



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:44 AM UTC

PDB ID : 1YCA / pdb_00001yca
Title : DISTAL POCKET POLARITY IN LIGAND BINDING TO MYOGLOBIN:
DEOXY AND CARBONMONOXY FORMS OF A THREONINE68 (E11)
MUTANT INVESTIGATED BY X-RAY CRYSTALLOGRAPHY AND IN-
FRARED SPECTROSCOPY
Authors : Cameron, A.D.; Smerdon, S.J.; Wilkinson, A.J.; Habash, J.; Helliwell, J.R.
Deposited on : 1993-08-10
Resolution : 2.90 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

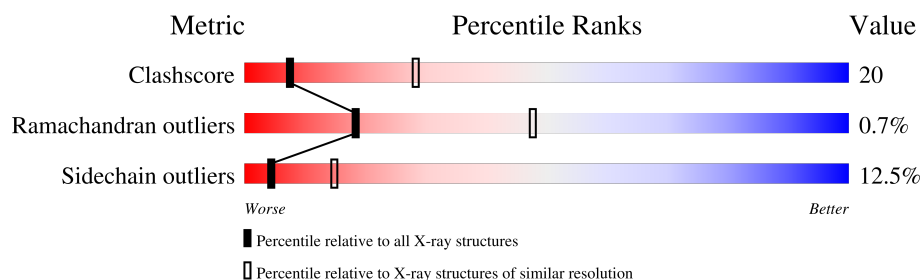
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2591 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.

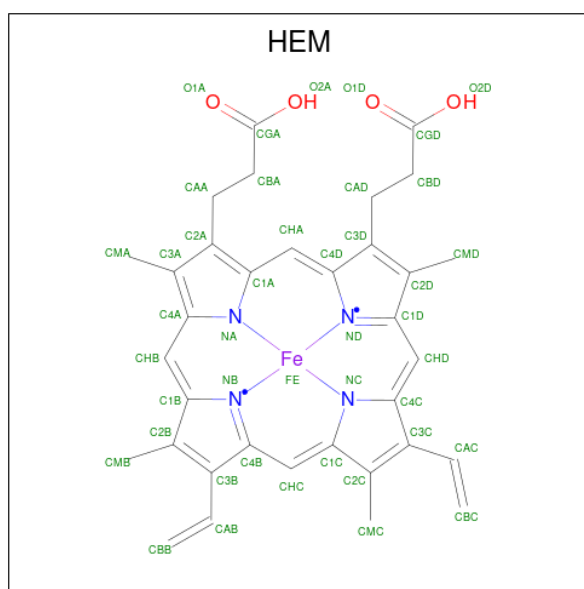
- Molecule 1 is a protein called MYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	42	0	0
			1197	763	208	223	3			
1	B	153	Total	C	N	O	S	48	0	0
			1197	763	208	223	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	THR	VAL	conflict	UNP P02189
B	68	THR	VAL	conflict	UNP P02189

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



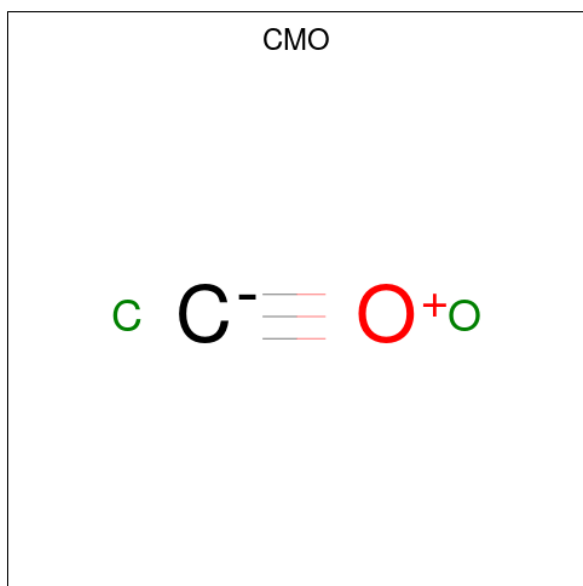
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 3 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			2	1	1		
3	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 4 is water.

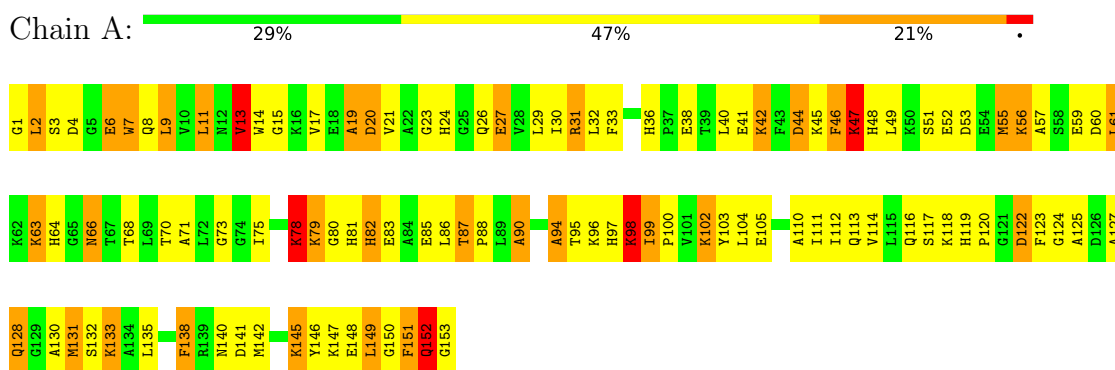
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	58	Total	O	0	0
			58	58		

3 Residue-property plots

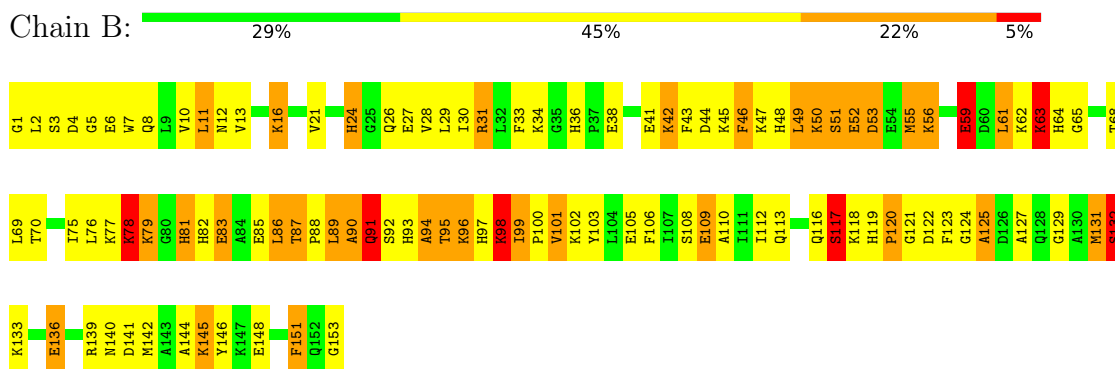
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: MYOGLOBIN



