



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 2GNW / pdb_00002gnw
Title : Crystal structure of non-symbiotic plant hemoglobin from rice, B10 mutant F40W
Authors : Hoy, J.A.
Deposited on : 2006-04-11
Resolution : 2.40 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

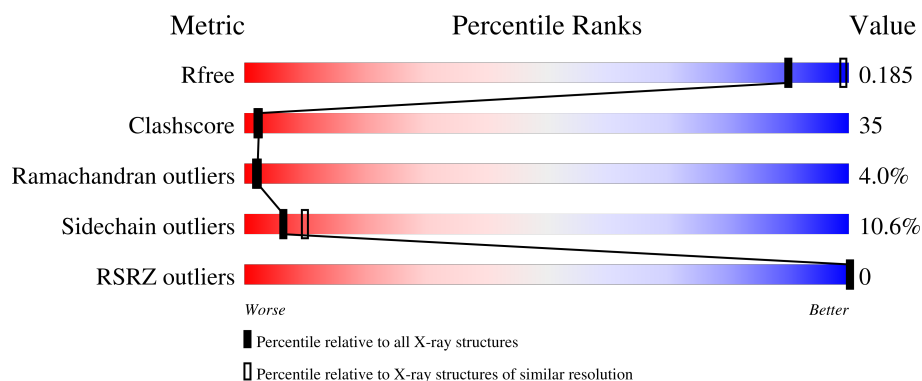
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

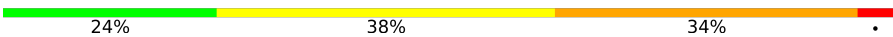
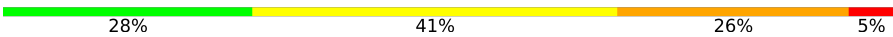
The reported resolution of this entry is 2.40 Å.

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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	165	 24% 38% 34% 5%
1	B	165	 28% 41% 26% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2765 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.

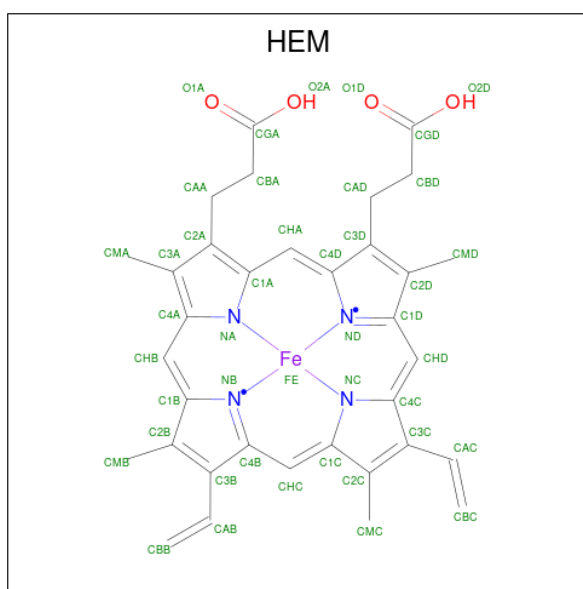
- Molecule 1 is a protein called Non-symbiotic hemoglobin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1291	829	217	238	7			
1	B	165	Total	C	N	O	S	0	0	0
			1291	829	217	238	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	TRP	PHE	engineered mutation	UNP O04986
B	40	TRP	PHE	engineered mutation	UNP O04986

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



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

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

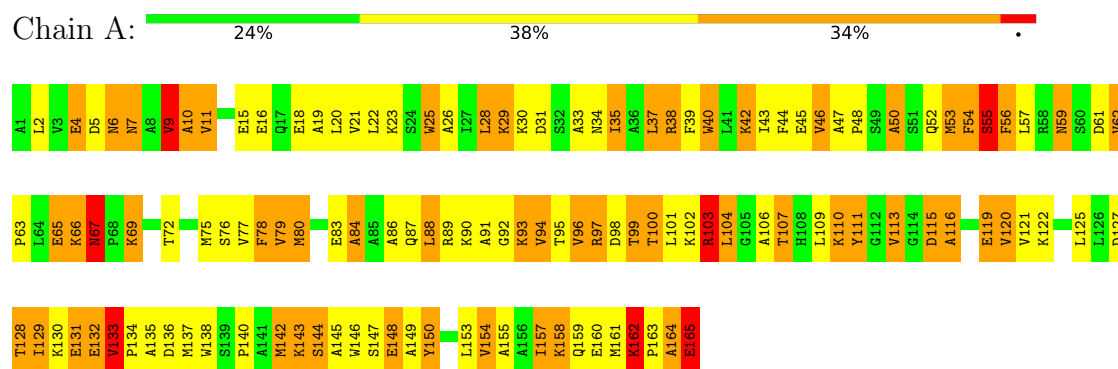
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	47	Total	O	0	0
			47	47		

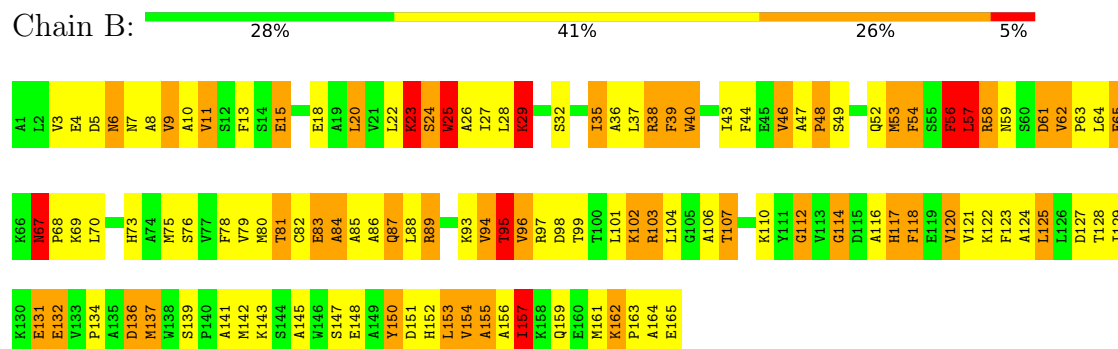
3 Residue-property plots

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: Non-symbiotic hemoglobin 1



• Molecule 1: Non-symbiotic hemoglobin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.68Å 125.68Å 56.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.40) 97.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.84Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.174 , 0.204 0.175 , 0.185	Depositor DCC
R_{free} test set	1599 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2765	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.78	98/1318 (7.4%)	1.95	38/1781 (2.1%)
1	B	2.61	74/1318 (5.6%)	1.97	36/1781 (2.0%)
All	All	2.70	172/2636 (6.5%)	1.96	74/3562 (2.1%)

