



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:02 PM UTC

PDB ID : 1MYG / pdb_00001myg
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 : 1.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

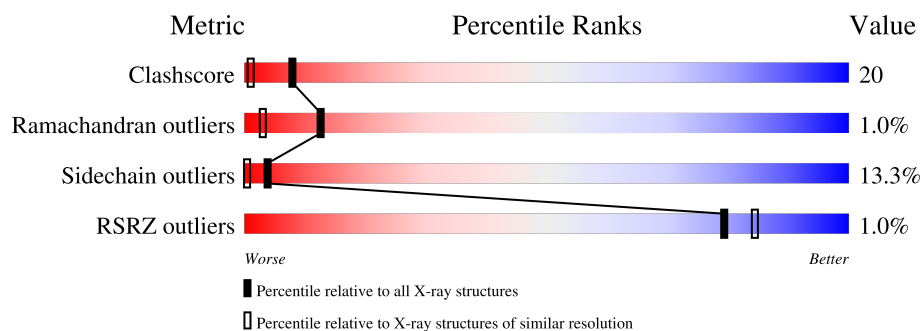
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	153	24% 56% 16% .
1	B	153	27% 47% 20% 7%

2 Entry composition [i](#)

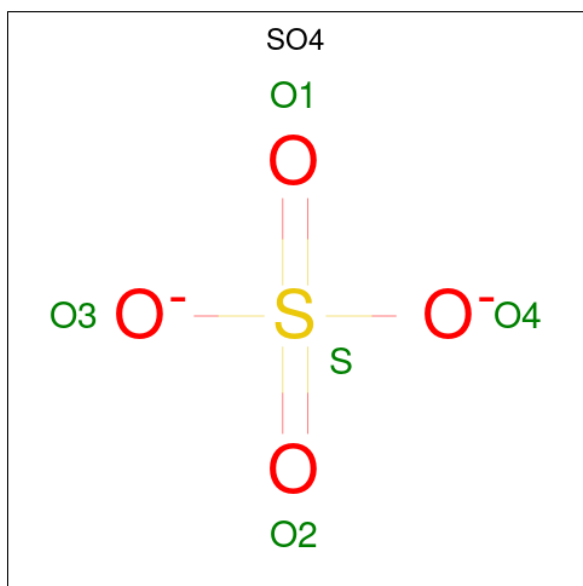
There are 4 unique types of molecules in this entry. The entry contains 2746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

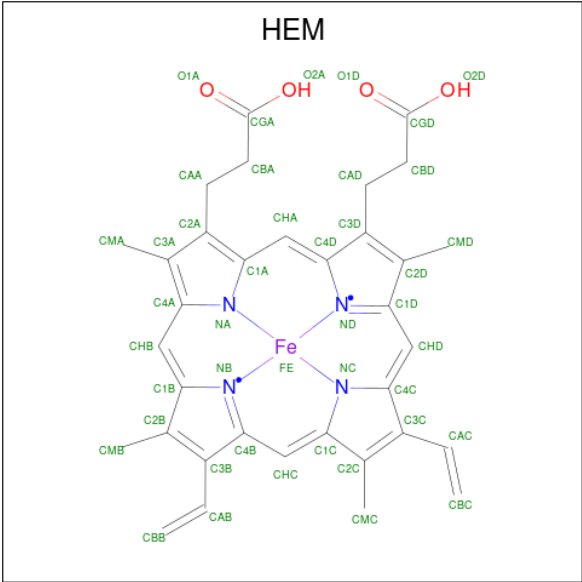
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	3	0
			1210	772	212	223	3			
1	B	153	Total	C	N	O	S	0	3	0
			1207	771	210	223	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

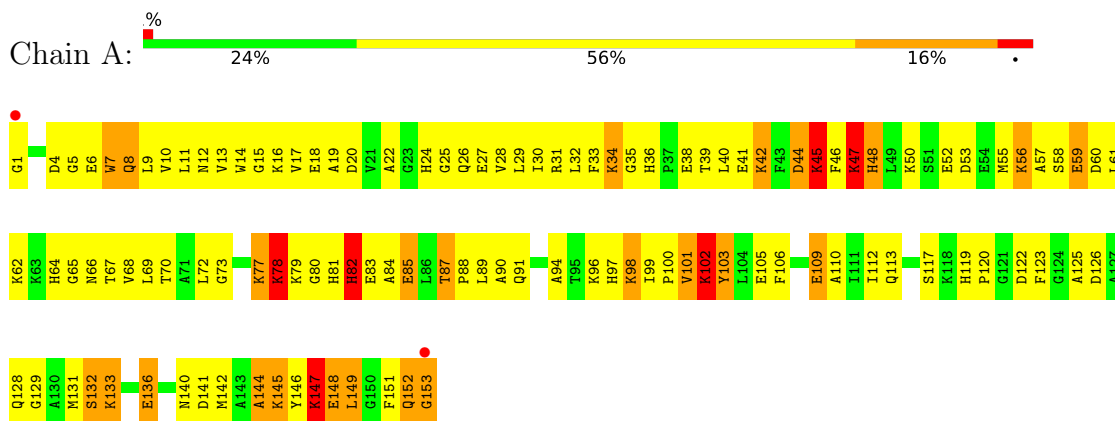
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		
4	B	122	Total	O	0	2
			122	122		

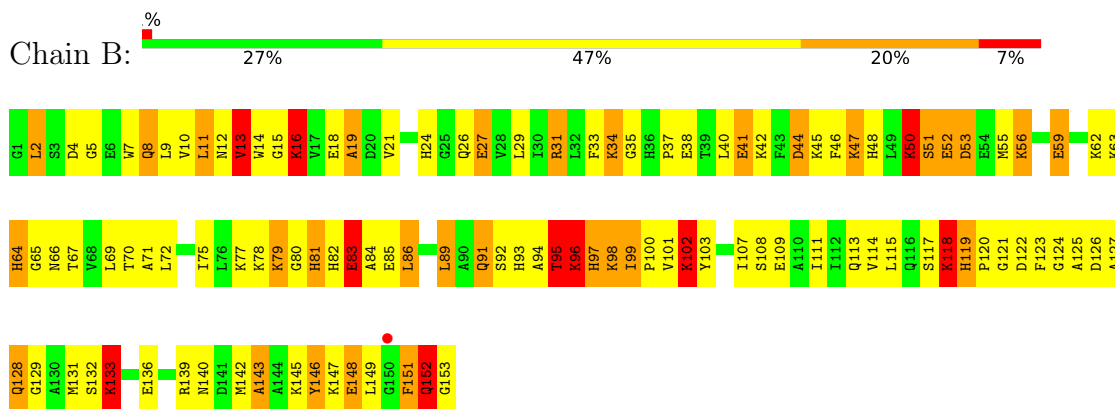
3 Residue-property plots

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: 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	125.26Å 42.49Å 92.37Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	10.00 – 1.75 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.75) 92.6 (10.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 1.79Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.198 , (Not available) 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.169 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2746	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: SO4, 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	1.70	11/1251 (0.9%)	3.19	187/1675 (11.2%)
1	B	1.73	7/1248 (0.6%)	3.21	199/1671 (11.9%)
All	All	1.71	18/2499 (0.7%)	3.20	386/3346 (11.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	ILE	CA-CB	8.34	1.64	1.54
1	B	5	GLY	C-N	-7.46	1.24	1.33
1	A	119	HIS	CA-CB	6.60	1.61	1.53
1	A	87	THR	CA-CB	6.28	1.61	1.53
1	A	5	GLY	N-CA	6.22	1.53	1.45
1	A	99	ILE	CA-CB	5.97	1.61	1.54
1	A	72	LEU	C-N	-5.95	1.25	1.33
1	A	16	LYS	C-O	5.93	1.31	1.24
1	A	26	GLN	N-CA	5.80	1.53	1.46
1	B	133	LYS	N-CA	5.63	1.53	1.46
1	B	81	HIS	N-CA	5.57	1.53	1.46
1	B	33	PHE	C-N	-5.48	1.26	1.33
1	A	15	GLY	C-N	-5.46	1.26	1.33
1	A	7	TRP	C-O	5.40	1.30	1.24
1	A	67	THR	CA-CB	5.37	1.61	1.53
1	A	47	LYS	N-CA	5.29	1.53	1.46
1	B	15	GLY	C-N	-5.08	1.27	1.33
1	B	67	THR	C-N	-5.03	1.27	1.33

