



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 05:23 PM BST

PDB ID : 1MYH
Title : HIGH RESOLUTION X-RAY STRUCTURES OF PIG METMYOGLOBIN AND TWO CD3 MUTANTS MB(LYS45-> ARG) AND MB(LYS45-> SER)
Authors : Smerdon, S.J.; Oldfield, T.J.; Wilkinson, A.J.; Dauter, Z.; Petratos, K.; Wilson, K.S.
Deposited on : 1992-02-27
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

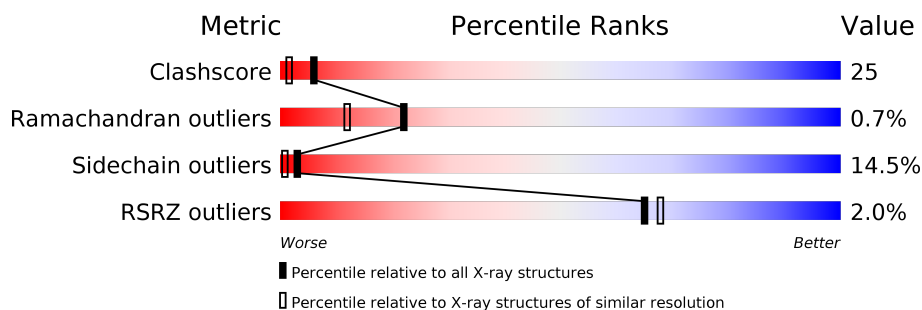
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	153	<div> <div>2%</div> <div>25%</div> <div>52%</div> <div>15%</div> <div>8%</div> </div>
1	B	153	<div> <div>2%</div> <div>26%</div> <div>48%</div> <div>19%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2590 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 MYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	13	0	0
			1199	764	210	222	3			
1	B	153	Total	C	N	O	S	0	0	0
			1199	764	210	222	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ARG	LYS	CONFLICT	UNP P02189
B	45	ARG	LYS	CONFLICT	UNP P02189

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



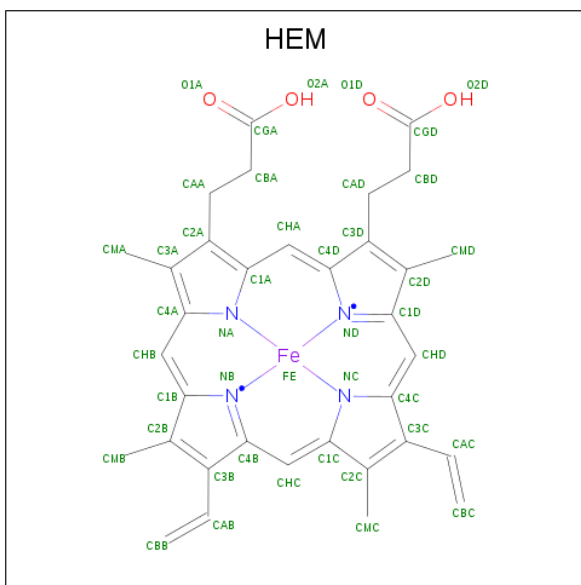
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

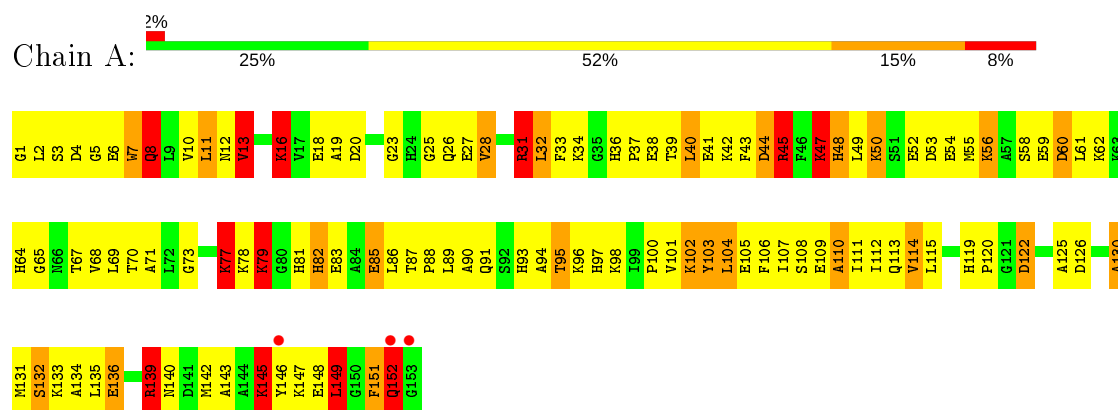
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	52	Total O 52 52	0	0
4	B	44	Total O 44 44	0	0

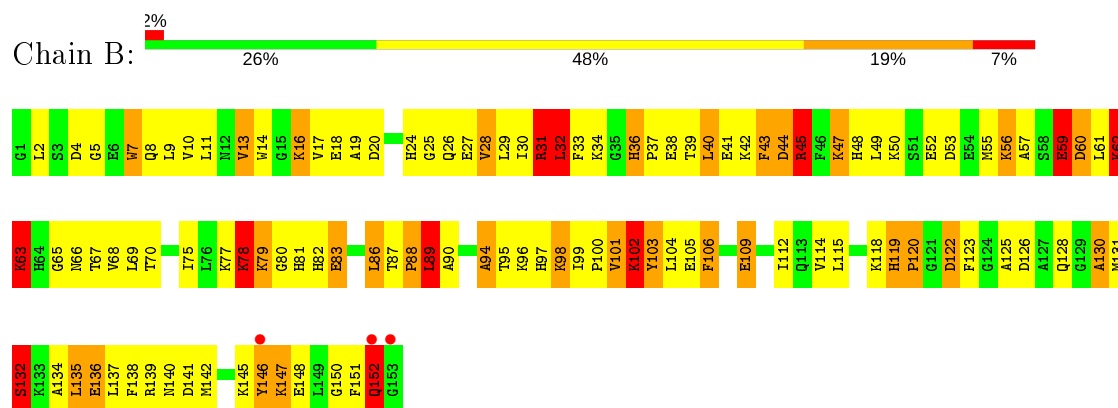
3 Residue-property plots [i](#)

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: MYOGLOBIN



• Molecule 1: MYOGLOBIN



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.70Å 42.88Å 92.83Å 90.00° 92.93° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 15.25 – 1.88	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 67.8 (15.25-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.88Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.227 , (Not available) 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 124.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.239 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2590	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 100.00 % 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 0.0000e+00.*

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, SO4

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	1.61	7/1224 (0.6%)	3.12	141/1640 (8.6%)
1	B	1.67	7/1224 (0.6%)	3.35	162/1640 (9.9%)
All	All	1.64	14/2448 (0.6%)	3.24	303/3280 (9.2%)

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	A	0	3
1	B	0	1
All	All	0	4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	LYS	CG-CD	-9.07	1.21	1.52
1	A	34	LYS	CB-CG	7.69	1.73	1.52
1	A	16	LYS	C-O	6.88	1.36	1.23
1	A	1	GLY	N-CA	6.69	1.56	1.46
1	B	27	GLU	CD-OE1	6.38	1.32	1.25
1	B	123	PHE	CE2-CZ	5.76	1.48	1.37
1	B	28	VAL	CB-CG2	5.75	1.65	1.52
1	B	59	GLU	CD-OE2	5.59	1.31	1.25
1	A	19	ALA	N-CA	5.35	1.57	1.46
1	A	131	MET	CA-CB	5.34	1.65	1.53
1	B	66	ASN	C-O	5.34	1.33	1.23
1	A	25	GLY	N-CA	5.28	1.53	1.46
1	B	70	THR	C-O	5.21	1.33	1.23
1	B	25	GLY	N-CA	5.16	1.53	1.46