• Molecule 1: MYOGLOBIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.20 Å 42.50 Å 92.10 Å 90.00° 92.20° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2591	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, 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	1.74	14/1222 (1.1%)	2.83	139/1637 (8.5%)
1	B	1.65	8/1222 (0.7%)	2.96	133/1637 (8.1%)
All	All	1.69	22/2444 (0.9%)	2.89	272/3274 (8.3%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLY	C-OXT	-21.48	0.80	1.23
1	B	151	PHE	C-N	-19.00	1.06	1.33
1	A	152	GLN	CA-CB	-11.06	1.34	1.53
1	A	83	GLU	CB-CG	7.62	1.75	1.52
1	A	87	THR	CA-CB	7.39	1.60	1.54
1	A	1	GLY	N-CA	6.74	1.56	1.45
1	A	123	PHE	N-CA	6.33	1.54	1.46
1	A	56	LYS	CE-NZ	6.22	1.68	1.49
1	B	34	LYS	CD-CE	-6.11	1.34	1.52
1	B	129	GLY	N-CA	5.98	1.53	1.45
1	A	63	LYS	CD-CE	5.66	1.69	1.52
1	A	127	ALA	N-CA	5.27	1.52	1.46
1	B	112	ILE	N-CA	5.21	1.52	1.46
1	B	127	ALA	N-CA	5.18	1.52	1.46
1	A	20	ASP	N-CA	5.17	1.52	1.46
1	A	81	HIS	N-CA	5.12	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	GLU	N-CA	5.11	1.52	1.46
1	A	15	GLY	C-O	5.08	1.30	1.23
1	B	153	GLY	C-OXT	-5.06	1.13	1.23
1	B	29	LEU	N-CA	5.05	1.52	1.46
1	A	31	ARG	CD-NE	5.01	1.53	1.46
1	A	7	TRP	C-O	5.00	1.30	1.24

