



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 4KLC / pdb_00004klc
Title : E343D/F110A Double mutant of human ferrochelatase
Authors : Lanzilotta, W.N.; Medlock, A.E.
Deposited on : 2013-05-07
Resolution : 2.40 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

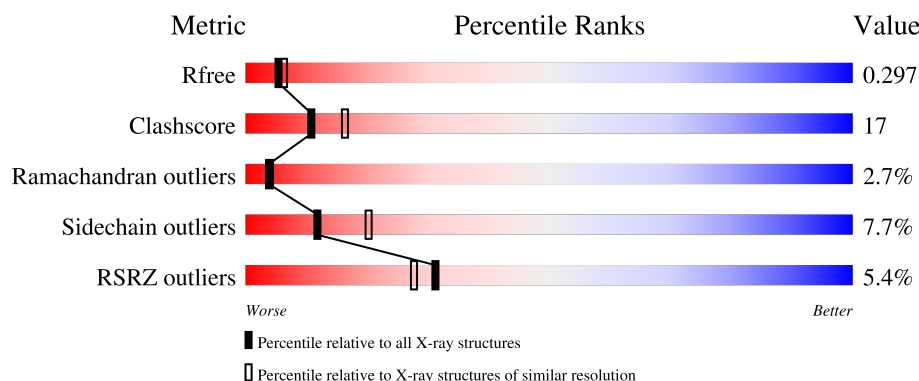
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	370	5% 64% 28% 5% . .
1	B	370	5% 66% 26% 5% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	502[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6182 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 Ferrochelatase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2884	1834	503	529	18			
1	B	359	Total	C	N	O	S	0	0	0
			2884	1834	503	529	18			

There are 26 discrepancies between the modelled and reference sequences:

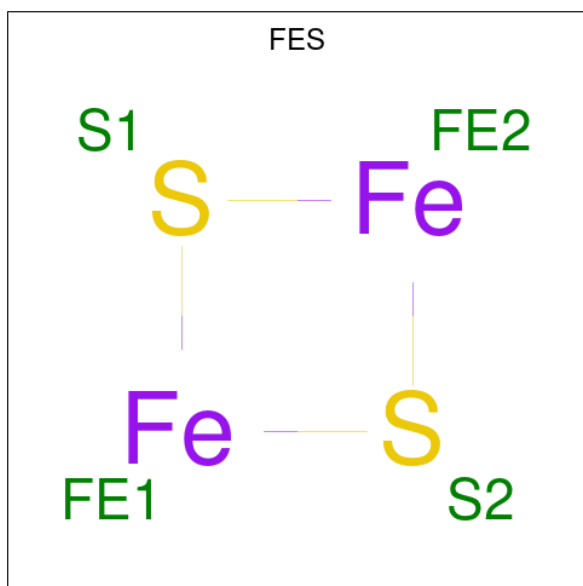
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP P22830
A	55	GLY	-	expression tag	UNP P22830
A	56	GLY	-	expression tag	UNP P22830
A	57	SER	-	expression tag	UNP P22830
A	58	HIS	-	expression tag	UNP P22830
A	59	HIS	-	expression tag	UNP P22830
A	60	HIS	-	expression tag	UNP P22830
A	61	HIS	-	expression tag	UNP P22830
A	62	HIS	-	expression tag	UNP P22830
A	63	HIS	-	expression tag	UNP P22830
A	64	GLY	-	expression tag	UNP P22830
A	110	ALA	PHE	engineered mutation	UNP P22830
A	343	ASP	GLU	engineered mutation	UNP P22830
B	54	MET	-	expression tag	UNP P22830
B	55	GLY	-	expression tag	UNP P22830
B	56	GLY	-	expression tag	UNP P22830
B	57	SER	-	expression tag	UNP P22830
B	58	HIS	-	expression tag	UNP P22830
B	59	HIS	-	expression tag	UNP P22830
B	60	HIS	-	expression tag	UNP P22830
B	61	HIS	-	expression tag	UNP P22830
B	62	HIS	-	expression tag	UNP P22830
B	63	HIS	-	expression tag	UNP P22830
B	64	GLY	-	expression tag	UNP P22830
B	110	ALA	PHE	engineered mutation	UNP P22830

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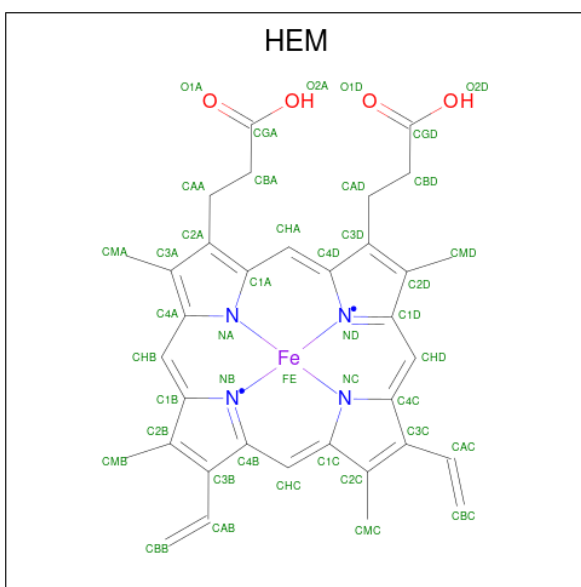
Chain	Residue	Modelled	Actual	Comment	Reference
B	343	ASP	GLU	engineered mutation	UNP P22830

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



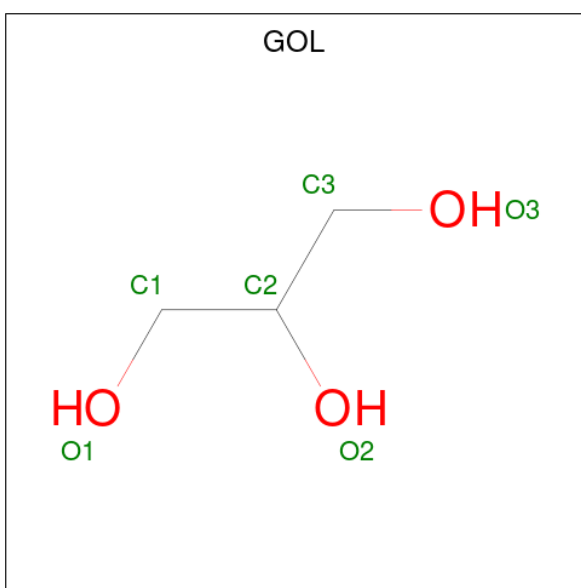
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	1
			12	6	6		