All (386) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLN	CA-C-N	12.38	143.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLN	C-N-CA	12.38	143.98	121.70
1	B	59	GLU	CA-CB-CG	12.33	138.76	114.10
1	B	15	GLY	CA-C-N	11.96	137.42	120.79
1	B	15	GLY	C-N-CA	11.96	137.42	120.79
1	B	89[A]	LEU	CA-C-O	11.87	133.13	120.55
1	B	89[B]	LEU	CA-C-O	11.87	133.13	120.55
1	A	89	LEU	CA-C-O	11.50	132.61	120.42
1	A	53	ASP	CA-CB-CG	-11.03	101.57	112.60
1	A	122	ASP	CA-CB-CG	-10.59	102.01	112.60
1	A	35	GLY	CA-C-N	10.53	133.90	122.74
1	A	35	GLY	C-N-CA	10.53	133.90	122.74
1	A	117	SER	O-C-N	10.49	134.10	122.15
1	A	6	GLU	CA-C-O	-10.46	109.84	120.82
1	B	18	GLU	CA-C-O	-10.15	107.21	119.49
1	A	120	PRO	CA-C-N	10.14	133.09	120.22
1	A	120	PRO	C-N-CA	10.14	133.09	120.22
1	B	52	GLU	CA-C-O	10.09	131.25	120.55
1	B	33	PHE	CA-C-O	-10.09	109.73	120.42
1	A	59	GLU	OE1-CD-OE2	10.08	147.09	122.90
1	A	38	GLU	CA-CB-CG	9.94	133.98	114.10
1	A	84	ALA	O-C-N	9.93	132.65	122.12
1	B	55	MET	CA-C-O	9.77	130.91	120.55
1	B	34	LYS	CA-C-N	9.65	130.62	120.00
1	B	34	LYS	C-N-CA	9.65	130.62	120.00
1	A	128	GLN	OE1-CD-NE2	9.63	132.23	122.60
1	B	12	ASN	OD1-CG-ND2	9.60	132.20	122.60
1	B	26	GLN	O-C-N	-9.59	112.20	122.07
1	A	117	SER	CA-C-O	-9.46	110.39	120.42
1	B	89[A]	LEU	O-C-N	-9.43	112.12	122.12
1	B	89[B]	LEU	O-C-N	-9.43	112.12	122.12
1	B	86	LEU	CA-C-O	9.38	130.94	119.31
1	B	16	LYS	CB-CA-C	-9.35	96.05	110.92
1	A	132	SER	O-C-N	9.23	131.91	122.12
1	B	24	HIS	CA-C-N	9.22	130.18	119.94
1	B	24	HIS	C-N-CA	9.22	130.18	119.94
1	B	31	ARG	CA-C-O	-9.13	110.87	120.55
1	A	81	HIS	CA-CB-CG	-9.09	104.71	113.80
1	A	77	LYS	CA-C-O	-9.06	108.24	119.38
1	A	132	SER	CB-CA-C	-8.97	95.90	110.79
1	A	87	THR	CA-C-O	8.83	126.75	118.63
1	A	36	HIS	CA-CB-CG	-8.83	104.97	113.80
1	B	125	ALA	CA-C-O	8.76	130.02	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ASN	CA-CB-CG	-8.76	103.84	112.60
1	A	40	LEU	O-C-N	8.74	134.14	122.43
1	A	67	THR	CA-CB-OG1	-8.73	96.50	109.60
1	A	112	ILE	CB-CG1-CD1	-8.73	95.47	113.80
1	A	9	LEU	CA-C-O	-8.72	111.31	120.55
1	A	26	GLN	CB-CG-CD	-8.72	97.78	112.60
1	A	27	GLU	CA-C-O	-8.70	111.33	120.55
1	B	132	SER	CB-CA-C	-8.69	96.37	110.79
1	A	55	MET	CA-C-O	8.66	129.92	120.82
1	B	72	LEU	CA-C-O	-8.65	111.25	120.42
1	A	77	LYS	O-C-N	8.40	133.69	122.43
1	B	33	PHE	CA-CB-CG	8.37	122.17	113.80
1	B	142	MET	CA-C-O	8.33	129.38	120.55
1	A	55	MET	O-C-N	-8.31	113.51	122.07
1	A	98	LYS	CA-CB-CG	-8.23	97.64	114.10
1	A	48[A]	HIS	CA-CB-CG	-8.23	105.57	113.80
1	A	48[B]	HIS	CA-CB-CG	-8.23	105.57	113.80
1	A	136	GLU	CA-CB-CG	-8.14	97.82	114.10
1	A	117	SER	CB-CA-C	-8.10	97.08	110.85
1	B	80	GLY	N-CA-C	-8.06	105.48	115.08
1	B	84	ALA	O-C-N	8.06	130.38	122.07
1	B	122	ASP	CA-C-O	7.92	128.18	119.15
1	A	117	SER	N-CA-CB	7.91	121.86	110.16
1	A	78	LYS	CA-CB-CG	7.90	129.90	114.10
1	A	1	GLY	CA-C-N	7.87	136.03	122.64
1	A	1	GLY	C-N-CA	7.87	136.03	122.64
1	B	9	LEU	CA-C-O	-7.87	112.21	120.55
1	B	77	LYS	CA-C-O	-7.81	109.77	119.38
1	B	151	PHE	CA-CB-CG	-7.81	105.99	113.80
1	A	84	ALA	CA-C-O	-7.80	112.28	120.55
1	B	126	ASP	N-CA-C	7.79	119.41	111.07
1	B	55	MET	O-C-N	-7.75	113.91	122.12
1	A	20	ASP	CA-CB-CG	-7.72	104.88	112.60
1	B	117	SER	O-C-N	7.70	130.41	122.09
1	B	148	GLU	N-CA-CB	-7.70	98.35	110.28
1	B	8[A]	GLN	CB-CA-C	-7.65	98.87	110.88
1	B	8[B]	GLN	CB-CA-C	-7.65	98.87	110.88
1	B	12	ASN	CB-CG-OD1	-7.64	105.51	120.80
1	B	93	HIS	CA-C-N	7.64	131.02	120.63
1	B	93	HIS	C-N-CA	7.64	131.02	120.63
1	A	119	HIS	CA-C-O	-7.64	113.74	121.07
1	B	108	SER	CA-C-O	7.62	128.62	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	PHE	O-C-N	7.60	131.62	122.27
1	B	123	PHE	O-C-N	7.57	134.18	122.67
1	B	132	SER	CA-CB-OG	-7.57	95.96	111.10
1	A	125	ALA	CA-C-O	7.49	128.72	120.63
1	A	61	LEU	CD1-CG-CD2	-7.45	94.40	110.80
1	A	31	ARG	CD-NE-CZ	7.45	134.82	124.40
1	B	27	GLU	CB-CG-CD	-7.43	99.96	112.60
1	B	47	LYS	CB-CG-CD	-7.43	94.22	111.30
1	B	15	GLY	N-CA-C	-7.40	103.86	112.73
1	A	132	SER	CA-CB-OG	-7.39	96.32	111.10
1	A	151	PHE	CA-CB-CG	-7.37	106.43	113.80
1	B	80	GLY	CA-C-N	-7.35	111.05	122.08
1	B	80	GLY	C-N-CA	-7.35	111.05	122.08
1	A	100	PRO	CA-C-O	7.35	130.63	121.67
1	B	122	ASP	OD1-CG-OD2	7.34	140.51	122.90
1	A	18	GLU	CA-C-O	-7.31	110.39	119.38
1	A	96	LYS	O-C-N	7.31	130.81	122.19
1	A	4	ASP	O-C-N	7.28	131.22	122.27
1	B	46	PHE	O-C-N	7.26	130.77	122.20
1	B	13	VAL	CA-C-O	-7.24	113.42	120.95
1	A	33	PHE	CA-C-O	-7.22	111.66	119.97
1	A	19	ALA	N-CA-C	-7.20	104.47	113.18
1	B	18	GLU	O-C-N	7.20	131.74	122.39
1	A	90	ALA	CA-C-O	-7.19	112.80	120.42
1	A	8[A]	GLN	CB-CG-CD	7.15	124.75	112.60
1	A	8[B]	GLN	CB-CG-CD	7.15	124.75	112.60
1	B	4	ASP	CA-CB-CG	-7.11	105.49	112.60
1	A	7	TRP	O-C-N	-7.11	114.58	122.12
1	B	151	PHE	CA-C-N	7.07	135.03	121.54
1	B	151	PHE	C-N-CA	7.07	135.03	121.54
1	A	78	LYS	CB-CA-C	-7.06	95.89	109.95
1	B	102	LYS	O-C-N	7.04	130.23	122.20
1	A	12	ASN	CB-CG-ND2	-7.03	105.86	116.40
1	B	46	PHE	CA-C-N	-7.02	109.00	120.72
1	B	46	PHE	C-N-CA	-7.02	109.00	120.72
1	A	22	ALA	CA-C-N	6.98	135.09	121.41
1	A	22	ALA	C-N-CA	6.98	135.09	121.41
1	B	117	SER	CB-CA-C	-6.97	99.89	110.90
1	B	4	ASP	CA-C-N	6.97	127.67	119.94
1	B	4	ASP	C-N-CA	6.97	127.67	119.94
1	B	33	PHE	CA-C-N	6.96	130.17	120.29
1	B	33	PHE	C-N-CA	6.96	130.17	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	GLU	O-C-N	-6.94	114.76	122.12
1	B	86	LEU	N-CA-CB	-6.93	99.10	110.40
1	B	64	HIS	O-C-N	-6.93	114.25	122.15
1	B	118	LYS	CA-C-O	-6.93	111.16	119.27