All (272) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	PHE	O-C-N	-34.08	77.26	122.59
1	B	136	GLU	CB-CG-CD	13.31	135.22	112.60
1	A	152	GLN	N-CA-CB	11.89	130.59	110.49
1	A	31	ARG	CD-NE-CZ	-11.55	108.24	124.40
1	A	60	ASP	CA-C-N	11.49	135.38	120.44
1	A	60	ASP	C-N-CA	11.49	135.38	120.44
1	B	26	GLN	OE1-CD-NE2	11.19	133.79	122.60
1	B	151	PHE	CA-C-N	10.72	140.47	121.92
1	B	151	PHE	C-N-CA	10.72	140.47	121.92
1	A	66	ASN	CA-C-O	10.61	131.96	120.82
1	A	49	LEU	CB-CA-C	10.42	126.83	109.84
1	A	132	SER	CA-CB-OG	-10.13	90.85	111.10
1	B	123	PHE	CA-C-O	-9.58	109.68	122.51
1	B	151	PHE	CA-C-O	-9.50	106.92	120.51
1	B	105	GLU	CA-C-O	9.49	130.48	120.42
1	B	98	LYS	CA-C-N	-9.34	113.31	123.02
1	B	98	LYS	C-N-CA	-9.34	113.31	123.02
1	A	81	HIS	CA-CB-CG	-9.14	104.66	113.80
1	B	124	GLY	O-C-N	-9.06	115.02	122.81
1	A	116	GLN	O-C-N	-9.04	112.54	122.12
1	A	113	GLN	CA-C-O	8.82	129.90	120.55
1	A	31	ARG	NE-CZ-NH1	-8.81	112.69	121.50
1	A	51	SER	O-C-N	8.67	132.36	123.26
1	B	132	SER	CA-CB-OG	-8.65	93.80	111.10
1	A	44	ASP	CA-CB-CG	-8.45	104.15	112.60
1	B	140	ASN	OD1-CG-ND2	-8.40	114.20	122.60
1	A	26	GLN	OE1-CD-NE2	-8.39	114.20	122.60
1	A	49	LEU	O-C-N	8.39	132.85	123.04
1	B	108	SER	N-CA-C	-8.36	102.17	111.28
1	B	81	HIS	CA-CB-CG	-8.05	105.75	113.80
1	B	48	HIS	CA-CB-CG	-8.01	105.79	113.80
1	A	48	HIS	CA-CB-CG	7.92	121.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLY	CA-C-N	-7.91	110.35	122.05
1	A	80	GLY	C-N-CA	-7.91	110.35	122.05
1	B	44	ASP	CA-CB-CG	-7.86	104.74	112.60
1	B	4	ASP	O-C-N	7.86	131.41	122.22
1	A	73	GLY	CA-C-N	7.86	130.20	120.22
1	A	73	GLY	C-N-CA	7.86	130.20	120.22
1	B	142	MET	N-CA-C	-7.84	102.67	111.14
1	B	112	ILE	CB-CG1-CD1	-7.84	97.34	113.80
1	A	78	LYS	CA-CB-CG	7.76	129.62	114.10
1	A	79	LYS	CA-C-O	-7.69	113.04	122.03
1	B	124	GLY	CA-C-N	7.68	130.91	120.54
1	B	124	GLY	C-N-CA	7.68	130.91	120.54
1	B	64	HIS	CA-CB-CG	-7.65	106.15	113.80
1	B	144	ALA	O-C-N	7.63	129.93	122.07
1	A	150	GLY	O-C-N	7.56	131.19	122.34
1	A	3	SER	O-C-N	-7.53	113.39	122.65
1	B	26	GLN	O-C-N	-7.51	114.22	122.03
1	A	102	LYS	CA-CB-CG	-7.50	99.11	114.10
1	B	82	HIS	CA-CB-CG	7.46	121.26	113.80
1	A	133	LYS	CA-C-O	7.44	128.31	120.42
1	B	94	ALA	O-C-N	7.44	132.48	122.59
1	B	12	ASN	CB-CG-ND2	7.38	127.47	116.40
1	B	99	ILE	O-C-N	7.36	127.20	121.46
1	A	46	PHE	O-C-N	7.35	130.87	122.20
1	B	103	TYR	O-C-N	7.34	131.30	122.27
1	B	21	VAL	N-CA-C	7.34	117.43	110.53
1	A	127	ALA	O-C-N	-7.33	114.35	122.12
1	A	60	ASP	CA-C-O	-7.26	111.62	119.97
1	A	82	HIS	N-CA-C	7.19	123.08	112.94
1	A	27	GLU	CB-CG-CD	-7.15	100.44	112.60
1	A	13	VAL	CA-C-O	7.14	128.42	120.85
1	B	139	ARG	CA-C-O	-7.12	113.34	120.82
1	B	81	HIS	N-CA-C	-7.09	101.72	110.65
1	A	146	TYR	CA-C-N	7.09	130.09	120.38
1	A	146	TYR	C-N-CA	7.09	130.09	120.38
1	A	9	LEU	N-CA-CB	-7.07	99.73	110.12
1	B	131	MET	CA-C-O	-7.06	113.07	120.55
1	A	6	GLU	CA-C-O	-7.05	113.64	120.90
1	A	64	HIS	CA-CB-CG	-7.03	106.77	113.80
1	B	79	LYS	CA-C-O	-7.00	113.84	122.03
1	A	36	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	125	ALA	CA-C-O	6.98	128.37	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	LYS	CB-CA-C	-6.97	99.21	110.79
1	B	132	SER	CB-CA-C	-6.93	97.35	110.67
1	B	27	GLU	CB-CG-CD	-6.93	100.83	112.60
1	B	59	GLU	CA-C-O	-6.90	112.03	119.97
1	B	69	LEU	CA-C-O	-6.90	112.31	120.10
1	B	29	LEU	CA-C-O	6.84	127.80	120.55
1	B	10	VAL	N-CA-CB	6.79	118.02	110.62
1	B	139	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	A	119	HIS	CA-CB-CG	-6.74	107.06	113.80
1	A	20	ASP	CA-CB-CG	-6.74	105.86	112.60
1	A	99	ILE	CA-C-O	-6.72	113.16	119.62
1	A	128	GLN	CA-C-O	6.69	128.06	120.90
1	B	43	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	33	PHE	CA-C-O	-6.67	111.93	119.79
1	A	8	GLN	OE1-CD-NE2	-6.66	115.94	122.60
