



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:57 PM EDT

PDB ID : 1I3D / pdb_00001i3d
Title : HUMAN CARBONMONOXY HEMOGLOBIN BART'S (GAMMA4)
Authors : Kidd, R.D.; Baker, H.M.; Mathews, A.J.; Brittain, T.; Baker, E.N.
Deposited on : 2001-02-15
Resolution : 1.70 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

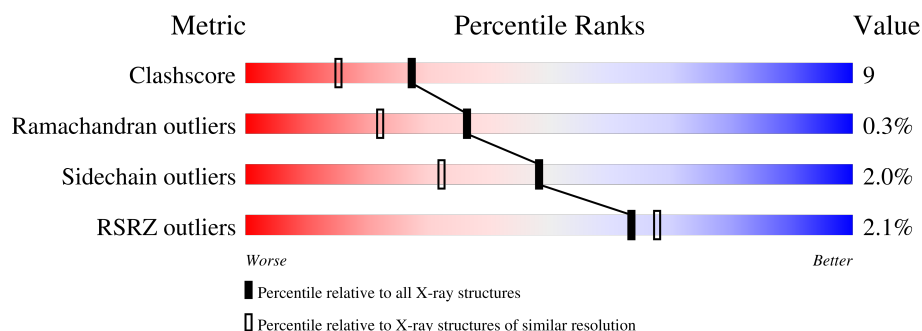
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	146	42% 51% 7%
1	B	146	3% 38% 51% 10%

2 Entry composition [i](#)

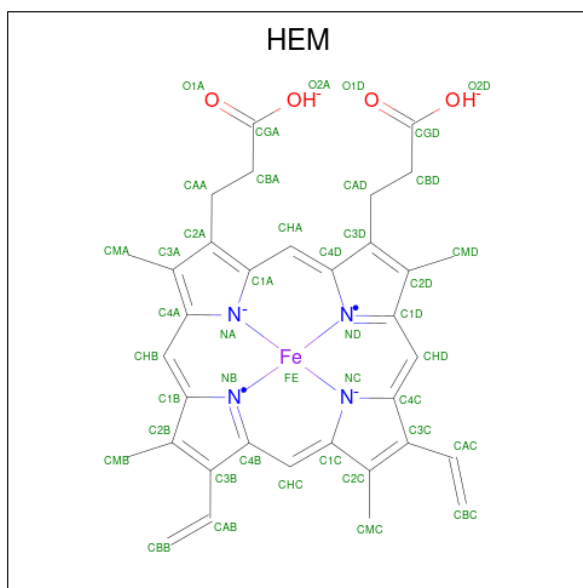
There are 4 unique types of molecules in this entry. The entry contains 2638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMOGLOBIN GAMMA CHAINS.

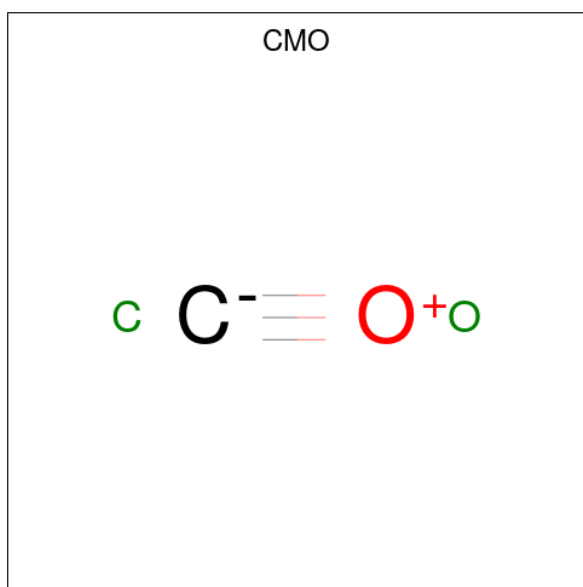
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	7	0	0
			1131	724	193	211	3			
1	B	146	Total	C	N	O	S	5	0	0
			1131	724	193	211	3			

- 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		
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		

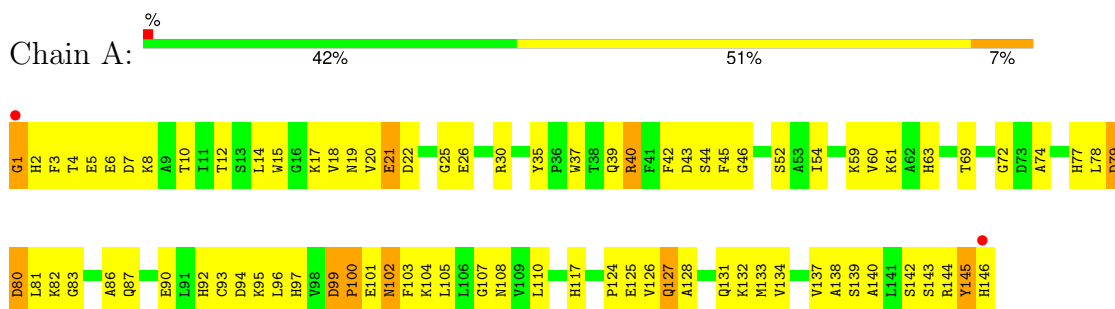
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	143	Total	O	0	0
			143	143		

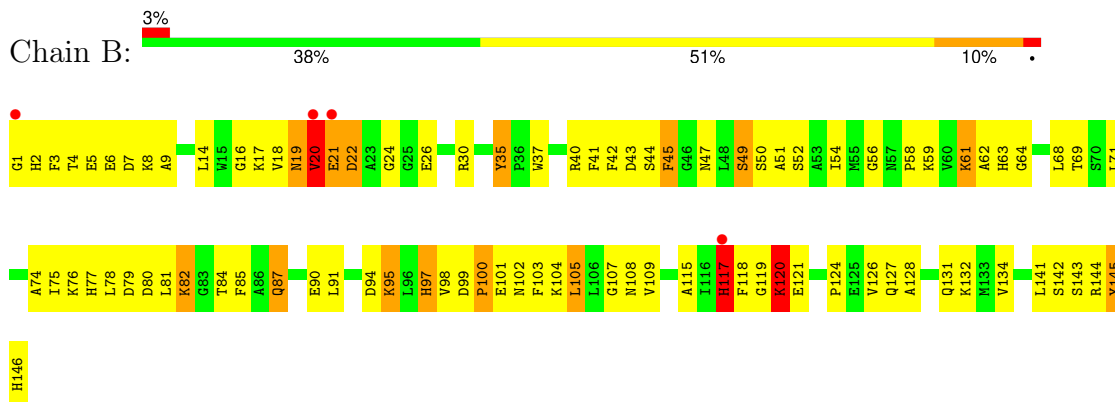
3 Residue-property plots

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: HEMOGLOBIN GAMMA CHAINS



• Molecule 1: HEMOGLOBIN GAMMA CHAINS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.62Å 82.84Å 53.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.5 (20.00-1.70) 88.6 (20.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.244 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2638	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	3.60	152/1157 (13.1%)	2.14	48/1565 (3.1%)
1	B	3.55	147/1157 (12.7%)	2.13	47/1565 (3.0%)
All	All	3.58	299/2314 (12.9%)	2.13	95/3130 (3.0%)