1	B	9	LEU	O-C-N	6.93	129.47	122.12
1	B	69	LEU	CA-C-O	-6.88	111.67	119.79
1	A	146	TYR	CA-C-N	6.88	129.50	120.28
1	A	146	TYR	C-N-CA	6.88	129.50	120.28
1	B	140	ASN	CA-C-O	-6.87	113.60	120.82
1	A	31	ARG	NE-CZ-NH2	-6.86	113.03	119.20
1	A	148	GLU	CA-CB-CG	6.84	127.78	114.10
1	B	27	GLU	OE1-CD-OE2	6.84	139.32	122.90
1	B	14	TRP	CA-C-N	6.84	127.57	119.98
1	B	14	TRP	C-N-CA	6.84	127.57	119.98
1	B	62	LYS	CA-CB-CG	-6.82	100.47	114.10
1	A	87	THR	N-CA-C	6.81	122.11	113.25
1	B	136	GLU	CA-CB-CG	-6.81	100.47	114.10
1	A	30	ILE	CA-C-N	6.78	129.25	120.44
1	A	30	ILE	C-N-CA	6.78	129.25	120.44
1	B	11	LEU	CB-CA-C	6.78	122.04	110.79
1	A	113	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	A	90	ALA	N-CA-C	-6.75	104.00	111.36
1	A	142	MET	N-CA-C	-6.75	103.84	111.07
1	B	44	ASP	CB-CG-OD2	-6.74	102.91	118.40
1	B	26	GLN	CA-C-O	6.73	127.88	120.82
1	B	86	LEU	N-CA-C	6.73	121.23	112.89
1	B	149	LEU	CA-C-N	6.73	131.73	121.51
1	B	149	LEU	C-N-CA	6.73	131.73	121.51
1	A	31	ARG	N-CA-C	-6.71	103.89	111.07
1	A	59	GLU	CA-C-O	6.71	127.53	120.42
1	B	85	GLU	CA-C-O	-6.70	113.45	120.55
1	B	119	HIS	O-C-N	6.69	126.82	121.20
1	A	83	GLU	CB-CG-CD	6.69	123.97	112.60
1	A	133	LYS	CG-CD-CE	6.67	126.65	111.30
1	B	41	GLU	CA-C-O	6.66	127.66	120.20
1	B	140	ASN	CB-CG-ND2	6.66	126.39	116.40
1	A	65	GLY	CA-C-N	6.63	129.06	120.44
1	A	65	GLY	C-N-CA	6.63	129.06	120.44
1	A	132	SER	N-CA-CB	6.63	119.86	110.12
1	B	7	TRP	CA-C-N	6.63	129.05	120.44
1	B	7	TRP	C-N-CA	6.63	129.05	120.44
1	B	113	GLN	OE1-CD-NE2	-6.61	115.99	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	HIS	O-C-N	6.60	131.78	122.41
1	B	79	LYS	CA-C-O	-6.56	114.23	121.84
1	A	110	ALA	N-CA-CB	-6.55	100.50	110.12
1	B	12	ASN	CB-CA-C	-6.50	100.63	110.90
1	B	95	THR	N-CA-C	6.50	121.48	112.45
1	B	107	ILE	CA-C-O	-6.49	113.46	120.47
1	A	34	LYS	N-CA-CB	6.47	119.74	110.16
1	A	1	GLY	O-C-N	-6.45	112.68	123.00
1	B	2	LEU	O-C-N	6.43	130.50	123.10
1	B	38	GLU	CA-CB-CG	6.43	126.96	114.10
1	B	80	GLY	CA-C-O	-6.43	112.59	119.27
1	B	132	SER	O-C-N	6.41	128.92	122.12
1	B	5	GLY	O-C-N	6.39	128.32	122.18
1	A	8[A]	GLN	CA-C-N	6.39	128.84	120.28
1	A	8[A]	GLN	C-N-CA	6.39	128.84	120.28
1	A	8[B]	GLN	CA-C-N	6.39	128.84	120.28
1	A	8[B]	GLN	C-N-CA	6.39	128.84	120.28
1	B	115	LEU	O-C-N	-6.39	115.35	122.12
1	A	16	LYS	N-CA-C	-6.38	103.84	111.69
1	B	148	GLU	CA-CB-CG	6.37	126.84	114.10
1	B	98	LYS	CA-C-N	-6.36	116.40	123.02
1	B	98	LYS	C-N-CA	-6.36	116.40	123.02
1	A	103	TYR	O-C-N	6.35	129.66	122.22
1	A	25	GLY	O-C-N	6.35	128.35	122.19
1	B	121	GLY	O-C-N	-6.32	115.39	122.28
1	B	92	SER	O-C-N	6.31	129.34	122.15
1	B	132	SER	N-CA-CB	6.30	119.39	110.12
1	B	53	ASP	O-C-N	-6.29	115.59	122.07
1	B	44	ASP	CA-CB-CG	-6.29	106.31	112.60
1	B	97	HIS	ND1-CG-CD2	-6.29	99.81	106.10
1	A	28	VAL	CA-C-N	-6.28	111.37	120.29
1	A	28	VAL	C-N-CA	-6.28	111.37	120.29
1	B	117	SER	CA-CB-OG	-6.27	98.56	111.10
1	A	26	GLN	CA-CB-CG	-6.27	101.57	114.10
1	B	16	LYS	N-CA-CB	6.26	119.34	109.82
1	A	39	THR	N-CA-C	-6.24	105.16	112.89
1	A	136	GLU	CG-CD-OE1	-6.23	104.08	118.40
1	B	83	GLU	O-C-N	-6.22	115.52	122.12
1	B	103	TYR	O-C-N	6.20	129.90	122.27
1	A	46	PHE	O-C-N	6.20	128.99	122.23
1	A	85	GLU	N-CA-CB	6.16	119.27	110.16
1	A	45	LYS	CA-C-O	-6.15	111.71	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	HIS	CA-CB-CG	6.15	119.95	113.80
1	A	126	ASP	O-C-N	6.13	128.71	122.09
1	B	85	GLU	CB-CG-CD	-6.12	102.20	112.60
1	A	80	GLY	CA-C-O	-6.12	113.14	119.20
1	B	15	GLY	O-C-N	-6.11	116.32	122.19
1	B	24	HIS	CG-CD2-NE2	6.11	113.31	107.20
1	A	152	GLN	OE1-CD-NE2	6.10	128.70	122.60
1	A	61	LEU	N-CA-C	-6.09	104.72	111.36
1	A	8[A]	GLN	N-CA-CB	6.08	118.82	110.01
1	A	8[B]	GLN	N-CA-CB	6.08	118.82	110.01
1	A	72	LEU	CA-C-N	6.06	126.70	119.98
1	A	72	LEU	C-N-CA	6.06	126.70	119.98
1	B	35	GLY	CA-C-O	-6.06	114.24	120.66
1	A	44	ASP	CA-C-O	6.04	127.71	121.07
1	B	97	HIS	CG-CD2-NE2	6.02	113.22	107.20
1	A	47	LYS	CA-CB-CG	-6.01	102.07	114.10
1	A	6	GLU	O-C-N	6.00	128.25	122.07
1	B	64	HIS	CA-CB-CG	-6.00	107.80	113.80
1	B	34	LYS	N-CA-CB	5.98	119.01	110.16
1	B	71	ALA	O-C-N	-5.97	115.92	122.07
1	A	69	LEU	CA-C-O	-5.97	113.11	119.97
1	A	80	GLY	CA-C-N	-5.96	113.23	122.05
1	A	80	GLY	C-N-CA	-5.96	113.23	122.05
1	B	126	ASP	N-CA-CB	-5.96	101.37	110.01
1	A	15	GLY	CA-C-N	5.92	130.71	120.58
1	A	15	GLY	C-N-CA	5.92	130.71	120.58
1	B	27	GLU	CA-CB-CG	-5.92	102.26	114.10
1	B	67	THR	CA-CB-OG1	-5.92	100.72	109.60
1	B	72	LEU	N-CA-C	-5.92	104.91	111.36
1	B	148	GLU	CB-CG-CD	-5.92	102.54	112.60
1	A	113	GLN	CG-CD-NE2	5.91	125.26	116.40
1	B	44	ASP	CA-C-O	5.87	126.98	120.82
1	B	139	ARG	NE-CZ-NH2	-5.85	113.94	119.20
1	A	11	LEU	CA-C-O	5.84	126.70	120.10
1	A	70	THR	N-CA-C	-5.84	105.00	111.36
1	A	8[A]	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	8[B]	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	B	31	ARG	CA-CB-CG	-5.83	102.44	114.10
1	A	72	LEU	CA-C-O	-5.83	114.25	120.42
1	B	21	VAL	CA-CB-CG1	5.83	120.30	110.40
1	A	59	GLU	CG-CD-OE1	-5.82	105.01	118.40
1	A	126	ASP	CA-C-O	-5.82	114.71	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	99	ILE	CA-CB-CG2	5.81	120.37	110.50
1	A	82	HIS	N-CA-CB	-5.80	101.63	111.20
1	A	50	LYS	CA-C-O	-5.80	112.57	119.35
1	B	129	GLY	O-C-N	-5.78	116.64	122.19
1	B	41	GLU	CG-CD-OE1	5.76	131.64	118.40
1	B	146	TYR	CA-C-N	5.74	128.28	120.54
1	B	146	TYR	C-N-CA	5.74	128.28	120.54
1	B	31	ARG	CA-C-N	5.73	127.89	120.44
1	B	31	ARG	C-N-CA	5.73	127.89	120.44
1	A	89	LEU	N-CA-CB	-5.72	101.69	110.16
