



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:07 AM UTC

PDB ID : 2QLS / pdb_00002qls
Title : crystal structure of hemoglobin from dog (*Canis familiaris*) at 3.5 Angstrom resolution
Authors : Packianathan, C.; Sundaresan, S.; Palani, K.; Neeelagandan, K.; Ponnuswamy, M.N.
Deposited on : 2007-07-13
Resolution : 3.50 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

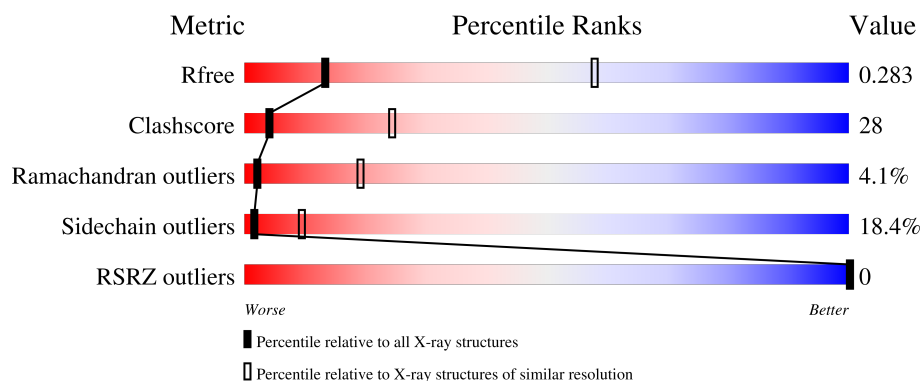
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	141	 23% 42% 25% 11%
1	C	141	 25% 47% 21% 7%
2	B	146	 18% 42% 26% 13%
2	D	146	 21% 53% 23% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4588 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.

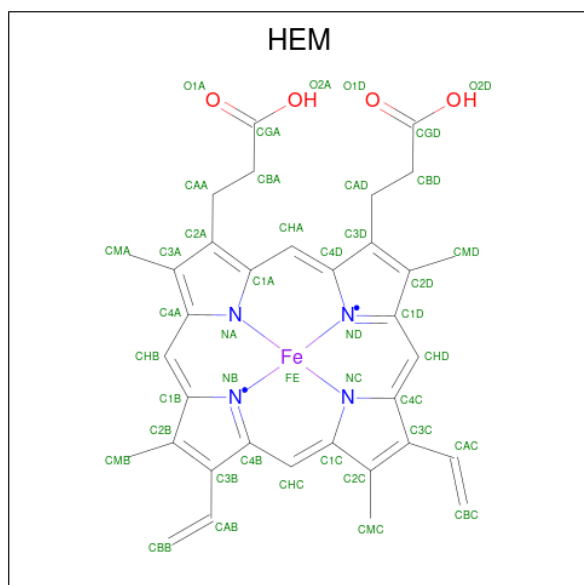
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1077	691	184	200	2			
1	C	141	Total	C	N	O	S	0	0	0
			1077	691	184	200	2			

- Molecule 2 is a protein called Hemoglobin subunit beta.

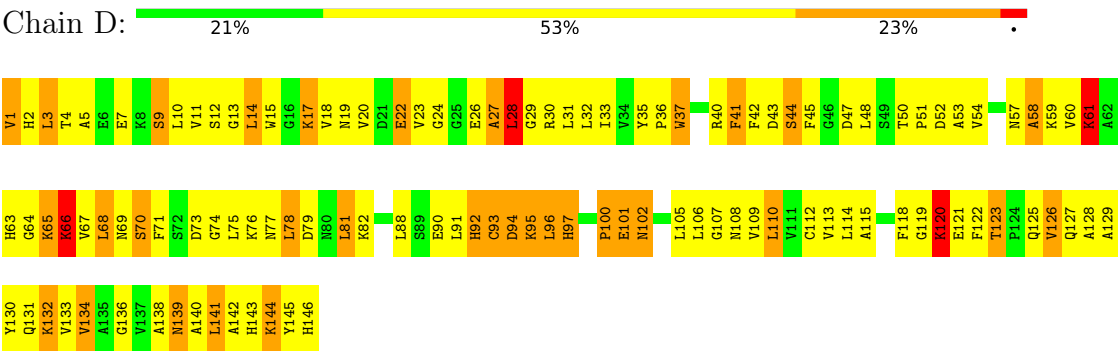
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1131	727	196	205	3			
2	D	146	Total	C	N	O	S	0	0	0
			1131	727	196	205	3			