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 (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	CA-CB	22.53	1.65	1.54
1	A	53	MET	SD-CE	-18.66	1.32	1.79
1	B	147	SER	CA-C	-13.47	1.36	1.52
1	A	21	VAL	C-O	-13.06	1.09	1.24
1	B	47	ALA	CA-CB	-11.48	1.38	1.53
1	A	66	LYS	C-O	9.91	1.36	1.24
1	B	43	ILE	C-O	-9.87	1.11	1.23
1	B	62	VAL	CA-C	9.35	1.62	1.52
1	B	137	MET	SD-CE	-9.33	1.56	1.79
1	B	153	LEU	C-O	-9.17	1.13	1.24
1	B	117	HIS	C-O	-8.87	1.13	1.24
1	B	13	PHE	C-O	-8.79	1.13	1.23
1	A	38	ARG	CA-C	8.78	1.65	1.52
1	A	127	ASP	N-CA	8.78	1.57	1.46
1	A	46	VAL	C-O	-8.75	1.14	1.24
1	A	122	LYS	C-O	-8.73	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PHE	N-CA	8.35	1.56	1.46
1	B	157	ILE	C-O	-8.34	1.14	1.24
1	B	165	GLU	CD-OE1	8.10	1.40	1.25
1	B	145	ALA	C-O	-8.09	1.14	1.24
1	B	62	VAL	CA-CB	8.03	1.64	1.54
1	A	143	LYS	CA-C	-7.96	1.42	1.52
1	A	121	VAL	C-O	-7.90	1.13	1.24
1	B	148	GLU	C-O	-7.87	1.15	1.24
1	A	54	PHE	CA-C	7.82	1.63	1.52
1	A	53	MET	CA-C	7.76	1.63	1.52
1	B	154	VAL	C-O	-7.75	1.14	1.24
1	B	22	LEU	C-O	-7.74	1.15	1.24
1	A	150	TYR	C-O	-7.71	1.15	1.24
1	A	43	ILE	C-O	-7.71	1.14	1.24
1	B	57	LEU	CA-C	7.52	1.62	1.52
1	B	75	MET	C-O	-7.50	1.14	1.24
1	A	63	PRO	C-O	7.50	1.33	1.24
1	B	141	ALA	C-O	-7.43	1.15	1.24
1	A	50	ALA	C-O	-7.42	1.15	1.24
1	A	21	VAL	N-CA	7.42	1.55	1.46
1	B	81	THR	CA-CB	7.40	1.65	1.53
1	A	28	LEU	C-O	-7.39	1.14	1.24
1	A	115	ASP	CA-C	-7.38	1.42	1.52
1	A	67	ASN	CA-C	7.37	1.61	1.53
1	A	46	VAL	N-CA	7.32	1.55	1.46
1	B	123	PHE	CA-CB	7.31	1.64	1.53
1	A	7	ASN	CA-C	7.30	1.61	1.52
1	A	28	LEU	CA-C	-7.26	1.43	1.52
1	A	142	MET	SD-CE	-7.25	1.61	1.79
1	B	162	LYS	C-O	7.24	1.31	1.24
1	A	4	GLU	CA-C	7.21	1.62	1.52
1	A	153	LEU	C-O	-7.21	1.15	1.24
1	B	139	SER	N-CA	-7.17	1.39	1.46
1	A	113	VAL	CA-C	7.16	1.61	1.52
1	A	104	LEU	CA-C	-7.15	1.43	1.52
1	A	162	LYS	CA-C	-7.13	1.45	1.52
1	A	93	LYS	CA-C	7.08	1.61	1.52
1	A	164	ALA	CA-C	-7.03	1.43	1.52
1	B	39	PHE	N-CA	7.00	1.54	1.46
1	A	120	VAL	CA-CB	-6.99	1.44	1.54
1	A	145	ALA	C-O	-6.95	1.15	1.24
1	B	85	ALA	N-CA	-6.91	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	VAL	CA-C	-6.86	1.42	1.52
1	A	9	VAL	CA-CB	6.86	1.63	1.54
1	B	54	PHE	CA-C	6.85	1.61	1.52
1	B	57	LEU	CA-CB	6.78	1.61	1.52
1	A	26	ALA	C-O	-6.78	1.16	1.24
1	A	53	MET	N-CA	6.77	1.55	1.46
1	A	44	PHE	C-O	-6.75	1.15	1.24
1	B	38	ARG	NE-CZ	6.75	1.40	1.33
1	B	46	VAL	CA-CB	6.74	1.63	1.54
1	B	58	ARG	N-CA	6.72	1.55	1.46
1	B	13	PHE	CA-C	-6.70	1.43	1.53
1	B	25	TRP	CA-C	-6.70	1.44	1.52
1	A	130	LYS	CA-C	-6.70	1.44	1.52
1	B	114	GLY	C-O	-6.69	1.15	1.23
1	B	9	VAL	C-N	6.68	1.43	1.33
1	A	6	ASN	CA-CB	6.67	1.64	1.53
1	A	59	ASN	CA-C	6.64	1.61	1.52
1	B	85	ALA	CA-CB	-6.59	1.43	1.53
1	A	115	ASP	C-O	-6.52	1.16	1.24
1	A	106	ALA	CA-CB	-6.49	1.42	1.53
1	B	73	HIS	C-O	-6.49	1.16	1.24
1	A	96	VAL	CA-CB	6.46	1.62	1.54
1	A	40	TRP	CB-CG	6.42	1.70	1.50
1	A	77	VAL	C-O	-6.33	1.17	1.24
1	A	96	VAL	CA-C	6.33	1.59	1.52
1	B	35	ILE	CA-CB	6.30	1.62	1.54
1	A	84	ALA	CA-C	-6.29	1.44	1.52
1	A	21	VAL	CA-C	-6.26	1.45	1.52
1	A	26	ALA	CA-CB	6.22	1.62	1.53
1	B	61	ASP	CA-C	6.22	1.61	1.52
1	A	56	PHE	CA-C	6.20	1.60	1.52
1	A	78	PHE	CA-C	-6.17	1.44	1.52
1	A	91	ALA	CA-CB	-6.17	1.45	1.54
1	B	128	THR	C-O	-6.12	1.16	1.24
1	B	153	LEU	CG-CD1	-6.12	1.32	1.52
1	B	87	GLN	CA-C	-6.12	1.45	1.52
1	B	120	VAL	N-CA	6.12	1.54	1.46
1	B	118	PHE	CA-C	-6.12	1.44	1.52
1	B	156	ALA	N-CA	6.10	1.53	1.46
1	A	54	PHE	CA-CB	6.09	1.63	1.53
1	A	35	ILE	C-O	-6.05	1.17	1.24
1	A	6	ASN	CA-C	6.04	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	THR	CA-CB	6.01	1.63	1.53
1	A	88	LEU	CA-C	-6.00	1.45	1.52
1	B	123	PHE	CA-C	-5.99	1.45	1.52
1	A	69	LYS	CE-NZ	5.97	1.67	1.49
1	B	161	MET	SD-CE	-5.96	1.64	1.79
1	A	62	VAL	C-O	5.95	1.29	1.24
1	B	59	ASN	CA-C	5.92	1.60	1.52
1	A	128	THR	C-O	5.91	1.30	1.24
1	B	88	LEU	CG-CD2	-5.88	1.33	1.52
1	B	9	VAL	CA-C	5.86	1.60	1.52
1	A	19	ALA	CA-CB	5.86	1.63	1.53
1	B	46	VAL	C-O	-5.85	1.17	1.24
1	A	56	PHE	C-N	5.85	1.41	1.33
1	B	27	ILE	CA-CB	5.85	1.62	1.54
1	B	47	ALA	N-CA	-5.85	1.40	1.46
1	A	111	TYR	CZ-OH	5.84	1.50	1.38
1	A	22	LEU	CA-C	-5.82	1.45	1.52
1	A	129	ILE	N-CA	-5.82	1.39	1.46
1	A	7	ASN	N-CA	5.80	1.52	1.46
1	A	39	PHE	CE1-CZ	-5.80	1.21	1.38
1	A	155	ALA	N-CA	5.78	1.53	1.46
1	B	95	THR	CA-CB	5.72	1.63	1.53
1	A	157	ILE	CA-CB	5.72	1.61	1.54
1	A	146	TRP	C-O	-5.71	1.17	1.24
1	B	124	ALA	C-O	5.71	1.31	1.24
1	A	132	GLU	N-CA	5.68	1.53	1.46
1	B	131	GLU	N-CA	-5.68	1.39	1.46
1	A	165	GLU	CD-OE2	5.67	1.36	1.25
1	A	149	ALA	C-O	-5.67	1.17	1.24