1	A	117	SER	CA-CB-OG	-5.71	99.68	111.10
1	A	149	LEU	CA-C-O	5.70	126.38	119.31
1	B	18	GLU	CB-CG-CD	-5.70	102.91	112.60
1	A	9	LEU	O-C-N	5.68	128.15	122.12
1	B	31	ARG	CD-NE-CZ	-5.68	116.44	124.40
1	B	81	HIS	O-C-N	-5.67	114.85	122.68
1	A	44	ASP	CB-CG-OD1	5.66	131.42	118.40
1	A	47	LYS	CA-C-O	5.66	126.23	119.10
1	B	29	LEU	N-CA-CB	-5.65	101.82	110.12
1	A	105	GLU	N-CA-C	-5.65	105.20	111.36
1	A	125	ALA	O-C-N	-5.64	116.14	122.12
1	A	58	SER	CA-CB-OG	-5.62	99.85	111.10
1	B	82	HIS	N-CA-C	5.62	120.13	112.88
1	B	11	LEU	O-C-N	-5.62	116.17	122.12
1	B	117	SER	CA-C-N	-5.61	111.79	121.66
1	B	117	SER	C-N-CA	-5.61	111.79	121.66
1	B	10	VAL	N-CA-CB	5.60	117.10	110.55
1	A	28	VAL	O-C-N	5.58	127.38	121.91
1	B	93	HIS	CA-C-O	5.57	126.37	119.97
1	B	26	GLN	OE1-CD-NE2	5.56	128.16	122.60
1	B	96	LYS	O-C-N	-5.56	115.93	122.32
1	B	109	GLU	N-CA-CB	-5.56	101.94	110.16
1	A	98	LYS	CB-CG-CD	5.55	124.07	111.30
1	A	123	PHE	O-C-N	5.55	129.97	122.59
1	B	62	LYS	O-C-N	-5.52	116.39	122.07
1	A	42	LYS	CA-CB-CG	-5.51	103.08	114.10
1	A	141	ASP	O-C-N	-5.51	115.87	122.15
1	B	151	PHE	CB-CA-C	5.51	119.68	109.54
1	A	16	LYS	CA-C-O	-5.50	114.13	120.24
1	B	19	ALA	N-CA-C	-5.50	106.52	113.18
1	B	107	ILE	O-C-N	5.50	128.02	121.80
1	B	97	HIS	CA-CB-CG	-5.48	108.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CA-C-O	5.47	126.35	120.55
1	A	87	THR	CA-CB-OG1	-5.47	101.40	109.60
1	B	109	GLU	CA-C-O	-5.47	114.63	120.42
1	B	123	PHE	CA-C-O	-5.47	113.62	122.20
1	B	27	GLU	CG-CD-OE1	-5.45	105.86	118.40
1	B	143	ALA	CA-C-O	-5.45	114.77	120.55
1	B	98	LYS	O-C-N	-5.45	116.40	123.32
1	B	81	HIS	N-CA-C	-5.44	103.11	110.68
1	A	17	VAL	CA-C-O	5.44	126.61	120.85
1	B	14	TRP	CE2-CD2-CE3	5.44	124.24	118.80
1	B	62	LYS	CA-C-O	5.44	126.53	120.82
1	B	126	ASP	CA-C-N	5.44	127.51	120.44
1	B	126	ASP	C-N-CA	5.44	127.51	120.44
1	A	62	LYS	O-C-N	-5.43	116.47	122.07
1	B	149	LEU	CA-C-O	5.43	126.11	119.05
1	B	111	ILE	O-C-N	5.43	127.23	121.91
1	B	77	LYS	CA-CB-CG	-5.42	103.26	114.10
1	A	15	GLY	O-C-N	-5.40	117.01	122.19
1	A	5	GLY	CA-C-N	5.39	127.45	120.44
1	A	5	GLY	C-N-CA	5.39	127.45	120.44
1	A	56	LYS	O-C-N	5.39	128.52	122.22
1	B	50	LYS	CG-CD-CE	-5.38	98.92	111.30
1	A	34	LYS	CA-C-N	5.38	127.12	120.34
1	A	34	LYS	C-N-CA	5.38	127.12	120.34
1	B	96	LYS	CA-C-O	5.35	127.03	120.56
1	B	8[A]	GLN	CB-CG-CD	-5.34	103.52	112.60
1	B	8[B]	GLN	CB-CG-CD	-5.34	103.52	112.60
1	B	59	GLU	N-CA-C	-5.34	105.54	111.36
1	B	2	LEU	CD1-CG-CD2	5.33	122.53	110.80
1	B	40	LEU	CA-C-N	5.33	128.17	120.38
1	B	40	LEU	C-N-CA	5.33	128.17	120.38
1	A	50	LYS	CD-CE-NZ	-5.32	94.87	111.90
1	B	96	LYS	CD-CE-NZ	5.32	128.91	111.90
1	B	128	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	B	125	ALA	O-C-N	-5.30	116.61	122.07
1	A	94	ALA	O-C-N	5.30	128.58	122.17
1	A	56	LYS	N-CA-CB	5.29	118.37	110.22
1	A	30	ILE	O-C-N	-5.29	116.73	121.91
1	B	89[A]	LEU	N-CA-CB	-5.29	102.35	110.12
1	B	89[B]	LEU	N-CA-CB	-5.29	102.35	110.12
1	B	12	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	151	PHE	O-C-N	5.28	131.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	O-C-N	-5.27	116.76	121.87
1	B	66	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	A	82	HIS	ND1-CE1-NE2	-5.25	103.15	108.40
1	A	34	LYS	CB-CA-C	-5.24	101.95	110.85
1	B	143	ALA	O-C-N	5.24	127.67	122.12
1	B	70	THR	CA-CB-OG1	-5.23	101.75	109.60
1	A	40	LEU	CD1-CG-CD2	-5.21	99.34	110.80
1	A	82	HIS	N-CA-C	5.21	119.18	112.41
1	A	66	ASN	CA-C-O	5.20	126.28	120.82
1	B	51	SER	O-C-N	5.20	128.61	123.46
1	B	31	ARG	N-CA-CB	5.19	117.75	110.12
1	B	46	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	97	HIS	N-CA-C	5.17	119.30	112.89
1	A	126	ASP	CA-CB-CG	-5.17	107.44	112.60
1	A	29	LEU	CA-C-O	-5.14	114.97	120.42
1	A	40	LEU	CA-C-O	-5.14	113.06	119.38
1	A	48[A]	HIS	CA-C-O	5.13	125.49	119.28
1	A	48[B]	HIS	CA-C-O	5.13	125.49	119.28
1	B	117	SER	N-CA-CB	5.12	117.50	110.07
1	A	102[A]	LYS	CA-C-O	-5.12	114.47	120.20
1	A	102[B]	LYS	CA-C-O	-5.12	114.47	120.20
1	A	39	THR	CA-CB-CG2	5.11	119.19	110.50
1	A	132	SER	CA-C-N	-5.10	113.05	120.29
1	A	132	SER	C-N-CA	-5.10	113.05	120.29
1	A	6	GLU	CA-CB-CG	-5.09	103.92	114.10
1	A	89	LEU	O-C-N	-5.08	116.36	122.15
1	A	12	ASN	CB-CA-C	-5.08	102.87	110.90
1	B	65	GLY	N-CA-C	-5.07	106.64	112.73
1	B	81	HIS	CB-CA-C	5.06	119.02	111.88
1	B	152	GLN	CB-CA-C	-5.06	100.36	110.42
1	A	140	ASN	CA-CB-CG	-5.05	107.55	112.60
1	B	127	ALA	CA-C-O	-5.05	115.51	120.82
1	A	136	GLU	CB-CG-CD	-5.05	104.01	112.60
1	B	24	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
1	B	85	GLU	CG-CD-OE2	-5.04	106.80	118.40
1	A	153	GLY	N-CA-C	-5.04	98.69	113.30
1	A	60	ASP	CA-C-O	-5.03	114.18	119.97
1	A	48[A]	HIS	N-CA-CB	-5.03	102.75	110.44
1	A	48[B]	HIS	N-CA-CB	-5.03	102.75	110.44
1	A	144	ALA	N-CA-CB	-5.03	102.72	110.16
1	A	109	GLU	CB-CA-C	5.02	119.39	110.85
1	A	32	LEU	CA-C-O	-5.02	115.55	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	HIS	CB-CG-ND1	5.02	130.23	122.70
1	B	7	TRP	O-C-N	-5.02	116.80	122.12
1	A	68	VAL	O-C-N	5.01	126.82	121.91
1	B	56	LYS	CB-CA-C	-5.01	102.47	110.79
1	B	131	MET	CA-C-N	-5.01	113.57	120.28
1	B	131	MET	C-N-CA	-5.01	113.57	120.28
1	A	147	LYS	O-C-N	5.00	127.42	122.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1210	0	1221	49	1
1	B	1207	0	1221	49	1
2	A	5	0	0	1	0
2	B	5	0	0	1	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
4	A	111	0	0	3	0
4	B	122	0	0	8	0
All	All	2746	0	2502	99	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 20.