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	1

All (299) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ASP	CA-CB	25.10	1.88	1.53
1	A	40	ARG	CD-NE	24.50	1.80	1.46
1	A	117	HIS	CG-CD2	-20.79	1.12	1.35
1	B	117	HIS	CE1-NE2	19.25	1.51	1.32
1	B	21	GLU	N-CA	18.21	1.71	1.46
1	A	144	ARG	CZ-NH2	17.47	1.56	1.33
1	A	1	GLY	C-N	17.07	1.57	1.33
1	A	146	HIS	CE1-NE2	17.00	1.49	1.32
1	A	40	ARG	NE-CZ	-16.63	1.14	1.33
1	A	2	HIS	CG-CD2	15.95	1.53	1.35
1	B	117	HIS	CD2-NE2	-14.80	1.21	1.37
1	A	101	GLU	CD-OE1	14.71	1.53	1.25
1	B	2	HIS	CG-CD2	14.33	1.51	1.35
1	B	2	HIS	N-CA	-14.18	1.27	1.46
1	B	40	ARG	NE-CZ	14.15	1.48	1.33
1	B	97	HIS	CE1-NE2	13.56	1.46	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ARG	CZ-NH2	13.53	1.51	1.33
1	A	117	HIS	CD2-NE2	13.35	1.52	1.37
1	B	94	ASP	C-N	13.30	1.51	1.33
1	B	26	GLU	CD-OE1	13.11	1.50	1.25
1	B	79	ASP	C-N	-12.98	1.17	1.33
1	B	101	GLU	CD-OE1	12.94	1.50	1.25
1	B	98	VAL	CA-CB	12.73	1.70	1.54
1	B	19	ASN	CG-ND2	-12.67	1.06	1.33
1	B	40	ARG	CZ-NH1	-12.29	1.15	1.32
1	B	2	HIS	CE1-NE2	12.06	1.44	1.32
1	A	78	LEU	CA-C	-12.03	1.35	1.52
1	B	49	SER	C-N	11.80	1.48	1.33
1	B	26	GLU	CD-OE2	-11.70	1.03	1.25
1	B	90	GLU	CD-OE1	11.47	1.47	1.25
1	B	47	ASN	CA-CB	11.35	1.70	1.53
1	B	20	VAL	CB-CG1	-11.13	1.15	1.52
1	A	80	ASP	CA-C	-11.04	1.41	1.53
1	A	1	GLY	N-CA	10.79	1.62	1.45
1	B	146	HIS	CE1-NE2	10.74	1.43	1.32
1	A	94	ASP	N-CA	10.67	1.59	1.46
1	B	21	GLU	C-O	10.38	1.37	1.24
1	B	146	HIS	C-O	10.28	1.44	1.23
1	B	99	ASP	CG-OD2	10.04	1.44	1.25
1	B	4	THR	CA-C	-9.85	1.39	1.53
1	B	94	ASP	N-CA	9.76	1.58	1.46
1	A	117	HIS	ND1-CE1	9.72	1.42	1.32
1	A	6	GLU	CD-OE1	9.61	1.43	1.25
1	A	43	ASP	CG-OD2	9.57	1.43	1.25
1	A	80	ASP	CB-CG	9.46	1.75	1.52
1	A	44	SER	CA-C	-9.43	1.39	1.52
1	B	99	ASP	CB-CG	-9.39	1.28	1.52
1	A	101	GLU	CA-C	9.32	1.65	1.52
1	A	146	HIS	CD2-NE2	-9.30	1.27	1.37
1	A	18	VAL	CA-CB	9.23	1.65	1.54
1	B	42	PHE	CA-CB	9.20	1.65	1.53
1	B	19	ASN	CG-OD1	9.13	1.40	1.23
1	A	117	HIS	CB-CG	9.08	1.62	1.50
1	A	19	ASN	C-N	-9.06	1.22	1.33
1	B	117	HIS	CG-CD2	-9.06	1.25	1.35
1	A	69	THR	N-CA	9.03	1.57	1.46
1	B	3	PHE	CA-C	-9.03	1.41	1.52
1	B	120	LYS	CD-CE	-8.94	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	HIS	CG-CD2	8.94	1.45	1.35
1	B	54	ILE	N-CA	8.90	1.57	1.46
1	A	77	HIS	CE1-NE2	8.83	1.41	1.32
1	A	82	LYS	CA-CB	8.82	1.67	1.53
1	A	21	GLU	CD-OE2	8.82	1.42	1.25
1	B	2	HIS	CB-CG	-8.81	1.37	1.50
1	B	8	LYS	CA-C	-8.80	1.41	1.52
1	B	3	PHE	N-CA	8.72	1.57	1.46
1	B	22	ASP	CG-OD2	8.68	1.41	1.25
1	B	101	GLU	CG-CD	-8.66	1.30	1.52
1	A	146	HIS	CB-CG	-8.66	1.38	1.50
1	B	121	GLU	CA-C	8.54	1.64	1.52
1	B	49	SER	CA-CB	8.49	1.68	1.53
1	B	22	ASP	CG-OD1	-8.48	1.09	1.25
1	B	98	VAL	CA-C	-8.44	1.43	1.52
1	B	44	SER	CA-CB	-8.44	1.39	1.53
1	B	142	SER	N-CA	8.42	1.57	1.46
1	B	19	ASN	CA-C	8.35	1.63	1.52
1	A	93	CYS	N-CA	8.34	1.56	1.46
1	A	20	VAL	N-CA	8.31	1.56	1.46
1	A	2	HIS	C-O	-8.28	1.13	1.24
1	A	6	GLU	CD-OE2	-8.27	1.09	1.25
1	B	1	GLY	C-N	8.18	1.45	1.33
1	B	5	GLU	N-CA	-8.09	1.36	1.46
1	A	4	THR	N-CA	8.07	1.56	1.45
1	B	56	GLY	CA-C	8.04	1.64	1.51
1	A	2	HIS	CA-C	8.01	1.63	1.52
1	A	6	GLU	C-N	-7.97	1.23	1.33
1	A	87	GLN	CD-NE2	7.93	1.50	1.33
1	B	4	THR	N-CA	-7.92	1.35	1.45
1	A	6	GLU	CG-CD	7.90	1.71	1.52
1	B	94	ASP	C-O	-7.88	1.14	1.24
1	A	5	GLU	CD-OE1	7.85	1.40	1.25
1	B	146	HIS	CG-ND1	7.82	1.46	1.38
1	A	145	TYR	CA-CB	-7.71	1.40	1.53
1	B	51	ALA	C-N	7.71	1.44	1.33
1	B	47	ASN	CA-C	7.69	1.62	1.52
1	B	45	PHE	CE1-CZ	7.65	1.61	1.38
1	A	82	LYS	C-N	7.60	1.43	1.33
1	B	132	LYS	C-N	-7.57	1.23	1.33
1	B	41	PHE	C-N	-7.53	1.22	1.33
1	B	100	PRO	N-CA	-7.51	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	HIS	CA-C	7.49	1.62	1.52
1	A	86	ALA	C-O	7.49	1.32	1.24
1	A	60	VAL	C-O	7.46	1.32	1.24
1	B	75	ILE	CA-CB	7.44	1.64	1.54
1	A	37	TRP	NE1-CE2	-7.43	1.29	1.37
1	B	115	ALA	CA-CB	7.40	1.65	1.53
1	A	80	ASP	C-O	7.39	1.36	1.23
1	B	18	VAL	CA-CB	7.39	1.64	1.54
1	B	47	ASN	CG-OD1	7.37	1.37	1.23
1	B	6	GLU	CA-C	7.36	1.62	1.52
1	A	72	GLY	N-CA	7.32	1.55	1.45
1	A	77	HIS	ND1-CE1	-7.30	1.25	1.32
1	B	117	HIS	CB-CG	7.27	1.60	1.50
1	B	20	VAL	N-CA	7.22	1.55	1.46
1	A	107	GLY	C-N	-7.21	1.24	1.34
1	A	4	THR	CA-CB	-7.17	1.42	1.53
1	A	12	THR	C-N	-7.11	1.24	1.33
1	A	25	GLY	C-N	7.10	1.43	1.34
1	A	3	PHE	C-O	7.08	1.32	1.24
1	A	95	LYS	C-O	7.06	1.33	1.23
1	A	104	LYS	C-O	7.05	1.32	1.24
1	A	22	ASP	N-CA	7.04	1.55	1.46
1	B	52	SER	CA-CB	7.02	1.64	1.53
1	B	119	GLY	C-O	-7.01	1.14	1.24
1	A	45	PHE	CA-C	7.00	1.62	1.52
1	A	86	ALA	N-CA	6.98	1.54	1.46
1	B	119	GLY	N-CA	6.94	1.54	1.45
1	A	61	LYS	N-CA	6.92	1.54	1.46
1	A	80	ASP	CG-OD2	-6.92	1.12	1.25
1	A	90	GLU	CD-OE2	6.92	1.38	1.25
1	A	43	ASP	CA-CB	6.90	1.64	1.53
1	A	19	ASN	C-O	6.87	1.32	1.23
1	A	2	HIS	CD2-NE2	6.84	1.45	1.37
1	B	63	HIS	CE1-NE2	6.83	1.39	1.32
1	A	2	HIS	ND1-CE1	6.80	1.39	1.32
1	A	45	PHE	C-O	-6.78	1.14	1.24
1	A	108	ASN	CG-OD1	6.75	1.36	1.23
1	A	20	VAL	CA-C	-6.75	1.44	1.52
1	A	99	ASP	CG-OD1	6.68	1.38	1.25
1	B	51	ALA	CA-C	-6.68	1.44	1.52
1	A	100	PRO	CA-CB	6.67	1.63	1.53
1	B	37	TRP	C-N	6.65	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	74	ALA	N-CA	-6.65	1.38	1.46
1	B	103	PHE	C-O	-6.65	1.16	1.24
1	A	144	ARG	CZ-NH1	-6.62	1.23	1.32
1	B	117	HIS	CG-ND1	-6.62	1.30	1.38