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH2	-30.59	105.00	120.30
1	B	31	ARG	CD-NE-CZ	26.21	160.29	123.60
1	B	31	ARG	NE-CZ-NH1	-22.26	109.17	120.30
1	B	45	ARG	NE-CZ-NH1	-17.16	111.72	120.30
1	A	60	ASP	CB-CG-OD2	-16.77	103.20	118.30
1	B	60	ASP	CB-CG-OD2	-16.19	103.73	118.30
1	A	139	ARG	NE-CZ-NH1	16.13	128.36	120.30
1	A	126	ASP	CB-CG-OD2	-16.05	103.85	118.30
1	B	83	GLU	CB-CG-CD	15.40	155.77	114.20
1	A	31	ARG	NE-CZ-NH1	-14.85	112.88	120.30
1	A	44	ASP	CB-CG-OD2	-14.62	105.14	118.30
1	B	44	ASP	CB-CG-OD2	-14.53	105.23	118.30
1	A	126	ASP	CB-CG-OD1	13.99	130.89	118.30
1	A	122	ASP	CB-CG-OD2	-13.00	106.60	118.30
1	B	68	VAL	CA-CB-CG1	12.93	130.30	110.90
1	A	83	GLU	OE1-CD-OE2	-12.49	108.31	123.30
1	B	140	ASN	CB-CA-C	12.40	135.21	110.40
1	A	83	GLU	CB-CG-CD	12.07	146.79	114.20
1	B	103	TYR	O-C-N	12.04	141.97	122.70
1	B	89	LEU	CA-CB-CG	11.87	142.60	115.30
1	B	59	GLU	CA-CB-CG	11.83	139.43	113.40
1	B	125	ALA	CB-CA-C	11.81	127.82	110.10
1	B	131	MET	CG-SD-CE	11.49	118.58	100.20
1	B	139	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	44	ASP	CB-CG-OD1	11.08	128.28	118.30
1	B	44	ASP	CB-CG-OD1	10.89	128.10	118.30
1	B	139	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	B	109	GLU	OE1-CD-OE2	10.57	135.99	123.30
1	B	105	GLU	OE1-CD-OE2	10.54	135.94	123.30
1	A	136	GLU	N-CA-CB	10.47	129.45	110.60
1	B	103	TYR	CD1-CE1-CZ	-10.41	110.43	119.80
1	A	43	PHE	CB-CG-CD2	-10.26	113.62	120.80
1	A	136	GLU	OE1-CD-OE2	10.16	135.49	123.30
1	B	45	ARG	NH1-CZ-NH2	10.11	130.52	119.40
1	A	43	PHE	CZ-CE2-CD2	-10.09	107.99	120.10
1	A	33	PHE	CB-CG-CD1	-10.00	113.80	120.80
1	B	33	PHE	CB-CG-CD2	9.99	127.79	120.80
1	B	148	GLU	OE1-CD-OE2	9.80	135.06	123.30
1	A	43	PHE	CG-CD1-CE1	-9.69	110.14	120.80
1	B	83	GLU	CA-CB-CG	9.67	134.67	113.40
1	B	132	SER	N-CA-CB	-9.63	96.05	110.50
1	A	54	GLU	CG-CD-OE2	9.58	137.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CB-CG-CD1	-9.32	95.15	111.00
1	A	131	MET	CA-CB-CG	-9.31	97.47	113.30
1	A	20	ASP	CB-CG-OD1	-9.26	109.96	118.30
1	A	90	ALA	O-C-N	9.19	137.40	122.70
1	B	50	LYS	O-C-N	9.18	137.38	122.70
1	A	54	GLU	OE1-CD-OE2	-9.11	112.37	123.30
1	B	122	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	B	5	GLY	O-C-N	9.03	137.14	122.70
1	A	113	GLN	CG-CD-OE1	9.01	139.61	121.60
1	B	103	TYR	CG-CD2-CE2	-8.94	114.15	121.30
1	B	69	LEU	CA-C-N	8.91	136.80	117.20
1	B	94	ALA	O-C-N	8.90	136.94	122.70
1	B	38	GLU	OE1-CD-OE2	-8.89	112.63	123.30
1	B	28	VAL	O-C-N	8.88	136.92	122.70
1	B	132	SER	CB-CA-C	8.87	126.95	110.10
1	B	80	GLY	C-N-CA	8.81	143.73	121.70
1	B	20	ASP	CB-CG-OD2	-8.75	110.43	118.30
1	A	83	GLU	CG-CD-OE1	8.73	135.76	118.30
1	B	19	ALA	N-CA-CB	8.67	122.23	110.10
1	B	11	LEU	CB-CG-CD2	8.63	125.67	111.00
1	B	83	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	B	140	ASN	OD1-CG-ND2	8.54	141.55	121.90
1	A	4	ASP	CB-CG-OD1	-8.53	110.62	118.30
1	B	102	LYS	N-CA-CB	8.51	125.92	110.60
1	A	82	HIS	CG-ND1-CE1	8.42	119.99	108.20
1	A	85	GLU	CG-CD-OE1	8.42	135.14	118.30
1	A	31	ARG	NH1-CZ-NH2	8.40	128.64	119.40
1	B	109	GLU	CG-CD-OE1	-8.37	101.56	118.30
1	A	53	ASP	CB-CG-OD1	-8.31	110.82	118.30
1	B	132	SER	O-C-N	-8.30	109.42	122.70
1	A	152	GLN	CA-CB-CG	8.22	131.48	113.40
1	A	122	ASP	CB-CG-OD1	8.21	125.69	118.30
1	B	136	GLU	O-C-N	-8.21	109.56	122.70
1	B	141	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	B	123	PHE	CB-CG-CD2	-8.09	115.14	120.80
1	B	122	ASP	OD1-CG-OD2	8.07	138.64	123.30
1	B	59	GLU	N-CA-CB	8.06	125.11	110.60
1	B	101	VAL	CB-CA-C	8.06	126.71	111.40
1	B	11	LEU	CA-CB-CG	8.00	133.70	115.30
1	B	9	LEU	O-C-N	7.93	135.39	122.70
1	B	122	ASP	CB-CG-OD1	-7.93	111.16	118.30
1	B	103	TYR	CG-CD1-CE1	7.87	127.60	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	VAL	CG1-CB-CG2	7.84	123.44	110.90
1	B	31	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	B	137	LEU	CB-CG-CD1	-7.76	97.80	111.00
1	B	70	THR	CA-CB-CG2	7.64	123.10	112.40
1	B	33	PHE	CZ-CE2-CD2	7.64	129.26	120.10
1	B	96	LYS	CB-CG-CD	-7.62	91.79	111.60
1	A	135	LEU	O-C-N	7.58	134.82	122.70
1	B	60	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	27	GLU	OE1-CD-OE2	-7.55	114.24	123.30
1	A	125	ALA	CB-CA-C	7.54	121.41	110.10
1	B	27	GLU	CG-CD-OE2	7.47	133.24	118.30
1	B	89	LEU	CB-CG-CD1	7.46	123.68	111.00
1	A	94	ALA	N-CA-CB	7.43	120.50	110.10
1	A	18	GLU	OE1-CD-OE2	7.42	132.21	123.30
1	A	19	ALA	CB-CA-C	7.39	121.19	110.10
1	B	9	LEU	CB-CG-CD1	7.34	123.48	111.00
1	A	82	HIS	ND1-CG-CD2	-7.32	95.75	106.00