All (99) 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:47:LYS:NZ	1:A:47:LYS:HB2	1.65	1.09
1:A:47:LYS:HB2	1:A:47:LYS:HZ2	1.17	1.07
1:B:16:LYS:HE2	1:B:16:LYS:HA	1.41	1.00
1:A:47:LYS:NZ	1:A:47:LYS:CB	2.25	0.99
1:A:78:LYS:HA	1:A:78:LYS:HE2	1.41	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG2	1:A:56:LYS:HE3	1.55	0.87
1:B:16:LYS:HA	1:B:16:LYS:CE	2.07	0.84
1:A:45:LYS:O	1:A:48[A]:HIS:HE1	1.64	0.80
1:B:59:GLU:O	1:B:63[A]:LYS:HD3	1.83	0.79
1:A:102[B]:LYS:HD2	1:A:103:TYR:CE1	2.20	0.76
1:A:102[A]:LYS:NZ	1:A:153:GLY:C	2.44	0.75
1:B:8[B]:GLN:NE2	4:B:329:HOH:O	2.22	0.73
1:B:96:LYS:HD2	1:B:97:HIS:CE1	2.24	0.72
1:B:146:TYR:CD2	1:B:151:PHE:HD2	2.07	0.71
1:A:47:LYS:CB	1:A:47:LYS:HZ3	2.02	0.71
1:A:78:LYS:HE2	1:A:78:LYS:CA	2.06	0.70
1:A:87:THR:HB	1:A:88:PRO:HD3	1.72	0.70
1:A:102[A]:LYS:HZ1	1:A:153:GLY:C	2.01	0.69
1:A:45:LYS:O	1:A:48[A]:HIS:CE1	2.44	0.69
1:B:45:LYS:O	1:B:48:HIS:HE1	1.74	0.69
1:B:146:TYR:HB2	1:B:153:GLY:OXT	1.91	0.69
1:B:83:GLU:HB3	4:B:377:HOH:O	1.91	0.68
1:B:63[A]:LYS:NZ	4:B:320:HOH:O	2.24	0.67
1:B:114:VAL:HG13	1:B:118:LYS:HD2	1.78	0.66
3:B:154:HEM:HBC2	3:B:154:HEM:HMC2	1.78	0.65
1:B:16:LYS:HE2	1:B:16:LYS:CA	2.16	0.65
1:A:73:GLY:O	1:A:77:LYS:HG3	1.96	0.65
1:B:83:GLU:CD	1:B:83:GLU:H	2.03	0.65
1:B:16:LYS:CE	1:B:16:LYS:CA	2.72	0.65
1:A:52:GLU:O	1:A:56:LYS:HG3	1.99	0.63
1:B:31:ARG:HD2	4:B:303:HOH:O	1.99	0.63
1:B:2:LEU:HG	1:B:133:LYS:HE2	1.82	0.62
1:B:143:ALA:O	1:B:153:GLY:OXT	2.18	0.62
1:B:95:THR:O	1:B:98:LYS:HE2	2.00	0.61
1:A:47:LYS:HB2	1:A:47:LYS:HZ3	1.61	0.61
1:B:45:LYS:O	1:B:48:HIS:CE1	2.55	0.60
1:B:146:TYR:CD2	1:B:151:PHE:CD2	2.89	0.60
1:B:44:ASP:HA	1:B:47:LYS:HE2	1.86	0.58
1:A:10:VAL:O	1:A:13:VAL:HG22	2.06	0.56
1:A:102[A]:LYS:HZ3	1:A:153:GLY:C	2.13	0.56
1:B:146:TYR:CB	1:B:153:GLY:OXT	2.53	0.56
1:B:146:TYR:O	1:B:151:PHE:N	2.33	0.56
1:A:102[B]:LYS:HD2	1:A:103:TYR:CD1	2.40	0.56
1:B:83:GLU:N	1:B:83:GLU:OE1	2.39	0.56
1:A:47:LYS:HZ3	1:A:47:LYS:HB3	1.71	0.55
1:B:91:GLN:O	1:B:95:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:CG	1:B:151:PHE:HD2	2.25	0.55
1:A:87:THR:CB	1:A:88:PRO:HD3	2.37	0.55
1:A:78:LYS:HG3	1:A:82:HIS:HA	1.88	0.55
1:B:19:ALA:HB1	4:B:391:HOH:O	2.07	0.55
1:A:78:LYS:HG3	1:A:82:HIS:CA	2.37	0.55
1:A:64:HIS:ND1	2:A:301:SO4:O2	2.40	0.54
1:A:7:TRP:CG	1:A:79:LYS:HG2	2.44	0.53
1:B:50:LYS:O	1:B:51:SER:HB3	2.09	0.53
1:A:102[A]:LYS:NZ	1:A:153:GLY:O	2.41	0.53
1:B:81:HIS:HD2	4:B:374:HOH:O	1.92	0.53
1:A:57:ALA:HB3	4:A:318:HOH:O	2.08	0.52
1:B:114:VAL:CG1	1:B:118:LYS:HD2	2.39	0.52
1:A:132:SER:HB2	4:A:394:HOH:O	2.09	0.51
1:B:11:LEU:CD1	1:B:79:LYS:HE3	2.41	0.51
1:A:78:LYS:HG3	1:A:82:HIS:HB3	1.94	0.50
1:B:11:LEU:HD11	1:B:79:LYS:HE3	1.93	0.50
1:A:13:VAL:HG23	1:A:14:TRP:N	2.28	0.49
1:A:87:THR:N	1:A:88:PRO:CD	2.75	0.49
1:A:129:GLY:O	1:A:133:LYS:HG3	2.13	0.49
1:A:88:PRO:HA	1:A:91:GLN:HE21	1.79	0.48
1:B:64:HIS:ND1	2:B:300:SO4:O3	2.43	0.48
1:A:136:GLU:O	1:A:136:GLU:HG2	2.14	0.48
1:A:13:VAL:HG21	1:A:131:MET:CE	2.44	0.47
1:B:151:PHE:O	1:B:153:GLY:N	2.47	0.47
1:A:78:LYS:HD2	1:A:85:GLU:CD	2.40	0.47
1:A:147:LYS:CB	1:A:147:LYS:NZ	2.78	0.47
1:B:75:ILE:HD11	1:B:89[A]:LEU:HD23	1.97	0.46
1:A:44:ASP:O	1:A:47:LYS:HG2	2.15	0.46
1:B:42:LYS:HG2	1:B:99:ILE:CD1	2.45	0.46
1:B:81:HIS:CD2	4:B:374:HOH:O	2.69	0.45
1:B:100:PRO:HB2	1:B:102:LYS:HG2	1.98	0.45
1:B:133:LYS:HB3	1:B:133:LYS:HE3	1.39	0.45
1:A:144:ALA:HA	1:A:147:LYS:HE3	1.99	0.45
1:A:106:PHE:O	1:A:109:GLU:HG2	2.17	0.44
1:B:42:LYS:HG2	1:B:99:ILE:HD12	1.99	0.44
1:A:78:LYS:HG3	1:A:82:HIS:CB	2.49	0.43
1:B:13:VAL:O	1:B:16:LYS:HG2	2.18	0.43
1:B:78:LYS:HA	1:B:78:LYS:HD2	1.65	0.43
1:B:52:GLU:O	1:B:56:LYS:HG3	2.19	0.42
1:A:13:VAL:CG2	1:A:14:TRP:N	2.82	0.42
1:A:78:LYS:CA	1:A:78:LYS:CE	2.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:TRP:CD2	1:A:79:LYS:HG2	2.54	0.42
1:B:119:HIS:N	1:B:120:PRO:CD	2.82	0.42
1:A:42:LYS:H	1:A:42:LYS:HG2	1.52	0.42
1:B:124:GLY:O	1:B:128:GLN:HG3	2.19	0.41
1:B:94:ALA:O	1:B:98:LYS:HD2	2.20	0.41
1:B:119:HIS:N	1:B:120:PRO:HD3	2.36	0.41
1:A:145:LYS:HD3	1:A:148:GLU:CG	2.50	0.41
1:B:27:GLU:HG2	4:B:340:HOH:O	2.21	0.40
1:A:78:LYS:HE3	4:A:362:HOH:O	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:A:48[A]:HIS:CD2	1:B:48:HIS:CD2[1_546]	2.19	0.01

