



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:52 AM UTC

PDB ID : 1MYH / pdb_00001myh
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 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

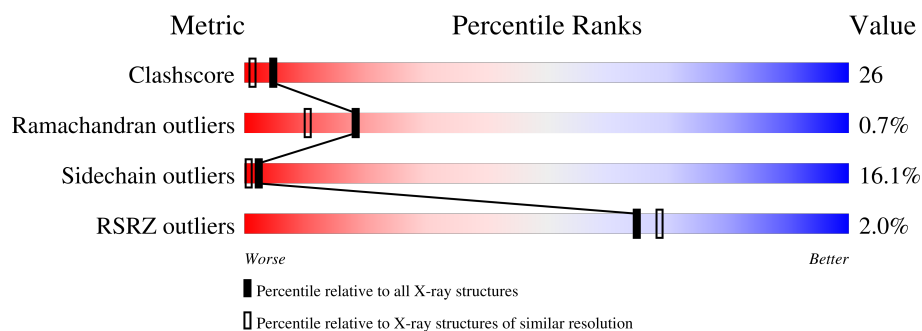
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	2% 7% 54% 30% 9%
1	B	153	2% 7% 55% 27% 10%

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.

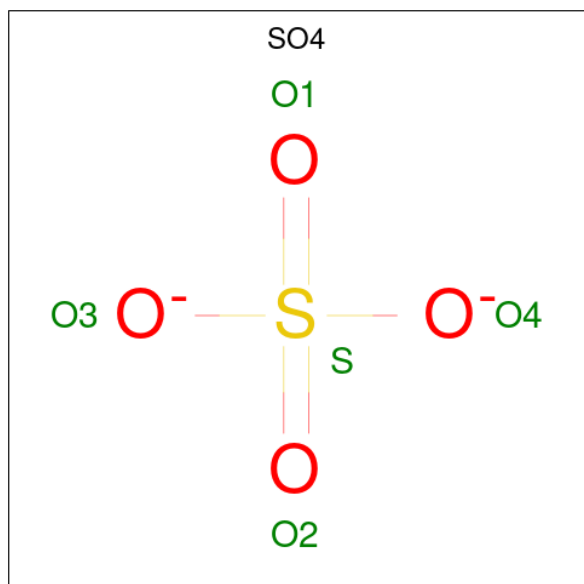
- Molecule 1 is a protein called MYOGLOBIN.

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 (CCD ID: SO4) (formula: O₄S).



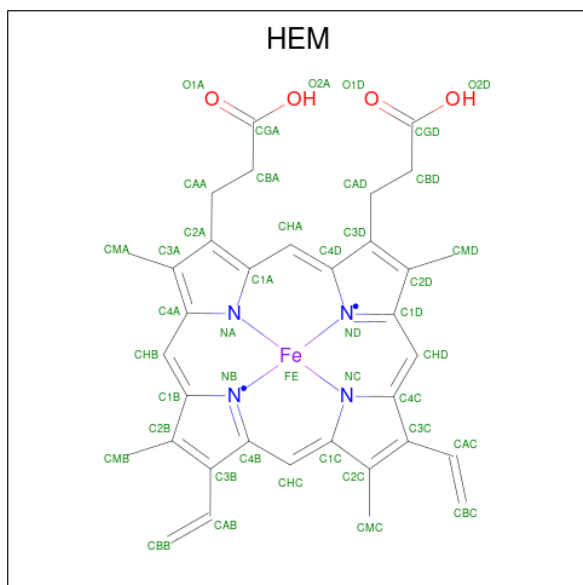
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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

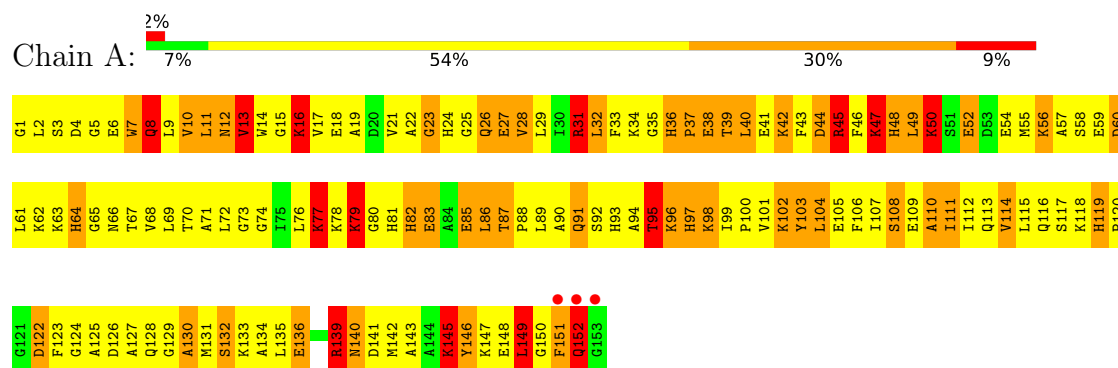
- Molecule 4 is water.

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

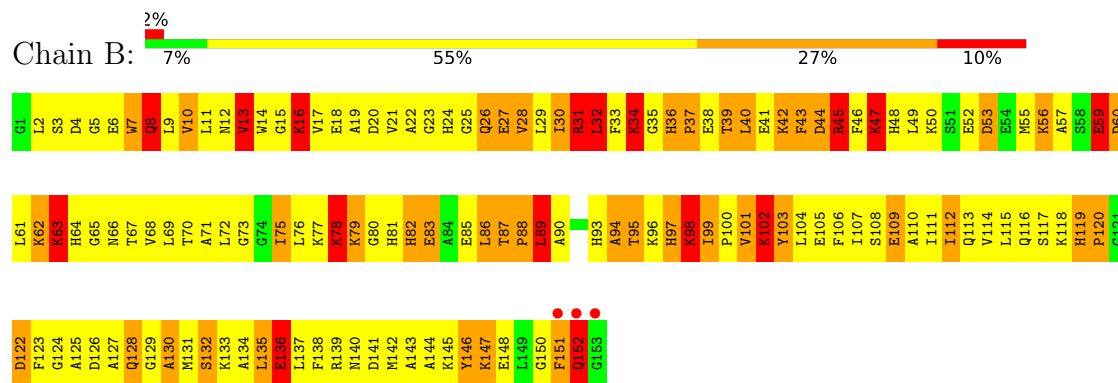
3 Residue-property plots [i](#)

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 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 68.4 (10.00-1.90)	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) (Not available) , (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)	0.47 , 139.8	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

5.1 Standard geometry

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	2.13	41/1224 (3.3%)	3.93	318/1640 (19.4%)
1	B	2.25	55/1224 (4.5%)	4.13	314/1640 (19.1%)
All	All	2.19	96/2448 (3.9%)	4.03	632/3280 (19.3%)

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	A	0	3
1	B	0	1
All	All	0	4

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	LYS	C-O	10.61	1.36	1.24
1	A	98	LYS	CG-CD	-10.28	1.21	1.52
1	B	24	HIS	CA-C	8.63	1.63	1.52
1	A	19	ALA	N-CA	8.21	1.57	1.46
1	B	66	ASN	C-O	8.19	1.33	1.24
1	A	87	THR	CA-CB	8.09	1.63	1.53
1	A	131	MET	CA-CB	7.95	1.65	1.53
1	A	28	VAL	N-CA	7.81	1.55	1.46
1	B	70	THR	C-O	7.79	1.33	1.24
1	B	87	THR	N-CA	7.73	1.53	1.46
1	B	130	ALA	C-N	-7.65	1.24	1.33
1	B	9	LEU	CA-C	7.65	1.62	1.52
1	B	29	LEU	N-CA	7.38	1.54	1.46
1	B	16	LYS	C-O	7.32	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	ILE	CA-CB	7.27	1.62	1.54
1	A	64	HIS	CA-CB	7.02	1.64	1.53
1	A	34	LYS	CB-CG	6.95	1.73	1.52
1	B	87	THR	CA-CB	6.95	1.62	1.53
1	B	99	ILE	CA-CB	6.82	1.60	1.53
1	A	91	GLN	C-N	6.67	1.43	1.33
1	A	25	GLY	N-CA	6.62	1.53	1.45
1	A	1	GLY	N-CA	6.58	1.56	1.45
1	B	63	LYS	C-N	-6.52	1.25	1.33
1	B	90	ALA	N-CA	6.51	1.54	1.46
1	B	124	GLY	N-CA	6.45	1.51	1.45
1	B	130	ALA	CA-C	6.44	1.60	1.52
1	B	25	GLY	N-CA	6.38	1.53	1.45
1	A	26	GLN	C-O	6.33	1.31	1.24
1	A	25	GLY	C-N	6.31	1.42	1.33
1	A	76	LEU	C-N	-6.30	1.25	1.34
1	B	64	HIS	CE1-NE2	6.27	1.38	1.32
1	A	23	GLY	C-N	6.19	1.42	1.33
1	B	64	HIS	N-CA	-6.15	1.39	1.46
1	A	146	TYR	CA-C	6.12	1.60	1.52
1	B	67	THR	C-N	-6.11	1.26	1.33
1	B	134	ALA	CA-C	6.01	1.60	1.52
1	A	67	THR	C-N	-6.00	1.26	1.33
1	B	93	HIS	C-O	5.99	1.31	1.24
1	B	64	HIS	ND1-CE1	-5.98	1.26	1.32
1	B	66	ASN	C-N	-5.98	1.26	1.33
1	B	10	VAL	N-CA	5.96	1.53	1.46
1	B	93	HIS	ND1-CE1	5.96	1.38	1.32
1	A	24	HIS	CA-C	5.95	1.60	1.52
1	B	39	THR	CA-CB	5.91	1.63	1.53
1	B	108	SER	N-CA	5.90	1.53	1.46
1	B	86	LEU	C-O	5.88	1.31	1.24
1	A	79	LYS	C-O	5.87	1.30	1.23
1	B	31	ARG	CD-NE	-5.87	1.38	1.46
1	A	113	GLN	N-CA	5.86	1.53	1.46
1	B	111	ILE	CA-C	5.84	1.59	1.52
1	A	103	TYR	C-O	5.83	1.31	1.24
1	B	110	ALA	C-O	5.81	1.30	1.24
1	A	74	GLY	N-CA	5.77	1.52	1.45
1	A	99	ILE	CA-CB	5.74	1.60	1.54
1	A	21	VAL	N-CA	5.74	1.53	1.46
1	B	15	GLY	N-CA	5.74	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	VAL	C-O	5.71	1.30	1.24
1	B	141	ASP	C-N	-5.71	1.26	1.33
1	A	67	THR	CA-CB	5.71	1.62	1.53
1	A	29	LEU	N-CA	5.65	1.53	1.46
1	B	98	LYS	C-N	5.64	1.38	1.33
1	A	93	HIS	CB-CG	5.63	1.58	1.50
1	B	117	SER	C-O	5.62	1.30	1.24
1	B	61	LEU	CA-C	5.61	1.60	1.52
1	A	96	LYS	CA-C	-5.61	1.45	1.52
1	A	72	LEU	C-O	5.55	1.31	1.24
1	B	65	GLY	N-CA	5.54	1.52	1.45
1	B	57	ALA	N-CA	5.53	1.53	1.46
1	A	98	LYS	C-N	5.47	1.38	1.33
1	A	11	LEU	N-CA	-5.46	1.39	1.46
1	B	135	LEU	N-CA	5.44	1.53	1.46
1	A	110	ALA	C-N	5.42	1.40	1.33
1	B	21	VAL	CA-C	5.39	1.59	1.52
1	A	112	ILE	CB-CG1	5.38	1.64	1.53
1	A	114	VAL	CA-CB	5.38	1.61	1.54
1	B	13	VAL	CA-C	5.38	1.59	1.52
1	A	91	GLN	C-O	5.36	1.30	1.24
1	B	8	GLN	CA-CB	5.36	1.61	1.53
1	B	95	THR	CA-CB	5.34	1.62	1.53
1	B	47	LYS	N-CA	5.30	1.53	1.46
1	A	106	PHE	C-O	5.28	1.30	1.24
1	B	67	THR	CA-CB	5.27	1.61	1.53
1	B	62	LYS	C-N	-5.25	1.27	1.33
1	B	69	LEU	C-N	-5.24	1.27	1.33
1	B	15	GLY	C-N	-5.20	1.27	1.33
1	A	5	GLY	C-N	-5.17	1.27	1.33
1	B	93	HIS	CA-CB	5.17	1.61	1.53
1	B	131	MET	SD-CE	-5.14	1.66	1.79
1	B	75	ILE	CA-CB	5.13	1.61	1.54
1	B	143	ALA	C-N	-5.12	1.26	1.33
1	A	39	THR	CA-CB	5.12	1.61	1.53
1	B	125	ALA	C-O	5.11	1.30	1.24
1	B	22	ALA	N-CA	5.07	1.52	1.46
1	A	63	LYS	CA-C	5.04	1.59	1.52
1	A	63	LYS	C-N	-5.04	1.27	1.33
1	A	74	GLY	C-N	-5.03	1.27	1.33