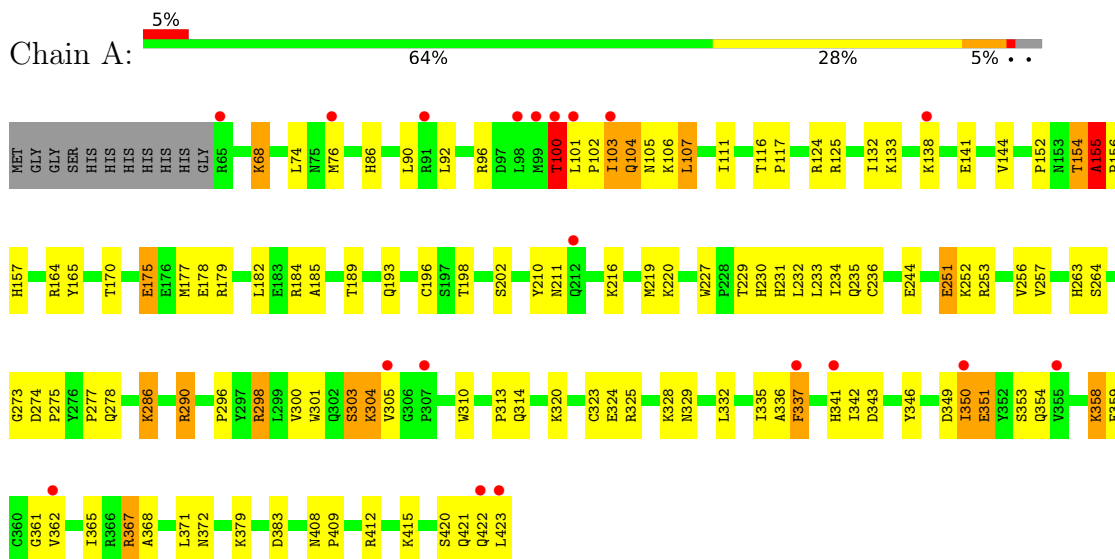
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total 173	O 173	0	0
5	B	135	Total 135	O 135	0	0

3 Residue-property plots [i](#)

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

• Molecule 1: Ferrochelatase, mitochondrial



• Molecule 1: Ferrochelatase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	62.66Å 133.40Å 136.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	136.78 – 2.40 136.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (136.78-2.40) 98.1 (136.78-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.255 , 0.299 0.255 , 0.297	Depositor DCC
R_{free} test set	2255 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6182	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 79.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5885e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	1/2953 (0.0%)	1.20	8/4001 (0.2%)
1	B	1.05	2/2953 (0.1%)	1.15	5/4001 (0.1%)
All	All	1.08	3/5906 (0.1%)	1.18	13/8002 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	THR	CA-CB	8.63	1.64	1.54
1	B	155	ALA	CA-C	-6.24	1.45	1.52
1	B	187	ALA	CA-CB	5.03	1.59	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	ILE	N-CA-C	-9.15	99.87	110.21
1	A	408	ASN	CA-C-N	7.02	126.72	119.56
1	A	408	ASN	C-N-CA	7.02	126.72	119.56
1	A	155	ALA	N-CA-C	6.88	125.01	109.81
1	A	154	THR	N-CA-C	-6.85	104.05	112.88
1	B	280	VAL	N-CA-C	-6.83	103.86	110.42
1	A	233	LEU	N-CA-C	-6.66	104.10	111.36
1	B	250	LEU	N-CA-C	5.70	118.23	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	VAL	N-CA-C	5.50	116.14	110.36
1	B	142	GLY	N-CA-C	-5.47	106.17	112.73
1	B	165	TYR	N-CA-C	5.25	119.65	112.88
1	A	86	HIS	N-CA-C	5.10	116.53	110.97
1	B	384	LEU	N-CA-C	5.08	117.48	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	THR	Peptide

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	2884	0	2893	108	0
1	B	2884	0	2893	91	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	43	0	30	9	0
3	B	43	0	30	8	0
4	B	12	0	16	5	0
5	A	173	0	0	9	1
5	B	135	0	0	2	1
All	All	6182	0	5862	195	2

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 17.