1	B	90	ALA	CA-C-O	6.59	127.40	120.42
1	B	129	GLY	CA-C-N	-6.57	111.51	120.44
1	B	129	GLY	C-N-CA	-6.57	111.51	120.44
1	B	33	PHE	CA-C-O	-6.55	113.95	120.70
1	A	40	LEU	CA-C-O	-6.49	112.77	120.10
1	A	31	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	A	73	GLY	O-C-N	-6.46	115.39	122.24
1	A	118	LYS	CA-C-N	-6.45	115.67	122.89
1	A	118	LYS	C-N-CA	-6.45	115.67	122.89
1	A	17	VAL	N-CA-C	-6.43	104.06	110.62
1	A	99	ILE	O-C-N	6.41	127.08	121.12
1	B	34	LYS	O-C-N	-6.37	114.89	122.15
1	A	19	ALA	N-CA-C	-6.37	105.48	113.18
1	A	40	LEU	O-C-N	6.35	129.65	122.22
1	B	48	HIS	CB-CA-C	6.35	121.68	110.37
1	B	85	GLU	O-C-N	6.35	130.08	122.27
1	A	117	SER	CA-C-O	-6.35	113.69	120.42
1	B	117	SER	CA-CB-OG	-6.35	98.40	111.10
1	A	80	GLY	N-CA-C	-6.35	107.53	115.08
1	A	142	MET	N-CA-CB	6.35	119.55	110.16
1	A	29	LEU	CA-C-O	-6.33	113.84	120.55
1	B	63	LYS	N-CA-CB	6.26	119.09	110.01
1	A	21	VAL	CA-CB-CG1	6.26	121.04	110.40
1	A	85	GLU	CA-C-O	-6.26	112.40	119.79
1	A	147	LYS	O-C-N	6.25	128.75	122.12
1	B	123	PHE	N-CA-CB	-6.25	103.35	110.35
1	A	47	LYS	CA-C-O	6.24	127.04	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	GLN	CA-C-O	6.21	127.14	120.55
1	A	68	THR	CA-C-O	-6.18	114.34	120.70
1	B	75	ILE	CA-C-N	6.16	128.86	120.54
1	B	75	ILE	C-N-CA	6.16	128.86	120.54
1	B	48	HIS	CA-C-N	-6.14	113.53	122.19
1	B	48	HIS	C-N-CA	-6.14	113.53	122.19
1	A	53	ASP	N-CA-C	-6.13	104.67	111.71
1	A	142	MET	N-CA-C	-6.12	104.69	111.36
1	A	19	ALA	O-C-N	-6.09	113.54	122.43
1	B	29	LEU	N-CA-CB	-6.08	101.18	110.12
1	B	106	PHE	N-CA-CB	6.08	119.16	110.16
1	B	136	GLU	CA-CB-CG	6.08	126.26	114.10
1	B	127	ALA	O-C-N	-6.08	115.68	122.12
1	A	4	ASP	N-CA-C	-6.06	104.74	111.71
1	B	49	LEU	CB-CA-C	6.03	119.68	109.80
1	B	36	HIS	O-C-N	6.02	126.29	121.17
1	B	106	PHE	CA-C-O	-6.01	114.05	120.42
1	A	145	LYS	N-CA-C	-6.01	104.85	111.82
1	A	138	PHE	CB-CA-C	6.00	120.76	110.79
1	A	138	PHE	N-CA-C	-5.99	104.75	111.28
1	B	132	SER	O-C-N	5.96	129.60	122.27
1	A	104	LEU	CA-C-O	5.93	126.81	120.10
1	B	36	HIS	CA-CB-CG	-5.92	107.88	113.80
1	B	148	GLU	N-CA-CB	-5.91	101.41	110.16
1	B	141	ASP	CA-CB-CG	-5.88	106.72	112.60
1	B	77	LYS	O-C-N	-5.87	115.35	122.22
1	B	8	GLN	CA-C-O	-5.86	114.21	120.42
1	B	56	LYS	N-CA-C	5.85	119.68	112.54
1	A	66	ASN	CA-CB-CG	-5.84	106.76	112.60
1	B	63	LYS	N-CA-C	-5.84	104.82	111.07
1	A	100	PRO	CA-C-O	-5.82	114.63	122.08
1	B	62	LYS	CA-C-N	5.82	128.00	120.44
1	B	62	LYS	C-N-CA	5.82	128.00	120.44
1	A	125	ALA	N-CA-CB	-5.80	101.30	109.94
1	A	127	ALA	CB-CA-C	5.79	120.39	110.79
1	B	52	GLU	CB-CG-CD	5.76	122.39	112.60
1	A	111	ILE	O-C-N	-5.73	116.29	121.91
1	B	91	GLN	N-CA-CB	-5.73	101.54	109.91
1	A	116	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	B	120	PRO	CA-C-O	5.72	129.09	120.05
1	B	31	ARG	CB-CG-CD	5.72	124.45	111.30
1	B	34	LYS	CG-CD-CE	5.71	124.44	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	GLU	N-CA-CB	-5.68	101.76	110.12
1	A	21	VAL	CA-C-N	-5.67	112.24	120.29
1	A	21	VAL	C-N-CA	-5.67	112.24	120.29
1	A	14	TRP	CA-C-O	-5.66	113.70	120.10
1	B	46	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	51	SER	O-C-N	5.61	129.02	123.46
1	B	85	GLU	CA-C-O	-5.61	113.52	119.97
1	A	122	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	44	ASP	CA-C-O	5.60	127.23	121.07
1	A	120	PRO	CA-C-O	5.58	128.87	120.05
1	A	102	LYS	CG-CD-CE	5.57	124.11	111.30
1	A	61	LEU	N-CA-C	-5.57	105.11	111.07
1	A	149	LEU	N-CA-C	-5.57	106.26	113.16
1	B	16	LYS	CA-C-N	-5.57	112.52	120.42
1	B	16	LYS	C-N-CA	-5.57	112.52	120.42
1	B	65	GLY	O-C-N	-5.55	116.85	122.18
1	B	86	LEU	CA-C-O	-5.53	112.80	119.27
1	B	125	ALA	N-CA-CB	-5.53	101.69	109.94
1	B	87	THR	CA-C-O	5.53	124.15	118.73
1	B	68	THR	CA-CB-OG1	-5.51	101.33	109.60
1	A	149	LEU	CA-C-O	5.48	125.91	119.28
1	A	123	PHE	CA-C-N	5.47	129.36	121.54