1	B	107	THR	C-O	-5.67	1.17	1.24
1	A	100	THR	C-O	-5.66	1.17	1.24
1	B	9	VAL	C-O	5.64	1.31	1.24
1	A	21	VAL	CA-CB	5.64	1.60	1.54
1	A	55	SER	C-O	5.62	1.31	1.24
1	A	153	LEU	N-CA	5.61	1.53	1.46
1	A	48	PRO	C-O	-5.59	1.16	1.24
1	B	23	LYS	CA-C	-5.58	1.45	1.52
1	B	53	MET	CA-C	5.48	1.60	1.52
1	A	65	GLU	CD-OE2	5.47	1.35	1.25
1	A	39	PHE	CE2-CZ	-5.46	1.22	1.38
1	A	33	ALA	CA-CB	-5.44	1.44	1.53
1	B	107	THR	CA-C	-5.42	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	VAL	C-N	-5.42	1.26	1.33
1	A	144	SER	C-O	-5.39	1.17	1.24
1	B	151	ASP	C-O	-5.38	1.17	1.24
1	B	56	PHE	CA-C	5.34	1.59	1.52
1	A	42	LYS	C-O	-5.34	1.17	1.24
1	A	57	LEU	CA-CB	5.33	1.62	1.53
1	A	165	GLU	CD-OE1	5.33	1.35	1.25
1	A	79	VAL	CA-C	-5.32	1.46	1.52
1	B	7	ASN	C-O	5.31	1.30	1.24
1	B	143	LYS	C-O	-5.30	1.17	1.24
1	B	78	PHE	CD2-CE2	5.30	1.54	1.38
1	A	80	MET	C-O	-5.29	1.17	1.24
1	A	72	THR	CA-CB	5.26	1.61	1.53
1	B	102	LYS	N-CA	5.26	1.52	1.46
1	B	131	GLU	C-O	-5.26	1.18	1.24
1	B	94	VAL	CA-CB	5.22	1.60	1.54
1	A	148	GLU	C-O	-5.19	1.18	1.24
1	A	11	VAL	CA-CB	5.19	1.59	1.53
1	A	133	VAL	N-CA	5.18	1.52	1.46
1	A	94	VAL	CA-C	5.17	1.58	1.52
1	B	6	ASN	C-N	5.17	1.40	1.34
1	B	145	ALA	CA-C	-5.16	1.46	1.52
1	B	38	ARG	CD-NE	5.15	1.53	1.46
1	A	148	GLU	CA-C	-5.14	1.46	1.52
1	A	37	LEU	N-CA	-5.12	1.39	1.46
1	B	8	ALA	C-O	5.12	1.29	1.23
1	B	59	ASN	N-CA	5.11	1.52	1.46
1	A	47	ALA	N-CA	-5.07	1.40	1.46
1	B	7	ASN	N-CA	5.06	1.52	1.46
1	A	77	VAL	N-CA	-5.02	1.40	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	GLU	N-CA-C	9.80	121.73	111.14
1	A	131	GLU	N-CA-C	9.59	121.81	111.36
1	B	155	ALA	N-CA-C	9.46	121.59	111.28
1	B	84	ALA	N-CA-C	8.64	120.31	111.07
1	B	83	GLU	CA-C-N	8.55	131.56	120.44
1	B	83	GLU	C-N-CA	8.55	131.56	120.44
1	B	107	THR	N-CA-C	-8.44	101.10	111.40
1	A	56	PHE	N-CA-C	8.38	122.83	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ILE	N-CA-C	-8.29	102.80	111.58
1	B	68	PRO	N-CA-C	8.19	124.10	114.03
1	A	77	VAL	N-CA-C	-7.80	102.93	110.42
1	A	67	ASN	N-CA-C	7.58	120.40	109.48
1	A	38	ARG	N-CA-C	7.49	121.52	112.38
1	B	132	GLU	N-CA-C	7.20	119.21	111.36
1	A	23	LYS	N-CA-C	7.09	119.01	111.28
1	A	119	GLU	N-CA-C	6.96	118.66	111.14
1	A	103	ARG	CA-C-N	6.82	129.98	120.29
1	A	103	ARG	C-N-CA	6.82	129.98	120.29
1	B	96	VAL	N-CA-C	-6.76	102.58	110.21
1	A	155	ALA	CA-C-N	6.75	129.62	120.44
1	A	155	ALA	C-N-CA	6.75	129.62	120.44
1	A	38	ARG	CA-C-N	6.53	129.51	120.63
1	A	38	ARG	C-N-CA	6.53	129.51	120.63
1	B	15	GLU	N-CA-C	-6.34	104.46	111.82
1	A	158	LYS	N-CA-C	6.27	118.92	111.71
1	B	11	VAL	CB-CA-C	-6.21	103.46	111.53
1	B	40	TRP	N-CA-C	6.15	118.06	111.36
1	B	67	ASN	CA-C-N	6.06	126.17	119.87
1	B	67	ASN	C-N-CA	6.06	126.17	119.87
1	A	154	VAL	N-CA-C	6.05	116.83	110.72
1	A	147	SER	N-CA-C	5.96	118.27	111.11
1	B	9	VAL	N-CA-C	5.91	118.13	108.97
1	B	35	ILE	CA-C-N	5.89	128.76	120.28
1	B	35	ILE	C-N-CA	5.89	128.76	120.28
1	A	86	ALA	CA-C-N	5.88	128.41	120.65
1	A	86	ALA	C-N-CA	5.88	128.41	120.65
1	A	116	ALA	N-CA-C	5.84	117.73	111.36
1	B	162	LYS	N-CA-C	-5.78	98.87	108.23
1	B	32	SER	N-CA-C	5.75	118.01	111.11
1	A	66	LYS	CA-C-N	-5.72	112.87	120.65
1	A	66	LYS	C-N-CA	-5.72	112.87	120.65
1	B	57	LEU	N-CA-C	5.69	118.69	107.98
1	A	62	VAL	N-CA-CB	5.68	114.32	110.52
1	B	24	SER	N-CA-C	5.66	117.45	111.28
1	A	99	THR	N-CA-C	5.65	117.89	111.11
1	A	34	ASN	N-CA-C	5.62	117.40	111.28
1	B	58	ARG	N-CA-C	5.58	118.21	107.44
1	B	150	TYR	N-CA-C	-5.52	105.26	111.28
1	A	94	VAL	N-CA-C	-5.50	101.50	108.93
1	A	107	THR	N-CA-C	5.45	119.10	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	GLU	CB-CA-C	-5.41	102.33	110.92
1	B	48	PRO	CA-C-N	5.38	128.03	120.28
1	B	48	PRO	C-N-CA	5.38	128.03	120.28
1	B	136	ASP	N-CA-C	5.36	119.87	113.23
1	A	40	TRP	CA-C-O	5.33	125.98	119.05
1	A	53	MET	CA-C-O	5.30	125.19	119.15
1	A	99	THR	CA-C-N	5.29	127.37	120.28
1	A	99	THR	C-N-CA	5.29	127.37	120.28
1	A	52	GLN	CA-C-N	5.26	131.36	122.26
1	A	52	GLN	C-N-CA	5.26	131.36	122.26
1	B	162	LYS	O-C-N	5.26	125.53	121.85
1	B	35	ILE	O-C-N	5.24	126.95	121.87
1	B	157	ILE	CB-CA-C	-5.24	105.16	112.02
1	A	96	VAL	CB-CA-C	5.24	117.96	111.15
1	B	20	LEU	N-CA-C	5.24	116.99	111.28
1	A	25	TRP	CA-C-N	5.23	127.24	120.44
1	A	25	TRP	C-N-CA	5.23	127.24	120.44
1	B	112	GLY	N-CA-C	-5.14	107.16	115.08
1	B	29	LYS	CA-C-N	5.13	127.47	120.54
1	B	29	LYS	C-N-CA	5.13	127.47	120.54
1	B	23	LYS	N-CA-C	5.13	116.56	111.07
1	A	119	GLU	CB-CA-C	-5.07	102.89	110.90
1	B	147	SER	CA-C-O	-5.03	115.72	121.00
1	B	99	THR	N-CA-CB	5.01	117.27	110.01

