HEM	CAC-C3C	3.10	1.55	1.47
2	B	4000	HEM	CAB-C3B	3.09	1.55	1.47
2	D	4000	HEM	CAB-C3B	3.09	1.55	1.47
2	A	4000	HEM	CAB-C3B	3.08	1.55	1.47
2	A	4000	HEM	FE-NA	3.00	2.05	1.95
2	D	4000	HEM	FE-NC	3.00	2.05	1.95
2	B	4000	HEM	FE-NA	2.80	2.04	1.95
2	C	4000	HEM	CMC-C2C	2.15	1.55	1.50
2	B	4000	HEM	CMC-C2C	2.08	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	HEM	CMC-C2C	2.04	1.54	1.50
2	A	4000	HEM	CMD-C2D	2.04	1.54	1.50
2	D	4000	HEM	CMA-C3A	2.04	1.54	1.50
2	A	4000	HEM	CMB-C2B	2.02	1.54	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4000	HEM	C4D-ND-C1D	5.83	112.11	105.21
2	C	4000	HEM	C4D-ND-C1D	5.74	112.00	105.21
2	B	4000	HEM	C4D-ND-C1D	5.73	111.99	105.21
2	A	4000	HEM	C4D-ND-C1D	5.65	111.90	105.21
2	B	4000	HEM	CAA-CBA-CGA	-2.90	105.98	113.67
2	A	4000	HEM	CAA-CBA-CGA	-2.82	106.17	113.67
2	D	4000	HEM	CAA-CBA-CGA	-2.71	106.46	113.67
2	C	4000	HEM	CAA-CBA-CGA	-2.69	106.52	113.67
2	B	4000	HEM	C2A-C1A-NA	-2.51	107.36	110.15
2	A	4000	HEM	C2A-C1A-NA	-2.51	107.36	110.15
2	D	4000	HEM	C3B-C2B-C1B	2.49	108.28	106.41
2	D	4000	HEM	C2A-C1A-NA	-2.49	107.39	110.15
2	C	4000	HEM	C2A-C1A-NA	-2.43	107.45	110.15
2	C	4000	HEM	C3B-C2B-C1B	2.40	108.22	106.41
2	B	4000	HEM	C3B-C2B-C1B	2.39	108.20	106.41
2	B	4000	HEM	CHD-C1D-ND	2.32	126.92	124.42
2	C	4000	HEM	CHD-C1D-ND	2.27	126.86	124.42
2	A	4000	HEM	CHD-C1D-ND	2.16	126.75	124.42
2	D	4000	HEM	C1B-NB-C4B	2.16	107.76	105.21
2	B	4000	HEM	CAD-C3D-C4D	2.14	128.43	124.70
2	C	4000	HEM	CAA-C2A-C1A	2.13	129.09	124.94
2	A	4000	HEM	C3B-C2B-C1B	2.09	107.98	106.41
2	B	4000	HEM	C1B-NB-C4B	2.07	107.66	105.21
2	C	4000	HEM	C1B-NB-C4B	2.04	107.62	105.21
2	A	4000	HEM	CAD-C3D-C4D	2.03	128.23	124.70
2	D	4000	HEM	CHD-C1D-ND	2.02	126.59	124.42

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4000	HEM	C1A-C2A-CAA-CBA
2	C	4000	HEM	C3A-C2A-CAA-CBA
2	A	4000	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	4000	HEM	CAD-CBD-CGD-O1D
2	B	4000	HEM	CAD-CBD-CGD-O2D
2	D	4000	HEM	CAA-CBA-CGA-O1A
2	B	4000	HEM	CAD-CBD-CGD-O1D
2	A	4000	HEM	C1A-C2A-CAA-CBA
2	A	4000	HEM	CAA-CBA-CGA-O2A