1	A	123	PHE	C-N-CA	5.47	129.36	121.54
1	A	105	GLU	CA-CB-CG	5.47	125.04	114.10
1	A	113	GLN	OE1-CD-NE2	5.47	128.07	122.60
1	B	89	LEU	CA-C-N	5.46	128.04	120.29
1	B	89	LEU	C-N-CA	5.46	128.04	120.29
1	B	110	ALA	CA-C-O	5.46	126.55	120.82
1	A	2	LEU	N-CA-CB	-5.45	102.02	110.46
1	B	70	THR	CA-CB-OG1	-5.45	101.43	109.60
1	B	127	ALA	CA-C-O	5.44	126.32	120.55
1	A	36	HIS	O-C-N	5.44	125.62	121.27
1	B	78	LYS	N-CA-C	-5.43	106.63	113.20
1	B	85	GLU	CB-CG-CD	-5.43	103.37	112.60
1	B	109	GLU	CA-C-N	5.42	127.49	120.44
1	B	109	GLU	C-N-CA	5.42	127.49	120.44
1	B	125	ALA	O-C-N	-5.42	116.45	122.09
1	B	1	GLY	CA-C-N	-5.41	113.40	122.92
1	B	1	GLY	C-N-CA	-5.41	113.40	122.92
1	B	89	LEU	CB-CA-C	5.41	120.04	110.85
1	A	64	HIS	N-CA-C	-5.39	105.48	111.36
1	B	53	ASP	O-C-N	5.39	127.83	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	GLU	N-CA-C	-5.37	105.46	112.23
1	A	151	PHE	CA-C-O	-5.37	115.34	121.68
1	A	118	LYS	N-CA-C	5.37	119.00	112.23
1	A	70	THR	CA-C-O	-5.34	115.21	120.82
1	A	122	ASP	N-CA-C	-5.34	105.40	112.94
1	B	79	LYS	CB-CA-C	-5.33	103.96	111.95
1	A	46	PHE	CA-C-O	-5.32	112.90	119.18
1	B	41	GLU	CB-CA-C	-5.32	100.78	110.63
1	A	59	GLU	N-CA-CB	5.32	118.12	110.20
1	B	5	GLY	O-C-N	5.31	127.28	122.18
1	A	55	MET	N-CA-C	-5.30	105.41	111.14
1	A	24	HIS	CA-C-N	-5.30	114.17	120.00
1	A	24	HIS	C-N-CA	-5.30	114.17	120.00
1	A	38	GLU	CB-CG-CD	5.30	121.61	112.60
1	B	3	SER	CA-C-O	-5.29	115.56	121.81
1	A	32	LEU	N-CA-CB	-5.29	102.35	110.12
1	B	105	GLU	CA-C-N	-5.28	112.80	120.29
1	B	105	GLU	C-N-CA	-5.28	112.80	120.29
1	A	85	GLU	N-CA-CB	5.28	118.43	110.30
1	A	53	ASP	CA-C-N	-5.27	111.72	120.68
1	A	53	ASP	C-N-CA	-5.27	111.72	120.68
1	A	61	LEU	CD1-CG-CD2	-5.26	99.22	110.80
1	A	99	ILE	N-CA-C	5.26	113.73	107.73
1	B	87	THR	CA-CB-CG2	5.26	119.44	110.50
1	B	24	HIS	CA-CB-CG	-5.25	108.55	113.80
1	A	98	LYS	N-CA-CB	-5.24	103.36	111.65
1	A	49	LEU	N-CA-C	-5.24	101.43	109.76
1	B	102	LYS	N-CA-CB	5.24	118.29	110.22
1	A	145	LYS	N-CA-CB	5.23	118.39	110.28
1	A	33	PHE	O-C-N	5.22	129.32	122.33
1	A	57	ALA	O-C-N	5.22	129.61	122.46
1	A	112	ILE	CA-C-O	5.22	126.38	120.95
1	B	62	LYS	CG-CD-CE	-5.21	99.31	111.30
1	A	2	LEU	CA-C-O	-5.21	115.28	121.89
1	B	103	TYR	CA-C-O	-5.21	113.98	119.97
1	B	11	LEU	CA-C-O	-5.21	114.22	120.10
1	B	127	ALA	CB-CA-C	5.19	119.41	110.79
1	A	13	VAL	O-C-N	-5.19	116.48	121.83
1	A	94	ALA	CA-C-O	-5.19	115.00	120.55
1	B	61	LEU	N-CA-C	-5.19	105.69	112.23
1	B	132	SER	N-CA-C	5.17	117.82	111.82
1	B	55	MET	N-CA-C	-5.17	105.56	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	TYR	CA-C-O	-5.16	114.27	120.10
1	B	108	SER	CA-C-N	-5.16	112.46	120.31
1	B	108	SER	C-N-CA	-5.16	112.46	120.31
1	A	122	ASP	CA-C-N	-5.15	111.70	121.54
1	A	122	ASP	C-N-CA	-5.15	111.70	121.54
1	A	13	VAL	CA-CB-CG2	-5.15	101.65	110.40
1	B	144	ALA	N-CA-C	-5.15	105.56	111.07
1	B	96	LYS	CA-C-O	5.14	126.74	120.31
1	B	92	SER	CA-C-O	-5.11	115.14	120.55
1	A	13	VAL	CB-CA-C	5.11	119.27	112.22
1	A	90	ALA	N-CA-C	-5.10	105.80	111.36
1	A	87	THR	CA-C-O	5.10	123.23	118.44
1	B	12	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	85	GLU	CG-CD-OE1	5.09	130.10	118.40
1	B	122	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	113	GLN	CA-CB-CG	-5.08	103.94	114.10
1	A	71	ALA	N-CA-CB	5.08	117.67	110.16
1	A	105	GLU	CA-C-O	5.07	125.80	120.42
1	A	2	LEU	N-CA-C	-5.07	102.95	110.46
1	A	2	LEU	O-C-N	5.06	128.71	122.84
1	A	27	GLU	CG-CD-OE1	-5.05	106.78	118.40
1	A	44	ASP	CA-C-N	5.05	128.68	120.60
1	A	44	ASP	C-N-CA	5.05	128.68	120.60
1	B	83	GLU	O-C-N	-5.05	116.77	122.12
1	A	131	MET	CG-SD-CE	-5.04	89.81	100.90
1	A	24	HIS	N-CA-C	-5.03	105.99	111.82
1	A	11	LEU	CA-C-O	5.03	125.78	120.10
1	B	31	ARG	N-CA-C	-5.01	105.90	111.36
1	B	76	LEU	O-C-N	5.01	127.30	122.09
1	A	17	VAL	O-C-N	-5.01	117.01	121.87