All (632) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	ARG	CD-NE-CZ	25.64	160.29	124.40
1	B	83	GLU	CB-CG-CD	25.40	155.77	112.60
1	A	83	GLU	CB-CG-CD	20.11	146.79	112.60
1	B	140	ASN	OD1-CG-ND2	18.95	141.55	122.60
1	A	139	ARG	NE-CZ-NH2	-15.78	105.00	119.20
1	B	28	VAL	O-C-N	15.31	136.92	121.91
1	B	44	ASP	CA-CB-CG	-14.75	97.85	112.60
1	B	103	TYR	O-C-N	14.66	141.97	122.33
1	A	6	GLU	CA-C-O	-14.17	106.12	121.00
1	A	8	GLN	OE1-CD-NE2	-14.00	108.60	122.60
1	A	13	VAL	N-CA-CB	13.87	125.91	110.51
1	B	80	GLY	CA-C-N	13.80	143.73	123.17
1	B	80	GLY	C-N-CA	13.80	143.73	123.17
1	A	136	GLU	N-CA-CB	13.04	129.45	110.16
1	B	5	GLY	O-C-N	12.87	137.14	122.34
1	A	5	GLY	O-C-N	12.71	134.39	122.19
1	B	59	GLU	CA-CB-CG	12.67	139.43	114.10
1	B	9	LEU	O-C-N	12.52	135.39	122.12
1	B	31	ARG	NE-CZ-NH1	-12.33	109.17	121.50
1	A	90	ALA	O-C-N	12.30	137.40	122.27
1	B	66	ASN	CA-C-N	12.10	136.16	120.44
1	B	66	ASN	C-N-CA	12.10	136.16	120.44
1	B	63	LYS	CA-C-N	12.07	136.86	120.44
1	B	63	LYS	C-N-CA	12.07	136.86	120.44
1	B	140	ASN	CB-CA-C	12.06	135.21	109.99
1	A	35	GLY	CA-C-N	11.86	132.72	122.28
1	A	35	GLY	C-N-CA	11.86	132.72	122.28
1	B	8	GLN	OE1-CD-NE2	-11.80	110.80	122.60
1	A	71	ALA	CA-C-O	-11.77	108.58	120.70
1	B	146	TYR	CA-C-N	11.72	136.44	120.38
1	B	146	TYR	C-N-CA	11.72	136.44	120.38
1	B	68	VAL	CA-CB-CG1	11.71	130.30	110.40
1	A	69	LEU	CA-C-O	-11.50	106.22	119.79
1	B	50	LYS	O-C-N	11.42	137.38	122.42
1	B	122	ASP	CA-CB-CG	-11.38	101.22	112.60
1	A	70	THR	CA-C-O	11.20	132.42	120.55
1	B	132	SER	O-C-N	-11.17	109.42	122.15
1	B	108	SER	N-CA-C	-11.10	99.19	111.07
1	A	82	HIS	CA-CB-CG	11.08	124.88	113.80
1	A	28	VAL	CA-C-O	-10.94	109.26	120.85
1	A	93	HIS	CE1-NE2-CD2	10.90	119.90	109.00
1	B	4	ASP	O-C-N	10.84	135.60	122.27
1	B	136	GLU	O-C-N	-10.82	109.56	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	CA-C-O	-10.81	106.41	119.49
1	B	67	THR	O-C-N	10.79	133.19	122.07
1	B	87	THR	CA-C-O	10.77	129.28	118.73
1	B	24	HIS	O-C-N	10.76	133.16	122.07
1	B	119	HIS	O-C-N	10.60	133.51	121.32
1	B	101	VAL	CB-CA-C	10.50	126.71	112.22
1	B	104	LEU	CA-C-O	-10.41	109.38	120.42
1	B	67	THR	CA-C-O	-10.37	109.93	120.82
1	A	149	LEU	CA-C-O	10.36	131.97	119.43
1	A	82	HIS	ND1-CG-CD2	-10.35	95.75	106.10
1	B	83	GLU	CA-CB-CG	10.29	134.67	114.10
1	A	8	GLN	CG-CD-NE2	10.26	131.79	116.40
1	A	5	GLY	CA-C-N	10.21	134.13	120.65
1	A	5	GLY	C-N-CA	10.21	134.13	120.65
1	B	65	GLY	O-C-N	-10.17	112.43	122.19
1	B	77	LYS	CA-C-O	-10.08	109.75	120.63
1	B	36	HIS	CA-CB-CG	-10.02	103.78	113.80
1	B	94	ALA	O-C-N	9.97	136.94	122.28
1	B	68	VAL	N-CA-CB	9.97	121.48	110.62
1	B	13	VAL	CB-CA-C	-9.92	99.27	111.97
1	A	65	GLY	O-C-N	-9.88	112.71	122.19
1	B	45	ARG	NE-CZ-NH1	-9.78	111.72	121.50
1	B	135	LEU	O-C-N	9.72	133.23	122.15
1	A	135	LEU	O-C-N	9.68	134.82	122.23
1	A	147	LYS	CA-C-O	-9.67	110.09	120.92
1	A	67	THR	CA-C-O	-9.65	110.69	120.82
1	A	113	GLN	OE1-CD-NE2	-9.65	112.95	122.60
1	A	93	HIS	CG-CD2-NE2	-9.63	97.56	107.20
1	B	59	GLU	N-CA-CB	9.57	125.11	110.28
1	B	132	SER	N-CA-CB	-9.54	96.05	110.16
1	A	145	LYS	CA-C-O	9.50	131.00	119.79
1	B	66	ASN	O-C-N	-9.48	112.23	122.09
1	A	70	THR	O-C-N	-9.48	112.07	122.12
1	B	103	TYR	CA-C-O	-9.48	108.61	119.79
1	B	132	SER	CB-CA-C	9.47	126.95	110.85
1	B	7	TRP	O-C-N	-9.47	112.24	122.09
1	A	61	LEU	O-C-N	-9.41	112.14	122.12
1	A	113	GLN	CG-CD-OE1	9.41	139.61	120.80
1	B	63	LYS	O-C-N	-9.39	112.17	122.12
1	A	81	HIS	CA-C-N	9.39	137.25	122.60
1	A	81	HIS	C-N-CA	9.39	137.25	122.60
1	B	33	PHE	O-C-N	9.36	133.78	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	O-C-N	9.31	132.14	122.09
1	A	151	PHE	CA-C-N	9.24	139.20	121.54
1	A	151	PHE	C-N-CA	9.24	139.20	121.54
1	A	128	GLN	CA-C-N	9.22	130.41	119.99
1	A	128	GLN	C-N-CA	9.22	130.41	119.99
1	B	102	LYS	N-CA-CB	9.18	125.92	110.32
1	A	116	GLN	N-CA-C	-9.17	101.26	111.07
1	B	125	ALA	CA-C-O	9.16	133.60	120.51
1	A	44	ASP	CA-CB-CG	-9.14	103.46	112.60
1	A	36	HIS	O-C-N	9.10	128.22	121.12
1	A	42	LYS	CA-C-O	-9.09	107.47	119.11
1	A	87	THR	CA-C-O	9.08	127.71	119.08
1	B	98	LYS	CA-C-N	-9.06	116.07	122.59
1	B	98	LYS	C-N-CA	-9.06	116.07	122.59
1	B	5	GLY	CA-C-O	-9.05	110.41	120.09
1	B	70	THR	O-C-N	-9.05	112.53	122.12
1	A	140	ASN	CA-CB-CG	-9.05	103.55	112.60
1	A	58	SER	CA-CB-OG	-9.04	93.01	111.10
1	A	28	VAL	CA-C-N	-9.04	108.69	120.44
1	A	28	VAL	C-N-CA	-9.04	108.69	120.44
1	B	25	GLY	O-C-N	8.99	130.81	122.18
1	B	32	LEU	CD1-CG-CD2	8.98	130.55	110.80
1	A	140	ASN	OD1-CG-ND2	-8.97	113.63	122.60
1	A	115	LEU	N-CA-CB	-8.95	96.92	110.16
1	A	129	GLY	CA-C-N	8.95	132.46	120.65
1	A	129	GLY	C-N-CA	8.95	132.46	120.65
1	B	132	SER	CA-C-N	8.93	132.25	120.28
1	B	132	SER	C-N-CA	8.93	132.25	120.28
1	A	11	LEU	O-C-N	8.93	134.40	122.43
1	B	81	HIS	CA-C-N	8.91	136.50	122.60
1	B	81	HIS	C-N-CA	8.91	136.50	122.60
1	A	93	HIS	ND1-CE1-NE2	-8.87	99.53	108.40
1	B	28	VAL	CA-C-O	-8.87	111.77	121.17
1	A	142	MET	O-C-N	8.85	131.65	122.09
1	A	33	PHE	O-C-N	8.81	132.19	122.15
1	A	125	ALA	CA-C-O	8.79	130.13	120.63
1	A	116	GLN	CA-C-O	-8.78	111.60	120.82
1	B	125	ALA	CB-CA-C	8.74	127.82	110.42
1	A	59	GLU	N-CA-CB	8.73	123.08	110.16
1	A	61	LEU	N-CA-C	-8.71	101.79	111.28
1	A	152	GLN	CA-CB-CG	8.69	131.48	114.10
1	B	130	ALA	O-C-N	8.68	131.47	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NH1-CZ-NH2	8.63	130.52	119.30
1	A	116	GLN	CA-C-N	8.63	132.04	120.65
1	A	116	GLN	C-N-CA	8.63	132.04	120.65
1	A	31	ARG	NE-CZ-NH1	-8.62	112.88	121.50
1	B	136	GLU	CA-C-N	8.60	132.33	120.63
1	B	136	GLU	C-N-CA	8.60	132.33	120.63
1	B	65	GLY	N-CA-C	-8.57	102.45	112.73
1	B	32	LEU	O-C-N	8.56	130.89	122.07
1	A	28	VAL	O-C-N	8.56	130.65	121.83
1	A	82	HIS	CG-CD2-NE2	8.56	115.76	107.20
1	A	123	PHE	CA-CB-CG	8.55	122.35	113.80
1	B	93	HIS	CA-CB-CG	-8.51	105.29	113.80
1	A	134	ALA	O-C-N	-8.49	113.11	122.12
1	B	96	LYS	CB-CG-CD	-8.48	91.79	111.30
1	A	112	ILE	CB-CG1-CD1	-8.45	96.05	113.80
1	A	109	GLU	N-CA-CB	8.45	122.26	110.01
1	B	130	ALA	CA-C-O	-8.43	112.01	120.70
1	B	19	ALA	CA-C-O	-8.43	108.86	119.31
1	A	55	MET	CA-C-O	-8.41	111.99	120.82
1	A	115	LEU	CA-C-N	8.41	131.37	120.44
1	A	115	LEU	C-N-CA	8.41	131.37	120.44
1	B	109	GLU	O-C-N	-8.40	113.22	122.12
1	A	44	ASP	CA-C-O	8.38	129.68	120.63
1	A	131	MET	CA-CB-CG	-8.31	97.47	114.10
1	B	86	LEU	CA-C-N	-8.29	109.14	120.26
1	B	86	LEU	C-N-CA	-8.29	109.14	120.26
1	A	54	GLU	CG-CD-OE2	8.29	137.46	118.40
1	A	90	ALA	CA-C-O	-8.29	110.44	119.97
1	B	94	ALA	CA-C-O	-8.27	109.91	120.00
1	A	133	LYS	CA-C-O	-8.27	111.66	120.42
1	A	13	VAL	CB-CA-C	-8.27	101.30	111.88
1	B	7	TRP	CA-C-O	8.26	129.74	120.90
1	A	31	ARG	CA-CB-CG	-8.19	97.72	114.10
1	B	126	ASP	O-C-N	8.18	130.93	122.09
1	A	47	LYS	CA-C-N	8.18	134.38	120.72
1	A	47	LYS	C-N-CA	8.18	134.38	120.72
1	A	136	GLU	CB-CG-CD	-8.16	98.73	112.60
1	B	83	GLU	O-C-N	-8.16	112.73	122.11
1	A	125	ALA	O-C-N	-8.13	113.50	122.12
1	B	69	LEU	CA-C-O	-8.13	110.63	119.97
1	A	6	GLU	N-CA-C	-8.09	102.15	110.97
1	A	133	LYS	CB-CG-CD	-8.06	92.76	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ASN	CB-CG-ND2	8.06	128.49	116.40
1	A	104	LEU	O-C-N	8.04	132.16	122.27
1	A	11	LEU	CA-C-O	-8.04	109.49	119.38
1	A	68	VAL	O-C-N	-8.04	113.66	121.94
1	B	131	MET	CG-SD-CE	8.04	118.58	100.90
1	A	146	TYR	CA-C-N	8.03	132.86	120.82
1	A	146	TYR	C-N-CA	8.03	132.86	120.82
1	B	104	LEU	O-C-N	8.03	131.30	122.15
1	A	136	GLU	CB-CA-C	-8.03	97.20	110.85
1	A	36	HIS	CA-C-N	7.99	128.74	119.47
1	A	36	HIS	C-N-CA	7.99	128.74	119.47
1	A	124	GLY	CA-C-N	7.98	131.31	120.38
1	A	124	GLY	C-N-CA	7.98	131.31	120.38
1	A	17	VAL	CA-C-O	-7.97	112.72	121.17
1	B	18	GLU	O-C-N	7.95	133.08	122.43
1	B	69	LEU	O-C-N	-7.93	112.51	122.27
1	A	2	LEU	N-CA-C	-7.91	96.51	109.40
1	A	70	THR	CA-C-N	7.90	131.19	120.44
1	A	70	THR	C-N-CA	7.90	131.19	120.44
1	A	27	GLU	CA-C-O	7.89	129.04	119.97
1	B	57	ALA	CA-C-O	7.87	129.02	119.97
1	B	112	ILE	N-CA-CB	7.84	119.72	110.55
1	A	55	MET	N-CA-CB	7.84	121.38	110.01
1	B	137	LEU	O-C-N	7.83	130.48	122.03
1	A	37	PRO	CA-C-N	7.82	131.80	120.38
1	A	37	PRO	C-N-CA	7.82	131.80	120.38
1	B	123	PHE	CA-C-N	-7.82	114.53	122.27
1	B	123	PHE	C-N-CA	-7.82	114.53	122.27
1	A	136	GLU	CA-C-O	-7.80	112.15	120.42
1	B	123	PHE	O-C-N	7.77	134.58	122.61
1	B	83	GLU	CA-C-O	7.70	129.54	120.92
1	B	15	GLY	N-CA-C	-7.69	103.06	113.37
1	B	40	LEU	O-C-N	7.69	130.92	122.15
1	B	130	ALA	CA-C-N	7.68	130.90	120.54
1	B	130	ALA	C-N-CA	7.68	130.90	120.54
1	A	147	LYS	CA-C-N	7.63	131.91	120.31
1	A	147	LYS	C-N-CA	7.63	131.91	120.31
1	B	72	LEU	CA-C-N	7.63	128.61	119.99
1	B	72	LEU	C-N-CA	7.63	128.61	119.99
1	B	29	LEU	CB-CA-C	7.61	122.68	110.96
1	A	111	ILE	CA-C-O	-7.60	113.05	120.95
1	B	102	LYS	CA-C-O	-7.58	110.31	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LEU	N-CA-CB	-7.58	99.48	110.47