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	SER	Peptide

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	1291	0	1313	99	3
1	B	1291	0	1313	91	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	50	0	0	11	3
3	B	47	0	0	14	2
All	All	2765	0	2686	190	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 35.

All (190) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LYS:HA	1:B:29:LYS:NZ	1.57	1.19
1:A:78:PHE:CE1	1:A:129:ILE:HD11	1.91	1.04
1:A:78:PHE:HE1	1:A:129:ILE:HD11	1.16	1.03
1:A:9:VAL:O	1:A:11:VAL:HG23	1.56	1.03
1:A:10:ALA:HB2	3:A:192:HOH:O	1.62	0.99
1:B:153:LEU:O	1:B:157:ILE:HD13	1.65	0.95
1:B:29:LYS:HA	1:B:29:LYS:HZ2	1.18	0.92
1:A:28:LEU:HD22	1:A:35:ILE:CD1	2.00	0.91
1:A:25:TRP:O	1:A:29:LYS:HG3	1.70	0.91
1:A:11:VAL:HG11	1:A:88:LEU:HD22	1.55	0.87
1:B:29:LYS:HZ2	1:B:29:LYS:CA	1.90	0.84
1:A:5:ASP:OD2	1:A:9:VAL:HG13	1.77	0.84
1:B:103:ARG:O	1:B:103:ARG:NH1	2.11	0.83
1:A:28:LEU:HD11	1:A:129:ILE:HD12	1.61	0.82
1:B:29:LYS:NZ	1:B:29:LYS:CA	2.43	0.82
1:A:10:ALA:CB	3:A:192:HOH:O	2.22	0.81
1:A:144:SER:O	1:A:148:GLU:HG2	1.80	0.80
1:B:96:VAL:HB	1:B:101:LEU:HG	1.63	0.80
1:A:20:LEU:O	1:A:142:MET:HE2	1.82	0.79
1:A:35:ILE:HD12	1:A:132:GLU:HG3	1.64	0.78
1:B:29:LYS:HA	1:B:29:LYS:HZ1	1.47	0.78
1:A:11:VAL:HG11	1:A:88:LEU:CD2	2.15	0.77
1:B:38:ARG:NE	1:B:132:GLU:OE1	2.18	0.76
1:A:2:LEU:HD22	3:A:199:HOH:O	1.85	0.76
1:B:76:SER:O	1:B:80:MET:HB2	1.85	0.76
1:A:103:ARG:HH11	1:A:103:ARG:HB3	1.51	0.76
1:B:127:ASP:OD1	3:B:186:HOH:O	2.05	0.74
1:A:11:VAL:CG1	1:A:88:LEU:HD22	2.17	0.73
1:A:31:ASP:O	1:A:35:ILE:HG22	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:O	1:A:80:MET:HB2	1.90	0.72
1:B:103:ARG:O	1:B:103:ARG:CZ	2.39	0.71
1:B:80:MET:HE1	1:B:104:LEU:HD11	1.73	0.71
1:A:18:GLU:OE2	1:A:89:ARG:HG2	1.91	0.70
1:B:103:ARG:NH2	1:B:106:ALA:HB3	2.07	0.69
1:A:28:LEU:HD22	1:A:35:ILE:HD11	1.74	0.69
1:A:28:LEU:HD22	1:A:35:ILE:HD12	1.74	0.69
1:A:59:ASN:HA	3:A:190:HOH:O	1.94	0.68
1:B:37:LEU:HD11	1:B:64:LEU:HD11	1.76	0.67
1:A:29:LYS:NZ	1:A:29:LYS:HB3	2.10	0.66
1:B:110:LYS:HE3	3:B:175:HOH:O	1.95	0.66
1:B:23:LYS:HB3	3:B:213:HOH:O	1.94	0.66
1:A:93:LYS:HE3	1:A:95:THR:HG22	1.75	0.66
1:B:54:PHE:HB3	1:B:69:LYS:HZ3	1.60	0.66
1:A:83:GLU:O	1:A:87:GLN:HG3	1.96	0.66
1:A:67:ASN:N	1:A:67:ASN:HD22	1.94	0.65
1:A:164:ALA:O	1:A:165:GLU:C	2.40	0.65
1:B:25:TRP:CD1	1:B:82:CYS:HG	2.14	0.65
1:B:96:VAL:HG22	3:B:184:HOH:O	1.97	0.65
1:A:116:ALA:O	1:A:120:VAL:HG23	1.97	0.63
1:A:133:VAL:HB	1:A:137:MET:HE2	1.81	0.63
1:B:120:VAL:HG12	1:B:120:VAL:O	1.98	0.63
1:B:5:ASP:HB2	1:B:155:ALA:HB1	1.80	0.62
1:A:35:ILE:CD1	1:A:132:GLU:HG3	2.30	0.62
1:A:28:LEU:HD11	1:A:129:ILE:CD1	2.30	0.61
1:A:2:LEU:HD12	1:A:5:ASP:H	1.65	0.61
1:A:42:LYS:O	1:A:46:VAL:HG23	2.01	0.61
1:B:103:ARG:HH22	1:B:106:ALA:HB3	1.65	0.60
1:A:29:LYS:HE2	3:A:185:HOH:O	2.02	0.59
1:B:94:VAL:HG23	1:B:152:HIS:HB3	1.84	0.59
1:A:2:LEU:HD13	1:A:5:ASP:HB2	1.84	0.59
1:B:96:VAL:HB	1:B:101:LEU:CG	2.32	0.59
1:A:101:LEU:CD2	1:A:157:ILE:HD13	2.33	0.59
1:B:131:GLU:HG3	3:B:171:HOH:O	2.03	0.58
1:A:80:MET:HE1	1:A:104:LEU:HD11	1.86	0.58
1:A:5:ASP:OD2	1:A:9:VAL:HG22	2.03	0.58
1:B:157:ILE:N	1:B:157:ILE:CD1	2.67	0.57
1:B:15:GLU:HG3	1:B:89:ARG:CZ	2.36	0.56
1:B:103:ARG:NH1	1:B:107:THR:OG1	2.38	0.56
1:B:35:ILE:HD12	1:B:36:ALA:N	2.22	0.55
1:B:137:MET:O	3:B:194:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HB3	1:B:65:GLU:HB2	1.89	0.55
1:A:29:LYS:HB3	1:A:29:LYS:HZ2	1.70	0.55
1:B:121:VAL:HG21	2:B:166:HEM:CMC	2.37	0.55
1:A:104:LEU:HD12	1:A:157:ILE:CD1	2.37	0.55
1:A:110:LYS:NZ	1:A:111:TYR:HE1	2.05	0.55
1:B:44:PHE:O	1:B:48:PRO:HG3	2.08	0.54
1:B:94:VAL:CG2	1:B:152:HIS:HB3	2.37	0.54
1:A:101:LEU:HD23	1:A:157:ILE:HD13	1.90	0.54
1:B:53:MET:HE1	1:B:117:HIS:NE2	2.22	0.54
1:A:110:LYS:NZ	1:A:111:TYR:CE1	2.76	0.53
1:B:157:ILE:N	1:B:157:ILE:HD12	2.24	0.53
1:B:54:PHE:HB3	1:B:69:LYS:NZ	2.22	0.53
1:A:61:ASP:HB3	1:A:66:LYS:HB3	1.89	0.53
1:B:3:VAL:HG12	1:B:4:GLU:N	2.24	0.53
1:B:103:ARG:NE	1:B:103:ARG:HA	2.24	0.53
1:B:125:LEU:O	1:B:129:ILE:HG13	2.09	0.53
1:A:30:LYS:NZ	3:A:189:HOH:O	2.41	0.52
1:A:67:ASN:HD22	1:A:67:ASN:H	1.57	0.52
1:A:84:ALA:O	1:A:88:LEU:HG	2.10	0.52
1:A:134:PRO:HB2	1:A:136:ASP:OD2	2.09	0.51
1:A:154:VAL:O	1:A:158:LYS:HG3	2.10	0.51
1:A:56:PHE:CZ	1:A:62:VAL:HG13	2.46	0.51
1:B:38:ARG:HH21	1:B:132:GLU:CD	2.18	0.50
1:B:9:VAL:O	1:B:11:VAL:HG23	2.11	0.50