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	151	PHE	Mainchain

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	1197	0	1203	44	0
1	B	1197	0	1202	50	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	49	0	0	4	0
4	B	58	0	0	4	0
All	All	2591	0	2465	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (96) 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:B:78:LYS:HZ3	1:B:78:LYS:HB3	1.30	0.94
1:B:31:ARG:HD2	4:B:176:HOH:O	1.68	0.93
1:B:78:LYS:HB3	1:B:78:LYS:NZ	1.93	0.80
1:A:96:LYS:HE2	4:A:191:HOH:O	1.81	0.79
2:B:154:HEM:HMC1	2:B:154:HEM:HBC2	1.65	0.79
1:A:42:LYS:NZ	1:A:98:LYS:O	2.18	0.75
1:A:42:LYS:HG2	1:A:99:ILE:CD1	2.20	0.72
1:B:46:PHE:HB3	1:B:49:LEU:HD12	1.71	0.71
1:B:42:LYS:HG2	1:B:99:ILE:CD1	2.20	0.71
1:A:87:THR:HB	1:A:88:PRO:HD3	1.72	0.70
2:A:154:HEM:HMC1	2:A:154:HEM:HBC2	1.73	0.69
1:B:87:THR:HB	1:B:88:PRO:HD3	1.76	0.68
1:B:42:LYS:HG2	1:B:99:ILE:HD12	1.75	0.67
1:A:96:LYS:HD3	1:A:97:HIS:CE1	2.30	0.67
1:B:87:THR:O	1:B:91:GLN:HB2	1.95	0.66
1:B:52:GLU:O	1:B:56:LYS:HG3	1.96	0.65
1:A:86:LEU:CD2	1:A:141:ASP:HB3	2.29	0.62
1:B:118:LYS:NZ	4:B:199:HOH:O	2.31	0.62
1:B:38:GLU:OE1	1:B:38:GLU:N	2.28	0.61
1:A:86:LEU:HD21	1:A:141:ASP:HB3	1.82	0.60
2:B:154:HEM:HBC2	2:B:154:HEM:CMC	2.31	0.60
1:A:46:PHE:CZ	1:A:61:LEU:HA	2.37	0.59
1:B:59:GLU:O	1:B:63:LYS:HD2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ALA:O	1:B:94:ALA:CB	2.50	0.59
1:B:11:LEU:CD1	1:B:79:LYS:HE3	2.32	0.59
1:A:31:ARG:NH1	4:A:171:HOH:O	2.35	0.57
1:B:132:SER:O	1:B:136:GLU:HB2	2.06	0.56
2:A:154:HEM:HBC2	2:A:154:HEM:CMC	2.35	0.55
1:B:11:LEU:HD11	1:B:79:LYS:HE3	1.89	0.55
1:A:149:LEU:O	1:B:91:GLN:OE1	2.24	0.55
1:B:86:LEU:HD23	1:B:145:LYS:HD3	1.89	0.54
1:B:52:GLU:HG2	1:B:56:LYS:HE3	1.89	0.54
1:B:87:THR:N	1:B:88:PRO:CD	2.71	0.54
1:A:110:ALA:O	1:A:114:VAL:HG23	2.08	0.53
1:B:90:ALA:O	1:B:94:ALA:HB2	2.09	0.53
1:B:101:VAL:HG12	1:B:146:TYR:CD2	2.43	0.52
1:A:42:LYS:HG2	1:A:99:ILE:HD13	1.90	0.52
1:B:61:LEU:C	1:B:61:LEU:HD23	2.35	0.52
1:A:87:THR:N	1:A:88:PRO:CD	2.74	0.51
1:A:124:GLY:O	1:A:128:GLN:HG3	2.11	0.51
1:A:30:ILE:HG12	1:A:55:MET:HB3	1.93	0.51
1:B:93:HIS:O	1:B:99:ILE:N	2.38	0.50
1:A:7:TRP:O	1:A:11:LEU:HG	2.12	0.49
1:A:19:ALA:O	1:A:20:ASP:HB2	2.12	0.49
1:B:120:PRO:O	1:B:121:GLY:C	2.53	0.48
1:B:78:LYS:HB3	1:B:81:HIS:O	2.14	0.48
1:B:61:LEU:HD23	1:B:61:LEU:O	2.13	0.48
1:A:75:ILE:O	1:A:78:LYS:HB2	2.14	0.47
1:A:140:ASN:ND2	4:A:201:HOH:O	2.46	0.47
1:A:44:ASP:O	1:A:47:LYS:HG3	2.14	0.47
1:B:96:LYS:HE3	4:B:213:HOH:O	2.14	0.47
1:A:131:MET:HE2	1:A:131:MET:HB2	1.59	0.47
1:B:78:LYS:NZ	1:B:81:HIS:O	2.47	0.46
1:B:96:LYS:HD2	1:B:97:HIS:CE1	2.50	0.46
1:A:87:THR:CB	1:A:88:PRO:HD3	2.44	0.46
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.71	0.46
1:A:99:ILE:HD12	2:A:154:HEM:CAC	2.46	0.46
1:B:2:LEU:HD23	1:B:6:GLU:HB3	1.98	0.46
1:B:78:LYS:O	1:B:79:LYS:C	2.58	0.46
1:A:31:ARG:HD2	4:A:171:HOH:O	2.16	0.46
1:B:30:ILE:HG12	1:B:55:MET:HB3	1.97	0.46
1:B:119:HIS:N	1:B:120:PRO:CD	2.78	0.46
1:A:23:GLY:O	1:A:27:GLU:HG3	2.15	0.45
1:A:7:TRP:CE3	1:A:7:TRP:HA	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD12	1:B:93:HIS:CE1	2.52	0.45
1:B:11:LEU:HD12	1:B:79:LYS:HE3	1.97	0.45
1:B:6:GLU:O	1:B:7:TRP:C	2.59	0.45
1:B:78:LYS:NZ	1:B:78:LYS:CB	2.59	0.45
1:A:97:HIS:NE2	2:A:154:HEM:O1A	2.41	0.45
1:B:83:GLU:O	1:B:83:GLU:HG3	2.16	0.44
1:B:24:HIS:O	1:B:28:VAL:HG23	2.17	0.44
1:A:2:LEU:HD23	1:A:6:GLU:HB3	2.00	0.44
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.65	0.44
1:A:87:THR:N	1:A:88:PRO:HD2	2.33	0.44
1:A:95:THR:HB	1:B:95:THR:HG21	1.98	0.44
1:A:42:LYS:HG2	1:A:99:ILE:HD11	1.97	0.44
1:A:52:GLU:O	1:A:56:LYS:HG3	2.17	0.44
1:A:95:THR:HG22	1:A:151:PHE:CZ	2.53	0.44
1:A:90:ALA:O	1:A:94:ALA:CB	2.66	0.43
1:B:42:LYS:CG	1:B:99:ILE:CD1	2.95	0.43
1:B:113:GLN:O	1:B:117:SER:HB3	2.18	0.43
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.72	0.43
1:B:131:MET:HB2	1:B:131:MET:HE2	1.67	0.43
1:B:101:VAL:HG12	1:B:146:TYR:HD2	1.85	0.42
1:B:50:LYS:O	1:B:51:SER:HB3	2.20	0.42
1:B:98:LYS:O	1:B:100:PRO:HD3	2.20	0.41
1:A:130:ALA:HA	1:A:133:LYS:HZ2	1.85	0.41
1:A:13:VAL:CG1	1:A:131:MET:CE	2.98	0.41
1:A:86:LEU:C	1:A:88:PRO:HD2	2.44	0.41
1:A:82:HIS:NE2	1:A:141:ASP:OD2	2.39	0.41
1:A:44:ASP:O	1:A:47:LYS:CG	2.68	0.41
1:A:52:GLU:HG2	1:A:56:LYS:CE	2.51	0.41
1:B:125:ALA:N	4:B:203:HOH:O	2.39	0.41
1:A:78:LYS:O	1:A:79:LYS:C	2.64	0.41
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.90	0.40
1:A:63:LYS:O	1:A:66:ASN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/153 (99%)	146 (97%)	4 (3%)	1 (1%)	18	48
1	B	151/153 (99%)	143 (95%)	7 (5%)	1 (1%)	18	48
All	All	302/306 (99%)	289 (96%)	11 (4%)	2 (1%)	18	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	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	124/124 (100%)	111 (90%)	13 (10%)	6	22
1	B	124/124 (100%)	106 (86%)	18 (14%)	3	10
All	All	248/248 (100%)	217 (88%)	31 (12%)	4	15

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	41	GLU
1	A	42	LYS
1	A	45	LYS
1	A	47	LYS
1	A	78	LYS
1	A	98	LYS
1	A	102	LYS
1	A	122	ASP
1	A	138	PHE

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Mol	Chain	Res	Type
1	A	145	LYS
1	A	148	GLU
1	A	152	GLN
1	B	13	VAL
1	B	16	LYS
1	B	42	LYS
1	B	47	LYS
1	B	50	LYS
1	B	53	ASP
1	B	59	GLU
1	B	63	LYS
1	B	78	LYS
1	B	91	GLN
1	B	95	THR
1	B	98	LYS
1	B	101	VAL
1	B	109	GLU
1	B	117	SER
1	B	132	SER
1	B	133	LYS
1	B	145	LYS