1	A	112	ILE	O-C-N	7.58	129.63	121.83
1	B	116	GLN	CA-C-N	7.55	130.26	120.44
1	B	116	GLN	C-N-CA	7.55	130.26	120.44
1	A	83	GLU	CG-CD-OE1	7.55	135.76	118.40
1	B	89	LEU	CA-CB-CG	7.52	142.60	116.30
1	A	98	LYS	CG-CD-CE	7.51	128.58	111.30
1	B	137	LEU	CA-C-O	-7.50	113.17	120.90
1	B	14	TRP	CE2-CD2-CE3	7.48	126.28	118.80
1	A	27	GLU	N-CA-C	7.46	120.47	111.82
1	A	148	GLU	CB-CA-C	-7.44	96.38	110.67
1	B	66	ASN	OD1-CG-ND2	-7.42	115.18	122.60
1	B	136	GLU	CB-CG-CD	-7.42	99.99	112.60
1	B	70	THR	CA-CB-CG2	7.41	123.10	110.50
1	A	62	LYS	CG-CD-CE	-7.41	94.25	111.30
1	B	6	GLU	CA-C-O	-7.41	113.07	120.70
1	A	66	ASN	CB-CG-ND2	7.38	127.47	116.40
1	B	125	ALA	O-C-N	-7.36	112.80	122.59
1	A	97	HIS	CA-C-O	7.35	127.86	119.27
1	A	5	GLY	CA-C-O	-7.33	112.69	120.90
1	A	95	THR	CA-CB-OG1	-7.33	98.61	109.60
1	B	109	GLU	CG-CD-OE1	-7.32	101.56	118.40
1	B	101	VAL	CA-C-O	-7.30	113.11	120.85
1	A	120	PRO	O-C-N	-7.29	113.85	122.24
1	B	18	GLU	CA-C-O	-7.29	110.41	119.38
1	A	126	ASP	CA-C-N	7.29	130.35	120.44
1	A	126	ASP	C-N-CA	7.29	130.35	120.44
1	A	85	GLU	CG-CD-OE1	7.28	135.14	118.40
1	A	22	ALA	CA-C-O	7.26	128.33	120.20
1	B	19	ALA	N-CA-CB	7.26	122.23	110.40
1	A	32	LEU	O-C-N	7.25	129.54	122.07
1	A	103	TYR	O-C-N	7.24	131.18	122.27
1	A	126	ASP	CA-C-O	-7.24	112.20	120.24
1	A	17	VAL	N-CA-C	-7.22	103.49	110.42
1	B	97	HIS	CA-CB-CG	-7.22	106.58	113.80
1	B	56	LYS	CB-CG-CD	7.22	127.90	111.30
1	A	27	GLU	CB-CG-CD	7.22	124.87	112.60
1	B	82	HIS	CA-C-N	7.21	131.63	120.82
1	B	82	HIS	C-N-CA	7.21	131.63	120.82
1	B	93	HIS	CA-C-O	7.21	128.26	119.97
1	A	152	GLN	CB-CG-CD	7.20	124.84	112.60
1	A	3	SER	O-C-N	-7.19	114.19	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NH1-CZ-NH2	7.18	128.64	119.30
1	B	12	ASN	CA-C-O	-7.18	113.31	120.70
1	B	105	GLU	CB-CA-C	-7.15	98.92	110.79
1	A	39	THR	CA-C-O	7.14	128.18	119.97
1	A	128	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	B	133	LYS	CA-C-O	-7.12	113.00	120.55
1	B	73	GLY	CA-C-N	7.12	127.88	119.98
1	B	73	GLY	C-N-CA	7.12	127.88	119.98
1	B	115	LEU	CA-C-O	-7.11	113.38	120.70
1	B	131	MET	O-C-N	7.10	129.47	122.09
1	A	60	ASP	CA-C-O	-7.09	111.82	119.97
1	A	34	LYS	CB-CA-C	7.08	123.93	109.55
1	B	45	ARG	N-CA-CB	-7.07	97.46	110.18
1	A	86	LEU	N-CA-C	7.06	120.01	111.82
1	B	136	GLU	CA-CB-CG	-7.04	100.01	114.10
1	B	26	GLN	CB-CG-CD	7.03	124.56	112.60
1	A	148	GLU	CB-CG-CD	7.03	124.54	112.60
1	A	28	VAL	N-CA-CB	7.02	121.11	110.58
1	A	94	ALA	N-CA-CB	7.01	120.50	110.13
1	B	152	GLN	CA-C-O	6.99	130.50	120.51
1	A	60	ASP	CA-C-N	6.98	129.63	120.28
1	A	60	ASP	C-N-CA	6.98	129.63	120.28
1	B	141	ASP	N-CA-CB	6.95	121.01	110.30
1	A	78	LYS	CG-CD-CE	6.95	127.28	111.30
1	B	142	MET	O-C-N	6.95	129.23	122.07
1	A	6	GLU	N-CA-CB	6.93	120.03	109.91
1	A	98	LYS	CA-C-N	-6.92	115.82	123.02
1	A	98	LYS	C-N-CA	-6.92	115.82	123.02
1	B	126	ASP	N-CA-C	6.91	118.60	111.14
1	B	61	LEU	CA-C-O	6.90	127.74	120.42
1	A	24	HIS	O-C-N	6.88	129.99	122.15
1	B	13	VAL	N-CA-CB	6.88	118.60	110.55
1	B	116	GLN	OE1-CD-NE2	-6.87	115.73	122.60
1	B	87	THR	N-CA-C	6.87	122.09	112.75
1	A	54	GLU	N-CA-C	-6.87	103.80	111.28
1	A	139	ARG	NE-CZ-NH1	6.86	128.36	121.50
1	B	89	LEU	N-CA-C	-6.86	103.86	111.82
1	B	42	LYS	CA-C-O	-6.86	110.14	119.05
1	B	140	ASN	CB-CG-OD1	-6.85	107.10	120.80
1	B	90	ALA	O-C-N	6.84	129.37	122.12
1	A	132	SER	N-CA-CB	-6.84	100.04	110.16
1	A	151	PHE	N-CA-CB	-6.83	99.27	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLY	N-CA-C	-6.82	104.31	113.24
1	B	33	PHE	CA-C-O	-6.80	112.15	119.97
1	A	120	PRO	CA-C-O	6.78	131.30	119.84
1	B	29	LEU	CA-C-O	-6.78	113.88	121.00
1	B	69	LEU	N-CA-C	-6.76	103.98	111.82
1	A	2	LEU	N-CA-CB	6.75	122.57	110.83
1	A	126	ASP	N-CA-C	6.75	119.99	111.69
1	B	61	LEU	CA-C-N	6.75	129.62	120.44
1	B	61	LEU	C-N-CA	6.75	129.62	120.44
1	A	22	ALA	N-CA-C	6.74	120.38	111.75
1	A	48	HIS	N-CA-C	-6.74	104.32	112.54
1	A	9	LEU	CA-C-N	6.72	129.03	120.56
1	A	9	LEU	C-N-CA	6.72	129.03	120.56
1	B	111	ILE	N-CA-CB	6.71	118.40	110.55
1	B	88	PRO	O-C-N	6.69	131.30	122.27
1	A	43	PHE	CZ-CE2-CD2	-6.67	107.99	120.00
1	B	119	HIS	CA-C-O	-6.67	111.02	120.16
1	A	31	ARG	CD-NE-CZ	6.66	133.73	124.40
1	B	89	LEU	O-C-N	6.65	130.45	122.27
1	A	91	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	B	12	ASN	CA-CB-CG	6.64	119.24	112.60
1	B	20	ASP	CA-CB-CG	-6.64	105.96	112.60
1	B	75	ILE	O-C-N	6.63	130.59	121.84
1	A	12	ASN	CA-C-O	-6.62	113.88	120.70
1	A	60	ASP	CB-CG-OD2	-6.61	103.20	118.40
1	B	22	ALA	N-CA-C	6.61	119.31	111.71
1	B	11	LEU	O-C-N	6.60	130.38	122.27
1	A	12	ASN	O-C-N	6.56	129.18	122.09
1	B	122	ASP	OD1-CG-OD2	6.56	138.64	122.90
1	A	63	LYS	CA-C-O	-6.51	113.52	120.42
1	A	80	GLY	CA-C-O	-6.50	112.15	119.04
1	A	130	ALA	CA-C-O	-6.48	114.20	121.00
1	A	42	LYS	O-C-N	6.47	131.88	122.43
1	A	70	THR	CA-CB-OG1	-6.47	99.89	109.60
1	B	130	ALA	N-CA-CB	6.46	119.43	110.07
1	B	27	GLU	CG-CD-OE2	6.45	133.24	118.40
1	A	13	VAL	O-C-N	6.45	128.39	121.94
1	A	104	LEU	CA-C-O	-6.45	112.56	119.97
1	B	135	LEU	CA-C-O	-6.43	113.60	120.42
1	B	94	ALA	N-CA-CB	6.42	119.82	110.26
1	B	6	GLU	N-CA-C	-6.41	104.21	111.14
1	B	87	THR	CA-CB-OG1	-6.40	100.00	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	PHE	CA-C-O	-6.40	113.64	120.42
1	A	98	LYS	CA-CB-CG	-6.40	101.30	114.10
1	B	53	ASP	CA-C-O	6.40	127.75	120.90
1	B	78	LYS	CA-C-O	-6.39	111.04	119.10
1	B	60	ASP	CB-CG-OD2	-6.38	103.73	118.40
1	A	87	THR	N-CA-C	6.36	121.14	112.55
1	B	75	ILE	CA-C-O	-6.35	113.92	120.71
1	B	148	GLU	CA-C-O	6.34	127.27	119.97
1	B	151	PHE	CA-C-N	6.34	133.66	121.54
1	B	151	PHE	C-N-CA	6.34	133.66	121.54
1	A	77	LYS	N-CA-CB	6.34	119.98	110.22
1	B	29	LEU	O-C-N	6.34	128.62	122.03
1	B	9	LEU	N-CA-C	-6.33	104.38	111.28
1	A	3	SER	CA-C-O	6.33	129.18	122.03
1	A	126	ASP	CB-CG-OD2	-6.33	103.85	118.40
1	B	139	ARG	CG-CD-NE	6.33	125.92	112.00
1	A	117	SER	CA-CB-OG	-6.32	98.45	111.10
1	A	55	MET	O-C-N	6.32	128.57	122.07
1	B	79	LYS	CA-CB-CG	6.32	126.73	114.10
1	A	93	HIS	N-CA-C	6.31	119.14	111.82
1	A	125	ALA	CB-CA-C	6.31	121.41	110.68
1	A	38	GLU	CB-CG-CD	6.30	123.31	112.60
1	B	14	TRP	CG-CD2-CE3	-6.30	127.60	133.90
1	B	27	GLU	CB-CG-CD	6.29	123.29	112.60
1	A	82	HIS	CG-ND1-CE1	6.29	119.99	109.30
1	B	4	ASP	CA-C-O	-6.23	112.81	119.97
1	B	31	ARG	CA-C-N	6.22	128.53	120.44
1	B	31	ARG	C-N-CA	6.22	128.53	120.44
1	A	43	PHE	CG-CD1-CE1	-6.21	110.14	120.70
1	B	80	GLY	O-C-N	-6.21	114.28	122.42
1	B	134	ALA	N-CA-CB	6.20	119.34	110.16
1	A	66	ASN	CA-C-N	6.20	128.50	120.44
1	A	66	ASN	C-N-CA	6.20	128.50	120.44
1	B	27	GLU	O-C-N	-6.19	114.98	122.22
1	B	4	ASP	CA-CB-CG	-6.18	106.42	112.60
1	B	139	ARG	CB-CA-C	-6.18	101.18	110.88
1	A	32	LEU	CD1-CG-CD2	6.17	124.37	110.80
1	B	150	GLY	CA-C-O	-6.17	111.56	119.58
1	B	70	THR	CA-CB-OG1	-6.16	100.36	109.60
1	B	115	LEU	CA-C-N	6.16	128.45	120.44
1	B	115	LEU	C-N-CA	6.16	128.45	120.44
1	A	52	GLU	CA-C-O	6.15	127.48	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	LYS	CA-C-N	6.13	129.00	120.29
1	A	63	LYS	C-N-CA	6.13	129.00	120.29
1	B	57	ALA	N-CA-CB	-6.12	100.79	110.28
1	A	126	ASP	N-CA-CB	-6.11	101.10	110.20
1	A	40	LEU	CB-CA-C	6.10	120.92	110.79
1	A	31	ARG	CG-CD-NE	-6.10	98.59	112.00
1	A	70	THR	CA-CB-CG2	6.10	120.86	110.50
1	B	94	ALA	CA-C-N	-6.09	111.38	121.92
1	B	94	ALA	C-N-CA	-6.09	111.38	121.92
1	B	9	LEU	CA-C-O	-6.09	114.09	120.55
1	A	115	LEU	CA-C-O	6.08	126.87	120.42
1	A	83	GLU	OE1-CD-OE2	-6.08	108.31	122.90
1	B	88	PRO	CB-CA-C	-6.08	103.24	112.11
1	B	43	PHE	CA-C-N	-6.08	112.14	120.28
1	B	43	PHE	C-N-CA	-6.08	112.14	120.28
1	B	107	ILE	CA-CB-CG2	6.07	120.82	110.50
1	A	108	SER	N-CA-C	-6.06	104.58	111.07
1	B	128	GLN	N-CA-CB	6.06	118.97	109.94
1	A	43	PHE	CA-CB-CG	6.05	119.85	113.80
1	A	18	GLU	O-C-N	6.05	130.48	122.43
1	B	17	VAL	N-CA-C	-6.05	104.45	110.62
1	B	38	GLU	N-CA-CB	6.04	119.53	110.22
1	B	75	ILE	CA-CB-CG2	6.04	120.77	110.50
1	B	133	LYS	CA-C-N	6.03	128.85	120.29
1	B	133	LYS	C-N-CA	6.03	128.85	120.29
1	B	144	ALA	N-CA-C	-6.02	104.64	112.23
1	A	48	HIS	O-C-N	-6.02	114.36	122.43
1	B	138	PHE	O-C-N	-6.02	115.83	122.09
1	A	111	ILE	N-CA-CB	6.01	118.72	110.54
1	B	71	ALA	O-C-N	6.01	130.04	122.23
1	B	59	GLU	CB-CG-CD	6.00	122.80	112.60
1	B	111	ILE	O-C-N	6.00	127.79	121.91
1	B	57	ALA	O-C-N	-6.00	114.90	122.27
1	B	152	GLN	CB-CG-CD	5.98	122.77	112.60
1	A	113	GLN	CG-CD-NE2	-5.98	107.43	116.40
1	A	151	PHE	CB-CA-C	5.97	119.73	109.51
1	A	63	LYS	O-C-N	5.97	128.96	122.15
1	A	4	ASP	O-C-N	5.97	129.20	122.22
1	B	36	HIS	CB-CA-C	-5.96	101.32	111.15
1	A	99	ILE	CA-CB-CG2	5.96	120.62	110.50
1	A	68	VAL	CA-CB-CG1	5.96	120.52	110.40
1	A	68	VAL	N-CA-C	-5.95	104.53	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	GLU	CA-CB-CG	5.94	125.99	114.10