1:A:101:LEU:HD23	1:A:157:ILE:CD1	2.41	0.50
1:B:23:LYS:O	1:B:26:ALA:HB3	2.12	0.50
1:B:40:TRP:CH2	1:B:65:GLU:HB3	2.47	0.50
1:B:112:GLY:HA2	3:B:211:HOH:O	2.11	0.50
1:B:116:ALA:O	1:B:120:VAL:HG23	2.12	0.50
1:B:132:GLU:OE2	1:B:132:GLU:HA	2.12	0.49
1:A:96:VAL:O	1:A:97:ARG:C	2.52	0.49
1:B:89:ARG:HD2	3:B:181:HOH:O	2.11	0.49
1:A:15:GLU:O	1:A:15:GLU:HG2	2.11	0.49
1:A:150:TYR:CE2	1:A:154:VAL:HG21	2.48	0.49
1:A:104:LEU:HD12	1:A:157:ILE:HD11	1.94	0.48
1:B:24:SER:O	1:B:28:LEU:HD13	2.14	0.48
1:A:38:ARG:HD3	1:A:128:THR:HG23	1.94	0.48
1:B:54:PHE:C	1:B:69:LYS:HZ1	2.21	0.48
1:A:103:ARG:HB3	1:A:103:ARG:NH1	2.26	0.48
1:A:140:PRO:O	1:A:143:LYS:HB3	2.14	0.48
1:B:26:ALA:HA	1:B:29:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PHE:HE1	1:B:125:LEU:HA	1.79	0.47
1:A:94:VAL:HG13	1:A:96:VAL:HG23	1.95	0.47
1:A:38:ARG:CD	1:A:132:GLU:OE1	2.62	0.47
1:A:109:LEU:N	1:A:161:MET:HE3	2.30	0.47
1:B:18:GLU:OE1	1:B:89:ARG:NE	2.47	0.47
1:B:35:ILE:HD12	1:B:35:ILE:C	2.40	0.47
1:A:15:GLU:HA	1:A:89:ARG:HD3	1.96	0.47
1:A:38:ARG:NH2	1:A:131:GLU:HG2	2.31	0.46
1:A:125:LEU:O	1:A:129:ILE:HG12	2.14	0.46
1:B:155:ALA:O	1:B:159:GLN:HG3	2.14	0.46
1:A:11:VAL:HB	1:A:92:GLY:O	2.15	0.46
1:B:11:VAL:HG13	3:B:206:HOH:O	2.13	0.46
1:B:20:LEU:HB3	1:B:142:MET:HG3	1.98	0.46
1:B:162:LYS:HE2	3:B:204:HOH:O	2.14	0.46
1:A:134:PRO:O	1:A:136:ASP:N	2.49	0.46
1:A:5:ASP:OD2	1:A:9:VAL:CG1	2.57	0.46
1:A:115:ASP:O	1:A:119:GLU:HG3	2.15	0.46
1:A:103:ARG:HH11	1:A:103:ARG:CB	2.25	0.46
1:A:98:ASP:OD2	1:A:98:ASP:C	2.59	0.46
1:B:106:ALA:O	1:B:110:LYS:HB2	2.16	0.46
1:A:2:LEU:CD1	1:A:5:ASP:HB2	2.46	0.45
1:A:28:LEU:CD1	1:A:129:ILE:HD12	2.41	0.45
1:B:64:LEU:O	1:B:65:GLU:HB3	2.14	0.45
1:B:54:PHE:CD2	1:B:70:LEU:HD23	2.51	0.45
1:B:122:LYS:HB2	1:B:150:TYR:CE2	2.52	0.45
1:A:50:ALA:HA	1:A:53:MET:HE2	1.98	0.45
1:A:67:ASN:H	1:A:67:ASN:ND2	2.15	0.45
1:B:49:SER:HA	1:B:52:GLN:HG3	1.98	0.45
1:B:83:GLU:O	1:B:87:GLN:HG3	2.17	0.45
1:B:157:ILE:CD1	1:B:157:ILE:H	2.28	0.45
1:B:29:LYS:CA	1:B:29:LYS:CE	2.94	0.45
1:A:134:PRO:O	1:A:137:MET:N	2.50	0.45
1:B:15:GLU:HG3	1:B:89:ARG:NH1	2.32	0.45
1:B:53:MET:HE1	1:B:117:HIS:CD2	2.52	0.44
1:A:38:ARG:HD2	1:A:132:GLU:OE1	2.17	0.44
1:A:67:ASN:N	1:A:67:ASN:ND2	2.61	0.44
1:A:100:THR:O	1:A:104:LEU:HG	2.17	0.44
1:A:113:VAL:HG13	2:A:166:HEM:HAC	1.99	0.44
1:A:101:LEU:HD22	1:A:157:ILE:HD13	1.98	0.44
1:A:90:LYS:HB2	3:A:186:HOH:O	2.18	0.44
1:B:114:GLY:N	1:B:117:HIS:ND1	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:HA	1:A:69:LYS:NZ	2.33	0.44
1:B:96:VAL:HB	1:B:101:LEU:CD1	2.48	0.44
1:A:79:VAL:O	1:A:83:GLU:HG3	2.17	0.44
1:B:121:VAL:HG21	2:B:166:HEM:HMC2	2.00	0.43
1:B:79:VAL:O	1:B:83:GLU:HG3	2.18	0.43
1:B:154:VAL:HG22	2:B:166:HEM:HBB1	2.00	0.43
1:B:118:PHE:HB2	3:B:172:HOH:O	2.19	0.43
1:B:6:ASN:CG	1:B:9:VAL:O	2.62	0.43
1:B:46:VAL:HG11	1:B:120:VAL:HG13	2.01	0.43
1:B:131:GLU:OE2	3:B:171:HOH:O	2.21	0.43
1:A:110:LYS:HZ2	1:A:110:LYS:HB3	1.84	0.43
1:A:104:LEU:CD1	1:A:157:ILE:CD1	2.96	0.43
1:A:104:LEU:CD1	1:A:157:ILE:HD12	2.48	0.43
1:B:20:LEU:HD22	3:B:194:HOH:O	2.18	0.43
1:A:104:LEU:CB	1:A:157:ILE:HD12	2.49	0.42
1:B:3:VAL:HG12	1:B:4:GLU:H	1.84	0.42
1:B:101:LEU:HD23	1:B:104:LEU:HD12	2.00	0.42
1:A:110:LYS:NZ	1:A:110:LYS:HB3	2.34	0.42
1:A:138:TRP:CZ2	1:A:143:LYS:HB2	2.55	0.42
1:B:81:THR:O	1:B:84:ALA:HB3	2.19	0.42
1:B:93:LYS:HE3	1:B:95:THR:CG2	2.49	0.42
1:B:101:LEU:HD22	1:B:157:ILE:HD12	2.01	0.42
1:A:115:ASP:OD1	3:A:177:HOH:O	2.22	0.41
1:B:134:PRO:C	1:B:136:ASP:H	2.28	0.41
1:B:150:TYR:O	1:B:154:VAL:HG23	2.20	0.41
1:A:15:GLU:O	1:A:15:GLU:CG	2.68	0.41
1:B:98:ASP:O	1:B:102:LYS:HB2	2.19	0.41
1:A:131:GLU:OE1	3:A:206:HOH:O	2.22	0.41
1:A:159:GLN:O	1:A:162:LYS:NZ	2.48	0.41
1:A:102:LYS:HG2	1:A:160:GLU:OE2	2.20	0.41
1:A:134:PRO:C	1:A:136:ASP:N	2.78	0.41
1:B:67:ASN:HD21	1:B:69:LYS:HG3	1.85	0.41
1:A:6:ASN:HD22	1:A:7:ASN:H	1.69	0.40
1:A:65:GLU:HA	3:A:178:HOH:O	2.20	0.40
1:B:38:ARG:NH2	1:B:132:GLU:OE1	2.53	0.40
1:B:97:ARG:NH1	3:B:182:HOH:O	2.54	0.40
1:A:138:TRP:CD1	3:A:170:HOH:O	2.73	0.40
1:B:18:GLU:OE2	1:B:86:ALA:HA	2.21	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)
3:A:202:HOH:O	3:A:203:HOH:O[3_564]	1.92	0.28
1:A:61:ASP:OD1	3:B:177:HOH:O[2_665]	2.03	0.17
1:A:89:ARG:NH1	3:B:176:HOH:O[2_664]	2.05	0.15
1:A:111:TYR:OH	3:A:171:HOH:O[4_555]	2.14	0.06
1:B:64:LEU:CD1	3:A:185:HOH:O[3_564]	2.18	0.02