All (195) 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:A:152:PRO:O	1:A:155:ALA:HB2	1.50	1.10
1:A:290:ARG:HH11	1:A:290:ARG:CG	1.66	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HG13	1:A:286:LYS:HD2	1.11	1.06
1:A:290:ARG:HG2	1:A:290:ARG:NH1	1.66	1.02
1:B:341:HIS:CE1	3:B:503:HEM:HMD3	1.96	1.00
1:A:290:ARG:HH11	1:A:290:ARG:HG2	0.83	0.98
1:A:234:ILE:HG13	1:A:286:LYS:CD	1.93	0.97
1:A:277:PRO:HB2	4:B:502[A]:GOL:H2	1.43	0.96
1:B:155:ALA:HB1	1:B:156:PRO:CD	1.96	0.96
1:A:104:GLN:HA	1:A:107:LEU:HB3	1.47	0.94
1:A:68:LYS:HG3	1:A:156:PRO:HD2	1.50	0.94
1:A:234:ILE:HG21	1:A:286:LYS:HD3	1.52	0.91
1:B:155:ALA:HB1	1:B:156:PRO:HD2	1.51	0.91
1:B:68:LYS:HE2	1:B:155:ALA:HB2	1.50	0.90
1:B:341:HIS:HE1	3:B:503:HEM:HMD3	1.37	0.86
1:B:68:LYS:HE2	1:B:155:ALA:CB	2.07	0.83
1:B:101:LEU:C	1:B:103:ILE:H	1.86	0.83
1:A:273:GLY:O	1:B:298:ARG:NH1	2.13	0.82
1:A:244:GLU:HG2	5:A:656:HOH:O	1.79	0.81
1:B:341:HIS:CE1	3:B:503:HEM:CMD	2.66	0.78
1:A:100:THR:O	1:A:102:PRO:HD3	1.83	0.77
1:B:276:TYR:HB3	1:B:277:PRO:HD3	1.64	0.77
1:B:350:ILE:O	1:B:351:GLU:HB3	1.84	0.76
1:A:152:PRO:O	1:A:155:ALA:CB	2.32	0.76
1:B:352:TYR:O	1:B:357:ALA:HB2	1.85	0.76
1:B:155:ALA:CB	1:B:156:PRO:CD	2.65	0.75
1:A:277:PRO:HB2	4:B:502[A]:GOL:C2	2.17	0.74
1:A:68:LYS:HG3	1:A:156:PRO:CD	2.18	0.74
1:A:296:PRO:HD3	1:B:397:LYS:HD2	1.69	0.73
1:B:68:LYS:CE	1:B:155:ALA:HB2	2.19	0.72
1:A:349:ASP:O	1:A:353:SER:HB2	1.90	0.71
1:A:141:GLU:OE1	5:A:716:HOH:O	2.09	0.70
1:A:252:LYS:HB3	1:A:329:ASN:ND2	2.08	0.69
1:B:76:MET:HG2	1:B:165:TYR:HE1	1.56	0.69
1:A:104:GLN:O	1:A:106:LYS:N	2.22	0.68
1:B:155:ALA:CB	1:B:156:PRO:HD2	2.21	0.68
1:A:415:LYS:HE3	5:A:761:HOH:O	1.93	0.67
1:A:290:ARG:CG	1:A:290:ARG:NH1	2.35	0.67
1:A:263:HIS:CD2	3:A:502:HEM:C4C	2.82	0.67
1:A:116:THR:N	1:A:117:PRO:HD2	2.10	0.67
1:B:316:ASP:HB3	1:B:352:TYR:CE1	2.30	0.67
1:A:335:ILE:O	1:A:335:ILE:HG13	1.94	0.66
1:A:323:CYS:SG	1:A:362:VAL:HG22	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:O	1:B:351:GLU:CB	2.44	0.65
1:B:76:MET:HG2	1:B:165:TYR:CE1	2.32	0.64
1:A:350:ILE:HA	1:A:354:GLN:OE1	1.98	0.63
1:A:300:VAL:HG12	1:A:313:PRO:HG2	1.81	0.63
1:A:343:ASP:OD1	5:A:750:HOH:O	2.16	0.63
1:A:244:GLU:HG3	1:A:368:ALA:HA	1.80	0.63
1:B:226:ARG:HD3	1:B:279:GLU:OE2	1.99	0.63
1:B:101:LEU:C	1:B:103:ILE:N	2.53	0.63
1:A:235:GLN:HG3	1:A:290:ARG:HH22	1.65	0.62
1:B:105:ASN:C	1:B:107:LEU:H	2.08	0.62
1:A:342:ILE:HG22	3:A:502:HEM:CAD	2.30	0.61
1:A:304:LYS:O	1:A:304:LYS:HG2	2.01	0.61
1:B:208:ARG:NH2	1:B:410:VAL:HG21	2.15	0.61
1:A:298:ARG:HG3	5:A:692:HOH:O	2.01	0.61
1:B:319:ILE:HD11	1:B:332:LEU:HD21	1.83	0.60
1:B:101:LEU:O	1:B:103:ILE:N	2.35	0.60
1:B:281:SER:OG	4:B:502[B]:GOL:H31	2.01	0.60
1:A:103:ILE:O	1:A:104:GLN:O	2.20	0.60
1:A:74:LEU:HD22	1:A:202:SER:HB3	1.84	0.59
1:B:213:VAL:HG13	1:B:215:ARG:HG2	1.84	0.59
1:A:346:TYR:O	1:A:350:ILE:O	2.20	0.59
1:B:75:ASN:OD1	1:B:132:ILE:HD11	2.03	0.59
1:B:101:LEU:O	1:B:101:LEU:HD22	2.03	0.59
1:A:220:LYS:HE3	1:A:423:LEU:O	2.03	0.58
1:B:365:ILE:O	1:B:365:ILE:HG23	2.04	0.58
1:A:342:ILE:HG22	3:A:502:HEM:HAD1	1.86	0.58
1:B:195:SER:HB2	1:B:276:TYR:HB2	1.87	0.57
1:B:182:LEU:HB2	1:B:219:MET:HE2	1.85	0.57
1:A:68:LYS:HG3	1:A:156:PRO:CG	2.36	0.56
1:B:320:LYS:HG2	1:B:360:CYS:SG	2.45	0.56
1:A:332:LEU:HD11	1:A:365:ILE:HD11	1.87	0.56
1:B:208:ARG:HH21	1:B:410:VAL:HG21	1.71	0.56
1:A:232:LEU:HD13	1:A:379:LYS:HG2	1.87	0.55
1:A:68:LYS:HG3	1:A:156:PRO:HG2	1.88	0.55
1:B:341:HIS:CE1	1:B:343:ASP:HB2	2.41	0.55
1:A:231:HIS:HD2	5:A:623:HOH:O	1.90	0.55
1:A:323:CYS:C	1:A:325:ARG:H	2.14	0.55
1:B:266:PRO:HD2	3:B:503:HEM:HAB	1.89	0.54
1:B:68:LYS:HB3	1:B:155:ALA:HB3	1.90	0.54
1:A:104:GLN:HG3	1:A:105:ASN:H	1.73	0.54
1:B:125:ARG:CZ	1:B:125:ARG:HA	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:CG	1:A:156:PRO:HD2	2.33	0.54
1:A:152:PRO:C	1:A:155:ALA:HB2	2.30	0.54
1:A:100:THR:C	1:A:102:PRO:HD3	2.32	0.53
1:B:122:GLN:NE2	1:B:346:TYR:CE2	2.77	0.53
1:A:252:LYS:HB3	1:A:329:ASN:HD22	1.72	0.53
1:B:122:GLN:HE21	1:B:346:TYR:HD2	1.48	0.53
1:B:207:TYR:CE1	1:B:413:GLU:HG3	2.44	0.53
1:A:337:PHE:HB2	5:A:759:HOH:O	2.09	0.52
1:A:341:HIS:HB2	3:A:502:HEM:O2D	2.10	0.52
1:B:99:MET:O	1:B:102:PRO:HD2	2.10	0.51
1:B:263:HIS:HD2	3:B:503:HEM:C1D	2.29	0.51
1:A:251:GLU:OE2	1:A:251:GLU:N	2.38	0.51