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	154/153 (101%)	148 (96%)	4 (3%)	2 (1%)	9	2
1	B	154/153 (101%)	147 (96%)	6 (4%)	1 (1%)	21	8
All	All	308/306 (101%)	295 (96%)	10 (3%)	3 (1%)	12	3

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	152	GLN
1	A	45	LYS

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	127/124 (102%)	112 (88%)	15 (12%)	5	0
1	B	127/124 (102%)	107 (84%)	20 (16%)	2	0
All	All	254/248 (102%)	219 (86%)	35 (14%)	4	0

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8[A]	GLN
1	A	8[B]	GLN
1	A	34	LYS
1	A	41	GLU
1	A	45	LYS
1	A	47	LYS
1	A	59	GLU
1	A	78	LYS
1	A	82	HIS
1	A	98	LYS
1	A	102[A]	LYS
1	A	102[B]	LYS
1	A	145	LYS
1	A	147	LYS
1	A	149	LEU
1	B	13	VAL
1	B	16	LYS
1	B	34	LYS
1	B	37	PRO
1	B	41	GLU
1	B	50	LYS
1	B	53	ASP
1	B	83	GLU
1	B	86	LEU
1	B	91	GLN
1	B	95	THR
1	B	96	LYS

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Mol	Chain	Res	Type
1	B	101	VAL
1	B	102	LYS
1	B	118	LYS
1	B	133	LYS
1	B	145	LYS
1	B	147	LYS
1	B	148	GLU
1	B	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	140	ASN
1	A	152	GLN
1	B	12	ASN
1	B	48	HIS
1	B	128	GLN
1	B	140	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	300	-	4,4,4	1.06	0	6,6,6	0.57	0
3	HEM	B	154	1,4	50,50,50	1.87	13 (26%)	67,82,82	2.42	23 (34%)
2	SO4	A	301	-	4,4,4	1.06	0	6,6,6	0.95	0
3	HEM	A	154	1,4	50,50,50	1.64	9 (18%)	67,82,82	2.01	22 (32%)

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	B	154	1,4	-	5/14/54/54	-
3	HEM	A	154	1,4	-	5/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	154	HEM	FE-NB	5.43	2.11	1.94
3	B	154	HEM	FE-NB	5.08	2.10	1.94
3	B	154	HEM	FE-ND	3.53	2.05	1.94
3	B	154	HEM	CAB-C3B	3.40	1.56	1.47
3	B	154	HEM	C3B-C2B	-3.39	1.30	1.37
3	B	154	HEM	C1B-NB	-3.34	1.34	1.40
3	B	154	HEM	CMB-C2B	3.33	1.57	1.50
3	A	154	HEM	CAB-C3B	3.23	1.56	1.47
3	B	154	HEM	CAC-C3C	3.11	1.55	1.47
3	B	154	HEM	CHC-C1C	3.09	1.44	1.38
3	B	154	HEM	CAA-C2A	2.82	1.58	1.51
3	A	154	HEM	CBD-CAD	2.56	1.60	1.51
3	B	154	HEM	O1A-CGA	2.46	1.30	1.22
3	B	154	HEM	C3D-C2D	-2.44	1.31	1.36
3	A	154	HEM	CMD-C2D	2.36	1.55	1.50
3	A	154	HEM	CAA-C2A	2.32	1.57	1.51
3	A	154	HEM	C4D-C3D	2.24	1.48	1.45
3	A	154	HEM	C4B-NB	-2.22	1.34	1.38
3	A	154	HEM	O1A-CGA	2.21	1.29	1.22
3	B	154	HEM	CMD-C2D	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	154	HEM	CBD-CAD	2.11	1.59	1.51
3	A	154	HEM	CMB-C2B	2.02	1.54	1.50

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	154	HEM	CBD-CAD-C3D	-6.00	95.95	112.53
3	B	154	HEM	CMD-C2D-C1D	-5.71	116.11	125.03
3	B	154	HEM	CAD-C3D-C4D	-5.52	115.07	124.70
3	B	154	HEM	C3B-C2B-C1B	5.04	110.19	106.41
3	A	154	HEM	CBD-CAD-C3D	-4.88	99.04	112.53
3	B	154	HEM	CAD-CBD-CGD	-4.62	101.41	113.67
3	B	154	HEM	CMB-C2B-C1B	-4.60	117.84	125.03
3	B	154	HEM	CMD-C2D-C3D	4.59	138.56	126.15
3	B	154	HEM	O1D-CGD-CBD	-4.54	108.69	123.09
3	B	154	HEM	C3D-C4D-ND	-4.42	105.33	110.17
3	A	154	HEM	CHB-C1B-NB	4.32	129.71	124.37
3	A	154	HEM	CMB-C2B-C1B	-4.23	118.42	125.03
3	B	154	HEM	C4D-C3D-C2D	4.19	112.99	106.89
3	B	154	HEM	O2A-CGA-CBA	4.12	127.03	114.00
3	A	154	HEM	C3B-C2B-C1B	4.04	109.44	106.41
3	A	154	HEM	O1D-CGD-CBD	-3.95	110.57	123.09
3	A	154	HEM	C3D-C4D-ND	-3.63	106.19	110.17
3	A	154	HEM	C4D-ND-C1D	3.59	109.46	105.21
3	A	154	HEM	C1B-NB-C4B	3.53	109.39	105.21
3	B	154	HEM	O2A-CGA-O1A	-3.51	114.30	123.33
3	A	154	HEM	CHA-C4D-ND	3.42	128.60	124.37
3	B	154	HEM	O2D-CGD-CBD	3.40	124.75	114.00
3	A	154	HEM	C2B-C1B-NB	-2.98	106.42	109.84
3	B	154	HEM	CHB-C1B-NB	2.90	127.96	124.37
3	A	154	HEM	CAD-CBD-CGD	-2.81	106.22	113.67
3	A	154	HEM	CAA-CBA-CGA	-2.73	106.43	113.67
3	A	154	HEM	CHC-C1C-NC	-2.62	121.60	124.45
3	B	154	HEM	C4D-ND-C1D	2.58	108.26	105.21
3	A	154	HEM	CAC-C3C-C4C	-2.47	118.92	124.82
3	A	154	HEM	CHB-C4A-NA	2.43	128.27	123.86
3	A	154	HEM	O2A-CGA-CBA	2.42	121.65	114.00
3	A	154	HEM	O2D-CGD-CBD	2.35	121.43	114.00
3	A	154	HEM	CHB-C4A-C3A	-2.34	120.63	127.43
3	A	154	HEM	C4A-CHB-C1B	-2.33	120.77	126.25
3	B	154	HEM	C2B-C1B-NB	-2.27	107.22	109.84
3	A	154	HEM	C1A-CHA-C4D	-2.26	120.92	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	154	HEM	O2A-CGA-O1A	-2.24	117.57	123.33
3	B	154	HEM	C4B-C3B-C2B	-2.24	105.22	107.28
3	B	154	HEM	CHA-C4D-C3D	2.14	129.17	125.23
3	A	154	HEM	CHD-C1D-ND	2.11	126.69	124.42
3	B	154	HEM	C1B-NB-C4B	2.10	107.69	105.21
3	B	154	HEM	CHC-C1C-NC	2.08	126.72	124.45
3	B	154	HEM	C4A-NA-C1A	-2.07	102.45	105.82
3	B	154	HEM	CHD-C4C-C3C	-2.06	121.74	125.21
3	B	154	HEM	CHB-C4A-C3A	-2.05	121.47	127.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	154	HEM	CAA-CBA-CGA-O2A
3	B	154	HEM	CAA-CBA-CGA-O2A
3	B	154	HEM	CAD-CBD-CGD-O2D
3	A	154	HEM	CAA-CBA-CGA-O1A
3	B	154	HEM	CAA-CBA-CGA-O1A
3	B	154	HEM	C4B-C3B-CAB-CBB
3	B	154	HEM	CAD-CBD-CGD-O1D
3	A	154	HEM	CAD-CBD-CGD-O1D
3	A	154	HEM	CAD-CBD-CGD-O2D
3	A	154	HEM	C2B-C3B-CAB-CBB