1	A	6	GLU	O-C-N	5.93	128.20	122.03
1	B	65	GLY	CA-C-N	5.92	128.54	120.54
1	B	65	GLY	C-N-CA	5.92	128.54	120.54
1	B	140	ASN	N-CA-C	-5.91	105.56	112.89
1	A	64	HIS	N-CA-CB	5.91	118.91	110.16
1	A	94	ALA	N-CA-C	-5.91	104.19	111.40
1	A	135	LEU	CA-C-O	-5.90	113.69	120.24
1	B	139	ARG	CA-C-O	-5.89	114.64	120.82
1	B	50	LYS	CA-C-N	-5.88	111.59	121.75
1	B	50	LYS	C-N-CA	-5.88	111.59	121.75
1	B	113	GLN	CA-C-N	5.87	128.76	120.42
1	B	113	GLN	C-N-CA	5.87	128.76	120.42
1	A	56	LYS	CA-CB-CG	5.86	125.83	114.10
1	B	88	PRO	CA-C-O	-5.86	110.72	119.34
1	B	50	LYS	CG-CD-CE	5.86	124.78	111.30
1	A	78	LYS	N-CA-C	-5.86	106.09	113.18
1	A	64	HIS	CA-CB-CG	-5.86	107.94	113.80
1	B	99	ILE	N-CA-C	5.85	113.67	107.76
1	B	37	PRO	CA-C-N	5.84	128.68	120.28
1	B	37	PRO	C-N-CA	5.84	128.68	120.28
1	A	63	LYS	CA-CB-CG	-5.82	102.46	114.10
1	A	140	ASN	O-C-N	5.80	128.05	122.07
1	A	21	VAL	CA-C-O	-5.80	114.45	121.18
1	B	117	SER	N-CA-C	5.78	117.25	111.07
1	B	115	LEU	O-C-N	5.78	128.33	122.09
1	B	34	LYS	CB-CG-CD	5.77	124.58	111.30
1	B	47	LYS	CA-C-N	5.77	128.59	120.28
1	B	47	LYS	C-N-CA	5.77	128.59	120.28
1	B	148	GLU	N-CA-CB	-5.77	101.34	110.28
1	A	44	ASP	CB-CG-OD2	-5.77	105.14	118.40
1	A	57	ALA	CA-C-O	5.76	126.45	119.31
1	A	33	PHE	N-CA-CB	5.75	118.67	110.16
1	B	114	VAL	CG1-CB-CG2	5.75	123.44	110.80
1	B	50	LYS	N-CA-CB	5.74	119.08	110.53
1	B	98	LYS	CA-C-O	5.74	129.25	122.14
1	A	4	ASP	CA-C-N	5.73	126.19	119.94
1	A	4	ASP	C-N-CA	5.73	126.19	119.94
1	A	31	ARG	N-CA-CB	5.73	118.47	109.94
1	B	44	ASP	CB-CG-OD2	-5.73	105.23	118.40
1	B	114	VAL	O-C-N	5.73	127.73	121.83
1	A	14	TRP	CA-C-O	5.72	126.61	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	GLY	CA-C-O	5.72	126.73	120.66
1	A	67	THR	CA-C-N	5.71	127.84	120.70
1	A	67	THR	C-N-CA	5.71	127.84	120.70
1	A	130	ALA	O-C-N	5.71	127.96	122.03
1	A	152	GLN	CA-C-N	5.70	131.97	121.70
1	A	152	GLN	C-N-CA	5.70	131.97	121.70
1	B	120	PRO	N-CA-CB	5.70	109.76	103.26
1	B	126	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	25	GLY	CA-C-O	-5.70	114.84	121.00
1	B	134	ALA	N-CA-C	-5.70	105.15	111.36
1	B	75	ILE	CB-CG1-CD1	-5.69	101.85	113.80
1	B	82	HIS	CG-CD2-NE2	5.68	112.88	107.20
1	A	122	ASP	O-C-N	5.68	130.21	122.37
1	A	152	GLN	CA-C-O	5.68	128.63	120.51
1	B	97	HIS	CB-CG-CD2	5.68	138.58	131.20
1	A	50	LYS	CA-C-N	-5.67	112.57	121.87
1	A	50	LYS	C-N-CA	-5.67	112.57	121.87
1	A	24	HIS	ND1-CG-CD2	5.66	111.76	106.10
1	A	147	LYS	CA-CB-CG	5.66	125.42	114.10
1	A	34	LYS	CG-CD-CE	5.66	124.32	111.30
1	A	99	ILE	O-C-N	-5.66	117.05	121.46
1	A	65	GLY	N-CA-C	-5.65	105.95	112.73
1	A	140	ASN	CA-C-O	-5.65	114.89	120.82
1	A	14	TRP	O-C-N	-5.64	115.77	122.20
1	A	77	LYS	CB-CA-C	-5.64	100.19	110.63
1	B	31	ARG	NH1-CZ-NH2	5.63	126.62	119.30
1	B	8	GLN	CA-C-O	-5.63	114.91	120.82
1	A	129	GLY	O-C-N	5.61	127.69	122.13
1	B	3	SER	O-C-N	-5.60	115.81	122.65
1	A	139	ARG	NH1-CZ-NH2	5.60	126.58	119.30
1	A	27	GLU	CA-C-N	-5.60	112.47	120.42
1	A	27	GLU	C-N-CA	-5.60	112.47	120.42
1	A	141	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	126	ASP	CA-C-O	-5.59	114.94	120.70
1	B	13	VAL	O-C-N	5.58	127.38	121.91
1	A	149	LEU	CA-C-N	5.58	131.84	120.80
1	A	149	LEU	C-N-CA	5.58	131.84	120.80
1	A	46	PHE	O-C-N	5.57	128.31	122.23
1	A	79	LYS	CB-CG-CD	-5.57	98.48	111.30
1	A	49	LEU	O-C-N	5.57	129.87	123.02
1	B	31	ARG	NE-CZ-NH2	5.55	124.20	119.20
1	B	82	HIS	CA-CB-CG	-5.55	108.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	LEU	CA-C-N	5.55	128.27	120.28
1	A	76	LEU	C-N-CA	5.55	128.27	120.28
1	B	76	LEU	CA-C-O	5.54	126.42	120.55
1	B	127	ALA	N-CA-C	-5.54	105.24	111.28
1	B	85	GLU	N-CA-CB	5.53	118.35	110.16
1	A	42	LYS	CA-C-N	-5.53	114.78	123.13
1	A	42	LYS	C-N-CA	-5.53	114.78	123.13
1	A	63	LYS	CG-CD-CE	5.53	124.01	111.30
1	A	97	HIS	CA-CB-CG	5.51	119.31	113.80
1	A	119	HIS	CA-C-O	-5.50	112.62	120.16
1	B	103	TYR	N-CA-C	-5.50	105.30	112.23
1	B	103	TYR	N-CA-CB	5.50	118.77	110.30
1	A	99	ILE	N-CA-C	5.50	113.93	107.77
1	B	16	LYS	CG-CD-CE	5.48	123.90	111.30
1	B	31	ARG	CG-CD-NE	5.47	124.05	112.00
1	B	68	VAL	O-C-N	-5.47	116.31	121.94
1	A	60	ASP	OD1-CG-OD2	5.46	136.02	122.90
1	B	21	VAL	CA-C-N	-5.46	112.42	120.28
1	B	21	VAL	C-N-CA	-5.46	112.42	120.28
1	A	110	ALA	N-CA-CB	-5.46	101.88	110.06
1	B	109	GLU	OE1-CD-OE2	5.45	135.99	122.90
1	B	93	HIS	N-CA-C	5.44	118.14	111.82
1	B	105	GLU	OE1-CD-OE2	5.43	135.94	122.90
1	A	126	ASP	CB-CG-OD1	5.43	130.89	118.40
1	B	14	TRP	CD2-CE3-CZ3	-5.43	111.54	118.60
1	A	38	GLU	CA-C-O	5.42	126.27	120.20
1	A	71	ALA	N-CA-C	-5.42	105.29	111.14
1	B	26	GLN	CB-CA-C	5.42	119.38	110.88
1	B	96	LYS	CA-CB-CG	-5.41	103.28	114.10
1	B	137	LEU	N-CA-C	-5.40	105.04	111.03
1	A	120	PRO	CB-CA-C	5.39	122.02	112.64
1	A	129	GLY	CA-C-O	-5.38	115.51	121.05
1	B	107	ILE	O-C-N	5.38	129.19	121.82
1	B	66	ASN	CA-C-O	-5.37	115.16	120.90
1	B	22	ALA	O-C-N	-5.37	115.94	122.22
1	B	82	HIS	O-C-N	-5.37	115.86	122.25
1	A	19	ALA	CB-CA-C	5.36	121.19	109.99
1	A	47	LYS	CA-C-O	5.36	125.98	119.49
1	A	45	ARG	CA-CB-CG	5.35	124.80	114.10
1	B	152	GLN	CA-C-N	5.35	131.33	121.70
1	B	152	GLN	C-N-CA	5.35	131.33	121.70
1	A	42	LYS	N-CA-CB	5.33	119.36	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	ASP	N-CA-CB	-5.33	102.64	111.96
1	B	104	LEU	N-CA-C	-5.33	105.56	111.36
1	B	64	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	59	GLU	CB-CA-C	-5.32	101.80	110.85
1	B	79	LYS	O-C-N	-5.32	115.96	122.55
1	A	58	SER	CA-C-O	-5.31	112.91	120.51
1	B	31	ARG	N-CA-C	5.30	117.06	111.28
1	A	14	TRP	CE2-CD2-CE3	5.30	124.10	118.80
1	A	2	LEU	O-C-N	5.30	130.12	123.23
1	A	72	LEU	O-C-N	-5.29	115.76	122.27
1	A	77	LYS	CA-C-N	5.29	131.89	121.58
1	A	77	LYS	C-N-CA	5.29	131.89	121.58
1	B	35	GLY	CA-C-N	5.29	128.34	122.74
1	B	35	GLY	C-N-CA	5.29	128.34	122.74
1	B	82	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	A	23	GLY	O-C-N	5.28	127.26	122.19
1	A	97	HIS	ND1-CE1-NE2	-5.28	103.12	108.40
1	B	61	LEU	O-C-N	-5.28	116.13	122.15
1	A	132	SER	CA-C-O	5.28	126.02	120.42
1	B	46	PHE	O-C-N	5.27	127.98	122.23
1	A	52	GLU	CB-CG-CD	5.26	121.54	112.60
1	A	126	ASP	O-C-N	5.25	129.06	122.23
1	B	138	PHE	CA-CB-CG	5.25	119.05	113.80
1	B	136	GLU	CB-CA-C	-5.25	100.92	110.63
1	A	130	ALA	N-CA-CB	5.25	117.57	109.91
1	A	136	GLU	OE1-CD-OE2	5.25	135.49	122.90
1	A	77	LYS	CA-C-O	-5.23	114.19	120.10
1	A	65	GLY	CA-C-O	5.23	126.14	120.75
1	B	27	GLU	CA-C-O	5.23	126.00	120.10
1	B	108	SER	CA-CB-OG	5.23	121.55	111.10
1	B	88	PRO	CA-C-N	-5.22	112.37	120.31
1	B	88	PRO	C-N-CA	-5.22	112.37	120.31
1	A	18	GLU	CB-CG-CD	-5.21	103.74	112.60
1	A	24	HIS	CA-C-N	5.21	125.88	119.99
1	A	24	HIS	C-N-CA	5.21	125.88	119.99
1	A	82	HIS	ND1-CE1-NE2	-5.21	103.19	108.40
1	A	136	GLU	CA-CB-CG	-5.20	103.70	114.10
1	B	93	HIS	ND1-CE1-NE2	-5.20	103.20	108.40
1	B	41	GLU	CG-CD-OE1	5.19	130.34	118.40
1	B	98	LYS	CB-CG-CD	5.19	123.23	111.30
1	B	142	MET	CA-C-N	5.19	127.49	120.38
1	B	142	MET	C-N-CA	5.19	127.49	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	HIS	O-C-N	-5.19	116.24	122.15
1	B	115	LEU	CB-CG-CD1	-5.18	95.15	110.70
1	A	93	HIS	CA-C-O	5.18	125.93	119.97
1	A	126	ASP	CA-CB-CG	5.17	117.78	112.60
1	B	81	HIS	CB-CA-C	-5.16	102.46	111.23
1	B	33	PHE	CZ-CE2-CD2	5.15	129.26	120.00
1	B	7	TRP	CA-C-N	5.14	127.12	120.44
1	B	7	TRP	C-N-CA	5.14	127.12	120.44
1	A	10	VAL	O-C-N	-5.13	116.88	121.91
1	A	93	HIS	ND1-CG-CD2	5.13	111.23	106.10
1	A	122	ASP	CB-CG-OD2	-5.13	106.60	118.40
1	A	96	LYS	CG-CD-CE	5.13	123.10	111.30
1	B	68	VAL	CG1-CB-CG2	-5.13	99.52	110.80
1	A	92	SER	O-C-N	-5.12	116.31	122.15
1	B	10	VAL	CB-CA-C	5.12	118.52	111.97
1	A	150	GLY	N-CA-C	-5.11	107.03	114.90
1	A	22	ALA	CA-C-N	5.10	125.50	119.94
1	A	22	ALA	C-N-CA	5.10	125.50	119.94
1	B	103	TYR	CD1-CE1-CZ	-5.10	110.43	119.60
1	B	129	GLY	CA-C-N	5.10	127.37	120.44
1	B	129	GLY	C-N-CA	5.10	127.37	120.44
1	A	6	GLU	CG-CD-OE1	-5.09	106.69	118.40
1	B	101	VAL	CA-CB-CG1	5.09	119.05	110.40
1	A	26	GLN	CA-C-N	-5.09	112.58	120.31
1	A	26	GLN	C-N-CA	-5.09	112.58	120.31
1	A	95	THR	OG1-CB-CG2	5.09	119.48	109.30
1	A	127	ALA	N-CA-C	-5.08	105.66	111.14
1	A	36	HIS	CB-CA-C	-5.08	103.81	110.87
1	B	105	GLU	CA-C-N	5.07	127.04	120.44
1	B	105	GLU	C-N-CA	5.07	127.04	120.44
1	A	119	HIS	O-C-N	5.07	127.15	121.32
1	B	148	GLU	OE1-CD-OE2	5.07	135.06	122.90
1	B	14	TRP	CB-CG-CD1	5.06	134.49	126.90
1	A	113	GLN	CA-C-O	-5.06	115.49	120.90
1	A	78	LYS	O-C-N	5.06	129.81	122.43
1	B	122	ASP	N-CA-CB	-5.04	102.54	110.46
1	B	66	ASN	N-CA-CB	5.04	117.45	109.94
1	B	137	LEU	CB-CA-C	5.04	118.76	110.95
1	A	7	TRP	CB-CG-CD2	5.02	133.82	126.80
1	A	69	LEU	O-C-N	5.02	129.05	122.33
1	A	7	TRP	O-C-N	-5.01	116.87	122.09
1	B	104	LEU	N-CA-CB	5.00	117.57	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	VAL	CG1-CB-CG2	5.00	121.80	110.80