1	A	11	LEU	O-C-N	7.31	134.40	122.70
1	A	5	GLY	O-C-N	7.31	134.39	122.70
1	B	136	GLU	OE1-CD-OE2	7.31	132.07	123.30
1	B	45	ARG	N-CA-CB	-7.30	97.46	110.60
1	B	4	ASP	O-C-N	7.29	135.60	123.20
1	B	140	ASN	CB-CG-OD1	-7.25	107.10	121.60
1	A	133	LYS	CB-CG-CD	-7.24	92.76	111.60
1	A	31	ARG	CD-NE-CZ	7.23	133.73	123.60
1	A	31	ARG	CA-CB-CG	-7.13	97.72	113.40
1	B	68	VAL	CG1-CB-CG2	-7.11	99.52	110.90
1	B	44	ASP	CA-CB-CG	-7.07	97.85	113.40
1	A	148	GLU	CB-CA-C	-7.01	96.38	110.40
1	A	151	PHE	C-N-CA	7.00	139.20	121.70
1	B	14	TRP	CG-CD2-CE3	-7.00	127.60	133.90
1	A	132	SER	N-CA-CB	-6.97	100.04	110.50
1	B	94	ALA	N-CA-CB	6.94	119.82	110.10
1	A	59	GLU	N-CA-CB	6.93	123.08	110.60
1	B	33	PHE	O-C-N	6.92	133.78	122.70
1	B	66	ASN	CA-C-N	6.88	132.34	117.20
1	A	28	VAL	CG1-CB-CG2	6.81	121.80	110.90
1	A	133	LYS	CD-CE-NZ	-6.81	96.04	111.70
1	B	50	LYS	CD-CE-NZ	6.81	127.36	111.70
1	A	114	VAL	CG1-CB-CG2	6.78	121.75	110.90
1	A	34	LYS	CB-CA-C	6.76	123.93	110.40
1	A	115	LEU	N-CA-CB	-6.74	96.92	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	SER	CA-CB-OG	-6.74	93.01	111.20
1	B	40	LEU	CB-CG-CD2	-6.72	99.57	111.00
1	B	139	ARG	CG-CD-NE	6.72	125.92	111.80
1	B	123	PHE	O-C-N	6.69	134.58	123.20
1	A	60	ASP	OD1-CG-OD2	6.69	136.02	123.30
1	B	32	LEU	CD1-CG-CD2	6.68	130.55	110.50
1	B	130	ALA	N-CA-CB	6.67	119.43	110.10
1	A	6	GLU	CA-C-O	-6.66	106.12	120.10
1	B	57	ALA	N-CA-CB	-6.65	100.79	110.10
1	A	70	THR	O-C-N	-6.64	112.07	122.70
1	A	82	HIS	CA-CB-CG	6.64	124.88	113.60
1	B	63	LYS	CA-C-N	6.62	131.77	117.20
1	A	69	LEU	CA-C-O	-6.61	106.22	120.10
1	A	61	LEU	O-C-N	-6.60	112.14	122.70
1	A	136	GLU	CB-CA-C	-6.60	97.20	110.40
1	B	134	ALA	N-CA-CB	6.60	119.34	110.10
1	B	63	LYS	O-C-N	-6.58	112.17	122.70
1	B	135	LEU	O-C-N	6.58	133.23	122.70
1	B	29	LEU	CB-CA-C	6.57	122.68	110.20
1	B	31	ARG	NH1-CZ-NH2	6.56	126.62	119.40
1	B	67	THR	O-C-N	6.55	133.19	122.70
1	A	13	VAL	N-CA-CB	6.55	125.91	111.50
1	B	66	ASN	O-C-N	-6.54	112.23	122.70
1	B	7	TRP	O-C-N	-6.54	112.24	122.70
1	B	119	HIS	O-C-N	6.53	133.51	121.10
1	A	139	ARG	NH1-CZ-NH2	6.53	126.58	119.40
1	A	45	ARG	CA-C-O	-6.52	106.41	120.10
1	A	45	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	71	ALA	CA-C-N	6.50	131.50	117.20
1	B	18	GLU	O-C-N	6.49	133.08	122.70
1	A	109	GLU	N-CA-CB	6.48	122.26	110.60
1	A	115	LEU	CB-CG-CD2	6.46	121.98	111.00
1	A	106	PHE	CB-CG-CD2	-6.45	116.28	120.80
1	B	125	ALA	CA-C-O	6.43	133.60	120.10
1	B	65	GLY	O-C-N	-6.42	112.43	122.70
1	A	68	VAL	CA-CB-CG1	6.42	120.52	110.90
1	B	13	VAL	CB-CA-C	-6.38	99.27	111.40
1	A	112	ILE	CB-CG1-CD1	-6.38	96.05	113.90
1	A	32	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	B	69	LEU	O-C-N	-6.37	112.51	122.70
1	B	70	THR	O-C-N	-6.36	112.53	122.70
1	B	14	TRP	CE2-CD2-CE3	6.32	126.28	118.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	CG-CD-NE	-6.29	98.59	111.80
1	A	151	PHE	N-CA-CB	-6.29	99.27	110.60
1	A	8	GLN	CG-CD-NE2	6.29	131.79	116.70
1	B	56	LYS	CB-CG-CD	6.27	127.90	111.60
1	A	44	ASP	CA-C-N	-6.25	103.45	117.20
1	A	65	GLY	O-C-N	-6.25	112.71	122.70
1	B	83	GLU	O-C-N	-6.23	112.73	122.70
1	A	81	HIS	C-N-CA	6.22	137.25	121.70
1	B	125	ALA	O-C-N	-6.19	112.80	122.70
1	B	33	PHE	CG-CD1-CE1	6.17	127.58	120.80
1	A	93	HIS	CG-CD2-NE2	-6.12	97.56	109.20
1	A	2	LEU	N-CA-CB	6.09	122.57	110.40
1	B	136	GLU	CA-CB-CG	-6.09	100.01	113.40
1	A	6	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	B	63	LYS	C-N-CA	6.06	136.86	121.70
1	B	79	LYS	CA-CB-CG	6.06	126.73	113.40
1	A	70	THR	CA-CB-CG2	6.04	120.86	112.40
1	A	103	TYR	CD1-CE1-CZ	-6.03	114.37	119.80
1	B	41	GLU	CG-CD-OE1	6.02	130.34	118.30
1	A	42	LYS	CA-C-O	-6.01	107.47	120.10
1	A	134	ALA	O-C-N	-5.99	113.11	122.70
1	A	55	MET	N-CA-CB	5.99	121.38	110.60
1	A	33	PHE	O-C-N	5.93	132.19	122.70
1	B	109	GLU	O-C-N	-5.92	113.22	122.70
1	B	81	HIS	C-N-CA	5.92	136.50	121.70
1	A	104	LEU	O-C-N	5.91	132.16	122.70
1	A	89	LEU	O-C-N	5.90	132.14	122.70
1	B	146	TYR	C-N-CA	5.89	136.44	121.70
1	B	90	ALA	CB-CA-C	5.89	118.93	110.10
1	A	62	LYS	CG-CD-CE	-5.88	94.25	111.90
1	A	110	ALA	N-CA-CB	-5.87	101.88	110.10
1	A	70	THR	CA-C-O	5.87	132.42	120.10
1	B	24	HIS	O-C-N	5.86	133.16	123.20
1	B	31	ARG	CG-CD-NE	5.83	124.05	111.80
1	A	61	LEU	CB-CG-CD2	5.81	120.87	111.00
1	A	6	GLU	CG-CD-OE1	-5.80	106.69	118.30
1	B	66	ASN	C-N-CA	5.79	136.16	121.70
1	B	141	ASP	N-CA-CB	5.78	121.01	110.60
1	A	8	GLN	OE1-CD-NE2	-5.78	108.60	121.90
1	B	36	HIS	CA-CB-CG	-5.77	103.78	113.60
1	B	14	TRP	CB-CG-CD1	5.76	134.49	127.00