1	A	133	MET	CA-C	6.60	1.61	1.52
1	A	143	SER	CA-CB	6.55	1.63	1.53
1	A	79	ASP	N-CA	-6.51	1.38	1.46
1	A	105	LEU	CB-CG	-6.47	1.40	1.53
1	A	137	VAL	CA-CB	6.47	1.62	1.54
1	A	78	LEU	C-O	6.47	1.32	1.24
1	A	20	VAL	C-N	6.46	1.42	1.34
1	B	77	HIS	N-CA	-6.46	1.36	1.46
1	A	145	TYR	C-O	6.43	1.32	1.24
1	A	86	ALA	C-N	-6.43	1.25	1.33
1	B	50	SER	C-N	-6.41	1.25	1.33
1	B	21	GLU	CA-C	-6.39	1.43	1.52
1	A	54	ILE	CA-C	-6.39	1.45	1.52
1	B	80	ASP	C-N	6.36	1.42	1.34
1	B	97	HIS	CB-CG	6.36	1.59	1.50
1	A	124	PRO	C-O	-6.34	1.16	1.24
1	B	95	LYS	C-O	6.34	1.31	1.23
1	A	5	GLU	CA-C	6.32	1.61	1.52
1	A	7	ASP	N-CA	6.30	1.53	1.46
1	A	92	HIS	C-N	-6.30	1.25	1.33
1	A	138	ALA	N-CA	6.28	1.53	1.46
1	B	42	PHE	C-N	6.28	1.43	1.33
1	B	76	LYS	C-O	6.26	1.32	1.24
1	B	21	GLU	CB-CG	-6.25	1.33	1.52
1	A	96	LEU	C-O	6.24	1.32	1.24
1	B	19	ASN	CB-CG	6.21	1.67	1.52
1	A	87	GLN	C-O	6.20	1.31	1.24
1	B	102	ASN	N-CA	-6.13	1.38	1.46
1	B	50	SER	N-CA	-6.13	1.38	1.45
1	A	26	GLU	CD-OE1	6.10	1.36	1.25
1	A	10	THR	CA-C	-6.08	1.45	1.52
1	B	44	SER	CB-OG	6.04	1.54	1.42
1	A	6	GLU	C-O	6.03	1.31	1.24
1	B	69	THR	C-N	6.03	1.42	1.34
1	B	95	LYS	CA-C	-6.01	1.45	1.53
1	A	110	LEU	C-N	-6.00	1.26	1.33
1	B	20	VAL	CA-CB	6.00	1.62	1.54
1	B	4	THR	C-O	5.99	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	18	VAL	N-CA	-5.98	1.39	1.46
1	B	81	LEU	N-CA	5.98	1.53	1.46
1	B	143	SER	N-CA	5.98	1.53	1.46
1	A	140	ALA	C-O	5.97	1.31	1.24
1	A	79	ASP	CG-OD1	5.96	1.36	1.25
1	A	4	THR	CA-C	-5.96	1.45	1.53
1	B	49	SER	CA-C	-5.94	1.44	1.52
1	A	80	ASP	CG-OD1	-5.93	1.14	1.25
1	B	16	GLY	C-N	-5.93	1.25	1.33
1	A	8	LYS	C-N	5.92	1.41	1.33
1	B	37	TRP	C-O	-5.91	1.16	1.24
1	A	134	VAL	CA-C	-5.89	1.45	1.52
1	A	81	LEU	CA-C	5.88	1.60	1.52
1	A	80	ASP	CA-CB	5.88	1.57	1.53
1	A	128	ALA	CA-C	-5.86	1.45	1.52
1	B	144	ARG	CZ-NH2	5.83	1.41	1.33
1	B	101	GLU	CB-CG	5.82	1.69	1.52
1	A	15	TRP	NE1-CE2	-5.81	1.31	1.37
1	A	142	SER	N-CA	5.80	1.53	1.46
1	A	146	HIS	CA-C	-5.80	1.40	1.52
1	B	47	ASN	CB-CG	-5.78	1.37	1.52
1	B	43	ASP	N-CA	5.77	1.54	1.46
1	A	63	HIS	CA-C	5.77	1.60	1.52
1	A	39	GLN	N-CA	5.73	1.53	1.46
1	B	97	HIS	C-N	5.72	1.41	1.33
1	B	2	HIS	CA-CB	5.72	1.63	1.53
1	B	59	LYS	CE-NZ	5.71	1.66	1.49
1	B	81	LEU	CA-CB	-5.71	1.43	1.53
1	A	137	VAL	CA-C	5.70	1.60	1.52
1	B	85	PHE	CA-CB	5.70	1.62	1.53
1	A	140	ALA	CA-C	-5.69	1.45	1.52
1	A	133	MET	CA-CB	5.69	1.62	1.53
1	A	74	ALA	C-N	5.67	1.40	1.34
1	A	21	GLU	CA-CB	5.66	1.62	1.53
1	B	59	LYS	C-N	-5.65	1.26	1.33
1	A	77	HIS	CD2-NE2	5.64	1.44	1.37
1	A	146	HIS	N-CA	5.64	1.56	1.46
1	A	14	LEU	C-N	5.63	1.41	1.34
1	A	105	LEU	CG-CD1	5.61	1.71	1.52
1	B	45	PHE	CA-CB	5.61	1.63	1.53
1	B	3	PHE	C-N	5.60	1.41	1.33
1	B	146	HIS	C-OXT	-5.60	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	GLU	CA-CB	5.60	1.62	1.53
1	B	105	LEU	CB-CG	-5.60	1.42	1.53
1	A	20	VAL	CB-CG1	-5.58	1.34	1.52
1	B	63	HIS	ND1-CE1	5.57	1.38	1.32
1	A	139	SER	CA-C	-5.54	1.45	1.52
1	A	6	GLU	N-CA	5.54	1.53	1.46
1	B	126	VAL	CA-C	5.53	1.59	1.52
1	B	64	GLY	N-CA	5.52	1.53	1.45
1	B	84	THR	CA-C	5.52	1.60	1.52
1	B	19	ASN	CA-CB	-5.52	1.46	1.52
1	A	14	LEU	CA-CB	5.50	1.62	1.53
1	A	103	PHE	C-O	5.46	1.30	1.24
1	B	52	SER	C-O	-5.45	1.17	1.24
1	B	58	PRO	N-CD	5.44	1.55	1.47
1	A	4	THR	CB-OG1	5.43	1.52	1.43
1	B	145	TYR	CE2-CZ	5.42	1.51	1.38
1	B	82	LYS	N-CA	5.42	1.52	1.46
1	B	54	ILE	CB-CG1	5.42	1.64	1.53
1	A	43	ASP	CB-CG	-5.42	1.38	1.52
1	A	40	ARG	CZ-NH1	-5.40	1.25	1.32
1	A	97	HIS	CD2-NE2	-5.38	1.31	1.37
1	B	42	PHE	N-CA	-5.38	1.40	1.46
1	A	42	PHE	C-N	5.38	1.41	1.34
1	B	54	ILE	CA-C	-5.37	1.46	1.52
1	B	17	LYS	C-N	5.36	1.49	1.33
1	A	52	SER	C-N	-5.35	1.26	1.33
1	A	59	LYS	CA-C	5.34	1.59	1.52
1	B	82	LYS	C-N	5.33	1.40	1.33
1	B	45	PHE	C-O	-5.32	1.17	1.24
1	B	41	PHE	C-O	5.32	1.31	1.24
1	B	71	LEU	C-N	-5.31	1.26	1.33
1	A	87	GLN	CG-CD	5.30	1.65	1.52
1	A	20	VAL	CA-CB	5.29	1.61	1.54
1	B	7	ASP	C-O	-5.27	1.18	1.24
1	A	99	ASP	CA-C	-5.27	1.46	1.52
1	B	87	GLN	CD-OE1	5.26	1.33	1.23
1	A	126	VAL	CA-C	5.26	1.59	1.52
1	B	141	LEU	CA-C	5.26	1.59	1.52
1	B	144	ARG	CA-C	5.26	1.60	1.52
1	A	15	TRP	CA-CB	5.25	1.61	1.53
1	A	134	VAL	N-CA	5.25	1.52	1.46
1	B	43	ASP	CG-OD1	-5.25	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	GLY	C-O	5.24	1.30	1.23
1	B	47	ASN	N-CA	-5.22	1.39	1.46
1	A	52	SER	CA-C	5.21	1.59	1.52
1	A	107	GLY	C-O	5.20	1.30	1.23
1	A	26	GLU	N-CA	-5.18	1.39	1.46
1	A	102	ASN	CG-OD1	-5.18	1.13	1.23
1	B	77	HIS	CB-CG	5.17	1.57	1.50
1	B	62	ALA	N-CA	-5.17	1.40	1.46
1	B	101	GLU	C-N	5.17	1.41	1.34
1	A	139	SER	C-O	5.17	1.30	1.24
1	A	10	THR	N-CA	5.16	1.52	1.46
1	B	79	ASP	CG-OD2	-5.15	1.15	1.25
1	B	9	ALA	N-CA	-5.13	1.40	1.46
1	B	143	SER	CA-C	-5.13	1.45	1.52
1	A	30	ARG	N-CA	5.11	1.52	1.46
1	A	60	VAL	C-N	-5.11	1.26	1.33
1	A	52	SER	CA-CB	5.11	1.61	1.53
1	A	99	ASP	CA-CB	5.10	1.63	1.53
1	A	94	ASP	CB-CG	-5.09	1.39	1.52
1	A	127	GLN	CD-NE2	5.07	1.43	1.33
1	B	143	SER	C-O	5.07	1.30	1.24
1	B	109	VAL	CA-CB	5.07	1.61	1.54
1	A	46	GLY	N-CA	5.06	1.52	1.45
1	A	143	SER	C-N	-5.05	1.27	1.33
1	A	146	HIS	ND1-CE1	5.04	1.37	1.32
1	B	8	LYS	C-N	5.03	1.40	1.33
1	B	47	ASN	C-O	-5.02	1.17	1.24
1	B	128	ALA	CA-CB	5.02	1.61	1.53
1	A	77	HIS	CG-ND1	5.01	1.43	1.38
1	B	85	PHE	CG-CD2	5.01	1.49	1.38
1	B	97	HIS	CG-ND1	-5.00	1.32	1.38