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	53	1
1	B	1199	0	1205	71	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	2470	126	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 26.

All (126) 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:O	1:B:152:GLN:NE2	2.01	0.93
1:A:88:PRO:HA	1:A:91:GLN:HE21	1.33	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:136:GLU:HG3	1.84	0.75
1:B:95:THR:C	1:B:98:LYS:HE3	2.13	0.74
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: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:30:ILE:HG22	1:B:34:LYS:HZ3	1.65	0.59
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:HBC2	3:A:155:HEM:HMC2	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:98:LYS:HZ2	1:B:98:LYS:HB2	1.72	0.53
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:HMC1	3:B:155:HEM:HBC2	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:78:LYS:HB2	1:B:82:HIS:HB3	1.92	0.50
1:B:101:VAL:HG23	1:B:146:TYR:CE2	2.46	0.50
1:B:32:LEU:HD22	1:B:32:LEU:C	2.37	0.50
1:B:2:LEU:HD12	1:B:2:LEU:N	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:8:GLN:HE22	1:B:79:LYS:HZ1	1.62	0.47
1:B:26:GLN:HG3	4:B:156:HOH:O	2.13	0.47
1:A:41:GLU:HA	1:A:47:LYS:NZ	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ALA:CB	1:B:151:PHE:CD2	2.98	0.46
1:B:99:ILE:HD12	3:B:155:HEM:CAC	2.47	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:HD2	1:A:16:LYS:HA	1.29	0.45
1:B:8:GLN:NE2	1:B:79:LYS:HZ1	2.15	0.45
1:B:98:LYS:HB2	1:B:98:LYS:NZ	2.31	0.44
1:B:43:PHE:O	1:B:44:ASP:C	2.59	0.44
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:45:ARG:O	1:B:48:HIS:CE1	2.71	0.43
1:B:94:ALA:HB1	1:B:151:PHE:CB	2.48	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:82:HIS:CD2	1:B:82:HIS:C	2.97	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:11:LEU:HD12	1:A:79:LYS:HZ3	1.84	0.42
1:A:108:SER:CB	1:A:139:ARG:HH11	2.30	0.42
1:B:62:LYS:HZ3	1:B:62:LYS:HG3	1.59	0.42
1:B:119:HIS:HB3	1:B:122:ASP:HB2	2.00	0.42
1:B:75:ILE:HG21	1:B:75:ILE:HD13	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:7:TRP:HB3	1:B:79:LYS:NZ	2.30	0.41
1:B:112:ILE:HD11	1:B:135:LEU:HD12	2.02	0.41
1:A:42:LYS:NZ	1:A:98:LYS:O	2.47	0.41
1:A:44:ASP:O	1:A:47:LYS:HG2	2.20	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:27:GLU:OE2	1:A:118:LYS:NZ	2.54	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 sym-