1	A	125	ALA	O-C-N	-5.75	113.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	GLU	CB-CA-C	-5.74	98.92	110.40
1	A	42	LYS	O-C-N	5.74	131.88	122.70
1	A	136	GLU	CB-CG-CD	-5.73	98.73	114.20
1	B	38	GLU	CA-CB-CG	5.72	125.99	113.40
1	B	115	LEU	CB-CG-CD2	5.72	120.73	111.00
1	B	56	LYS	CD-CE-NZ	5.71	124.83	111.70
1	B	5	GLY	CA-C-O	-5.66	110.41	120.60
1	A	68	VAL	O-C-N	-5.65	113.66	122.70
1	A	149	LEU	CA-C-O	5.65	131.97	120.10
1	B	62	LYS	CD-CE-NZ	-5.65	98.70	111.70
1	A	56	LYS	CA-CB-CG	5.65	125.83	113.40
1	A	40	LEU	CB-CA-C	5.64	120.92	110.20
1	B	61	LEU	CB-CG-CD1	5.60	120.53	111.00
1	A	142	MET	O-C-N	5.59	131.65	122.70
1	B	14	TRP	CD2-CE3-CZ3	-5.59	111.54	118.80
1	A	98	LYS	CG-CD-CE	5.56	128.58	111.90
1	B	106	PHE	CB-CG-CD1	-5.56	116.91	120.80
1	A	7	TRP	CB-CG-CD2	5.56	133.82	126.60
1	A	103	TYR	CG-CD1-CE1	5.55	125.74	121.30
1	B	122	ASP	CA-CB-CG	-5.54	101.22	113.40
1	B	9	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	B	78	LYS	CB-CA-C	-5.50	99.39	110.40
1	A	120	PRO	O-C-N	-5.50	113.85	123.20
1	A	98	LYS	CA-CB-CG	-5.50	101.30	113.40
1	A	71	ALA	CA-C-O	-5.49	108.58	120.10
1	B	130	ALA	O-C-N	5.48	131.47	122.70
1	B	41	GLU	CG-CD-OE2	-5.48	107.35	118.30
1	B	103	TYR	CA-C-O	-5.47	108.61	120.10
1	A	147	LYS	CA-CB-CG	5.47	125.42	113.40
1	B	33	PHE	CB-CG-CD1	-5.47	116.97	120.80
1	A	149	LEU	N-CA-CB	-5.46	99.48	110.40
1	B	17	VAL	CG1-CB-CG2	5.44	119.61	110.90
1	B	101	VAL	CA-CB-CG1	5.43	119.05	110.90
1	A	85	GLU	CG-CD-OE2	-5.39	107.51	118.30
1	A	1	GLY	N-CA-C	-5.39	99.62	113.10
1	B	120	PRO	N-CA-CB	5.38	109.76	103.30
1	B	104	LEU	O-C-N	5.38	131.30	122.70
1	B	88	PRO	O-C-N	5.37	131.30	122.70
1	A	2	LEU	N-CA-C	-5.37	96.51	111.00
1	B	19	ALA	CA-C-O	-5.35	108.86	120.10
1	A	20	ASP	O-C-N	5.34	131.24	122.70
1	A	130	ALA	N-CA-CB	5.33	117.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	146	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
1	A	28	VAL	CA-CB-CG1	5.33	118.89	110.90
1	B	146	TYR	CE1-CZ-CE2	5.32	128.31	119.80
1	A	93	HIS	CE1-NE2-CD2	5.32	119.90	106.60
1	A	3	SER	O-C-N	-5.32	114.19	122.70
1	A	13	VAL	CB-CA-C	-5.32	101.30	111.40
1	B	138	PHE	CB-CG-CD2	-5.31	117.08	120.80
1	B	146	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
1	A	103	TYR	O-C-N	5.30	131.18	122.70
1	B	77	LYS	CA-C-N	5.30	128.86	117.20
1	A	126	ASP	N-CA-CB	-5.28	101.10	110.60
1	A	43	PHE	CG-CD2-CE2	5.28	126.60	120.80
1	B	135	LEU	CA-CB-CG	-5.27	103.17	115.30
1	A	114	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	B	136	GLU	CB-CG-CD	-5.26	99.99	114.20
1	A	2	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	B	80	GLY	O-C-N	-5.26	114.28	122.70
1	A	6	GLU	N-CA-CB	5.24	120.03	110.60
1	B	7	TRP	CH2-CZ2-CE2	-5.23	112.17	117.40
1	B	152	GLN	CA-C-N	-5.22	105.75	116.20
1	A	7	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	A	48	HIS	O-C-N	-5.21	114.36	122.70
1	A	77	LYS	N-CA-CB	5.21	119.98	110.60
1	A	28	VAL	C-N-CA	-5.20	108.69	121.70
1	A	40	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	45	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	145	LYS	CA-C-O	5.19	131.00	120.10
1	A	45	ARG	CA-CB-CG	5.18	124.80	113.40
1	B	142	MET	CA-CB-CG	5.18	122.10	113.30
1	B	43	PHE	CG-CD1-CE1	-5.17	115.11	120.80
1	A	28	VAL	CA-C-O	-5.16	109.26	120.10
1	A	43	PHE	CD1-CG-CD2	5.15	125.00	118.30
1	A	67	THR	CA-C-N	5.14	128.52	117.20
1	B	148	GLU	N-CA-CB	-5.14	101.34	110.60
1	B	126	ASP	O-C-N	5.14	130.93	122.70
1	B	40	LEU	O-C-N	5.14	130.92	122.70
1	A	78	LYS	CG-CD-CE	5.13	127.28	111.90
1	B	32	LEU	O-C-N	5.12	130.89	122.70
1	B	104	LEU	CA-C-O	-5.11	109.38	120.10
1	A	77	LYS	CB-CA-C	-5.10	100.19	110.40
1	A	152	GLN	CB-CG-CD	5.09	124.84	111.60
1	A	47	LYS	C-N-CA	5.07	134.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	GLY	O-C-N	5.07	130.81	122.70
1	A	11	LEU	CA-C-O	-5.05	109.49	120.10
1	A	135	LEU	CB-CG-CD2	5.05	119.59	111.00
1	A	79	LYS	CB-CG-CD	-5.04	98.48	111.60
1	B	63	LYS	CD-CE-NZ	-5.04	100.11	111.70
1	B	103	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	B	86	LEU	C-N-CA	-5.02	109.14	121.70
1	B	150	GLY	CA-C-O	-5.02	111.56	120.60
1	B	57	ALA	CB-CA-C	5.01	117.61	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	31	ARG	Sidechain
1	A	45	ARG	Sidechain
1	B	45	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1199	0	1205	51	1
1	B	1199	0	1201	69	1
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	43	0	30	2	0
3	B	43	0	30	4	0
4	A	52	0	0	5	0
4	B	44	0	0	3	0
All	All	2590	0	2466	122	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 25.