1:A:182:LEU:HB2	1:A:219:MET:HE2	1.92	0.51
1:B:263:HIS:CD2	3:B:503:HEM:C1D	2.99	0.50
1:B:104:GLN:HA	1:B:104:GLN:OE1	2.11	0.50
1:B:346:TYR:O	1:B:350:ILE:O	2.30	0.50
1:A:177:MET:HE1	1:A:185:ALA:HB1	1.94	0.49
1:A:230:HIS:NE2	1:A:383:ASP:OD2	2.43	0.49
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.27	0.49
1:A:278:GLN:HG2	1:B:281:SER:HB3	1.94	0.49
1:B:193:GLN:HG2	1:B:280:VAL:HA	1.94	0.49
1:B:68:LYS:HE2	1:B:155:ALA:HB3	1.94	0.49
1:B:75:ASN:O	1:B:163:PHE:HA	2.13	0.49
1:A:320:LYS:O	1:A:324:GLU:HG3	2.13	0.49
1:B:305:VAL:HG11	3:B:503:HEM:HMA2	1.93	0.49
1:B:177:MET:HB3	1:B:219:MET:HE1	1.95	0.49
1:A:320:LYS:O	1:A:320:LYS:HG2	2.12	0.48
1:A:76:MET:HA	1:A:164:ARG:HB3	1.96	0.48
1:A:182:LEU:HB2	1:A:219:MET:CE	2.42	0.48
1:A:342:ILE:HG22	3:A:502:HEM:HAD2	1.96	0.48
1:B:155:ALA:HB1	1:B:156:PRO:HD3	1.93	0.48
1:B:110:ALA:O	1:B:114:ARG:HB2	2.13	0.47
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.95	0.47
1:B:106:LYS:HE3	1:B:106:LYS:H	1.79	0.47
1:A:236:CYS:HB3	1:A:371:LEU:HD22	1.95	0.47
1:A:409:PRO:HA	5:A:733:HOH:O	2.14	0.47
1:B:106:LYS:HA	1:B:109:PRO:HD2	1.96	0.47
1:A:301:TRP:O	1:A:314:GLN:HA	2.14	0.47
1:B:182:LEU:HD12	1:B:219:MET:HE1	1.97	0.47
1:B:243:LYS:HZ1	1:B:369:GLU:H	1.63	0.47
1:B:272:ARG:O	1:B:272:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:HIS:CD2	3:A:502:HEM:CHD	2.98	0.47
1:B:91:ARG:NH2	5:B:713:HOH:O	2.47	0.47
1:B:105:ASN:C	1:B:107:LEU:N	2.73	0.47
1:A:277:PRO:HB2	4:B:502[A]:GOL:C3	2.45	0.47
1:B:76:MET:HB2	1:B:191:TYR:OH	2.15	0.47
1:A:175:GLU:OE1	1:A:179:ARG:NH1	2.48	0.46
1:B:349:ASP:O	1:B:353:SER:HB2	2.15	0.46
1:A:92:LEU:C	1:A:92:LEU:HD23	2.41	0.46
1:B:407:VAL:O	1:B:409:PRO:HD3	2.15	0.45
1:A:354:GLN:O	1:A:358:LYS:HB2	2.16	0.45
1:A:102:PRO:O	1:A:103:ILE:HG22	2.16	0.45
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.82	0.45
1:B:75:ASN:CG	1:B:132:ILE:HD11	2.40	0.45
1:A:263:HIS:CD2	3:A:502:HEM:C1D	3.04	0.45
1:A:323:CYS:C	1:A:325:ARG:N	2.71	0.45
1:A:277:PRO:HB2	4:B:502[A]:GOL:H32	1.99	0.45
1:A:328:LYS:HD2	1:A:361:GLY:O	2.17	0.45
1:B:87:ASP:OD1	1:B:91:ARG:CZ	2.65	0.45
1:B:97:ASP:HB2	1:B:201:SER:OG	2.17	0.45
1:A:124:ARG:HG2	1:A:125:ARG:HH21	1.81	0.44
1:A:337:PHE:CE1	3:A:502:HEM:HMD1	2.52	0.44
1:B:262:ALA:HB1	1:B:276:TYR:OH	2.17	0.44
1:A:332:LEU:HB2	1:A:367:ARG:HG2	1.99	0.44
1:B:91:ARG:O	1:B:92:LEU:C	2.59	0.44
1:A:103:ILE:O	1:A:103:ILE:HG13	2.18	0.44
1:A:104:GLN:HG3	1:A:105:ASN:N	2.33	0.44
1:B:312:GLY:HA2	1:B:313:PRO:O	2.18	0.43
1:A:304:LYS:O	1:A:304:LYS:CG	2.65	0.43
1:A:337:PHE:CE1	3:A:502:HEM:CMD	3.02	0.43
1:A:253:ARG:O	1:A:256:VAL:HG23	2.18	0.43
1:A:304:LYS:HA	1:A:310:TRP:CD2	2.54	0.43
1:A:264:SER:HB3	1:A:310:TRP:HE3	1.82	0.43
1:B:283:THR:O	1:B:287:VAL:HG23	2.19	0.43
1:A:251:GLU:N	1:A:251:GLU:CD	2.76	0.43
1:B:107:LEU:O	1:B:111:ILE:HG13	2.19	0.43
1:B:398:GLN:HA	1:B:398:GLN:OE1	2.19	0.42
1:A:189:THR:O	1:A:189:THR:HG23	2.18	0.42
1:B:118:LYS:O	1:B:121:GLU:HB2	2.19	0.42
1:A:350:ILE:O	1:A:351:GLU:HB3	2.19	0.42
1:B:314:GLN:HB3	1:B:316:ASP:OD2	2.19	0.42
1:B:308:MET:HB3	1:B:309:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:O	1:A:104:GLN:C	2.61	0.42
1:B:149:GLU:HA	5:B:729:HOH:O	2.19	0.42
1:A:76:MET:HB2	1:A:165:TYR:CD1	2.55	0.42
1:A:132:ILE:HG23	1:A:133:LYS:N	2.34	0.42
1:A:196:CYS:SG	5:A:762:HOH:O	2.62	0.42
1:A:273:GLY:HA2	1:B:313:PRO:CG	2.49	0.42
1:B:408:ASN:OD1	1:B:410:VAL:HG23	2.19	0.42
1:A:234:ILE:HG21	1:A:286:LYS:CD	2.37	0.42
1:A:193:GLN:OE1	1:A:336:ALA:HA	2.20	0.41
1:B:89:LEU:HD11	1:B:119:ILE:HG13	2.02	0.41
1:B:102:PRO:HB3	1:B:105:ASN:OD1	2.20	0.41
1:A:251:GLU:CD	1:A:251:GLU:H	2.26	0.41
1:B:92:LEU:C	1:B:92:LEU:HD23	2.45	0.41
1:B:402:SER:O	1:B:403:CYS:C	2.61	0.41
1:A:231:HIS:CD2	1:A:231:HIS:H	2.39	0.41
1:A:323:CYS:O	1:A:325:ARG:N	2.53	0.41
1:B:263:HIS:CD2	3:B:503:HEM:C4C	3.08	0.41
1:A:412:ARG:HA	1:A:415:LYS:HE2	2.03	0.41
1:B:122:GLN:O	1:B:125:ARG:HB2	2.21	0.41
1:A:178:GLU:OE2	1:A:210:TYR:CE2	2.74	0.41
1:A:371:LEU:O	1:A:372:ASN:C	2.64	0.41
1:A:154:THR:OG1	1:A:157:HIS:NE2	2.49	0.40
1:B:171:GLU:H	1:B:171:GLU:CD	2.28	0.40
1:B:211:ASN:O	1:B:212:GLN:C	2.64	0.40
1:A:68:LYS:HB3	1:A:68:LYS:HE3	1.82	0.40
1:B:248:PHE:CZ	1:B:366:ARG:HG3	2.56	0.40
1:B:342:ILE:HD13	1:B:346:TYR:HB3	2.02	0.40
1:A:229:THR:O	1:A:230:HIS:C	2.61	0.40
1:B:391:SER:OG	1:B:393:GLU:HG2	2.22	0.40