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	HIS	ND1-CG-CD2	15.93	122.03	106.10
1	A	40	ARG	NE-CZ-NH2	-13.61	106.95	119.20
1	B	21	GLU	N-CA-C	-13.33	97.63	114.56
1	A	40	ARG	NE-CZ-NH1	12.99	134.50	121.50
1	B	20	VAL	CG1-CB-CG2	10.67	134.28	110.80
1	B	47	ASN	OD1-CG-ND2	-10.34	112.26	122.60
1	B	21	GLU	CA-C-O	-10.30	106.81	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	CB-CA-C	-10.27	94.49	111.02
1	A	144	ARG	NE-CZ-NH1	9.32	130.82	121.50
1	B	146	HIS	CA-C-O	-9.12	93.65	121.00
1	A	146	HIS	ND1-CE1-NE2	-8.69	99.71	108.40
1	B	117	HIS	CG-CD2-NE2	8.52	115.72	107.20
1	A	146	HIS	CG-CD2-NE2	7.99	115.19	107.20
1	B	45	PHE	CZ-CE2-CD2	7.79	134.01	120.00
1	A	79	ASP	CA-CB-CG	-7.76	104.84	112.60
1	B	101	GLU	OE1-CD-OE2	-7.54	104.81	122.90
1	A	43	ASP	CA-CB-CG	-7.25	105.34	112.60
1	A	131	GLN	N-CA-C	-7.21	103.50	111.36
1	A	117	HIS	CG-ND1-CE1	-6.97	97.45	109.30
1	B	21	GLU	N-CA-CB	-6.96	101.74	111.00
1	A	146	HIS	CA-CB-CG	6.94	120.74	113.80
1	A	81	LEU	CA-C-N	-6.93	111.00	120.28
1	A	81	LEU	C-N-CA	-6.93	111.00	120.28
1	B	43	ASP	CA-CB-CG	-6.93	105.67	112.60
1	B	19	ASN	CA-CB-CG	-6.91	105.69	112.60
1	B	49	SER	CA-C-O	6.86	127.89	119.11
1	B	94	ASP	CA-C-O	6.84	127.83	120.24
1	B	40	ARG	NH1-CZ-NH2	6.78	128.11	119.30
1	B	43	ASP	OD1-CG-OD2	-6.75	106.71	122.90
1	A	78	LEU	O-C-N	-6.68	113.70	122.39
1	B	98	VAL	N-CA-CB	-6.65	103.28	110.53
1	A	1	GLY	O-C-N	-6.64	112.37	123.00
1	B	97	HIS	ND1-CE1-NE2	-6.57	101.83	108.40
1	A	2	HIS	CA-C-N	-6.51	113.73	122.72
1	A	2	HIS	C-N-CA	-6.51	113.73	122.72
1	A	117	HIS	CB-CG-ND1	-6.41	113.09	122.70
1	A	52	SER	O-C-N	6.36	129.40	122.15
1	B	117	HIS	CE1-NE2-CD2	-6.31	102.69	109.00
1	A	6	GLU	CA-C-O	-6.13	113.44	120.24
1	B	117	HIS	ND1-CE1-NE2	-6.12	102.28	108.40
1	B	43	ASP	CB-CG-OD1	6.12	132.47	118.40
1	B	40	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	6	GLU	N-CA-C	-6.03	104.28	111.69
1	A	144	ARG	NE-CZ-NH2	-6.02	113.79	119.20
1	B	132	LYS	N-CA-C	-6.00	104.82	111.36
1	A	40	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	B	80	ASP	CB-CA-C	-5.91	102.27	112.44
1	A	80	ASP	CA-CB-CG	-5.91	106.69	112.60
1	B	97	HIS	CA-CB-CG	-5.79	108.01	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	SER	CA-C-O	-5.74	114.34	120.42
1	A	35	TYR	CA-C-N	5.74	126.13	119.47
1	A	35	TYR	C-N-CA	5.74	126.13	119.47
1	A	5	GLU	N-CA-C	-5.68	105.23	111.82
1	B	17	LYS	CA-C-N	-5.64	112.22	122.43
1	B	17	LYS	C-N-CA	-5.64	112.22	122.43
1	B	22	ASP	CA-CB-CG	-5.63	106.97	112.60
1	B	4	THR	O-C-N	-5.62	115.74	122.65
1	A	97	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	90	GLU	CA-C-O	5.59	126.47	120.55
1	B	3	PHE	O-C-N	-5.58	116.69	123.16
1	B	108	ASN	CA-CB-CG	-5.53	107.07	112.60
1	B	41	PHE	CA-C-O	-5.52	112.47	119.31
1	A	21	GLU	O-C-N	5.50	128.65	122.22
1	A	43	ASP	CB-CG-OD1	5.48	131.01	118.40
1	A	1	GLY	CA-C-O	5.48	132.30	120.80
1	A	87	GLN	CB-CG-CD	-5.46	103.32	112.60
1	B	43	ASP	N-CA-C	-5.45	106.70	113.19
1	A	146	HIS	CA-C-O	5.36	137.06	121.00
1	A	101	GLU	OE1-CD-OE2	-5.34	110.08	122.90
1	B	19	ASN	CB-CG-OD1	-5.33	110.13	120.80
1	A	146	HIS	CB-CA-C	5.32	120.21	110.10
1	B	146	HIS	CG-CD2-NE2	5.32	112.52	107.20
1	B	78	LEU	N-CA-C	5.29	117.79	111.71
1	B	42	PHE	CA-C-O	5.28	127.72	121.17
1	A	4	THR	O-C-N	-5.26	116.23	122.65
1	B	99	ASP	CB-CG-OD1	5.25	130.48	118.40
1	B	52	SER	N-CA-CB	-5.23	102.43	110.12
1	B	99	ASP	OD1-CG-OD2	-5.22	110.37	122.90
1	B	126	VAL	O-C-N	5.22	126.93	121.87
1	A	132	LYS	N-CA-C	-5.21	105.68	111.36
1	A	104	LYS	N-CA-C	-5.19	105.70	111.36
1	B	104	LYS	N-CA-C	-5.18	105.70	112.23
1	B	75	ILE	CA-CB-CG1	-5.17	101.61	110.40
1	A	101	GLU	N-CA-C	-5.16	105.78	111.71
1	B	97	HIS	CA-C-O	5.15	127.41	121.28
1	B	35	TYR	CA-C-N	5.10	126.22	119.84
1	B	35	TYR	C-N-CA	5.10	126.22	119.84
1	A	78	LEU	CA-C-N	-5.08	114.59	122.67
1	A	78	LEU	C-N-CA	-5.08	114.59	122.67
1	A	69	THR	N-CA-C	-5.08	105.93	111.82
1	A	105	LEU	CD1-CG-CD2	-5.07	99.65	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASN	CA-C-O	5.06	125.78	119.97
1	B	117	HIS	CB-CG-ND1	-5.03	115.15	122.70
1	A	17	LYS	N-CA-C	-5.03	106.83	113.17
1	B	98	VAL	CB-CA-C	-5.02	104.63	111.15