All (122) 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:102:LYS:HE3	1:A:103:TYR:CE1	1.88	1.09
1:A:102:LYS:HE3	1:A:103:TYR:HE1	1.10	1.08
1:B:152:GLN:NE2	1:B:152:GLN:O	2.01	0.93
1:A:88:PRO:HA	1:A:91:GLN:HE21	1.33	0.93
1:B:147:LYS:HG2	4:B:197:HOH:O	1.74	0.88
1:B:94:ALA:O	1:B:98:LYS:HD3	1.77	0.84
1:B:13:VAL:O	1:B:16:LYS:HB2	1.78	0.83
1:A:87:THR:HB	1:A:88:PRO:HD3	1.64	0.78
1:A:95:THR:HG22	1:A:151:PHE:CE2	2.20	0.77
1:A:102:LYS:CE	1:A:103:TYR:HE1	1.95	0.77
1:A:79:LYS:NZ	4:A:156:HOH:O	2.16	0.77
1:A:95:THR:HG22	1:A:151:PHE:HE2	1.49	0.77
1:B:136:GLU:HG3	1:B:136:GLU:O	1.84	0.75
1:B:30:ILE:HG22	1:B:34:LYS:NZ	2.04	0.72
1:B:95:THR:O	1:B:98:LYS:HE3	1.90	0.71
1:A:87:THR:N	1:A:88:PRO:HD2	2.05	0.70
1:B:95:THR:C	1:B:98:LYS:HE3	2.13	0.69
1:B:63:LYS:HE2	2:B:154:SO4:O4	1.92	0.69
1:A:102:LYS:CE	1:A:103:TYR:CE1	2.74	0.67
1:B:7:TRP:HB3	1:B:79:LYS:HZ3	1.59	0.66
1:A:143:ALA:O	1:A:146:TYR:HB2	1.97	0.65
1:A:88:PRO:HA	1:A:91:GLN:NE2	2.09	0.64
1:A:13:VAL:O	1:A:16:LYS:HB2	1.98	0.64
1:A:37:PRO:O	1:A:40:LEU:HB3	1.98	0.63
1:B:86:LEU:HD23	1:B:145:LYS:HD3	1.81	0.63
1:B:128:GLN:O	1:B:132:SER:HB3	1.98	0.63
1:A:107:ILE:O	1:A:111:ILE:HG13	1.99	0.63
1:B:94:ALA:HB2	1:B:146:TYR:CD1	2.34	0.63
1:A:82:HIS:HA	1:A:85:GLU:OE1	2.00	0.61
1:A:96:LYS:HD2	1:A:97:HIS:CE1	2.35	0.61
1:A:23:GLY:O	1:A:27:GLU:HG3	2.01	0.61
1:B:8:GLN:HE22	1:B:79:LYS:NZ	1.99	0.60
1:B:87:THR:OG1	1:B:145:LYS:HE3	2.02	0.60
1:B:52:GLU:O	1:B:56:LYS:HG3	2.01	0.59
1:A:108:SER:CB	1:A:139:ARG:NH1	2.65	0.59
1:A:100:PRO:HA	1:A:152:GLN:NE2	2.20	0.57
1:B:44:ASP:OD1	1:B:47:LYS:HE3	2.04	0.57
1:B:102:LYS:HD2	1:B:106:PHE:CE2	2.40	0.56
3:A:155:HEM:HMC2	3:A:155:HEM:HBC2	1.86	0.56
1:B:30:ILE:HG22	1:B:34:LYS:HZ3	1.70	0.56
1:A:87:THR:N	1:A:88:PRO:CD	2.68	0.56
1:B:7:TRP:CB	1:B:79:LYS:HZ3	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HG3	4:A:170:HOH:O	2.06	0.55
1:A:10:VAL:HG23	1:A:130:ALA:HB1	1.87	0.55
1:B:95:THR:O	1:B:98:LYS:CE	2.54	0.55
1:B:87:THR:OG1	1:B:145:LYS:CE	2.55	0.54
1:B:89:LEU:HD21	3:B:155:HEM:CHB	2.38	0.54
1:A:73:GLY:O	1:A:77:LYS:HD2	2.07	0.54
1:A:36:HIS:N	1:A:37:PRO:HD3	2.22	0.53
1:A:149:LEU:HD23	1:A:151:PHE:CD2	2.44	0.53
1:A:100:PRO:HA	1:A:152:GLN:HE22	1.74	0.52
1:A:52:GLU:O	1:A:56:LYS:N	2.30	0.52
3:B:155:HEM:HBC2	3:B:155:HEM:HMC1	1.90	0.52
1:B:94:ALA:HB1	1:B:151:PHE:CD2	2.43	0.52
1:A:11:LEU:HD12	1:A:79:LYS:NZ	2.25	0.52
1:A:110:ALA:O	1:A:114:VAL:HG23	2.09	0.52
1:B:10:VAL:HG23	1:B:130:ALA:HB1	1.92	0.51
1:B:89:LEU:HD11	3:B:155:HEM:C2B	2.45	0.51
1:A:64:HIS:NE2	4:A:184:HOH:O	2.33	0.51
1:B:87:THR:N	1:B:88:PRO:HD2	2.24	0.51
1:A:8:GLN:OE1	1:A:8:GLN:HA	2.07	0.50
1:B:101:VAL:HG23	1:B:146:TYR:CE2	2.46	0.50
1:B:78:LYS:HB2	1:B:82:HIS:HB3	1.92	0.50
1:B:2:LEU:N	1:B:2:LEU:HD12	2.26	0.50
1:A:48:HIS:NE2	1:A:49:LEU:HD21	2.27	0.50
1:B:101:VAL:CG2	1:B:146:TYR:CE2	2.95	0.50
1:A:101:VAL:O	1:A:104:LEU:N	2.42	0.49
1:B:119:HIS:N	1:B:120:PRO:HD3	2.27	0.49
1:B:94:ALA:HB1	1:B:151:PHE:CG	2.48	0.49
1:A:8:GLN:NE2	1:A:12:ASN:OD1	2.46	0.49
1:A:102:LYS:O	1:A:105:GLU:HB3	2.12	0.49
1:B:8:GLN:NE2	1:B:79:LYS:NZ	2.61	0.49
1:A:108:SER:HA	4:A:203:HOH:O	2.13	0.48
1:B:94:ALA:O	1:B:98:LYS:CD	2.57	0.48
1:B:101:VAL:CG2	1:B:146:TYR:CD2	2.96	0.48
1:B:78:LYS:N	1:B:78:LYS:HD2	2.28	0.47
1:B:26:GLN:HG3	4:B:156:HOH:O	2.13	0.47
1:B:8:GLN:HE22	1:B:79:LYS:HZ1	1.62	0.47
1:A:41:GLU:HA	1:A:47:LYS:NZ	2.30	0.47
1:B:30:ILE:HG22	1:B:34:LYS:HZ2	1.79	0.47
1:B:118:LYS:NZ	4:B:184:HOH:O	2.47	0.46
1:A:145:LYS:O	1:A:149:LEU:HB2	2.16	0.46
1:B:37:PRO:O	1:B:40:LEU:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:HIS:NE2	1:B:49:LEU:HD21	2.30	0.46
1:A:7:TRP:CD2	1:A:79:LYS:HB3	2.50	0.46
1:B:94:ALA:CB	1:B:151:PHE:CD2	2.98	0.46
1:B:98:LYS:HB2	1:B:98:LYS:NZ	2.31	0.45
1:B:99:ILE:HD12	3:B:155:HEM:CAC	2.47	0.45
1:B:32:LEU:C	1:B:32:LEU:HD22	2.37	0.45
1:A:32:LEU:HD11	1:A:39:THR:HG21	1.97	0.45
1:A:149:LEU:HD23	1:A:151:PHE:HD2	1.82	0.45
1:A:16:LYS:HA	1:A:16:LYS:HD2	1.29	0.45
1:B:8:GLN:NE2	1:B:79:LYS:HZ1	2.15	0.45
1:B:30:ILE:HG12	1:B:55:MET:HB3	1.98	0.44
1:B:48:HIS:CD2	1:B:49:LEU:CD2	3.01	0.44
1:B:86:LEU:CD2	1:B:145:LYS:HD3	2.44	0.44
1:B:94:ALA:HB1	1:B:151:PHE:CB	2.48	0.43
1:B:45:ARG:O	1:B:48:HIS:CE1	2.71	0.43
1:B:87:THR:N	1:B:88:PRO:CD	2.80	0.43
1:B:43:PHE:O	1:B:47:LYS:HG2	2.19	0.43
1:B:28:VAL:O	1:B:31:ARG:HB2	2.19	0.43
1:A:45:ARG:HH11	3:A:155:HEM:CGD	2.32	0.43
1:B:101:VAL:HG23	1:B:146:TYR:CD2	2.54	0.43
1:B:97:HIS:HB3	1:B:99:ILE:HD11	2.01	0.43
1:A:108:SER:CB	1:A:139:ARG:HH11	2.30	0.42
1:B:119:HIS:HB3	1:B:122:ASP:HB2	2.00	0.42
1:B:62:LYS:HG3	1:B:62:LYS:HZ3	1.59	0.42
1:B:75:ILE:HD13	1:B:75:ILE:HG21	1.78	0.42
1:B:94:ALA:HB2	1:B:146:TYR:CE1	2.54	0.42
1:B:36:HIS:CB	1:B:39:THR:HG23	2.49	0.42
1:A:26:GLN:HG3	4:A:165:HOH:O	2.18	0.42
1:A:132:SER:O	1:A:136:GLU:HG3	2.20	0.42
1:B:112:ILE:HD11	1:B:135:LEU:HD12	2.02	0.41
1:B:7:TRP:HB3	1:B:79:LYS:NZ	2.30	0.41
1:A:44:ASP:O	1:A:47:LYS:HG2	2.20	0.41
1:A:41:GLU:HA	1:A:47:LYS:HZ2	1.86	0.41
1:B:8:GLN:OE1	1:B:79:LYS:NZ	2.46	0.41
1:B:2:LEU:HB2	1:B:7:TRP:NE1	2.35	0.41
1:A:140:ASN:O	1:A:143:ALA:HB3	2.21	0.40
1:A:119:HIS:HB3	1:A:122:ASP:HB2	2.03	0.40
1:B:16:LYS:HA	1:B:16:LYS:HD2	1.28	0.40
1:B:100:PRO:HG2	1:B:103:TYR:CG	2.57	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:A:50:LYS:NZ	1:B:59:GLU:OE2[1_546]	1.48	0.72