All (2) 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)
5:B:729:HOH:O	5:B:730:HOH:O[2_555]	2.08	0.12
5:A:767:HOH:O	5:A:768:HOH:O[2_555]	2.09	0.11

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	357/370 (96%)	326 (91%)	21 (6%)	10 (3%)	4	3
1	B	357/370 (96%)	317 (89%)	31 (9%)	9 (2%)	4	5
All	All	714/740 (96%)	643 (90%)	52 (7%)	19 (3%)	4	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	THR
1	A	104	GLN
1	A	304	LYS
1	B	155	ALA
1	B	355	VAL
1	B	359	GLU
1	B	106	LYS
1	B	351	GLU
1	A	351	GLU
1	A	421	GLN
1	B	357	ALA
1	B	102	PRO
1	B	303	SER
1	A	155	ALA
1	A	227	TRP
1	A	303	SER
1	B	307	PRO
1	A	103	ILE
1	A	101	LEU

5.3.2 Protein sidechains [i](#)

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	323/331 (98%)	298 (92%)	25 (8%)	12	20
1	B	323/331 (98%)	298 (92%)	25 (8%)	12	20
All	All	646/662 (98%)	596 (92%)	50 (8%)	12	20

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS
1	A	90	LEU
1	A	96	ARG
1	A	100	THR
1	A	107	LEU
1	A	111	ILE
1	A	138	LYS
1	A	170	THR
1	A	175	GLU
1	A	184	ARG
1	A	211	ASN
1	A	216	LYS
1	A	251	GLU
1	A	257	VAL
1	A	286	LYS
1	A	290	ARG
1	A	298	ARG
1	A	303	SER
1	A	305	VAL
1	A	337	PHE
1	A	358	LYS
1	A	359	GLU
1	A	367	ARG
1	A	420	SER
1	A	422	GLN
1	B	90	LEU
1	B	100	THR
1	B	101	LEU
1	B	103	ILE
1	B	105	ASN
1	B	106	LYS
1	B	107	LEU
1	B	114	ARG

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Mol	Chain	Res	Type
1	B	125	ARG
1	B	126	ILE
1	B	137	SER
1	B	175	GLU
1	B	213	VAL
1	B	216	LYS
1	B	219	MET
1	B	243	LYS
1	B	250	LEU
1	B	251	GLU
1	B	257	VAL
1	B	314	GLN
1	B	320	LYS
1	B	339	SER
1	B	342	ILE
1	B	358	LYS
1	B	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	231	HIS
1	A	285	GLN
1	B	263	HIS
1	B	278	GLN
1	B	341	HIS
1	B	354	GLN
1	B	421	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	FES	B	501	1	0,4,4	-	-	-		
4	GOL	B	502[B]	-	5,5,5	0.83	0	5,5,5	1.38	1 (20%)
2	FES	A	501	1	0,4,4	-	-	-		
3	HEM	B	503	1	50,50,50	1.83	8 (16%)	67,82,82	1.62	13 (19%)
4	GOL	B	502[A]	-	5,5,5	0.45	0	5,5,5	1.13	0
3	HEM	A	502	1	50,50,50	2.12	10 (20%)	67,82,82	1.78	18 (26%)