metry 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%)	18	10
1	B	151/153 (99%)	143 (95%)	7 (5%)	1 (1%)	18	10
All	All	302/306 (99%)	288 (95%)	12 (4%)	2 (1%)	18	10

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%)	106 (86%)	18 (14%)	3	1
1	B	124/124 (100%)	102 (82%)	22 (18%)	2	0
All	All	248/248 (100%)	208 (84%)	40 (16%)	2	1

All (40) 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	83	GLU
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	8	GLN
1	B	13	VAL
1	B	16	LYS
1	B	27	GLU
1	B	31	ARG
1	B	32	LEU
1	B	34	LYS
1	B	42	LYS
1	B	47	LYS
1	B	53	ASP
1	B	59	GLU
1	B	60	ASP
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	136	GLU
1	B	147	LYS
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	97	HIS
1	A	113	GLN
1	A	140	ASN
1	B	48	HIS
1	B	66	ASN
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 oligosaccharides 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	0.83	0	6,6,6	1.69	1 (16%)
3	HEM	A	155	1,4	50,50,50	1.97	18 (36%)	67,82,82	2.64	31 (46%)
3	HEM	B	155	1,4	50,50,50	2.44	22 (44%)	67,82,82	2.89	31 (46%)
2	SO4	A	154	-	4,4,4	1.22	0	6,6,6	1.08	0

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	-	4/14/54/54	-
3	HEM	B	155	1,4	-	5/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	155	HEM	FE-NB	6.42	2.14	1.94
3	B	155	HEM	FE-ND	5.23	2.11	1.94
3	A	155	HEM	CMB-C2B	4.48	1.60	1.50
3	B	155	HEM	C4D-ND	-4.37	1.32	1.40
3	A	155	HEM	CBD-CAD	4.27	1.66	1.51
3	A	155	HEM	CAB-C3B	4.17	1.58	1.47
3	B	155	HEM	CAC-C3C	3.99	1.58	1.47
3	B	155	HEM	C4D-C3D	3.87	1.51	1.45
3	B	155	HEM	CAB-C3B	3.84	1.57	1.47
3	B	155	HEM	CAA-C2A	3.82	1.61	1.51
3	B	155	HEM	C3B-C2B	-3.51	1.30	1.37
3	A	155	HEM	FE-NB	3.51	2.05	1.94
3	B	155	HEM	CMA-C3A	3.31	1.57	1.50
3	A	155	HEM	CMA-C3A	3.30	1.57	1.50
3	B	155	HEM	O1A-CGA	3.22	1.32	1.22
3	B	155	HEM	CMD-C2D	3.20	1.57	1.50
3	A	155	HEM	CMD-C2D	3.20	1.57	1.50
3	B	155	HEM	CMB-C2B	2.96	1.56	1.50
3	A	155	HEM	O1A-CGA	2.94	1.31	1.22
3	A	155	HEM	C3B-C2B	-2.93	1.31	1.37
3	A	155	HEM	CAC-C3C	2.91	1.55	1.47
3	B	155	HEM	CBA-CAA	2.83	1.61	1.51
3	B	155	HEM	C1B-C2B	2.82	1.50	1.44
3	B	155	HEM	C2A-C3A	-2.78	1.31	1.38
3	A	155	HEM	C3D-C2D	-2.60	1.31	1.36
3	A	155	HEM	O1D-CGD	2.56	1.30	1.22
3	B	155	HEM	CHD-C1D	-2.51	1.33	1.39
3	A	155	HEM	CAA-C2A	2.50	1.57	1.51
3	A	155	HEM	CMC-C2C	2.47	1.55	1.50
3	B	155	HEM	O1D-CGD	2.41	1.30	1.22
3	B	155	HEM	C4C-NC	2.41	1.44	1.39
3	B	155	HEM	FE-NC	-2.39	1.87	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	155	HEM	C1B-NB	-2.27	1.36	1.40
3	A	155	HEM	CBA-CAA	2.17	1.59	1.51
3	A	155	HEM	CAD-C3D	2.14	1.56	1.51
3	B	155	HEM	C4B-NB	-2.14	1.34	1.38
3	B	155	HEM	C1C-C2C	-2.06	1.41	1.45
3	A	155	HEM	CHC-C1C	2.02	1.42	1.38
3	A	155	HEM	CBC-CAC	2.01	1.40	1.30
3	A	155	HEM	FE-ND	2.00	2.01	1.94