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	151/153 (99%)	145 (96%)	5 (3%)	1 (1%)	22	12
1	B	151/153 (99%)	143 (95%)	7 (5%)	1 (1%)	22	12
All	All	302/306 (99%)	288 (95%)	12 (4%)	2 (1%)	22	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	152	GLN

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	124/124 (100%)	107 (86%)	17 (14%)	3	1
1	B	124/124 (100%)	105 (85%)	19 (15%)	2	1
All	All	248/248 (100%)	212 (86%)	36 (14%)	3	1

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	13	VAL
1	A	16	LYS
1	A	28	VAL
1	A	31	ARG
1	A	38	GLU
1	A	47	LYS
1	A	50	LYS
1	A	60	ASP
1	A	77	LYS
1	A	79	LYS
1	A	86	LEU
1	A	95	THR
1	A	102	LYS
1	A	145	LYS
1	A	149	LEU
1	A	152	GLN
1	B	16	LYS
1	B	31	ARG
1	B	32	LEU
1	B	42	LYS
1	B	47	LYS
1	B	53	ASP
1	B	59	GLU
1	B	60	ASP
1	B	62	LYS
1	B	63	LYS
1	B	78	LYS
1	B	83	GLU
1	B	89	LEU
1	B	98	LYS
1	B	102	LYS
1	B	109	GLU
1	B	132	SER
1	B	147	LYS
1	B	152	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	91	GLN
1	A	113	GLN

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Mol	Chain	Res	Type
1	A	140	ASN
1	B	48	HIS
1	B	116	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	SO4	B	154	-	4,4,4	0.79	0	6,6,6	1.74	1 (16%)
2	SO4	A	154	-	4,4,4	1.19	0	6,6,6	1.14	1 (16%)
3	HEM	A	155	1,4	27,50,50	2.61	12 (44%)	17,82,82	3.17	8 (47%)
3	HEM	B	155	1,4	27,50,50	2.94	13 (48%)	17,82,82	2.81	8 (47%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	155	1,4	-	0/6/54/54	-
3	HEM	B	155	1,4	-	0/6/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	155	HEM	C3B-C2B	-7.46	1.30	1.40
3	A	155	HEM	C3B-C2B	-6.61	1.31	1.40
3	B	155	HEM	CAA-C2A	6.21	1.61	1.52
3	A	155	HEM	C3B-CAB	5.19	1.58	1.47
3	B	155	HEM	C3C-CAC	4.99	1.58	1.47
3	B	155	HEM	C3B-CAB	4.76	1.57	1.47
3	B	155	HEM	C4D-C3D	3.99	1.51	1.42
3	A	155	HEM	CAA-C2A	3.91	1.57	1.52
3	A	155	HEM	C3C-CAC	3.59	1.55	1.47
3	A	155	HEM	CMB-C2B	3.53	1.60	1.51
3	B	155	HEM	C1B-C2B	3.39	1.50	1.42
3	B	155	HEM	C1A-NA	3.23	1.42	1.36
3	A	155	HEM	C3C-C2C	-3.12	1.36	1.40
3	B	155	HEM	CMA-C3A	2.84	1.57	1.51
3	A	155	HEM	CMA-C3A	2.84	1.57	1.51
3	B	155	HEM	CMD-C2D	2.74	1.57	1.51
3	A	155	HEM	CMD-C2D	2.73	1.57	1.51
3	B	155	HEM	C1D-CHD	-2.71	1.33	1.41
3	B	155	HEM	C4A-NA	2.70	1.41	1.36
3	A	155	HEM	CAD-C3D	2.64	1.56	1.52
3	A	155	HEM	C1D-ND	2.40	1.41	1.36
3	A	155	HEM	C4A-NA	2.40	1.41	1.36
3	B	155	HEM	CMB-C2B	2.22	1.56	1.51
3	A	155	HEM	C3D-C2D	-2.19	1.31	1.37
3	B	155	HEM	C2A-C3A	-2.03	1.31	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	CBD-CAD-C3D	-7.59	98.49	112.48
3	A	155	HEM	CMD-C2D-C1D	-6.25	118.85	128.46
3	B	155	HEM	CMB-C2B-C3B	5.62	135.19	124.68
3	B	155	HEM	CMD-C2D-C1D	-5.09	120.65	128.46
3	A	155	HEM	CMD-C2D-C3D	4.38	133.21	124.94
3	B	155	HEM	CMD-C2D-C3D	4.38	133.20	124.94
3	A	155	HEM	CMA-C3A-C4A	-3.55	123.01	128.46
2	B	154	SO4	O4-S-O1	3.49	127.53	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	155	HEM	C3B-C4B-NB	-3.47	104.73	109.21
3	B	155	HEM	C4C-C3C-C2C	3.23	109.16	106.90
3	A	155	HEM	CMB-C2B-C3B	3.23	130.73	124.68
3	A	155	HEM	CAD-CBD-CGD	-2.93	107.75	112.67
3	B	155	HEM	CAD-CBD-CGD	2.85	117.45	112.67
3	A	155	HEM	C4C-C3C-C2C	-2.84	104.92	106.90
3	B	155	HEM	CMA-C3A-C4A	-2.65	124.38	128.46
3	B	155	HEM	CMC-C2C-C3C	-2.61	119.79	124.68
3	A	155	HEM	CMA-C3A-C2A	2.43	129.52	124.94
2	A	154	SO4	O3-S-O2	2.03	119.88	109.31

There are no chirality outliers.