- 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
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

● Molecule 2: Hemoglobin subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.09Å 88.49Å 66.37Å 90.00° 105.72° 90.00°	Depositor
Resolution (Å)	27.87 – 3.50 27.87 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.87-3.50) 96.9 (27.87-3.50)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.293 0.192 , 0.283	Depositor DCC
R_{free} test set	345 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 89.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4588	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.56% 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: 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	3.27	134/1107 (12.1%)	2.53	71/1507 (4.7%)
1	C	3.02	107/1107 (9.7%)	2.49	85/1507 (5.6%)
2	B	3.11	138/1157 (11.9%)	2.49	84/1564 (5.4%)
2	D	3.09	100/1157 (8.6%)	2.43	78/1564 (5.0%)
All	All	3.12	479/4528 (10.6%)	2.48	318/6142 (5.2%)

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	C	0	1

All (479) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	27	ALA	CA-CB	21.30	1.86	1.53
2	D	61	LYS	CE-NZ	15.63	1.96	1.49
1	A	88	ALA	C-O	-13.16	1.07	1.23
1	A	63	ALA	CA-CB	-13.09	1.30	1.53
1	C	82	ALA	CA-CB	-13.02	1.32	1.53
1	C	123	ALA	CA-CB	-13.01	1.32	1.53
2	D	115	ALA	CA-CB	-12.95	1.32	1.53
2	D	95	LYS	CA-C	-12.84	1.35	1.52
2	B	65	LYS	CE-NZ	12.81	1.87	1.49
2	B	105	LEU	N-CA	-12.22	1.30	1.46
1	A	3	SER	CB-OG	12.09	1.66	1.42
2	D	112	CYS	C-O	11.87	1.39	1.24
2	D	138	ALA	CA-CB	-11.82	1.35	1.53
1	C	141	ARG	NE-CZ	11.49	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	ASP	CA-C	-11.00	1.38	1.52
1	A	2	LEU	C-O	10.89	1.37	1.24
2	D	133	VAL	CA-CB	-10.74	1.41	1.54
2	D	132	LYS	CE-NZ	10.71	1.81	1.49
1	A	82	ALA	C-O	10.64	1.38	1.24
2	D	36	PRO	CA-CB	-10.36	1.39	1.53
2	D	30	ARG	N-CA	-10.07	1.34	1.46
1	A	4	PRO	N-CA	9.99	1.59	1.47
1	C	81	SER	N-CA	9.88	1.57	1.46
1	A	7	LYS	N-CA	-9.82	1.34	1.46
2	D	94	ASP	CA-C	-9.82	1.41	1.52
1	C	141	ARG	CD-NE	9.80	1.59	1.46
1	A	132	VAL	CA-CB	-9.79	1.41	1.54
1	A	3	SER	C-N	9.69	1.44	1.34
2	D	53	ALA	CA-CB	-9.67	1.38	1.53
2	B	66	LYS	CE-NZ	9.56	1.78	1.49
1	A	55	VAL	C-O	9.49	1.34	1.24
1	C	84	SER	N-CA	-9.39	1.34	1.46
2	B	108	ASN	C-O	9.30	1.35	1.24