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	CHD-C1D-ND	7.66	132.66	124.42
3	B	155	HEM	C4D-ND-C1D	7.51	114.11	105.21
3	B	155	HEM	C3B-C4B-NB	-6.60	104.73	109.47
3	B	155	HEM	C3D-C4D-ND	-6.58	102.95	110.17
3	B	155	HEM	C1B-NB-C4B	6.25	112.61	105.21
3	B	155	HEM	CHA-C4D-ND	5.88	131.63	124.37
3	B	155	HEM	CMC-C2C-C1C	5.47	134.36	124.73
3	A	155	HEM	C3B-C2B-C1B	5.27	110.37	106.41
3	A	155	HEM	CBD-CAD-C3D	-5.08	98.49	112.53
3	A	155	HEM	CHB-C4A-NA	4.74	132.46	123.86
3	A	155	HEM	C3D-C4D-ND	-4.58	105.14	110.17
3	B	155	HEM	CHD-C1D-ND	4.44	129.20	124.42
3	B	155	HEM	CMB-C2B-C1B	-4.40	118.15	125.03
3	A	155	HEM	CAD-C3D-C4D	-4.36	117.10	124.70
3	A	155	HEM	O1D-CGD-CBD	-4.25	109.60	123.09
3	B	155	HEM	O2A-CGA-CBA	4.25	127.42	114.00
3	B	155	HEM	C2B-C1B-NB	-4.19	105.03	109.84
3	B	155	HEM	C4A-NA-C1A	-4.17	99.02	105.82
3	A	155	HEM	C4C-CHD-C1D	-4.00	117.52	126.02
3	A	155	HEM	CMD-C2D-C1D	-3.96	118.85	125.03
3	A	155	HEM	CMB-C2B-C1B	-3.93	118.90	125.03
3	B	155	HEM	C4B-C3B-C2B	3.87	110.84	107.28
3	A	155	HEM	CHC-C1C-NC	3.83	128.62	124.45
3	A	155	HEM	CHB-C4A-C3A	-3.73	116.60	127.43
3	B	155	HEM	O2A-CGA-O1A	-3.72	113.76	123.33
3	A	155	HEM	C4D-ND-C1D	3.67	109.55	105.21
3	B	155	HEM	CMC-C2C-C3C	-3.57	119.79	128.43
3	B	155	HEM	CAD-C3D-C4D	-3.54	118.53	124.70
3	B	155	HEM	CAC-C3C-C4C	-3.50	116.47	124.82
3	A	155	HEM	CHD-C4C-C3C	-3.46	119.37	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	154	SO4	O4-S-O1	3.44	127.53	109.56
3	B	155	HEM	C2D-C1D-ND	-3.26	106.13	109.90
3	A	155	HEM	C3B-C4B-NB	-3.26	107.13	109.47
3	B	155	HEM	CHB-C1B-NB	3.23	128.37	124.37
3	A	155	HEM	O2D-CGD-O1D	3.15	131.44	123.33
3	A	155	HEM	C2D-C1D-ND	-3.14	106.28	109.90
3	A	155	HEM	C1C-CHC-C4B	-3.10	119.43	126.02
3	B	155	HEM	O2D-CGD-CBD	3.03	123.59	114.00
3	B	155	HEM	CAA-C2A-C1A	2.94	130.69	124.94
3	A	155	HEM	C4D-C3D-C2D	2.93	111.16	106.89
3	B	155	HEM	CMD-C2D-C1D	-2.81	120.65	125.03
3	B	155	HEM	CMB-C2B-C3B	2.80	135.19	128.43
3	B	155	HEM	O1D-CGD-CBD	-2.78	114.26	123.09
3	A	155	HEM	C1B-NB-C4B	2.78	108.50	105.21
3	A	155	HEM	CHC-C4B-NB	2.72	127.35	124.42
3	B	155	HEM	CHC-C4B-C3B	2.72	130.50	125.07
3	B	155	HEM	C4C-C3C-C2C	2.70	109.16	106.81
3	A	155	HEM	C3C-C2C-C1C	2.70	109.60	107.05
3	B	155	HEM	C4D-C3D-C2D	2.64	110.74	106.89
3	A	155	HEM	C2A-C1A-NA	2.63	113.06	110.15
3	A	155	HEM	CMD-C2D-C3D	2.61	133.21	126.15
3	B	155	HEM	CMD-C2D-C3D	2.61	133.20	126.15
3	A	155	HEM	CHD-C1D-C2D	-2.58	120.95	125.03
3	A	155	HEM	C4A-CHB-C1B	-2.57	120.20	126.25
3	A	155	HEM	C2B-C1B-NB	-2.49	106.98	109.84
3	B	155	HEM	C3A-C4A-NA	2.48	114.11	110.14
3	B	155	HEM	C1A-CHA-C4D	-2.47	120.43	126.25
3	A	155	HEM	CHD-C4C-NC	2.46	127.13	124.45
3	A	155	HEM	CAD-CBD-CGD	-2.23	107.75	113.67
3	A	155	HEM	CHA-C4D-ND	2.19	127.08	124.37
3	A	155	HEM	C4C-C3C-C2C	-2.19	104.92	106.81
3	B	155	HEM	CHC-C1C-C2C	-2.15	121.02	125.49
3	B	155	HEM	CAA-C2A-C3A	-2.13	122.29	127.07

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	155	HEM	CAA-CBA-CGA-O1A
3	B	155	HEM	CAA-CBA-CGA-O1A
3	A	155	HEM	CAD-CBD-CGD-O1D
3	B	155	HEM	CAD-CBD-CGD-O2D

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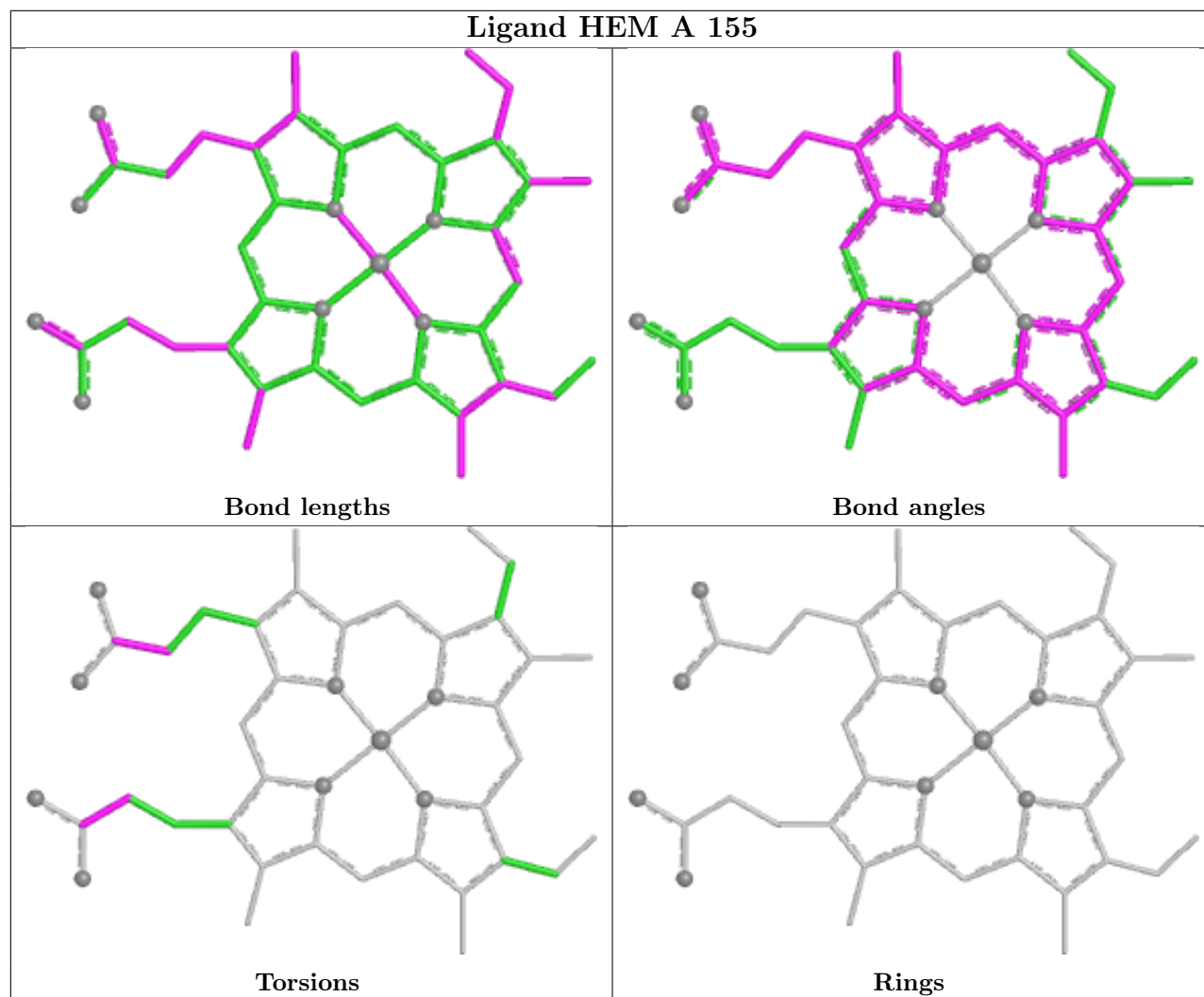
Mol	Chain	Res	Type	Atoms
3	A	155	HEM	CAD-CBD-CGD-O2D
3	A	155	HEM	CAA-CBA-CGA-O2A
3	B	155	HEM	CAD-CBD-CGD-O1D
3	B	155	HEM	CAA-CBA-CGA-O2A
3	B	155	HEM	C2A-CAA-CBA-CGA