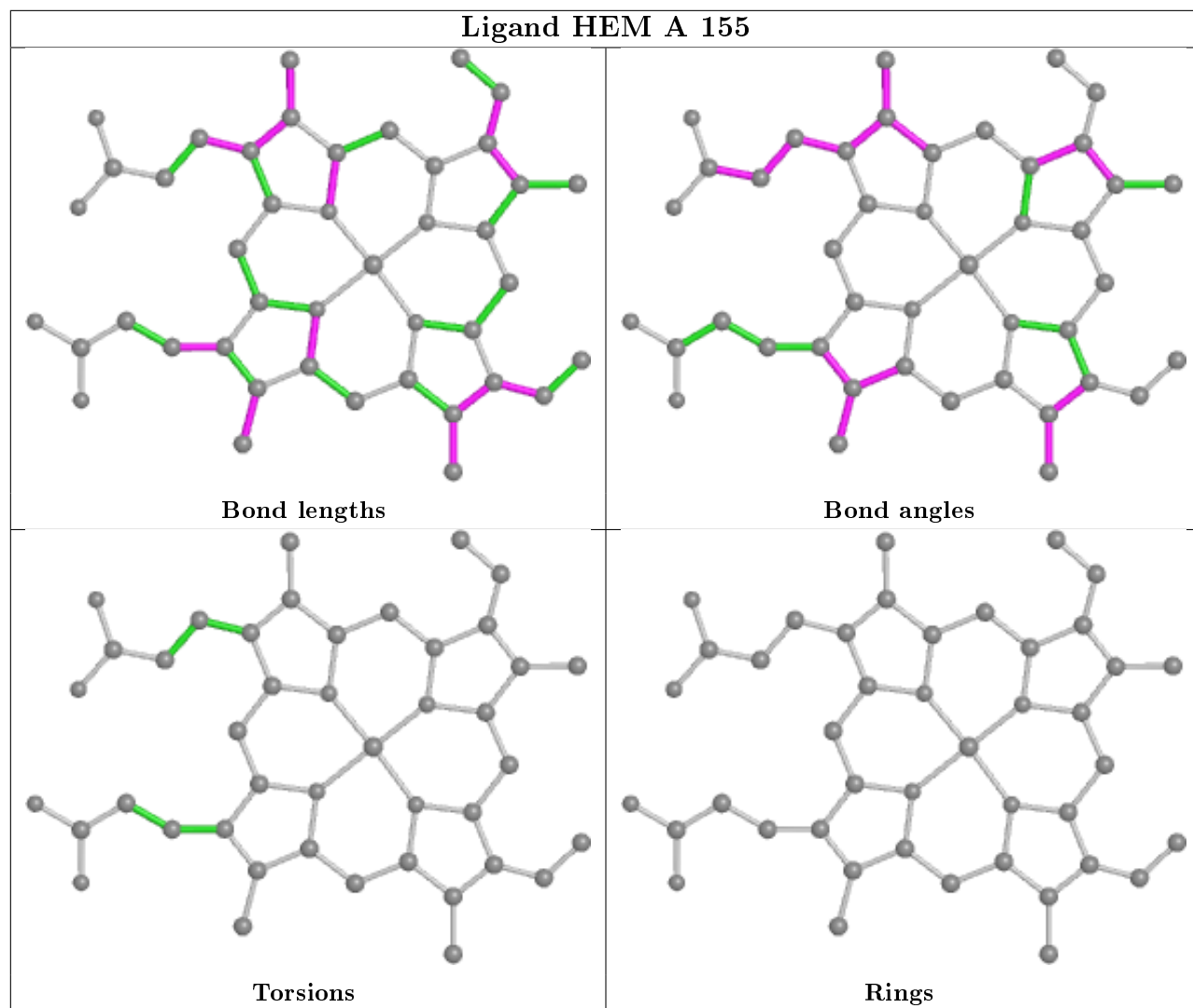
There are no torsion outliers.

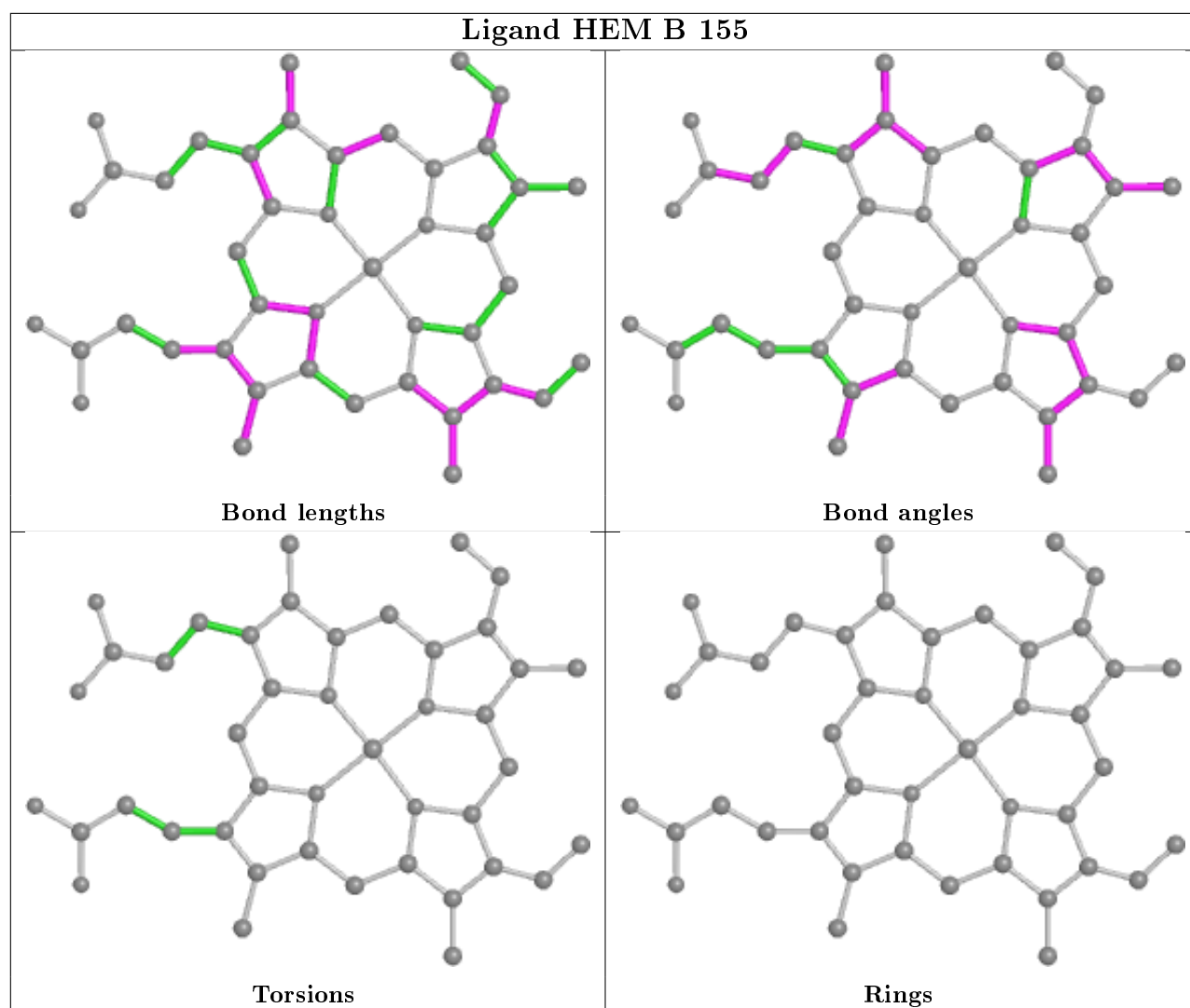
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	154	SO4	1	0
3	A	155	HEM	2	0
3	B	155	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.