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	B	26	GLN
1	B	36	HIS
1	B	81	HIS
1	B	116	GLN
1	B	128	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	154	1,3	50,50,50	1.49	11 (22%)	67,82,82	1.55	12 (17%)
2	HEM	B	154	1,3	50,50,50	1.46	7 (14%)	67,82,82	1.64	13 (19%)
3	CMO	A	155	2	0,1,1	-	-	-		
3	CMO	B	155	2	0,1,1	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	154	1,3	-	7/14/54/54	-
2	HEM	B	154	1,3	-	7/14/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	154	HEM	CAC-C3C	3.68	1.57	1.47
2	A	154	HEM	CMB-C2B	3.67	1.58	1.50
2	A	154	HEM	CAB-C3B	3.19	1.55	1.47
2	B	154	HEM	CAB-C3B	2.89	1.55	1.47
2	B	154	HEM	FE-NB	2.82	2.03	1.94
2	B	154	HEM	FE-ND	2.80	2.03	1.94
2	A	154	HEM	O1A-CGA	2.79	1.31	1.22
2	A	154	HEM	CAC-C3C	2.66	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	CMD-C2D	2.58	1.56	1.50
2	A	154	HEM	CMC-C2C	2.48	1.55	1.50
2	B	154	HEM	CMB-C2B	2.34	1.55	1.50
2	A	154	HEM	C3B-C2B	-2.31	1.32	1.37
2	A	154	HEM	FE-NB	2.23	2.01	1.94
2	A	154	HEM	FE-ND	2.06	2.01	1.94
2	A	154	HEM	O2D-CGD	-2.05	1.24	1.30
2	B	154	HEM	C2A-C3A	-2.03	1.33	1.38
2	A	154	HEM	CMA-C3A	2.02	1.54	1.50
2	B	154	HEM	O1A-CGA	2.01	1.28	1.22

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	O2A-CGA-O1A	-6.19	107.41	123.33
2	B	154	HEM	CHD-C1D-ND	4.02	128.75	124.42
2	B	154	HEM	CMB-C2B-C1B	-3.66	119.31	125.03
2	B	154	HEM	CBD-CAD-C3D	-3.50	102.86	112.53
2	A	154	HEM	CHB-C1B-NB	3.23	128.37	124.37
2	B	154	HEM	CHD-C4C-NC	3.09	127.82	124.45
2	B	154	HEM	CBB-CAB-C3B	-2.90	113.03	127.53
2	A	154	HEM	CAC-C3C-C4C	-2.86	117.99	124.82
2	A	154	HEM	O1A-CGA-CBA	2.84	132.09	123.09
2	B	154	HEM	O2D-CGD-CBD	2.83	122.93	114.00
2	B	154	HEM	C3D-C4D-ND	-2.80	107.09	110.17
2	B	154	HEM	C4C-CHD-C1D	-2.67	120.36	126.02
2	A	154	HEM	CHD-C1D-ND	2.65	127.27	124.42
2	A	154	HEM	CHD-C4C-NC	2.31	126.96	124.45
2	B	154	HEM	O2A-CGA-CBA	2.30	121.26	114.00
2	B	154	HEM	CMA-C3A-C2A	2.28	130.47	125.62
2	A	154	HEM	CBC-CAC-C3C	-2.28	116.15	127.53
2	A	154	HEM	O2D-CGD-CBD	2.20	120.94	114.00
2	A	154	HEM	C4C-C3C-C2C	2.17	108.69	106.81
2	A	154	HEM	C3B-C2B-C1B	2.05	107.95	106.41
2	A	154	HEM	O2A-CGA-CBA	2.05	120.48	114.00
2	B	154	HEM	C2B-C1B-NB	-2.04	107.49	109.84
2	B	154	HEM	CBC-CAC-C3C	-2.04	117.32	127.53
2	A	154	HEM	C4A-CHB-C1B	-2.04	121.45	126.25
2	B	154	HEM	O1D-CGD-CBD	-2.03	116.65	123.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

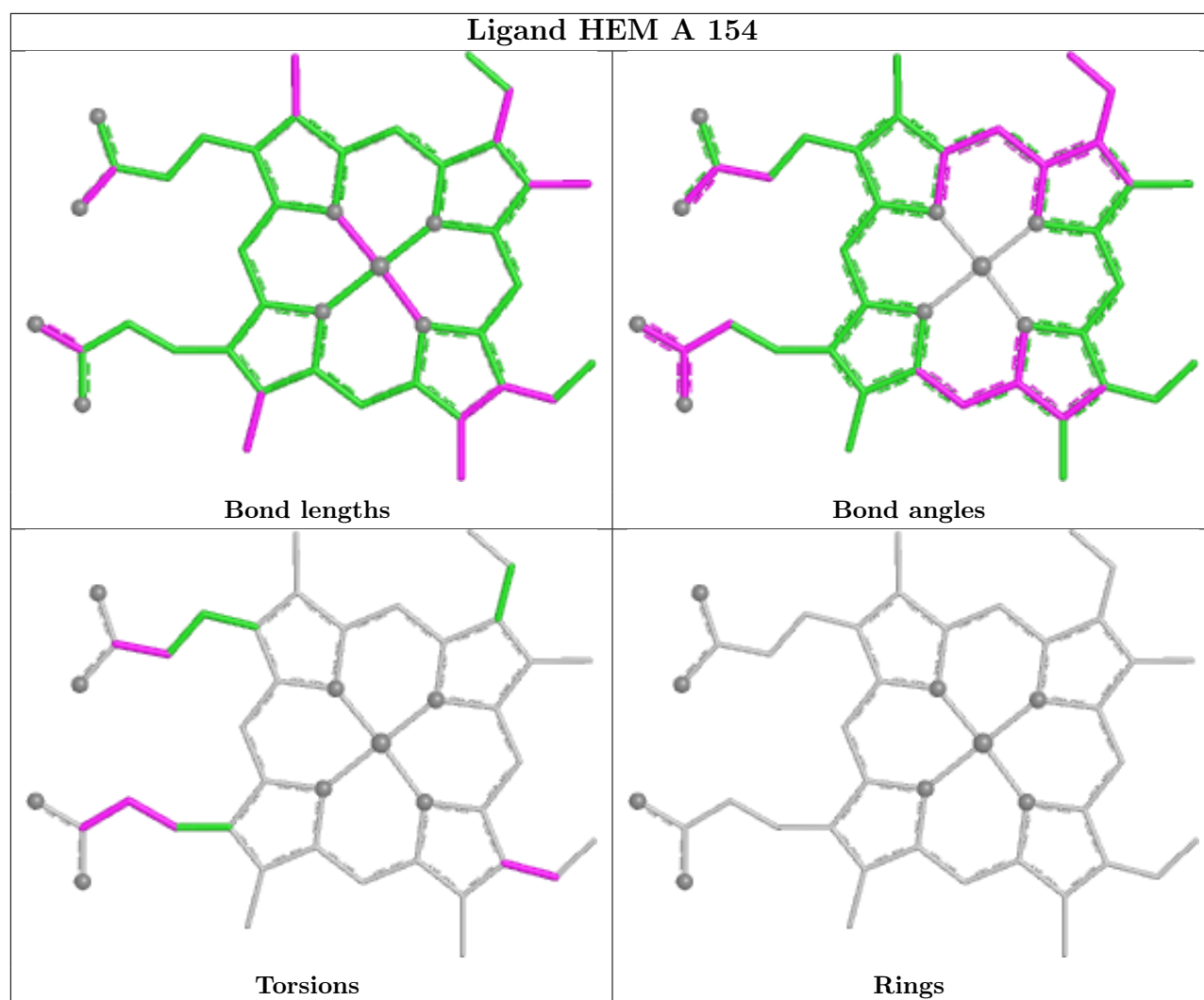
Mol	Chain	Res	Type	Atoms
2	A	154	HEM	C2B-C3B-CAB-CBB
2	A	154	HEM	C4B-C3B-CAB-CBB
2	A	154	HEM	C2A-CAA-CBA-CGA
2	B	154	HEM	C2A-CAA-CBA-CGA
2	B	154	HEM	C2B-C3B-CAB-CBB
2	B	154	HEM	C4B-C3B-CAB-CBB
2	A	154	HEM	CAA-CBA-CGA-O2A
2	B	154	HEM	CAA-CBA-CGA-O2A
2	A	154	HEM	CAA-CBA-CGA-O1A
2	A	154	HEM	CAD-CBD-CGD-O1D
2	A	154	HEM	CAD-CBD-CGD-O2D
2	B	154	HEM	CAA-CBA-CGA-O1A
2	B	154	HEM	CAD-CBD-CGD-O2D
2	B	154	HEM	CAD-CBD-CGD-O1D