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	GLY	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	1131	0	1128	14	3
1	B	1131	0	1128	29	1
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	143	0	0	2	0
4	B	143	0	0	4	5
All	All	2638	0	2316	42	5

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 9.

All (42) 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:80:ASP:CB	1:A:80:ASP:CG	1.75	1.53
1:A:79:ASP:CA	1:A:79:ASP:CB	1.88	1.51
1:B:61:LYS:NZ	1:B:61:LYS:HB2	1.52	1.17
1:B:87:GLN:NE2	4:B:341:HOH:O	1.82	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:HD2	1:B:120:LYS:H	1.09	1.09
1:A:40:ARG:NH2	4:A:376:HOH:O	1.87	1.05
1:B:61:LYS:HB2	1:B:61:LYS:HZ3	1.12	0.94
1:B:91:LEU:HA	1:B:95:LYS:HD2	1.47	0.93
1:B:120:LYS:H	1:B:120:LYS:CD	1.81	0.93
1:B:61:LYS:NZ	1:B:61:LYS:CB	2.31	0.92
1:B:120:LYS:HD2	1:B:120:LYS:N	1.90	0.84
1:A:79:ASP:CB	1:A:79:ASP:C	2.55	0.80
1:B:61:LYS:HB2	1:B:61:LYS:HZ2	1.45	0.79
1:B:20:VAL:C	1:B:21:GLU:CA	2.58	0.77
1:B:20:VAL:HG12	1:B:20:VAL:O	1.87	0.75
1:B:87:GLN:HG2	4:B:328:HOH:O	1.88	0.72
1:B:61:LYS:HZ3	1:B:61:LYS:CB	1.96	0.67
1:A:80:ASP:CG	1:A:80:ASP:CA	2.67	0.67
1:A:79:ASP:CB	1:A:79:ASP:N	2.58	0.66
1:A:79:ASP:CA	1:A:79:ASP:CG	2.69	0.65
1:B:100:PRO:HG3	1:B:145:TYR:CD2	2.35	0.61
1:A:80:ASP:CB	1:A:80:ASP:OD1	2.40	0.61
1:B:127:GLN:HE21	1:B:131:GLN:HE21	1.52	0.58
1:A:100:PRO:HG3	1:A:145:TYR:CD2	2.39	0.57
1:A:99:ASP:HB2	4:A:394:HOH:O	2.05	0.57
1:B:19:ASN:HD21	1:B:21:GLU:HB3	1.70	0.56
1:A:40:ARG:NE	1:A:40:ARG:CG	2.67	0.53
1:B:21:GLU:N	1:B:22:ASP:N	2.58	0.52
1:B:35:TYR:CZ	1:B:105:LEU:HD11	2.45	0.52
1:B:120:LYS:CD	1:B:120:LYS:N	2.63	0.51
1:B:107:GLY:HA3	1:B:134:VAL:HG13	1.93	0.51
1:A:21:GLU:H	1:A:21:GLU:CD	2.24	0.46
1:A:99:ASP:HB3	1:A:102:ASN:ND2	2.31	0.45
1:B:19:ASN:ND2	1:B:21:GLU:HB3	2.32	0.44
1:B:24:GLY:HA2	1:B:68:LEU:HD13	1.99	0.44
1:B:45:PHE:HE1	2:B:147:HEM:O1D	2.01	0.43
1:A:127:GLN:OE1	1:B:30:ARG:HD3	2.20	0.42
1:B:100:PRO:HG3	1:B:145:TYR:CE2	2.56	0.41
1:B:14:LEU:HD11	1:B:118:PHE:CG	2.56	0.40
1:B:24:GLY:N	1:B:68:LEU:HD22	2.36	0.40
1:B:49:SER:HA	4:B:454:HOH:O	2.20	0.40
1:B:97:HIS:HE1	4:B:426:HOH:O	2.03	0.40

All (5) 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:40:ARG:CD	4:B:298:HOH:O[2_565]	1.43	0.77
4:B:468:HOH:O	4:B:468:HOH:O[2_665]	1.76	0.44
1:A:40:ARG:NH1	4:B:291:HOH:O[2_565]	1.95	0.25
1:A:40:ARG:NE	4:B:298:HOH:O[2_565]	1.98	0.22
1:B:117:HIS:CE1	4:B:368:HOH:O[2_665]	2.01	0.19

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	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	B	144/146 (99%)	141 (98%)	2 (1%)	1 (1%)	18	7
All	All	288/292 (99%)	283 (98%)	4 (1%)	1 (0%)	36	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	VAL