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	FES	B	501	1	-	-	0/1/1/1
4	GOL	B	502[B]	-	-	0/4/4/4	-
2	FES	A	501	1	-	-	0/1/1/1
3	HEM	B	503	1	-	6/14/54/54	-
4	GOL	B	502[A]	-	-	2/4/4/4	-
3	HEM	A	502	1	-	6/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HEM	C3D-C2D	7.91	1.53	1.36
3	B	503	HEM	C3D-C2D	7.07	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	HEM	FE-NC	6.51	2.16	1.95
3	A	502	HEM	FE-ND	6.08	2.13	1.94
3	B	503	HEM	FE-ND	5.34	2.11	1.94
3	B	503	HEM	FE-NC	5.06	2.11	1.95
3	A	502	HEM	FE-NB	4.27	2.08	1.94
3	B	503	HEM	CAC-C3C	2.87	1.55	1.47
3	A	502	HEM	CAC-C3C	2.85	1.55	1.47
3	A	502	HEM	CAB-C3B	2.65	1.54	1.47
3	B	503	HEM	FE-NA	2.49	2.03	1.95
3	B	503	HEM	CAB-C3B	2.44	1.53	1.47
3	A	502	HEM	FE-NA	2.29	2.02	1.95
3	B	503	HEM	CMB-C2B	2.24	1.55	1.50
3	A	502	HEM	CMA-C3A	2.09	1.55	1.50
3	A	502	HEM	CMC-C2C	2.08	1.55	1.50
3	A	502	HEM	CAD-C3D	2.06	1.56	1.51
3	B	503	HEM	CMA-C3A	2.02	1.54	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	HEM	C4D-ND-C1D	6.05	112.38	105.21
3	B	503	HEM	C4D-ND-C1D	5.16	111.31	105.21
3	B	503	HEM	C3B-C4B-NB	-4.05	106.56	109.47
3	A	502	HEM	C3B-C2B-C1B	3.48	109.02	106.41
3	A	502	HEM	O2D-CGD-CBD	3.33	124.53	114.00
3	B	503	HEM	C1B-NB-C4B	3.11	108.89	105.21
3	A	502	HEM	C1B-NB-C4B	3.10	108.88	105.21
3	B	503	HEM	CHB-C1B-NB	3.08	128.18	124.37
3	A	502	HEM	CHD-C1D-ND	3.08	127.73	124.42
3	A	502	HEM	C2D-C1D-ND	-3.08	106.35	109.90
3	B	503	HEM	CBD-CAD-C3D	-2.92	104.45	112.53
3	A	502	HEM	CAD-C3D-C4D	2.88	129.72	124.70
3	A	502	HEM	CHC-C1C-NC	2.87	127.58	124.45
3	A	502	HEM	C3B-C4B-NB	-2.86	107.41	109.47
3	B	503	HEM	CHA-C4D-ND	2.77	127.79	124.37
3	A	502	HEM	C2B-C1B-NB	-2.63	106.81	109.84
3	B	503	HEM	CAA-CBA-CGA	-2.58	106.83	113.67
4	B	502[B]	GOL	O3-C3-C2	-2.48	99.20	110.38
3	B	503	HEM	CBA-CAA-C2A	-2.48	105.67	112.53
3	A	502	HEM	CAC-C3C-C4C	2.45	130.67	124.82
3	A	502	HEM	CHD-C4C-C3C	2.34	129.16	125.21
3	A	502	HEM	C3C-C2C-C1C	2.30	109.22	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	HEM	CAD-CBD-CGD	-2.27	107.65	113.67
3	A	502	HEM	CHB-C1B-NB	2.25	127.15	124.37
3	A	502	HEM	CAC-C3C-C2C	-2.21	121.23	128.43
3	B	503	HEM	C2A-C1A-NA	-2.21	107.70	110.15
3	A	502	HEM	C4D-C3D-C2D	-2.17	103.74	106.89
3	B	503	HEM	C4B-C3B-C2B	2.16	109.27	107.28
3	B	503	HEM	O1D-CGD-CBD	-2.07	116.53	123.09
3	B	503	HEM	C2B-C1B-NB	-2.05	107.48	109.84
3	A	502	HEM	O2D-CGD-O1D	-2.01	118.16	123.33
3	A	502	HEM	C4C-NC-C1C	2.00	109.09	105.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	HEM	C2B-C3B-CAB-CBB
3	A	502	HEM	C4B-C3B-CAB-CBB
3	B	503	HEM	C2B-C3B-CAB-CBB
3	B	503	HEM	C4B-C3B-CAB-CBB
4	B	502[A]	GOL	C1-C2-C3-O3
3	B	503	HEM	C4D-C3D-CAD-CBD
4	B	502[A]	GOL	O2-C2-C3-O3
3	A	502	HEM	C2A-CAA-CBA-CGA
3	B	503	HEM	C2C-C3C-CAC-CBC
3	A	502	HEM	C4C-C3C-CAC-CBC
3	B	503	HEM	C2D-C3D-CAD-CBD
3	B	503	HEM	C4C-C3C-CAC-CBC
3	A	502	HEM	CAD-CBD-CGD-O2D
3	A	502	HEM	CAD-CBD-CGD-O1D