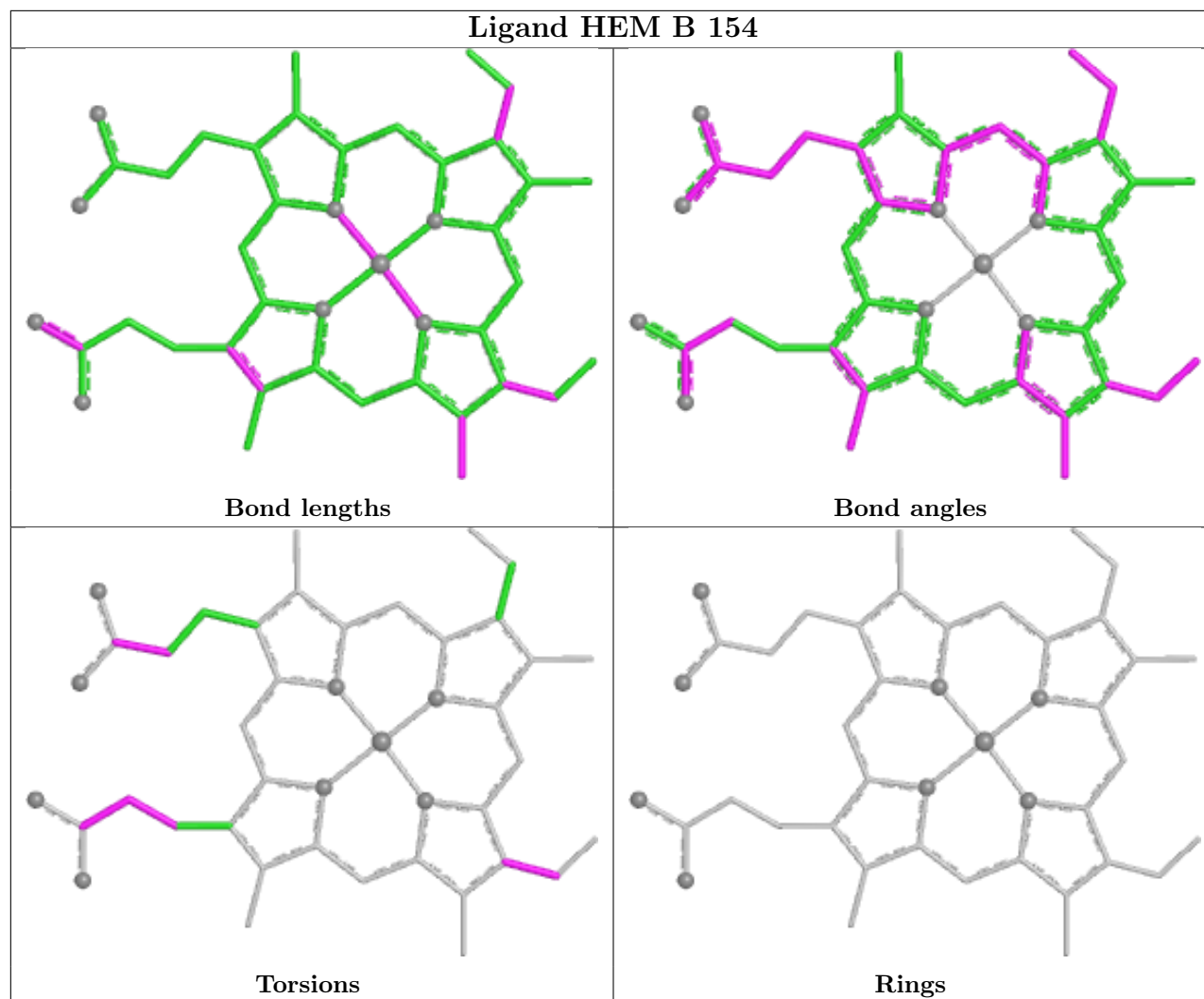
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	4	0
2	B	154	HEM	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	151:PHE	C	152:GLN	N	1.06

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.