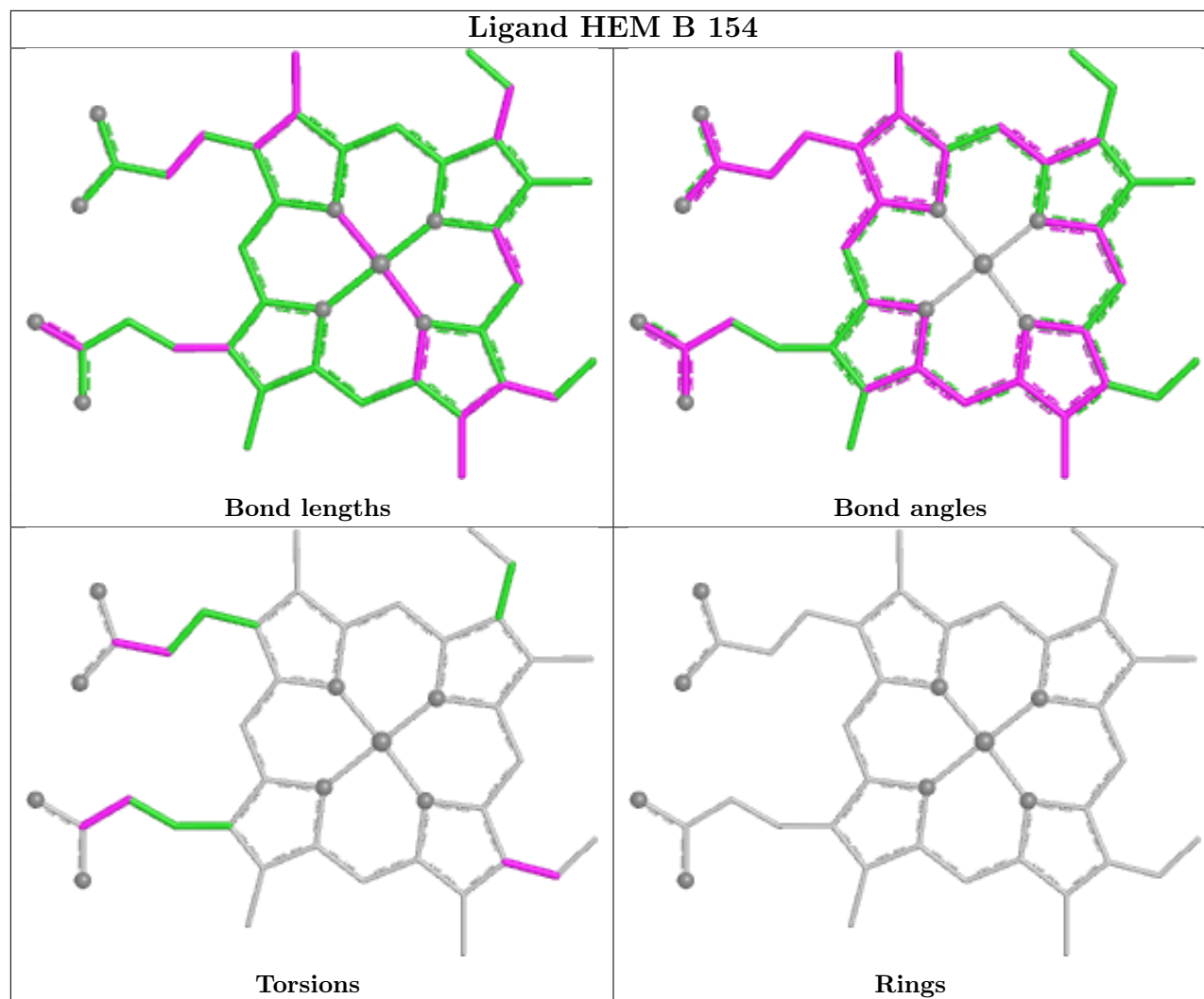
There are no ring outliers.

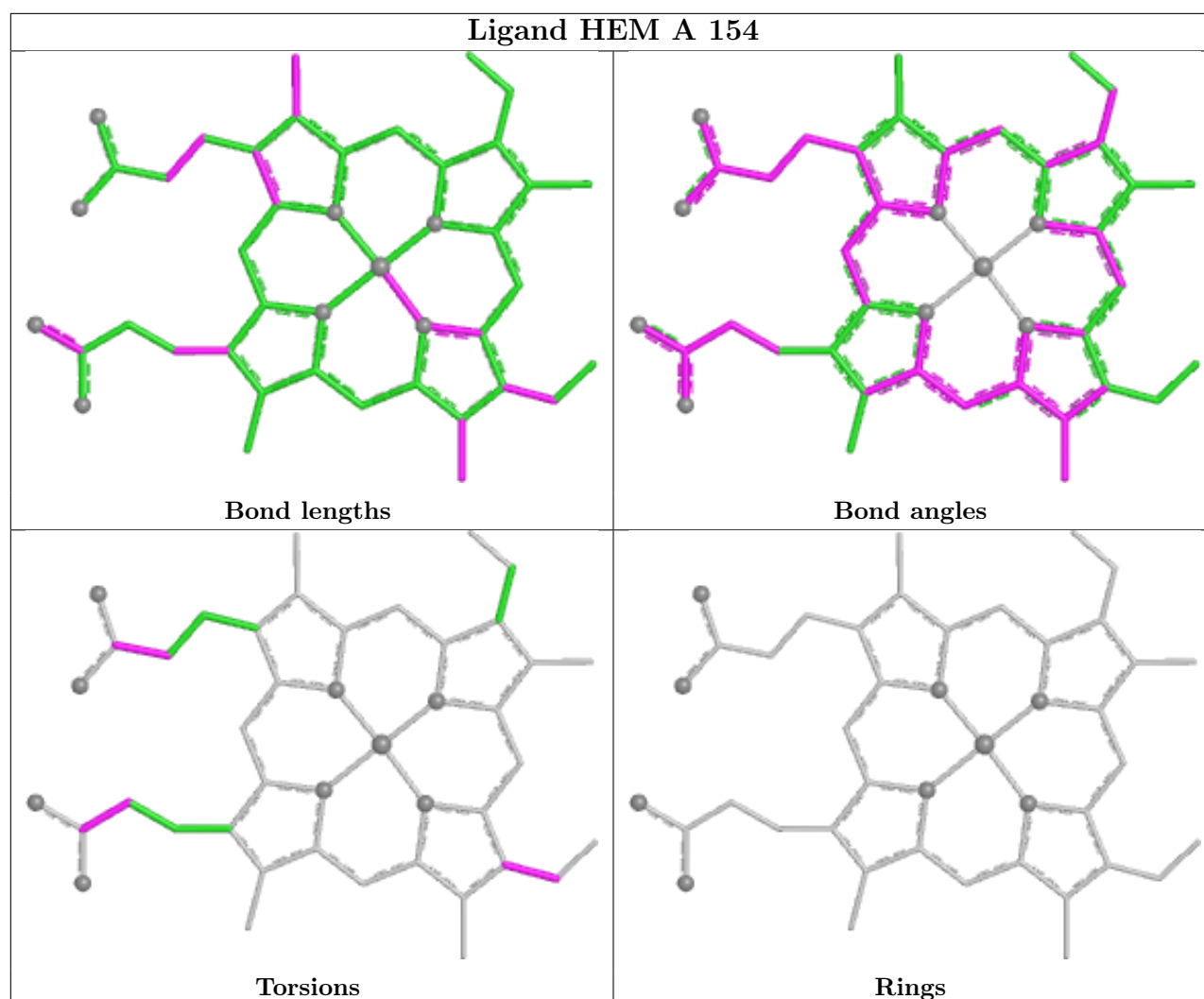
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	300	SO4	1	0
3	B	154	HEM	1	0
2	A	301	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.50	2 (1%) 75 81	13, 28, 56, 97	3 (1%)
1	B	153/153 (100%)	-0.53	1 (0%) 84 88	14, 27, 55, 88	3 (1%)
All	All	306/306 (100%)	-0.52	3 (0%) 79 84	13, 28, 56, 97	6 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	3.1
1	A	1	GLY	2.7
1	B	150	GLY	2.3