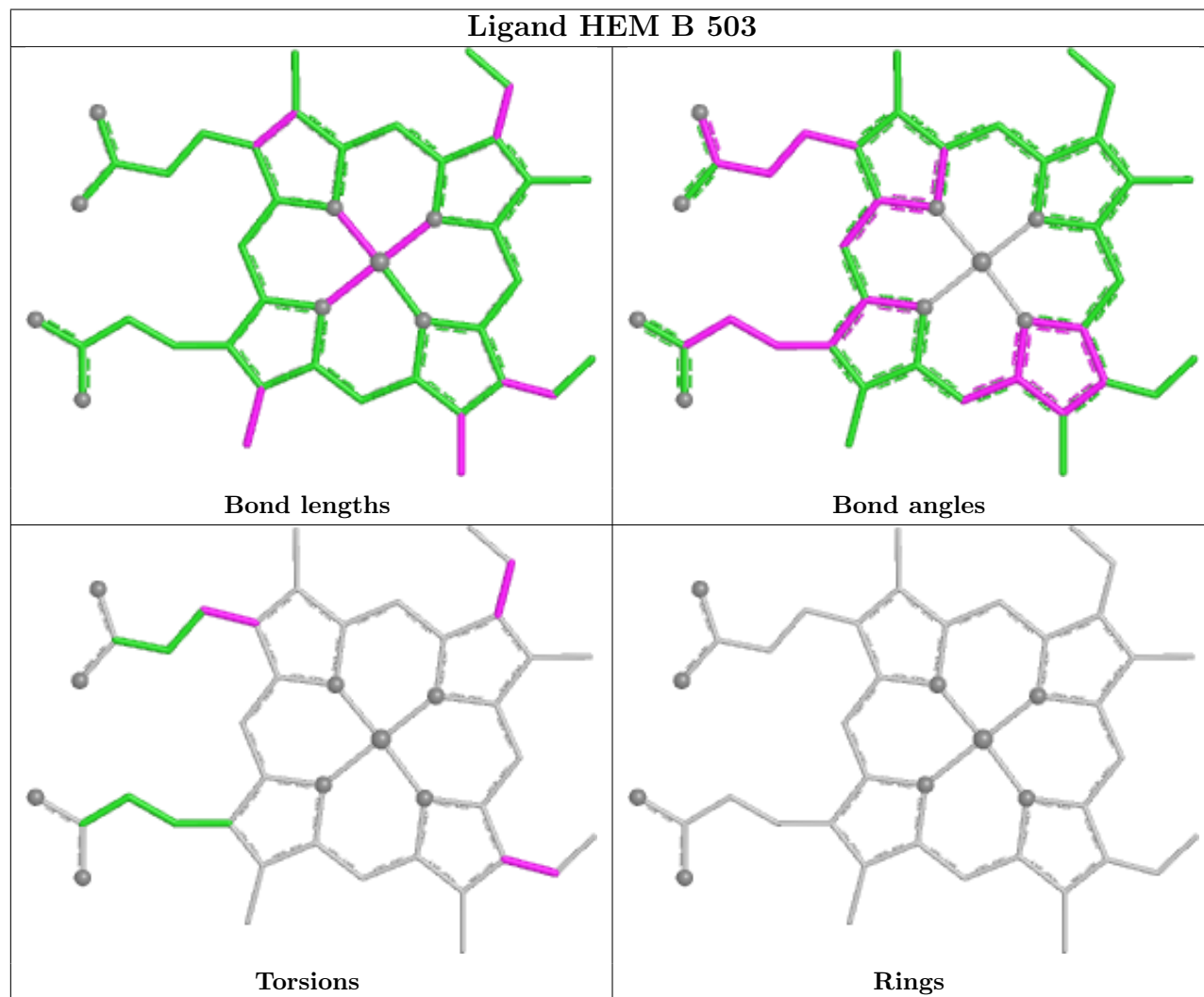
There are no ring outliers.

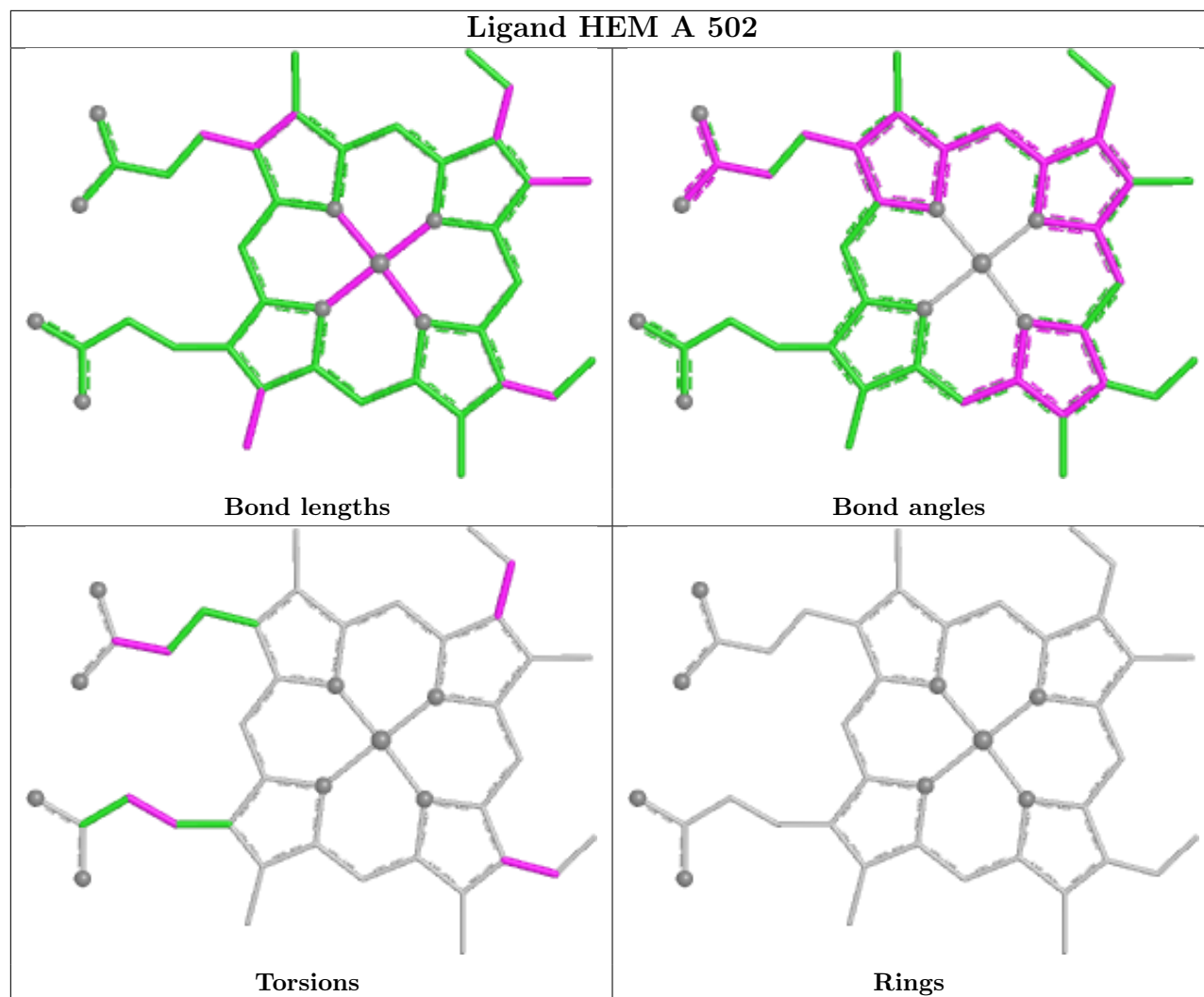
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	502[B]	GOL	1	0
3	B	503	HEM	8	0
4	B	502[A]	GOL	4	0
3	A	502	HEM	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	359/370 (97%)	0.10	19 (5%) 32 28	9, 27, 57, 74	4 (1%)
1	B	359/370 (97%)	0.10	20 (5%) 30 26	10, 29, 62, 76	4 (1%)
All	All	718/740 (97%)	0.10	39 (5%) 31 28	9, 28, 60, 76	8 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	5.0
1	B	423	LEU	4.5
1	A	101	LEU	4.4
1	A	212	GLN	4.3
1	A	91	ARG	3.6
1	B	99	MET	3.4
1	A	103	ILE	3.4
1	A	305	VAL	3.0
1	B	212	GLN	2.8
1	B	303	SER	2.8
1	B	91	ARG	2.8
1	B	110	ALA	2.7
1	B	103	ILE	2.6
1	B	350	ILE	2.6
1	A	76	MET	2.6
1	B	100	THR	2.6
1	A	307	PRO	2.4
1	B	102	PRO	2.4
1	A	341	HIS	2.4
1	A	99	MET	2.4
1	B	337	PHE	2.4
1	A	337	PHE	2.3
1	B	138	LYS	2.3
1	A	355	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	THR	2.3
1	B	101	LEU	2.3
1	B	106	LYS	2.3
1	A	65	ARG	2.2
1	A	422	GLN	2.2
1	A	98	LEU	2.2
1	A	350	ILE	2.2
1	B	353	SER	2.2
1	B	98	LEU	2.2
1	A	362	VAL	2.1
1	B	107	LEU	2.1
1	A	138	LYS	2.1
1	B	355	VAL	2.0
1	B	342	ILE	2.0
1	B	105	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