1	A	3	SER	C-O	9.29	1.38	1.23
1	C	56	LYS	CD-CE	9.24	1.80	1.52
1	A	139	LYS	CE-NZ	9.23	1.77	1.49
2	B	25	GLY	N-CA	9.19	1.58	1.45
2	D	122	PHE	N-CA	-9.17	1.35	1.46
1	A	130	ALA	CA-CB	9.09	1.67	1.53
2	B	61	LYS	CG-CD	8.98	1.79	1.52
1	A	11	LYS	CE-NZ	8.96	1.76	1.49
1	A	17	ILE	CA-CB	8.90	1.66	1.54
2	D	120	LYS	CB-CG	8.90	1.79	1.52
2	B	33	ILE	CA-CB	-8.88	1.43	1.54
2	B	91	LEU	C-O	8.87	1.34	1.24
2	D	105	LEU	N-CA	-8.84	1.35	1.46
1	A	54	GLN	C-O	8.80	1.34	1.24
2	B	22	GLU	CA-C	-8.79	1.41	1.52
1	C	46	PHE	C-O	8.74	1.34	1.23
1	C	17	ILE	C-O	8.73	1.35	1.24
2	B	111	VAL	C-O	8.72	1.33	1.24
2	B	19	ASN	CA-CB	-8.70	1.41	1.52
2	B	126	VAL	N-CA	8.64	1.56	1.46
1	A	106	LEU	N-CA	8.64	1.56	1.46
1	C	53	ALA	CA-CB	8.60	1.67	1.53
1	A	50	PRO	CG-CD	8.59	1.79	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	66	LYS	CD-CE	8.55	1.78	1.52
1	A	107	VAL	CA-CB	8.48	1.66	1.54
2	B	16	GLY	N-CA	8.42	1.56	1.45
2	D	93	CYS	CB-SG	8.39	2.08	1.81
2	B	76	LYS	CG-CD	8.39	1.77	1.52
1	C	54	GLN	C-O	8.37	1.33	1.24
2	B	91	LEU	N-CA	8.37	1.56	1.46
1	A	13	THR	N-CA	8.35	1.56	1.46
1	A	4	PRO	N-CD	8.34	1.59	1.47
2	B	127	GLN	C-O	8.25	1.34	1.24
2	D	17	LYS	CD-CE	8.25	1.77	1.52
1	A	6	ASP	CG-OD1	8.23	1.41	1.25
2	B	43	ASP	C-O	8.23	1.33	1.24
1	C	40	LYS	CA-CB	-8.18	1.38	1.53
1	A	11	LYS	CD-CE	8.16	1.76	1.52
2	B	54	VAL	CA-CB	-8.14	1.44	1.54
1	C	21	ALA	CA-CB	8.10	1.66	1.53
1	C	31	ARG	CZ-NH2	8.09	1.44	1.33
2	B	20	VAL	C-O	8.07	1.33	1.24
1	A	85	ASP	CA-C	-8.06	1.42	1.52
1	C	9	ASN	N-CA	-8.04	1.36	1.46
1	C	15	ASP	CG-OD2	7.99	1.40	1.25
1	A	141	ARG	CG-CD	7.97	1.76	1.52
1	A	125	LEU	CA-C	-7.96	1.42	1.52
2	D	14	LEU	CA-CB	-7.95	1.40	1.53
1	C	16	LYS	C-O	-7.84	1.14	1.24
1	A	67	THR	C-O	7.84	1.33	1.24
1	A	46	PHE	C-O	7.77	1.33	1.23
2	B	71	PHE	CA-CB	-7.75	1.41	1.53
1	C	127	LYS	CA-C	-7.74	1.43	1.52
2	D	69	ASN	C-O	7.71	1.33	1.24
1	C	50	PRO	C-O	7.69	1.33	1.24
1	A	70	VAL	C-O	7.68	1.32	1.24
1	C	69	ALA	C-O	7.65	1.32	1.24
2	B	124	PRO	CA-CB	-7.59	1.43	1.53
2	B	87	LYS	CA-C	7.56	1.62	1.52
1	A	12	SER	CA-C	-7.55	1.43	1.52
2	B	125	GLN	CG-CD	7.54	1.70	1.52
2	D	32	LEU	CG-CD2	-7.53	1.27	1.52
2	B	5	ALA	CA-CB	-7.51	1.40	1.53
1	A	52	SER	C-O	7.51	1.33	1.23
1	A	121	VAL	C-O	7.51	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ASN	N-CA	7.49	1.55	1.46
2	B	80	ASN	CA-C	7.46	1.61	1.53