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	122/122 (100%)	122 (100%)	0	100	100
1	B	122/122 (100%)	117 (96%)	5 (4%)	27	11
All	All	244/244 (100%)	239 (98%)	5 (2%)	48	32

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	LYS
1	B	82	LYS
1	B	117	HIS
1	B	120	LYS
1	B	124	PRO

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

Mol	Chain	Res	Type
1	A	102	ASN
1	B	2	HIS
1	B	19	ASN
1	B	39	GLN
1	B	97	HIS
1	B	131	GLN

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
3	CMO	B	148	-	0,1,1	-	-	-		
3	CMO	A	148	-	0,1,1	-	-	-		
2	HEM	A	147	1	50,50,50	2.72	26 (52%)	67,82,82	2.05	22 (32%)
2	HEM	B	147	1	50,50,50	2.31	15 (30%)	67,82,82	1.37	7 (10%)

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	147	1	-	8/14/54/54	-
2	HEM	B	147	1	-	3/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	147	HEM	CBA-CGA	7.28	1.67	1.50
2	A	147	HEM	CBA-CAA	-5.76	1.32	1.51
2	B	147	HEM	CBD-CGD	5.62	1.63	1.50
2	A	147	HEM	CHC-C1C	5.05	1.48	1.38
2	A	147	HEM	CAB-C3B	4.78	1.60	1.47
2	A	147	HEM	C1C-NC	-4.73	1.30	1.39
2	A	147	HEM	CBC-CAC	4.65	1.52	1.30
2	B	147	HEM	CBB-CAB	4.37	1.51	1.30
2	A	147	HEM	CBB-CAB	4.32	1.51	1.30
2	B	147	HEM	CMB-C2B	4.28	1.59	1.50
2	A	147	HEM	CHA-C4D	4.25	1.47	1.38
2	A	147	HEM	CMB-C2B	4.25	1.59	1.50
2	A	147	HEM	C4A-NA	4.23	1.47	1.39
2	B	147	HEM	CAD-C3D	4.07	1.61	1.51
2	B	147	HEM	O2D-CGD	-3.97	1.17	1.30
2	A	147	HEM	CMC-C2C	3.83	1.58	1.50
2	A	147	HEM	C3B-C2B	-3.64	1.29	1.37
2	A	147	HEM	O2D-CGD	-3.62	1.18	1.30
2	B	147	HEM	CMA-C3A	3.53	1.58	1.50
2	A	147	HEM	C4D-ND	-3.52	1.34	1.40
2	A	147	HEM	CBD-CGD	3.40	1.58	1.50
2	A	147	HEM	C1B-NB	3.40	1.46	1.40
2	B	147	HEM	CAC-C3C	3.34	1.56	1.47
2	B	147	HEM	C1D-ND	3.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	147	HEM	C1D-ND	3.12	1.45	1.38
2	A	147	HEM	CBD-CAD	-2.71	1.42	1.51
2	B	147	HEM	CMD-C2D	2.67	1.56	1.50
2	B	147	HEM	C1A-C2A	2.59	1.49	1.44
2	A	147	HEM	C3D-C2D	2.56	1.42	1.36
2	A	147	HEM	CAA-C2A	2.55	1.57	1.51
2	A	147	HEM	C3B-C4B	2.49	1.49	1.44
2	B	147	HEM	CBC-CAC	2.42	1.42	1.30
2	B	147	HEM	C1C-C2C	2.41	1.50	1.45
2	A	147	HEM	C1D-C2D	2.40	1.49	1.44
2	A	147	HEM	C1A-C2A	2.32	1.49	1.44
2	B	147	HEM	CHD-C4C	2.30	1.42	1.38
2	A	147	HEM	FE-NC	2.27	2.02	1.95
2	A	147	HEM	C2A-C3A	-2.09	1.33	1.38
2	A	147	HEM	CHB-C1B	2.09	1.42	1.38
2	A	147	HEM	CMA-C3A	2.06	1.55	1.50
2	B	147	HEM	CAB-C3B	2.02	1.52	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	147	HEM	C3D-C4D-ND	5.37	116.06	110.17
2	A	147	HEM	C1C-CHC-C4B	-4.35	116.77	126.02
2	A	147	HEM	C1D-C2D-C3D	-4.24	102.52	106.98
2	A	147	HEM	CHC-C1C-NC	4.14	128.97	124.45
2	B	147	HEM	C4C-C3C-C2C	4.07	110.34	106.81
2	A	147	HEM	CHD-C4C-NC	3.93	128.73	124.45
2	B	147	HEM	C3B-C4B-NB	3.80	112.20	109.47
2	A	147	HEM	CHC-C1C-C2C	-3.74	117.71	125.49
2	A	147	HEM	C4A-C3A-C2A	3.50	110.83	106.82
2	B	147	HEM	C3C-C2C-C1C	-3.50	103.73	107.05
2	A	147	HEM	CHC-C4B-NB	3.29	127.96	124.42
2	A	147	HEM	CAA-CBA-CGA	3.24	122.25	113.67
2	B	147	HEM	CHC-C1C-NC	3.11	127.84	124.45
2	A	147	HEM	C1B-NB-C4B	-3.09	101.55	105.21
2	A	147	HEM	CBA-CAA-C2A	3.07	121.03	112.53
2	A	147	HEM	O1D-CGD-CBD	-2.99	113.62	123.09
2	A	147	HEM	C4D-ND-C1D	-2.97	101.69	105.21
2	B	147	HEM	CAA-CBA-CGA	-2.92	105.93	113.67
2	A	147	HEM	C3B-C4B-NB	2.81	111.49	109.47
2	A	147	HEM	C2D-C1D-ND	2.54	112.84	109.90
2	A	147	HEM	CAD-CBD-CGD	2.46	120.19	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	147	HEM	CBB-CAB-C3B	-2.34	115.85	127.53
2	B	147	HEM	CHA-C1A-NA	2.29	128.02	123.86
2	A	147	HEM	CHC-C4B-C3B	-2.27	120.54	125.07
2	A	147	HEM	O2D-CGD-O1D	2.22	129.05	123.33
2	A	147	HEM	CHD-C4C-C3C	-2.19	121.52	125.21
2	A	147	HEM	CAD-C3D-C4D	2.17	128.47	124.70
2	B	147	HEM	CHC-C1C-C2C	-2.07	121.18	125.49
2	A	147	HEM	C3B-C2B-C1B	2.02	107.93	106.41

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	147	HEM	C2C-C3C-CAC-CBC
2	A	147	HEM	C2B-C3B-CAB-CBB
2	B	147	HEM	C2B-C3B-CAB-CBB
2	A	147	HEM	C4C-C3C-CAC-CBC
2	A	147	HEM	CAD-CBD-CGD-O2D
2	A	147	HEM	CAD-CBD-CGD-O1D
2	A	147	HEM	C4B-C3B-CAB-CBB
2	A	147	HEM	CAA-CBA-CGA-O1A
2	B	147	HEM	CAD-CBD-CGD-O1D
2	A	147	HEM	CAA-CBA-CGA-O2A
2	B	147	HEM	CAA-CBA-CGA-O2A