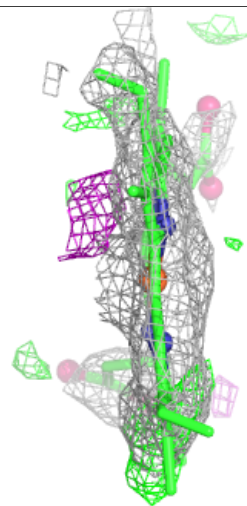
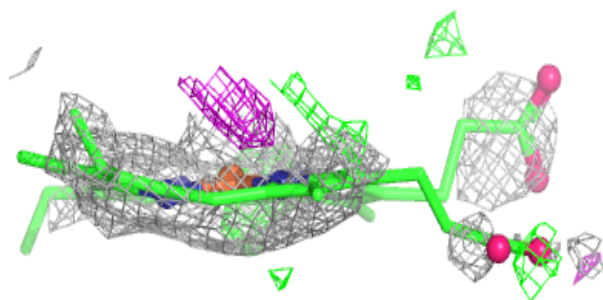
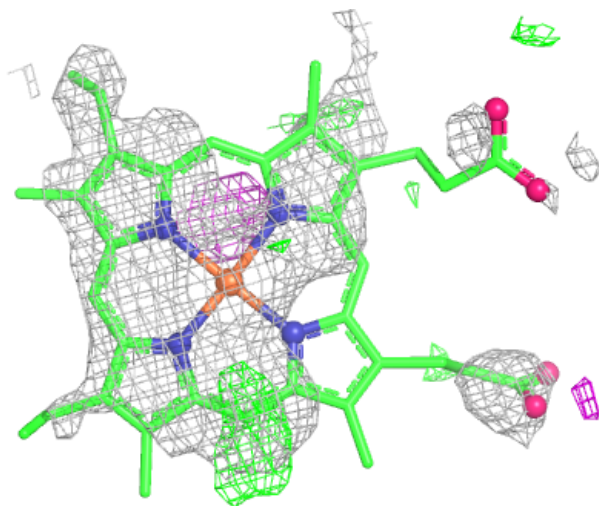
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HEM	B	503	43/43	0.82	0.31	36,42,45,46	43
3	HEM	A	502	43/43	0.83	0.25	19,33,34,35	43
4	GOL	B	502[A]	6/6	0.91	0.18	18,19,21,21	6
4	GOL	B	502[B]	6/6	0.91	0.18	18,19,20,20	6
2	FES	A	501	4/4	0.98	0.06	24,24,28,29	0
2	FES	B	501	4/4	0.98	0.05	29,30,31,32	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.

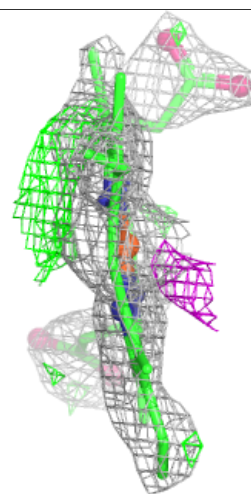
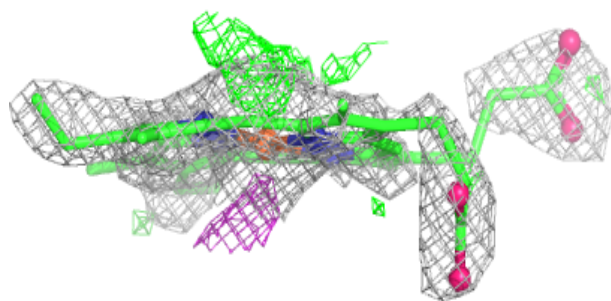
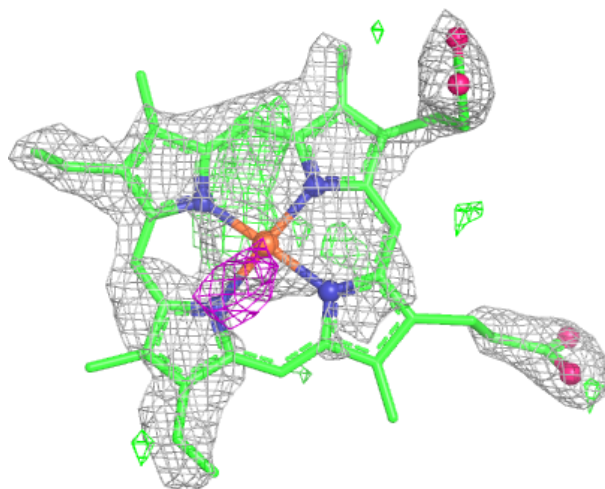
Electron density around HEM B 503:

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 502:

$2mF_o-DF_c$ (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.