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	163/165 (99%)	145 (89%)	12 (7%)	6 (4%)	2	2
1	B	163/165 (99%)	145 (89%)	11 (7%)	7 (4%)	2	1
All	All	326/330 (99%)	290 (89%)	23 (7%)	13 (4%)	2	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	B	56	PHE
1	B	61	ASP
1	B	164	ALA
1	A	4	GLU
1	A	135	ALA
1	B	163	PRO
1	B	65	GLU
1	A	55	SER
1	A	163	PRO
1	B	10	ALA
1	B	63	PRO
1	A	9	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/137 (100%)	121 (88%)	16 (12%)	5	7
1	B	137/137 (100%)	124 (90%)	13 (10%)	8	13
All	All	274/274 (100%)	245 (89%)	29 (11%)	6	10

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	29	LYS
1	A	37	LEU
1	A	40	TRP
1	A	45	GLU
1	A	55	SER
1	A	67	ASN
1	A	75	MET
1	A	97	ARG
1	A	99	THR
1	A	103	ARG
1	A	107	THR
1	A	110	LYS
1	A	133	VAL
1	A	162	LYS
1	A	165	GLU
1	B	23	LYS
1	B	25	TRP
1	B	29	LYS
1	B	56	PHE
1	B	57	LEU
1	B	58	ARG
1	B	62	VAL
1	B	67	ASN
1	B	89	ARG
1	B	95	THR
1	B	103	ARG

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Mol	Chain	Res	Type
1	B	125	LEU
1	B	157	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	34	ASN
1	A	67	ASN
1	B	7	ASN
1	B	159	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	166	1	50,50,50	2.29	19 (38%)	67,82,82	2.16	25 (37%)
2	HEM	B	166	1	50,50,50	2.28	15 (30%)	67,82,82	1.95	16 (23%)

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	166	1	-	6/14/54/54	-
2	HEM	B	166	1	-	8/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	166	HEM	C4D-ND	-7.04	1.28	1.40
2	B	166	HEM	CBD-CGD	5.25	1.62	1.50
2	B	166	HEM	FE-NB	5.24	2.11	1.94
2	B	166	HEM	FE-NA	5.15	2.12	1.95
2	B	166	HEM	C4C-NC	-4.94	1.30	1.39
2	A	166	HEM	FE-NB	4.60	2.09	1.94
2	B	166	HEM	C1D-ND	-4.39	1.30	1.38
2	A	166	HEM	C4C-NC	-4.21	1.31	1.39
2	B	166	HEM	CBC-CAC	3.97	1.49	1.30
2	B	166	HEM	C4D-ND	-3.96	1.33	1.40
2	A	166	HEM	C4A-NA	-3.94	1.32	1.39
2	A	166	HEM	FE-ND	3.81	2.06	1.94
2	B	166	HEM	C1A-NA	-3.63	1.32	1.39
2	A	166	HEM	CBB-CAB	3.57	1.47	1.30
2	A	166	HEM	CHC-C1C	3.39	1.45	1.38
2	B	166	HEM	CBB-CAB	3.33	1.46	1.30
2	A	166	HEM	C1D-ND	-3.16	1.32	1.38
2	A	166	HEM	FE-NA	3.15	2.05	1.95
2	A	166	HEM	O2D-CGD	-3.11	1.20	1.30
2	B	166	HEM	FE-NC	3.07	2.05	1.95
2	B	166	HEM	FE-ND	2.90	2.03	1.94
2	A	166	HEM	FE-NC	2.84	2.04	1.95
2	A	166	HEM	C1C-NC	-2.61	1.34	1.39
2	A	166	HEM	CMA-C3A	2.53	1.56	1.50
2	A	166	HEM	C3C-C4C	2.49	1.50	1.46
2	A	166	HEM	CHB-C4A	2.46	1.44	1.39
2	B	166	HEM	C4A-NA	-2.32	1.35	1.39
2	A	166	HEM	C1A-NA	-2.31	1.35	1.39
2	B	166	HEM	CBA-CAA	2.29	1.59	1.51
2	B	166	HEM	C1C-C2C	-2.28	1.40	1.45
2	A	166	HEM	C1B-NB	-2.19	1.36	1.40
2	A	166	HEM	CAD-C3D	2.17	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	166	HEM	CBC-CAC	2.14	1.40	1.30
2	B	166	HEM	O1D-CGD	2.11	1.29	1.22