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
2	SO4	B	300	5/5	0.94	0.10	74,74,77,77	0
2	SO4	A	301	5/5	0.95	0.09	76,77,77,80	0

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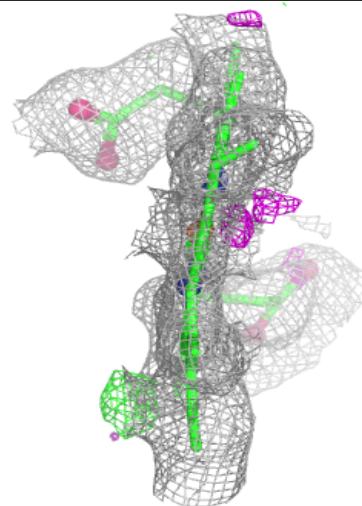
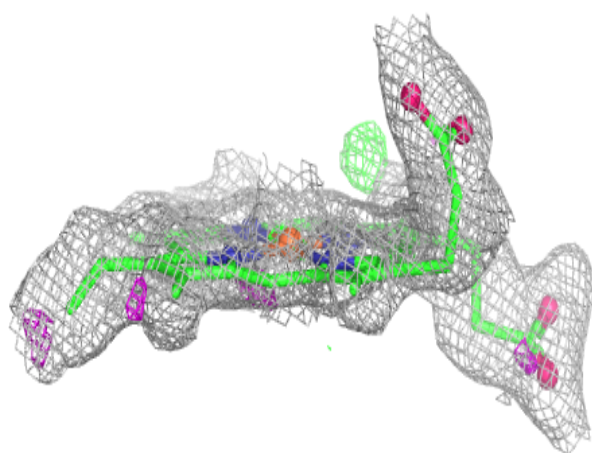
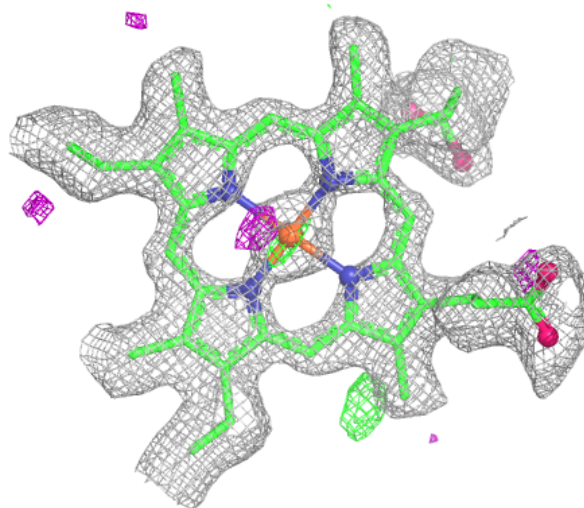
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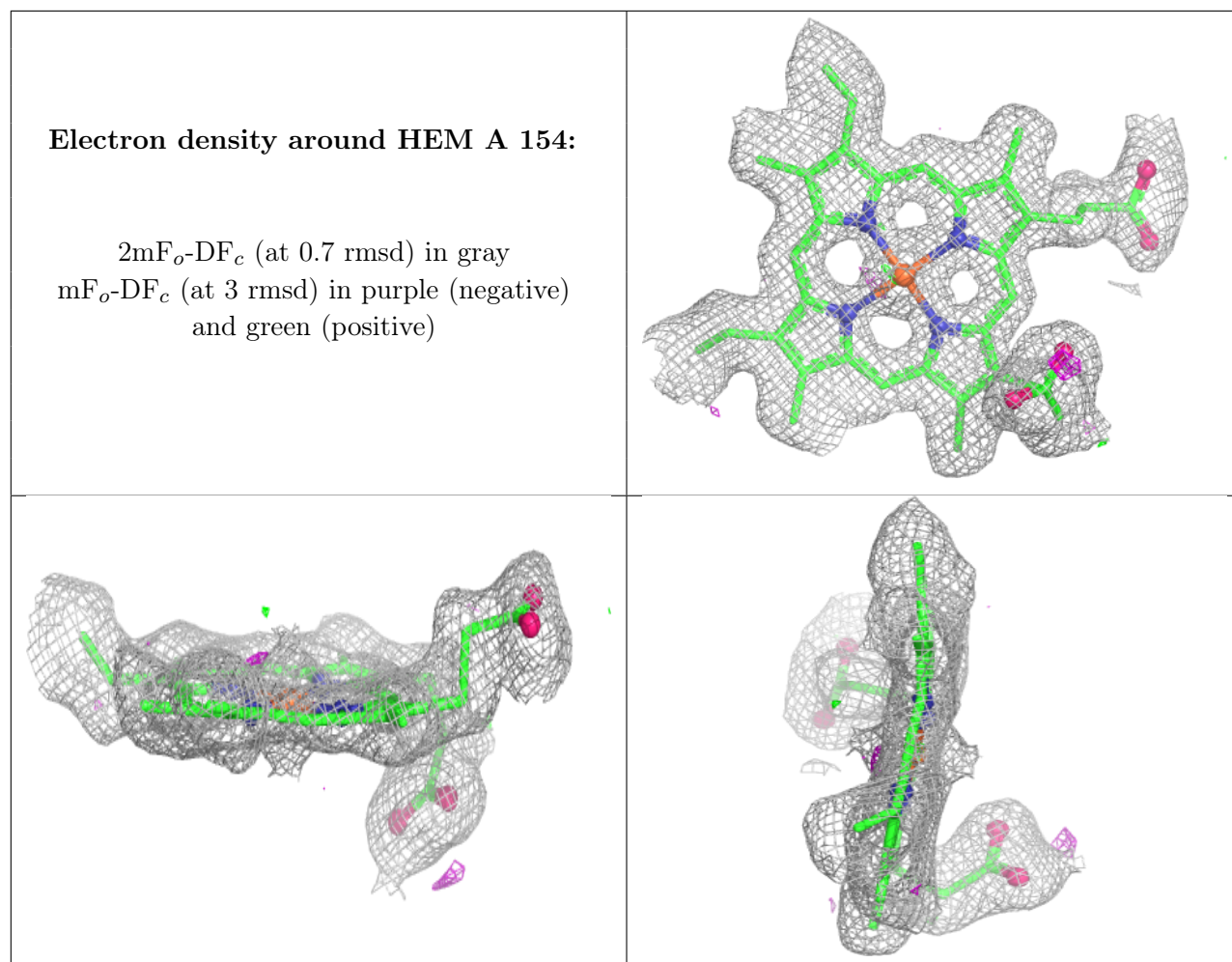
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	B	154	43/43	0.97	0.06	16,21,33,46	0
3	HEM	A	154	43/43	0.98	0.05	17,21,34,42	0

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 154:

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.