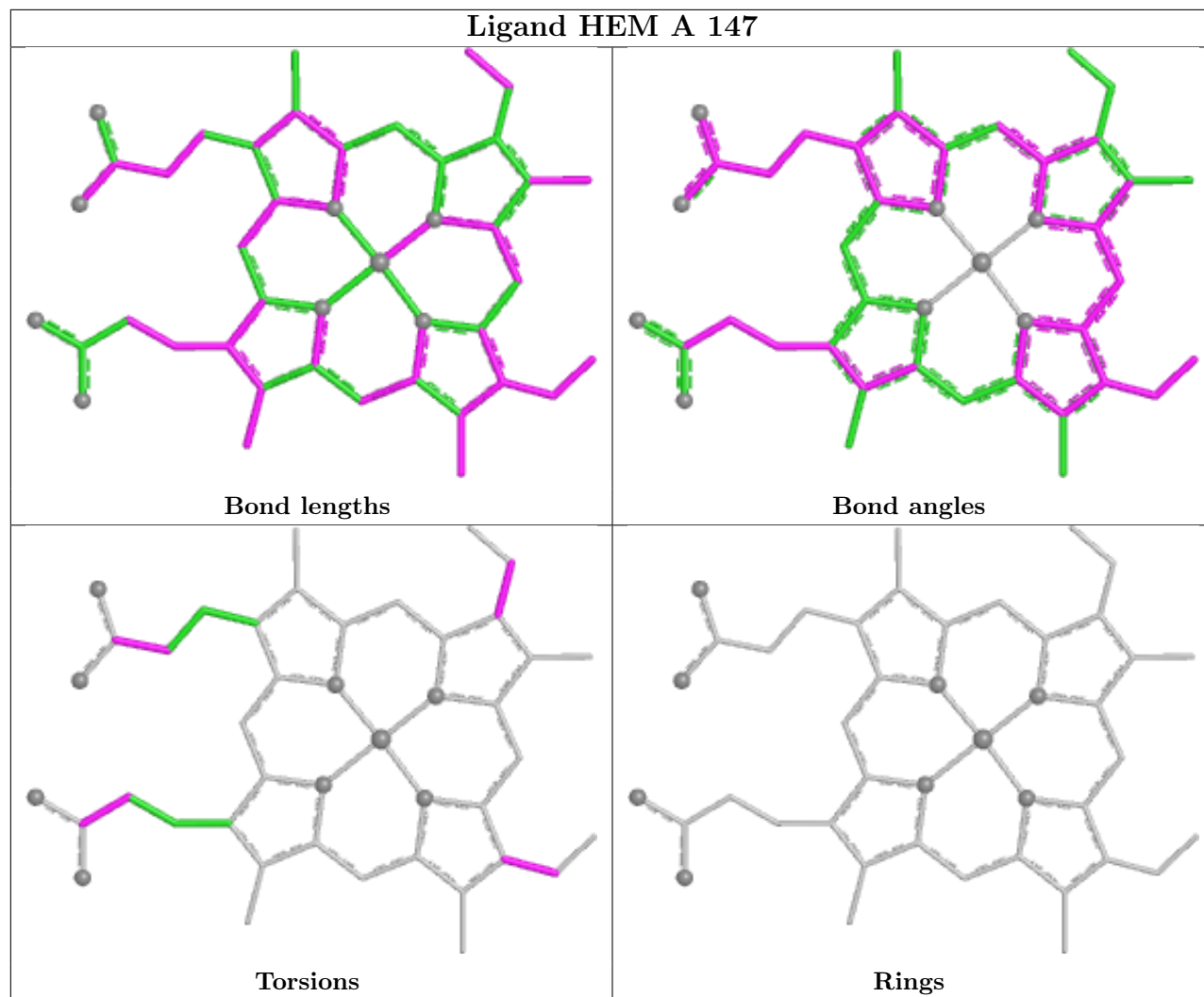
There are no ring outliers.

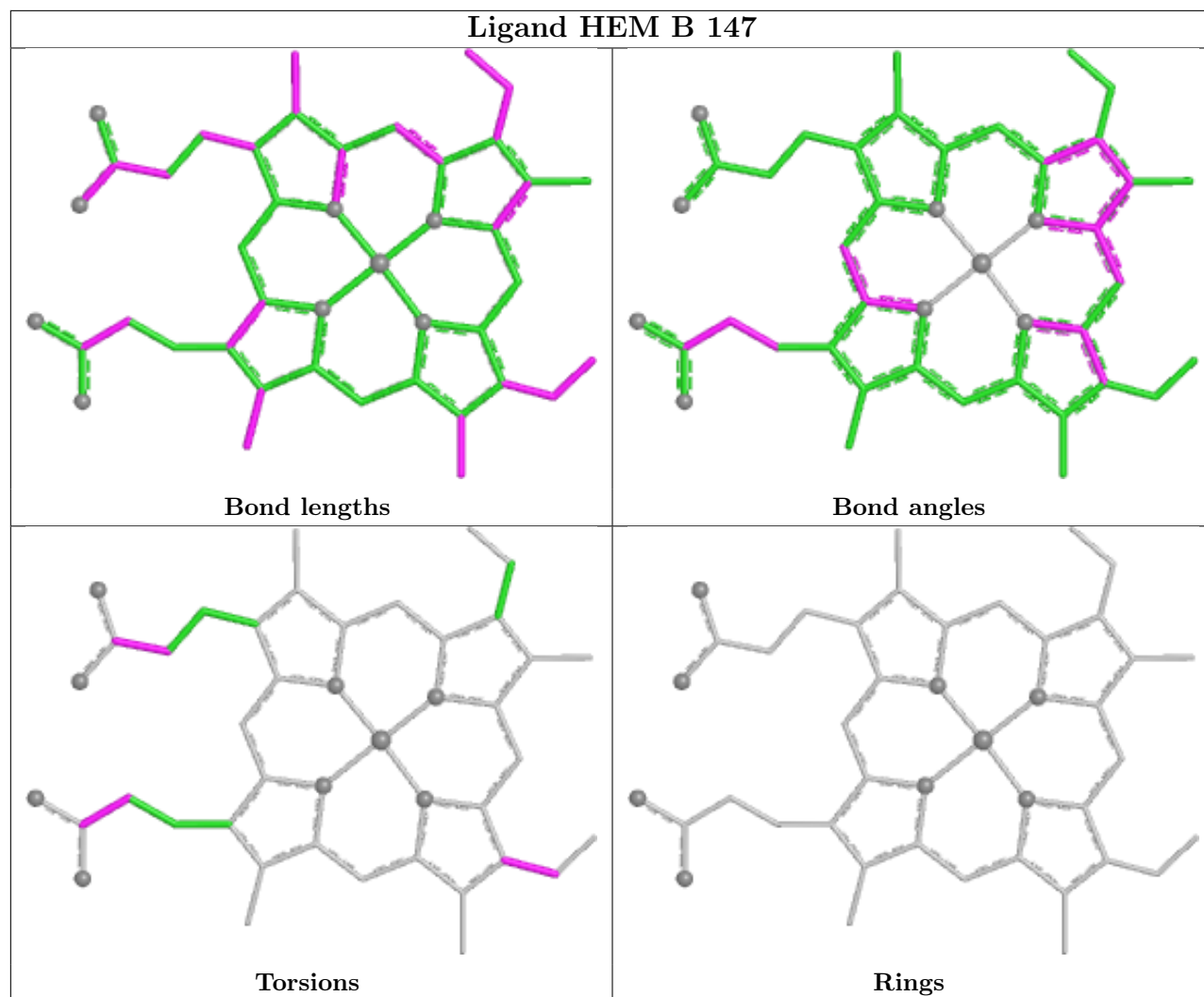
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	147	HEM	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](#)

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	79:ASP	C	80:ASP	N	1.17

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	146/146 (100%)	-0.01	2 (1%) 73 77	8, 15, 22, 28	11 (7%)
1	B	146/146 (100%)	0.14	4 (2%) 56 60	8, 15, 25, 30	15 (10%)
All	All	292/292 (100%)	0.06	6 (2%) 63 68	8, 15, 24, 30	26 (8%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	20	VAL	5.8
1	A	1	GLY	5.5
1	B	21	GLU	3.2
1	B	117	HIS	2.5
1	B	1	GLY	2.2
1	A	146	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