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	166	HEM	C4D-ND-C1D	5.42	111.63	105.21
2	A	166	HEM	C3B-C2B-C1B	5.38	110.45	106.41
2	A	166	HEM	C4B-C3B-C2B	-4.93	102.75	107.28
2	B	166	HEM	CHC-C1C-NC	4.88	129.76	124.45
2	B	166	HEM	CBA-CAA-C2A	4.60	125.25	112.53
2	A	166	HEM	CBA-CAA-C2A	4.46	124.87	112.53
2	A	166	HEM	CHA-C4D-ND	4.28	129.66	124.37
2	A	166	HEM	C3B-C4B-NB	4.07	112.39	109.47
2	A	166	HEM	CAD-C3D-C2D	4.01	135.37	127.87
2	B	166	HEM	O1A-CGA-CBA	-3.93	110.64	123.09
2	A	166	HEM	C4D-ND-C1D	3.81	109.72	105.21
2	B	166	HEM	C2D-C1D-ND	-3.80	105.51	109.90
2	B	166	HEM	CMD-C2D-C1D	3.68	130.78	125.03
2	B	166	HEM	CHA-C4D-ND	3.62	128.84	124.37
2	A	166	HEM	CHC-C1C-NC	3.23	127.97	124.45
2	A	166	HEM	CMB-C2B-C3B	-3.15	120.80	128.43
2	A	166	HEM	C2B-C1B-NB	-3.14	106.23	109.84
2	B	166	HEM	O2A-CGA-CBA	3.11	123.82	114.00
2	A	166	HEM	CHD-C4C-NC	3.02	127.74	124.45
2	A	166	HEM	CMA-C3A-C4A	-3.01	120.83	125.42
2	A	166	HEM	CAD-C3D-C4D	-2.90	119.64	124.70
2	B	166	HEM	CHC-C4B-NB	2.85	127.49	124.42
2	B	166	HEM	C4C-NC-C1C	2.76	110.33	105.82
2	A	166	HEM	C4C-NC-C1C	2.73	110.27	105.82
2	A	166	HEM	O2D-CGD-CBD	2.57	122.11	114.00
2	B	166	HEM	CHD-C1D-C2D	2.45	128.90	125.03
2	A	166	HEM	CHB-C4A-NA	2.42	128.25	123.86
2	A	166	HEM	C1B-NB-C4B	2.42	108.07	105.21
2	A	166	HEM	CHA-C4D-C3D	-2.41	120.79	125.23
2	B	166	HEM	O2D-CGD-CBD	2.39	121.54	114.00
2	B	166	HEM	O2D-CGD-O1D	-2.33	117.33	123.33
2	A	166	HEM	CMB-C2B-C1B	2.32	128.67	125.03
2	B	166	HEM	CHB-C4A-NA	2.28	127.99	123.86
2	A	166	HEM	CHC-C1C-C2C	-2.23	120.84	125.49
2	B	166	HEM	C1B-NB-C4B	2.23	107.85	105.21
2	A	166	HEM	C4A-C3A-C2A	2.19	109.33	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	166	HEM	CMD-C2D-C3D	-2.17	120.29	126.15
2	A	166	HEM	C3C-C2C-C1C	-2.13	105.03	107.05
2	A	166	HEM	O2D-CGD-O1D	-2.07	118.00	123.33
2	A	166	HEM	O2A-CGA-O1A	2.04	128.57	123.33
2	A	166	HEM	CBB-CAB-C3B	-2.01	117.49	127.53

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	166	HEM	C4B-C3B-CAB-CBB
2	A	166	HEM	C2C-C3C-CAC-CBC
2	A	166	HEM	C4C-C3C-CAC-CBC
2	B	166	HEM	C1A-C2A-CAA-CBA
2	B	166	HEM	C2B-C3B-CAB-CBB
2	B	166	HEM	C4B-C3B-CAB-CBB
2	B	166	HEM	C2C-C3C-CAC-CBC
2	B	166	HEM	C4C-C3C-CAC-CBC
2	B	166	HEM	C3A-C2A-CAA-CBA
2	B	166	HEM	C2A-CAA-CBA-CGA
2	A	166	HEM	C2B-C3B-CAB-CBB
2	B	166	HEM	C3D-CAD-CBD-CGD
2	A	166	HEM	CAA-CBA-CGA-O1A
2	A	166	HEM	CAA-CBA-CGA-O2A

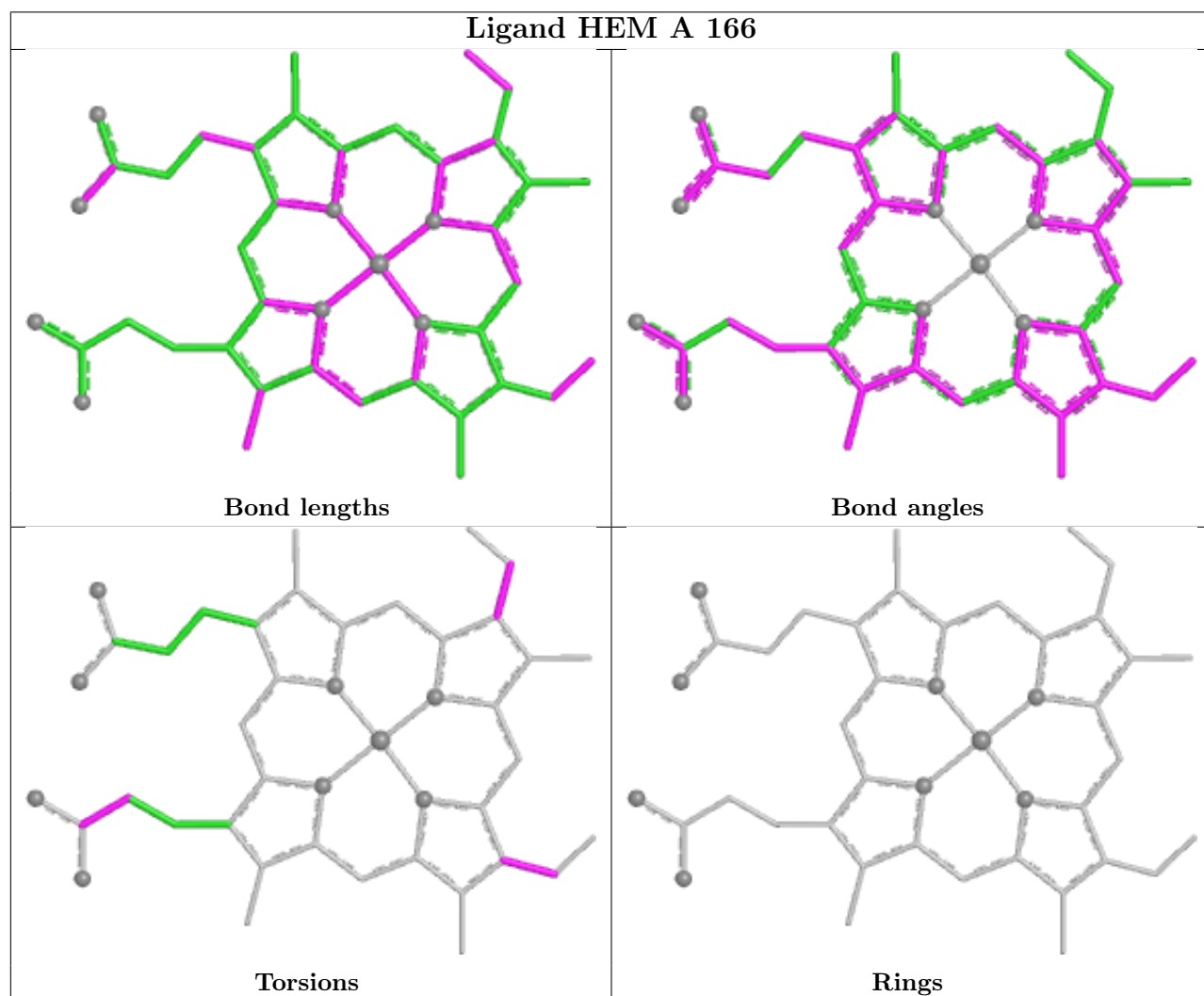
There are no ring outliers.