2	D	125	GLN	CD-NE2	7.46	1.49	1.33
2	D	73	ASP	N-CA	-7.44	1.37	1.46
2	D	101	GLU	CA-C	7.43	1.62	1.52
1	A	94	ASP	CA-CB	-7.39	1.41	1.53
2	D	101	GLU	CD-OE2	7.34	1.39	1.25
1	A	4	PRO	CG-CD	7.33	1.75	1.50
2	B	66	LYS	CD-CE	7.29	1.74	1.52
1	C	123	ALA	C-O	7.28	1.32	1.24
1	A	126	ASP	CA-C	-7.25	1.43	1.52
1	A	84	SER	N-CA	-7.24	1.37	1.46
1	A	4	PRO	C-O	7.23	1.33	1.24
2	D	92	HIS	CA-C	7.23	1.63	1.52
1	A	85	ASP	C-O	-7.22	1.13	1.23
1	C	60	LYS	CE-NZ	7.21	1.71	1.49
2	D	134	VAL	C-O	-7.20	1.16	1.24
2	B	132	LYS	CE-NZ	7.19	1.71	1.49
1	C	56	LYS	CA-C	-7.19	1.43	1.52
2	D	71	PHE	CA-CB	-7.17	1.41	1.53
1	C	132	VAL	CB-CG2	-7.17	1.28	1.52
2	D	94	ASP	CG-OD1	7.15	1.39	1.25
1	C	112	HIS	CA-C	-7.15	1.43	1.52
1	A	115	THR	N-CA	-7.14	1.36	1.46
1	A	16	LYS	CE-NZ	7.11	1.70	1.49
1	A	42	TYR	CZ-OH	7.11	1.52	1.38
1	A	69	ALA	C-O	7.11	1.32	1.24
2	B	61	LYS	CD-CE	7.11	1.73	1.52
1	A	77	PRO	CA-C	7.11	1.62	1.52
1	A	25	GLY	C-O	-7.10	1.15	1.23
1	C	16	LYS	CA-C	-7.09	1.43	1.52
1	A	97	ASN	C-O	-7.07	1.15	1.24
1	C	71	ALA	C-O	-7.04	1.15	1.24
2	B	112	CYS	N-CA	7.02	1.54	1.46
1	A	136	LEU	CA-C	7.02	1.62	1.52
2	B	76	LYS	CB-CG	7.02	1.73	1.52
2	B	13	GLY	N-CA	7.02	1.55	1.45
2	D	139	ASN	CG-ND2	7.01	1.48	1.33
2	D	41	PHE	CE1-CZ	6.97	1.59	1.38
2	B	134	VAL	C-O	6.96	1.32	1.24
2	D	24	GLY	C-O	6.93	1.32	1.23
2	D	120	LYS	CA-C	-6.92	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	111	VAL	CA-CB	-6.92	1.46	1.54
2	D	120	LYS	CE-NZ	6.92	1.70	1.49
2	B	59	LYS	CE-NZ	6.90	1.70	1.49
2	B	105	LEU	CA-C	-6.87	1.43	1.52
1	C	9	ASN	C-O	-6.87	1.16	1.24
1	A	127	LYS	CE-NZ	6.86	1.70	1.49
1	C	141	ARG	C-O	6.86	1.37	1.23
2	D	100	PRO	CA-C	-6.84	1.41	1.52
1	A	135	VAL	C-N	6.83	1.43	1.33
2	D	93	CYS	CA-C	-6.83	1.43	1.52
2	D	26	GLU	CA-CB	-6.82	1.42	1.53
2	B	28	LEU	CG-CD2	-6.81	1.30	1.52
1	A	135	VAL	C-O	6.81	1.32	1.24
1	A	24	TYR	CG-CD2	6.80	1.53	1.39
1	A	71	ALA	CA-CB	-6.78	1.42	1.53
1	C	87	HIS	CA-C	6.77	1.62	1.52
2	B	141	LEU	CA-C	6.76	1.61	1.52
1	A	19	GLY	C-O	6.76	1.31	1.23
2	B	125	GLN	N-CA	6.76	1.54	1.46
1	A	24	TYR	C-O	-6.75	1.15	1.24
1	A	6	ASP	CA-CB	6.75	1.64	1.53
1	A	42	TYR	C-O	-6.74	1.14	1.23
2	D	37	TRP	N-CA	6.72	1.54	1.46
1	C	74	ASP	CG-OD2	6.71	1.38	1.25
2	D	5	ALA	C-O	6.71	1.31	1.24
1	C	54	GLN	CA-C	6.69	1.61	1.52
1	C	100	LEU	CA-CB	-6.69	1.42	1.53
2	B	108	ASN	CG-ND2	6.69	1.47	1.33