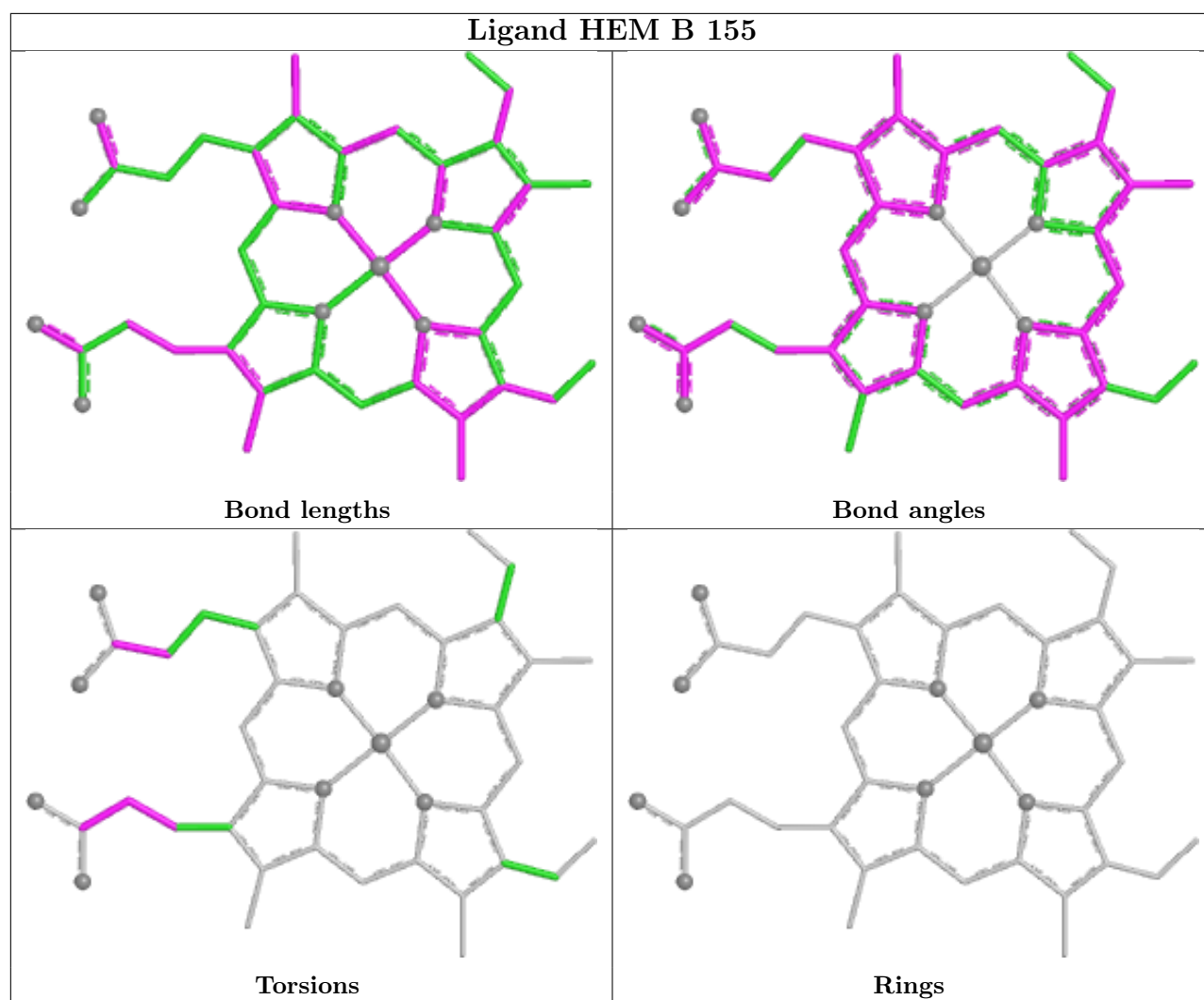
There are no ring outliers.

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%)	0.14	3 (1%) 65 69	7, 20, 38, 65	4 (2%)
1	B	153/153 (100%)	0.18	3 (1%) 65 69	7, 20, 37, 65	0
All	All	306/306 (100%)	0.16	6 (1%) 65 69	7, 20, 38, 65	4 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	GLY	4.8
1	A	153	GLY	4.0
1	B	151	PHE	3.2
1	B	152	GLN	2.8
1	A	152	GLN	2.4
1	A	151	PHE	2.2

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

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

6.3 Carbohydrates [i](#)

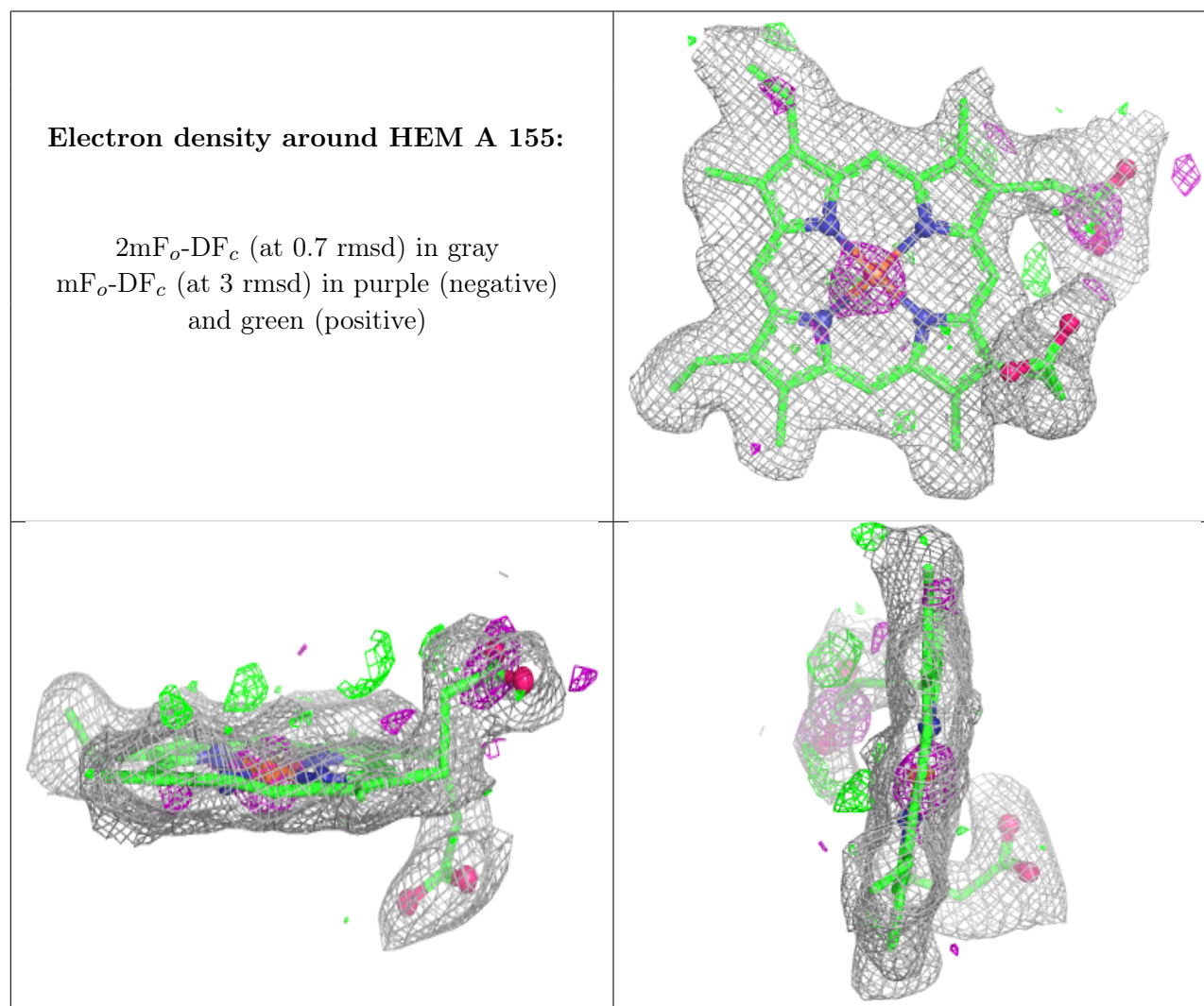
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

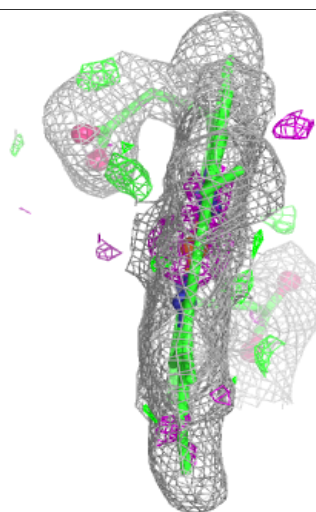
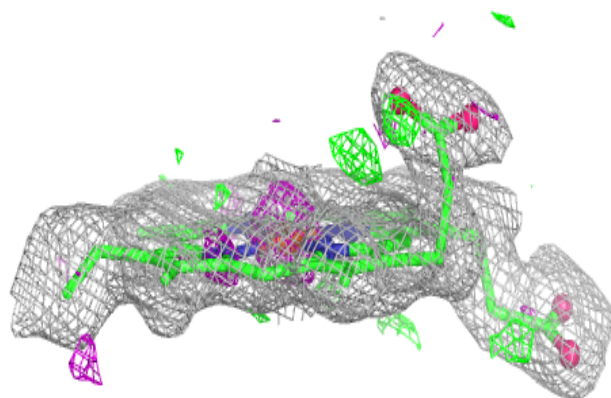
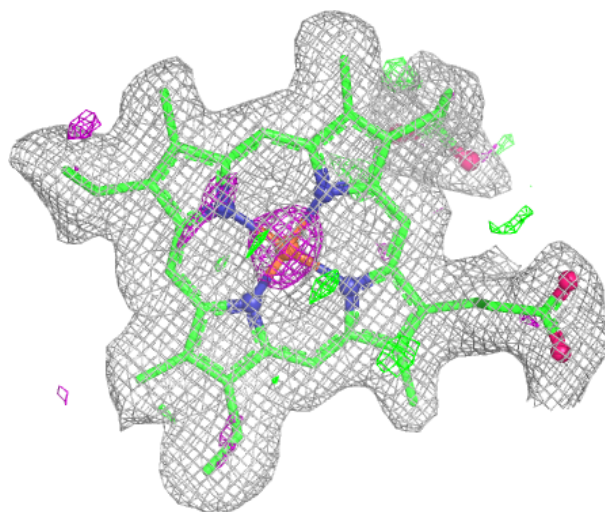
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	154	5/5	0.94	0.15	33,34,35,36	0
2	SO4	A	154	5/5	0.96	0.13	40,40,41,42	0
3	HEM	A	155	43/43	0.97	0.06	4,7,19,27	0
3	HEM	B	155	43/43	0.97	0.06	3,6,19,24	0

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 [i](#)

There are no such residues in this entry.