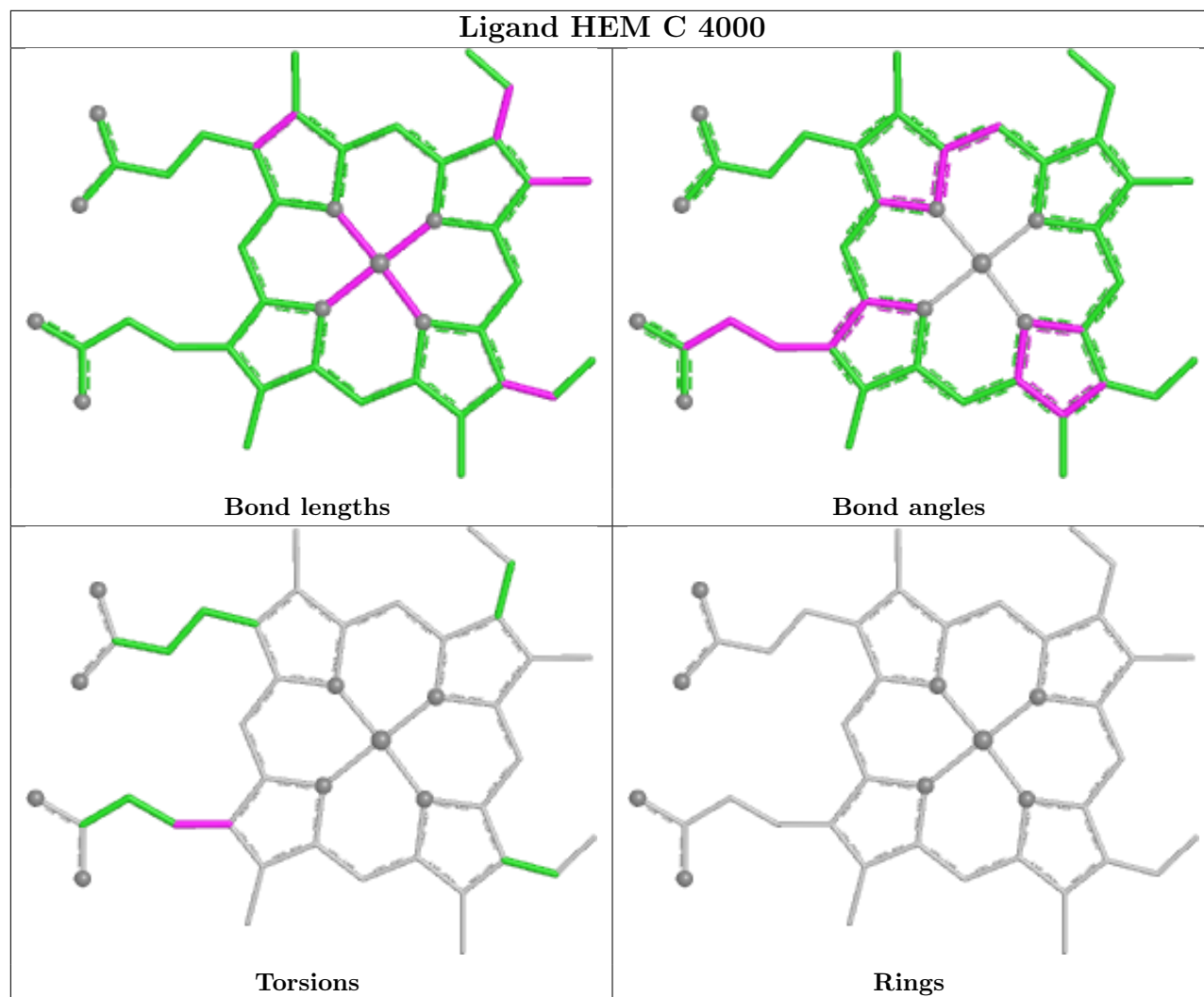
There are no ring outliers.

4 monomers are involved in 17 short contacts:

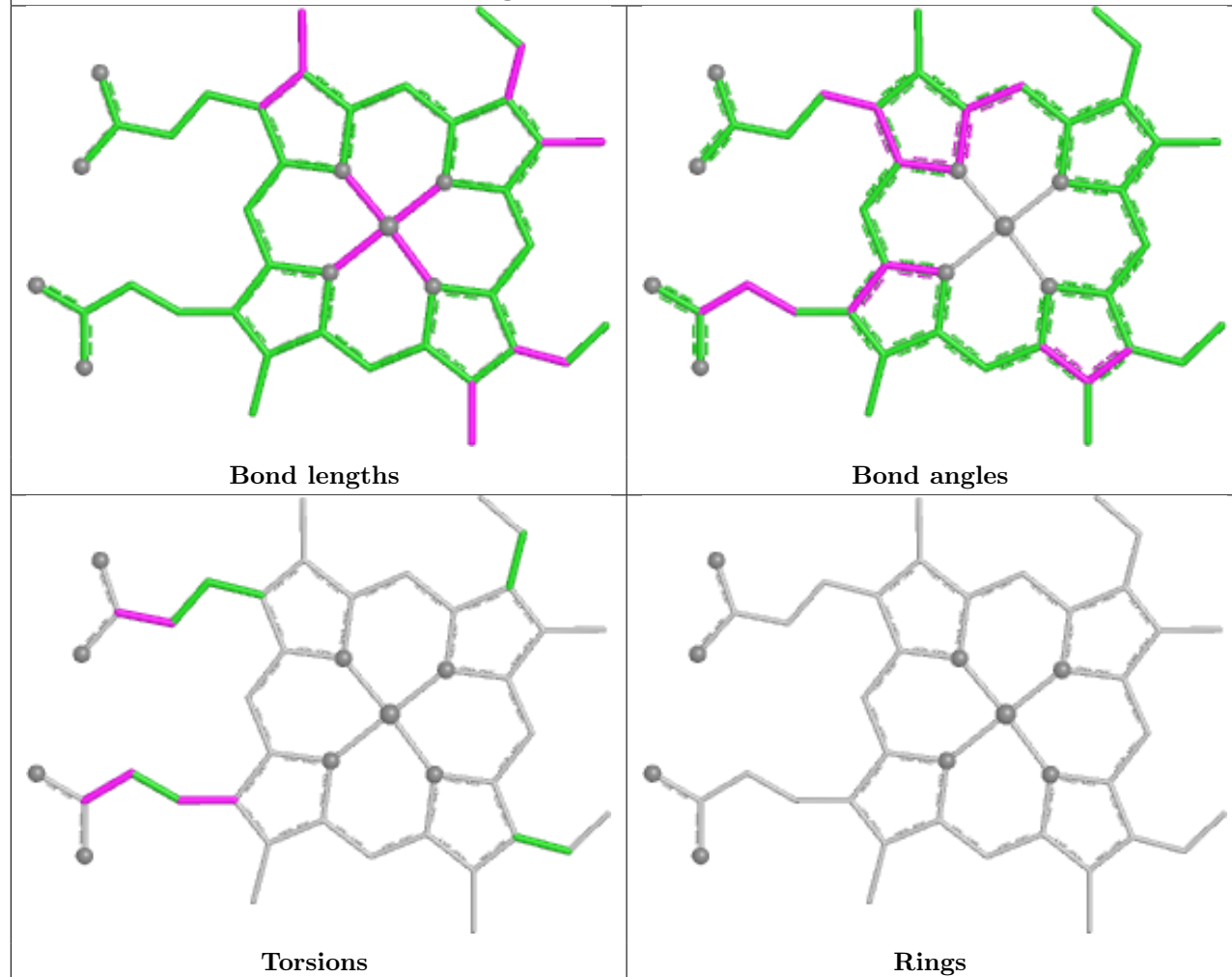
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4000	HEM	3	0
2	A	4000	HEM	3	0
2	B	4000	HEM	7	0
2	D	4000	HEM	4	0

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.