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	153/153 (100%)	0.16	3 (1%) 65 68	7, 20, 38, 65	4 (2%)
1	B	153/153 (100%)	0.18	3 (1%) 65 68	7, 20, 37, 65	0
All	All	306/306 (100%)	0.17	6 (1%) 65 68	7, 20, 38, 65	4 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	GLY	9.1
1	A	153	GLY	7.6
1	B	152	GLN	3.0
1	A	152	GLN	2.8
1	B	146	TYR	2.2
1	A	146	TYR	2.1

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](#)

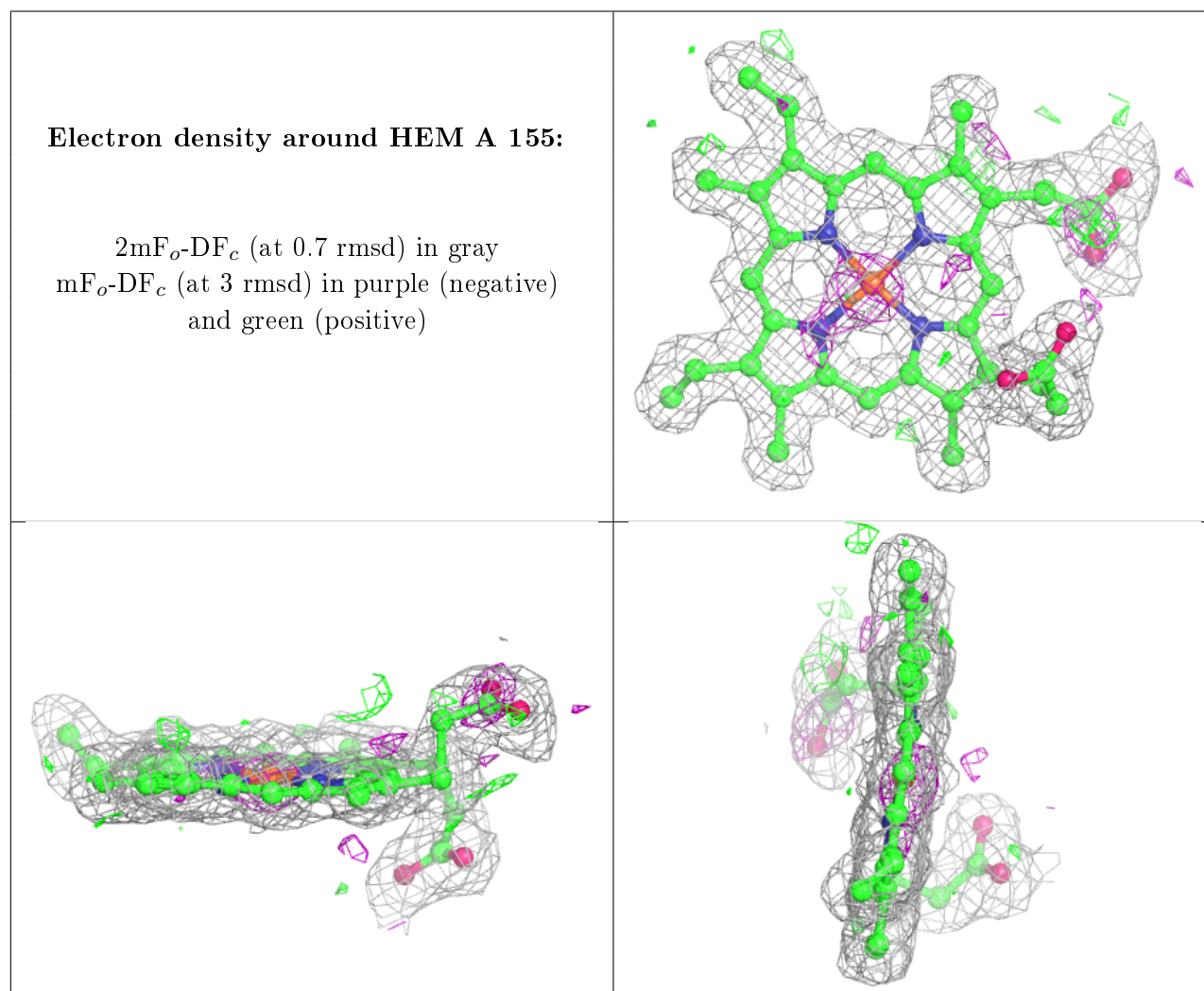
There are no monosaccharides in this entry.

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.

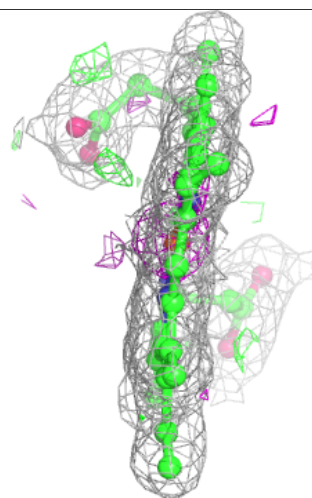
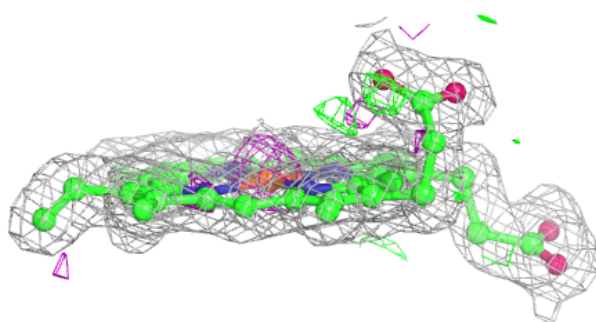
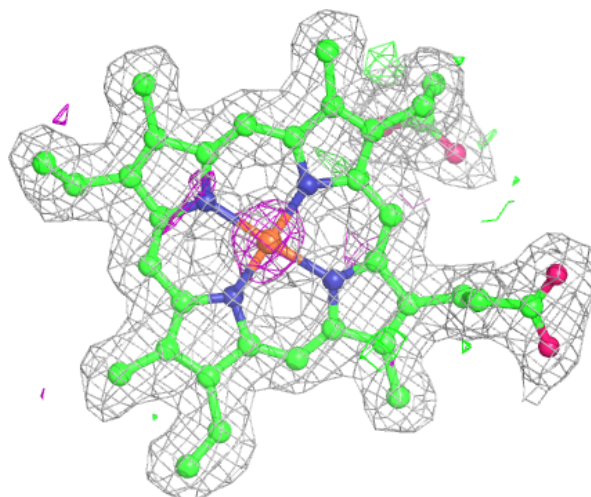
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	154	5/5	0.96	0.15	33,34,35,36	0
3	HEM	A	155	43/43	0.96	0.10	4,7,19,27	0
2	SO4	A	154	5/5	0.97	0.16	40,40,41,42	0
3	HEM	B	155	43/43	0.97	0.09	3,6,19,24	0

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 155:

$2mF_o-DF_c$ (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.