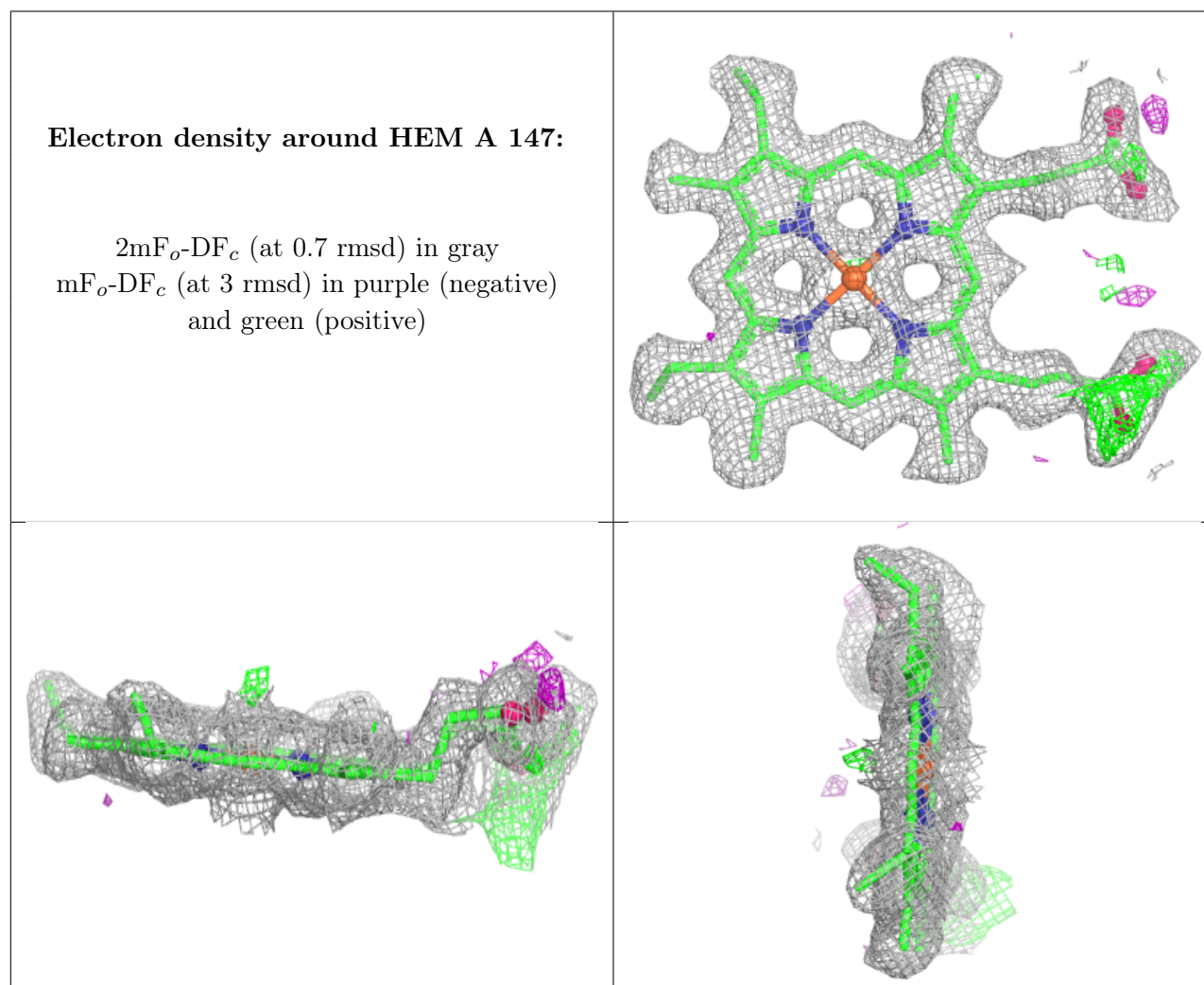
There are no oligosaccharides in this entry.

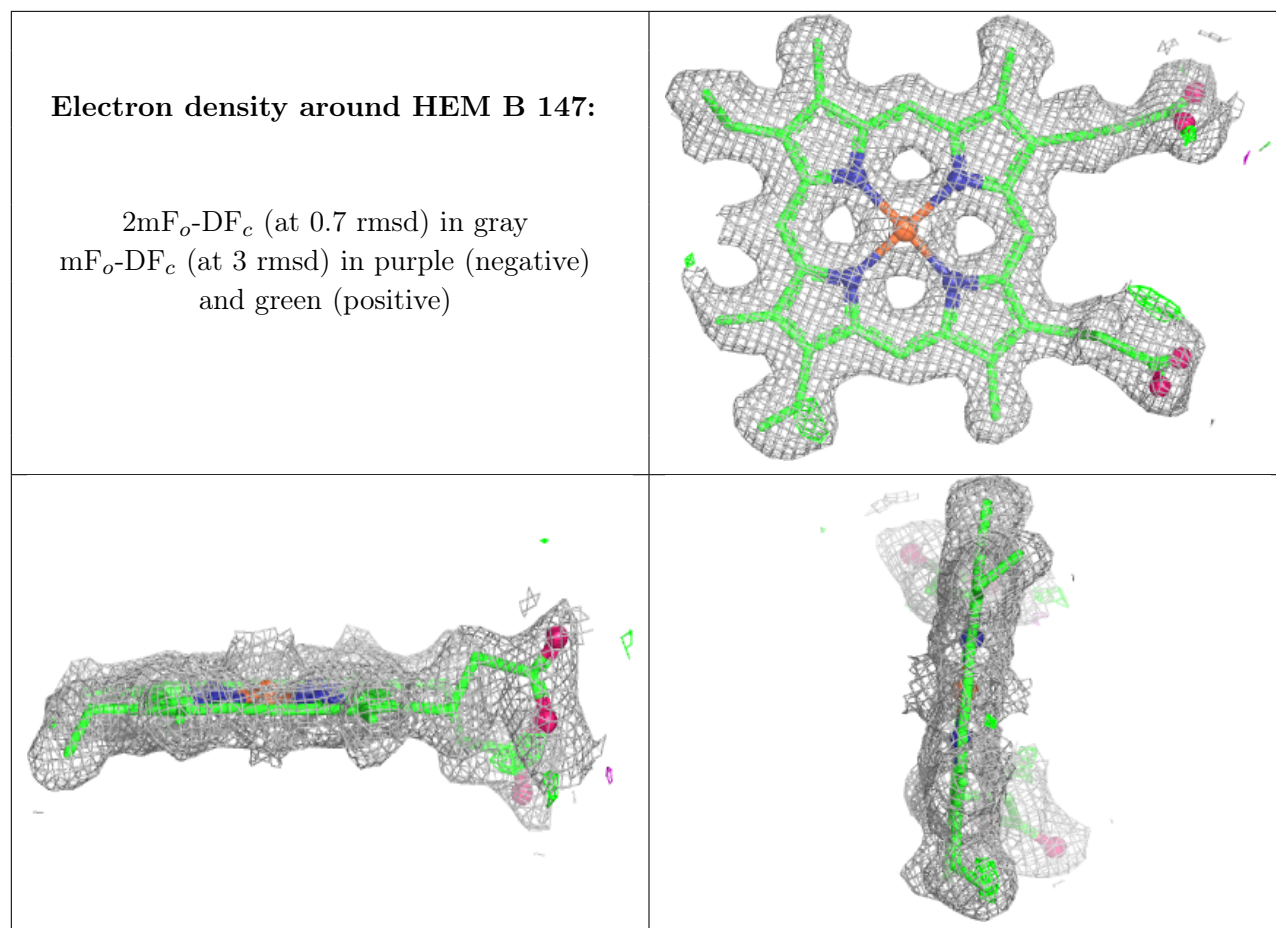
6.4 Ligands [i](#)

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
3	CMO	A	148	2/2	0.83	0.11	12,12,12,20	0
3	CMO	B	148	2/2	0.91	0.11	14,14,14,19	0
2	HEM	A	147	43/43	0.97	0.07	10,12,16,19	7
2	HEM	B	147	43/43	0.97	0.07	11,13,23,26	2

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.