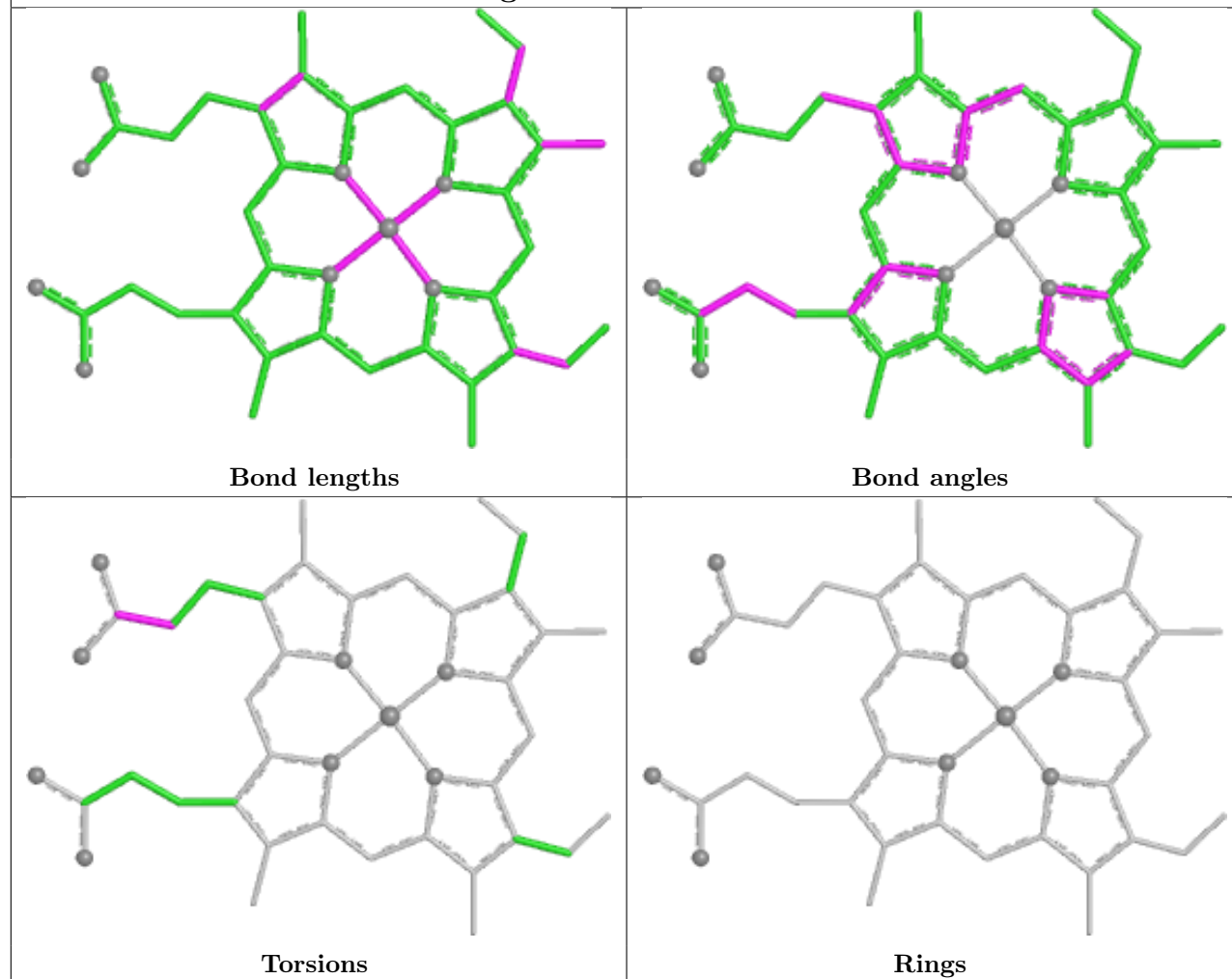
Ligand HEM C 4000

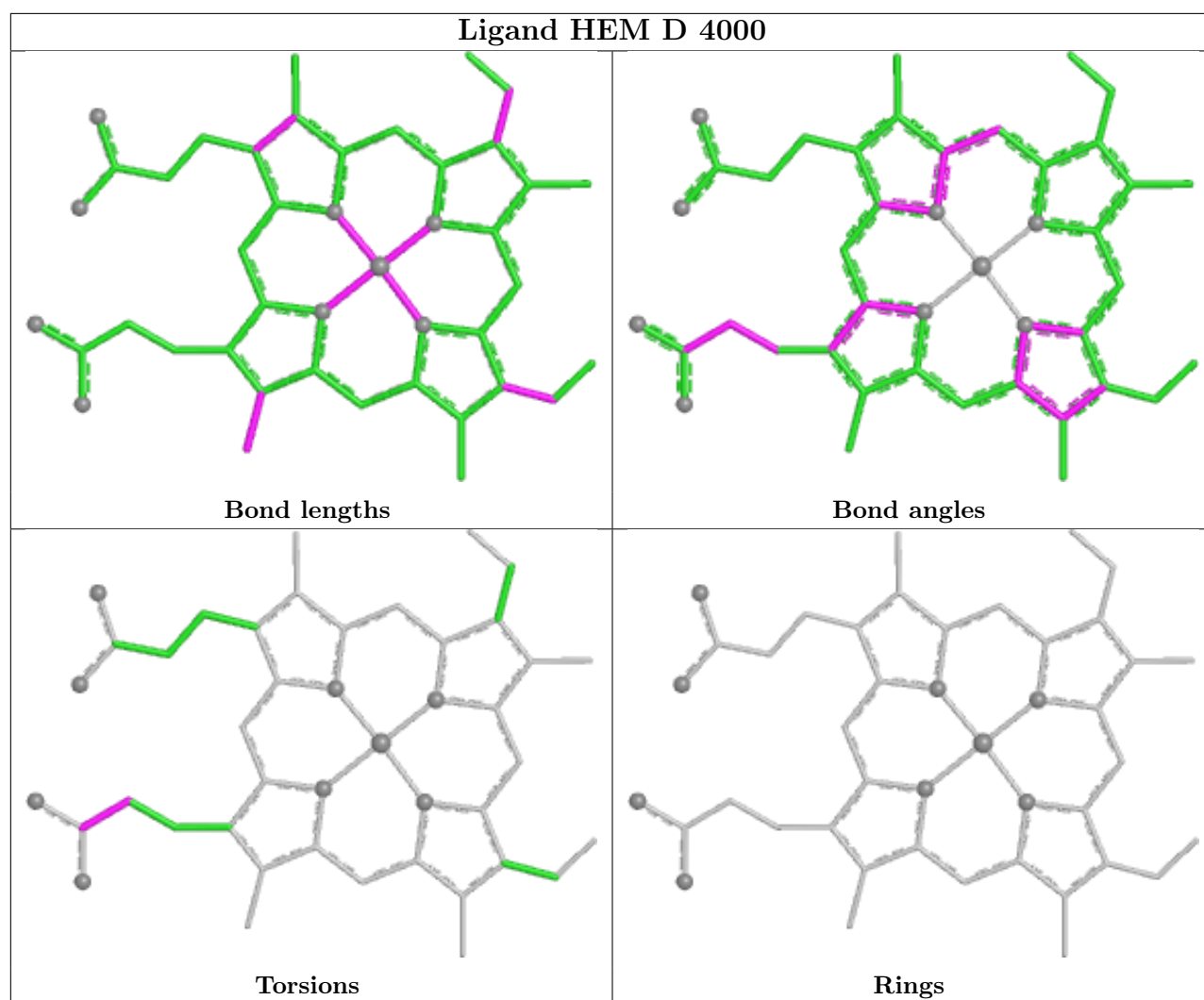


Ligand HEM A 4000



Ligand HEM B 4000





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	680/746 (91%)	0.03	6 (0%) 81 63	10, 40, 85, 128	0
1	B	681/746 (91%)	0.33	15 (2%) 62 41	16, 53, 105, 172	0
1	C	680/746 (91%)	-0.07	4 (0%) 85 70	5, 42, 78, 148	0
1	D	680/746 (91%)	0.07	4 (0%) 85 70	10, 44, 76, 165	0
All	All	2721/2984 (91%)	0.09	29 (1%) 78 59	5, 45, 89, 172	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	GLY	5.4
1	A	435	SER	5.4
1	C	716	ASP	3.1
1	B	630	GLY	2.9
1	B	715	GLY	2.9
1	B	545	PRO	2.9
1	D	716	ASP	2.8
1	A	690	ALA	2.7
1	B	625	VAL	2.6
1	B	640	ALA	2.6
1	C	636	SER	2.5
1	B	716	ASP	2.5
1	B	560	ASN	2.5
1	A	667	VAL	2.5
1	B	580	GLY	2.4
1	B	664	VAL	2.4
1	B	599	VAL	2.2
1	A	716	ASP	2.2
1	A	318	ASP	2.1
1	C	73	GLY	2.1
1	B	548	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	445	ALA	2.1
1	D	595	ASP	2.0
1	B	524	ILE	2.0
1	B	551	ASN	2.0
1	B	559	PHE	2.0
1	B	694	VAL	2.0
1	D	539	GLU	2.0
1	D	524	ILE	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](#)