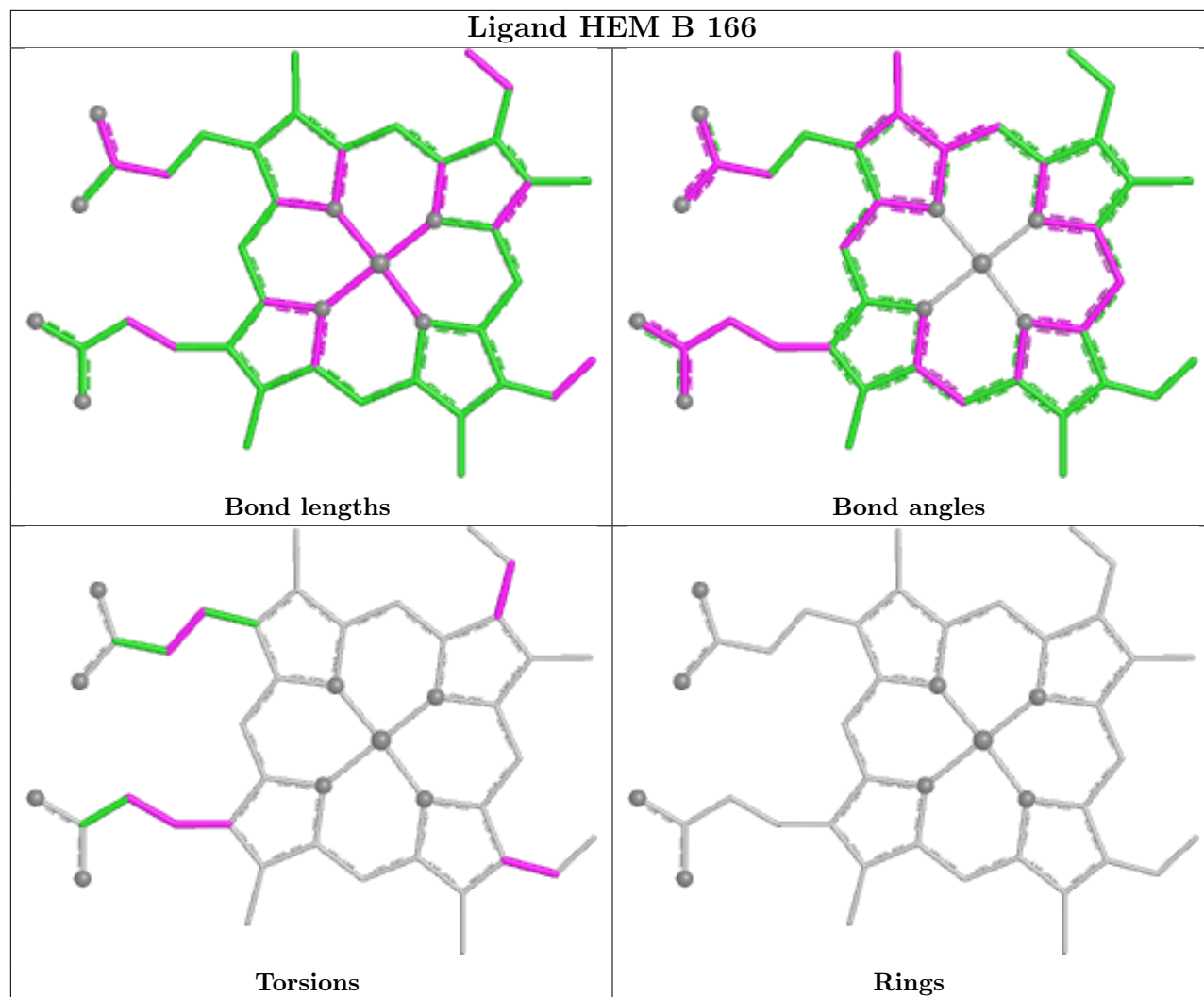
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	166	HEM	1	0
2	B	166	HEM	3	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	165/165 (100%)	-1.55	0 100 100	28, 40, 101, 107	0
1	B	165/165 (100%)	-1.50	0 100 100	25, 43, 105, 110	0
All	All	330/330 (100%)	-1.53	0 100 100	25, 42, 103, 110	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

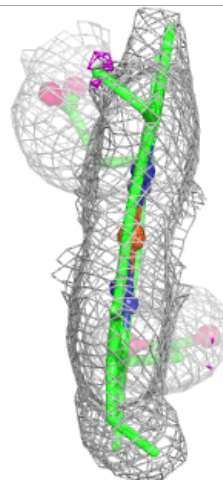
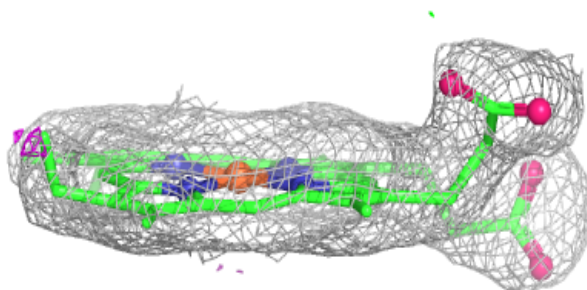
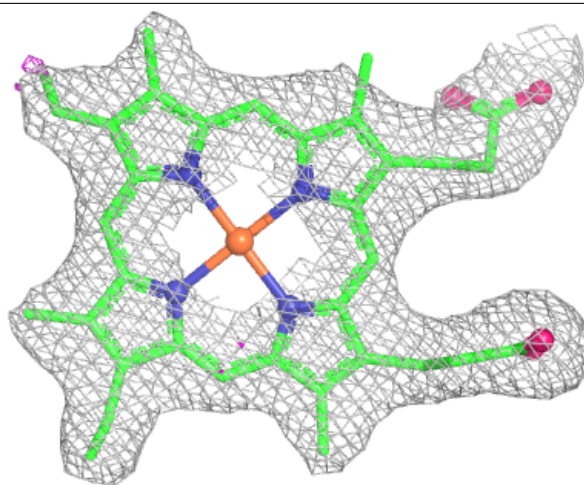
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	166	43/43	1.00	0.03	24,38,49,50	0
2	HEM	B	166	43/43	1.00	0.03	41,49,63,68	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.

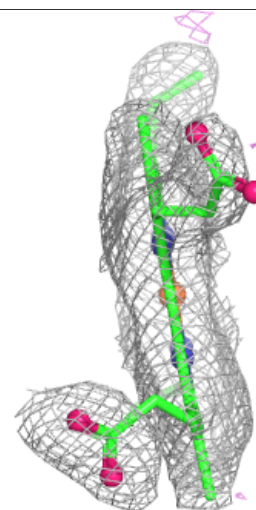
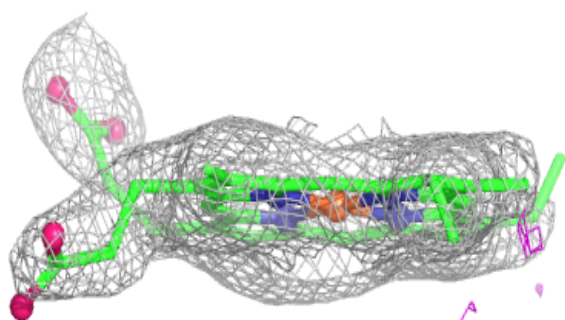
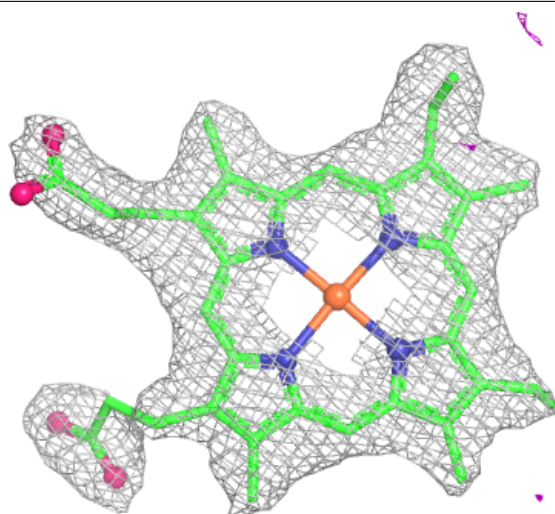
Electron density around HEM A 166:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 166:

$2mF_o-DF_c$ (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.