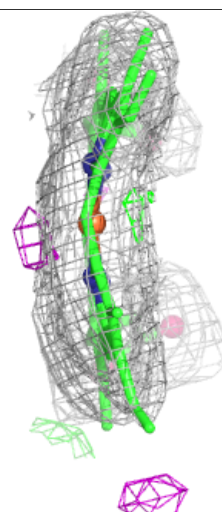
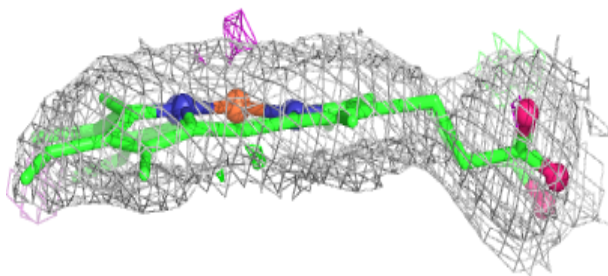
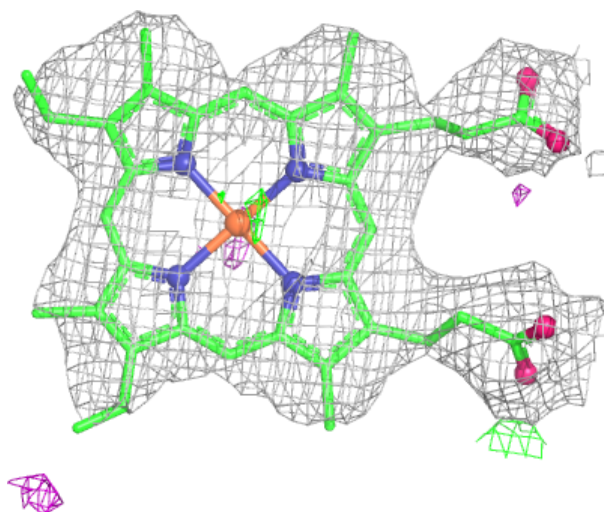
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	HEM	B	4000	43/43	0.95	0.10	25,36,45,58	0
2	HEM	A	4000	43/43	0.96	0.09	21,27,33,54	0
2	HEM	C	4000	43/43	0.96	0.08	18,25,35,37	0
2	HEM	D	4000	43/43	0.96	0.08	20,25,32,41	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.

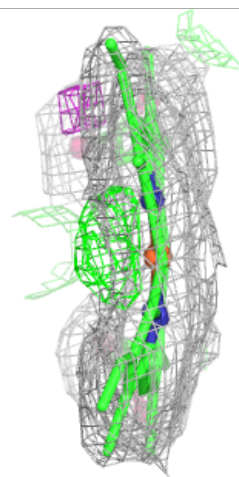
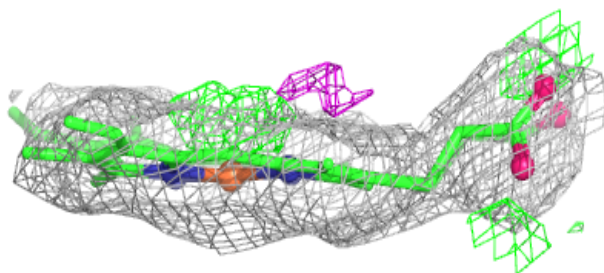
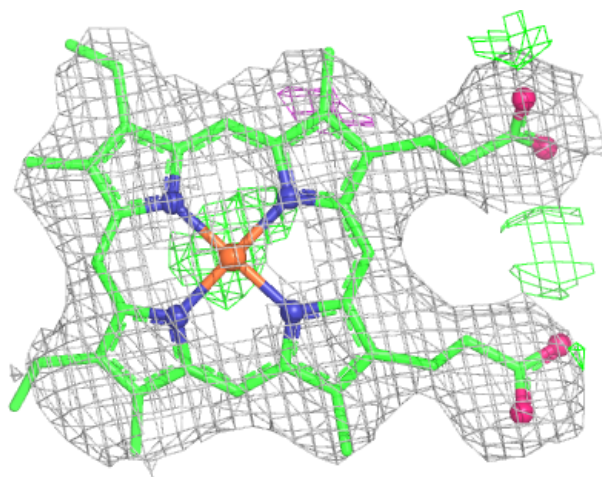
Electron density around HEM B 4000:

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



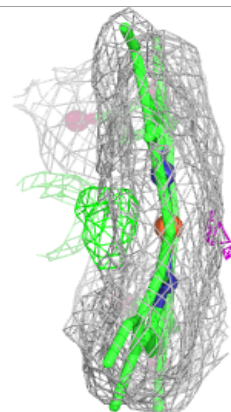
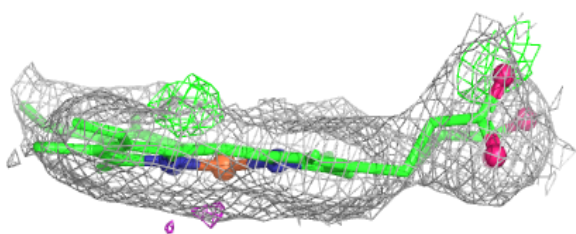
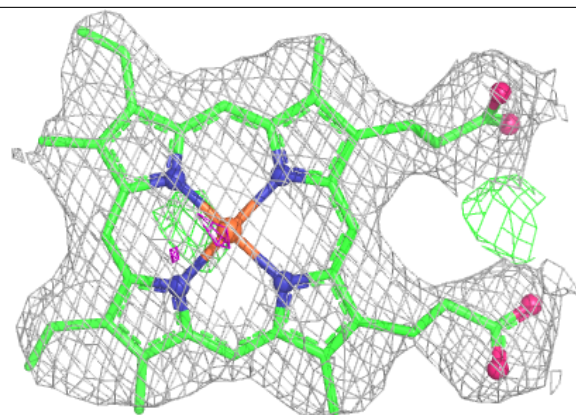
Electron density around HEM A 4000:

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

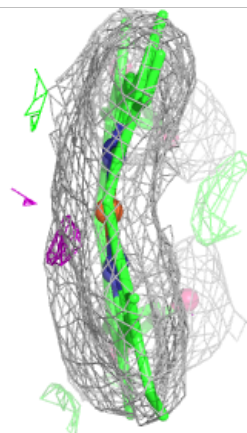
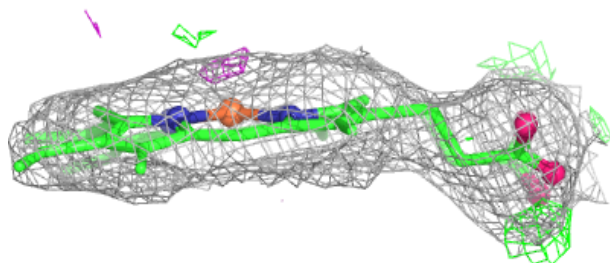
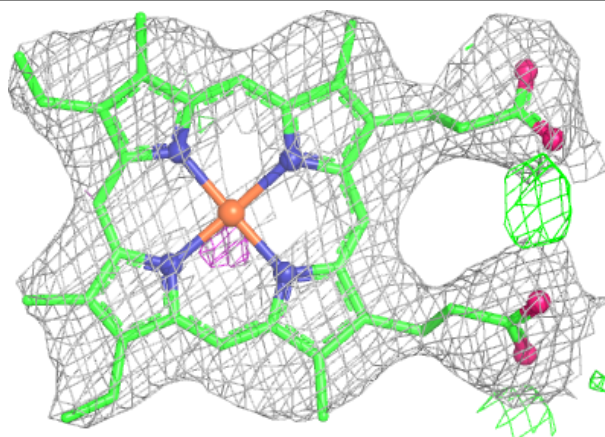


Electron density around HEM C 4000:

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

**Electron density around HEM D 4000:**

$2mF_o-DF_c$ (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.