2	B	107	GLY	C-O	6.67	1.31	1.23
1	A	7	LYS	CG-CD	6.66	1.72	1.52
2	B	104	LYS	CG-CD	6.66	1.72	1.52
2	D	118	PHE	CD1-CE1	6.65	1.58	1.38
1	C	2	LEU	CA-C	-6.64	1.43	1.52
2	D	119	GLY	N-CA	6.64	1.54	1.45
2	D	23	VAL	CA-CB	-6.62	1.47	1.54
1	C	21	ALA	CA-C	-6.62	1.44	1.52
1	A	6	ASP	CB-CG	6.61	1.68	1.52
2	B	83	GLY	C-O	6.60	1.32	1.23
1	A	61	LYS	CA-C	-6.59	1.43	1.52
1	A	64	ASP	N-CA	6.59	1.54	1.46
2	B	126	VAL	CA-CB	6.59	1.62	1.54
2	D	23	VAL	N-CA	-6.58	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	THR	C-O	6.58	1.32	1.24
1	C	79	ALA	CA-CB	6.58	1.64	1.53
2	B	133	VAL	CA-CB	-6.57	1.46	1.54
1	A	99	LYS	C-O	-6.56	1.16	1.24
2	D	128	ALA	CA-CB	-6.55	1.43	1.53
2	B	69	ASN	N-CA	6.53	1.54	1.46
1	A	118	THR	CA-C	6.52	1.61	1.53
1	C	100	LEU	N-CA	-6.52	1.37	1.46
2	B	79	ASP	CG-OD2	6.52	1.37	1.25
1	A	121	VAL	CA-C	6.51	1.60	1.52
2	D	118	PHE	CD2-CE2	6.51	1.58	1.38
2	B	73	ASP	CA-C	-6.50	1.43	1.52
2	B	146	HIS	C-O	6.50	1.36	1.23
1	C	62	VAL	CA-CB	-6.50	1.47	1.54
1	C	110	ALA	N-CA	6.49	1.54	1.46
2	D	22	GLU	CB-CG	6.49	1.72	1.52
2	D	94	ASP	C-O	-6.47	1.15	1.23
2	D	102	ASN	N-CA	-6.47	1.37	1.46
1	A	137	THR	N-CA	-6.43	1.37	1.46
2	D	32	LEU	CA-C	-6.43	1.44	1.52
2	B	61	LYS	CA-C	6.40	1.61	1.52
1	A	94	ASP	C-O	-6.39	1.16	1.24
1	C	31	ARG	C-O	-6.39	1.16	1.24
2	B	113	VAL	CB-CG2	-6.37	1.31	1.52
2	B	49	SER	CA-C	6.37	1.61	1.52
1	A	5	ALA	CA-CB	-6.36	1.43	1.53
2	D	101	GLU	CD-OE1	6.36	1.37	1.25
2	B	45	PHE	CA-C	-6.35	1.44	1.52
1	A	75	ASP	C-O	6.33	1.30	1.23
2	B	71	PHE	CB-CG	-6.33	1.36	1.50
1	A	16	LYS	CG-CD	6.33	1.71	1.52
2	B	68	LEU	N-CA	-6.32	1.38	1.46
2	B	116	HIS	CE1-NE2	6.32	1.38	1.32
2	B	139	ASN	C-O	-6.32	1.16	1.24
1	A	116	GLU	CD-OE2	6.31	1.37	1.25
2	B	101	GLU	N-CA	-6.31	1.38	1.46
1	C	13	THR	N-CA	-6.29	1.38	1.46
1	C	99	LYS	C-O	-6.28	1.16	1.24
2	B	143	HIS	CE1-NE2	6.27	1.38	1.32
1	C	100	LEU	C-O	6.27	1.32	1.24
1	A	93	VAL	CA-CB	6.26	1.61	1.54
1	C	50	PRO	CB-CG	6.25	1.80	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	LYS	CD-CE	6.25	1.71	1.52
1	A	70	VAL	CB-CG1	-6.24	1.31	1.52
2	B	70	SER	C-O	6.24	1.31	1.24
2	D	71	PHE	CA-C	-6.24	1.44	1.52
2	B	109	VAL	CA-CB	-6.24	1.45	1.54
2	D	66	LYS	CG-CD	6.22	1.71	1.52
2	B	131	GLN	N-CA	-6.21	1.38	1.46
1	C	56	LYS	CG-CD	6.21	1.71	1.52
1	C	70	VAL	CA-CB	-6.20	1.46	1.54
2	B	4	THR	N-CA	-6.19	1.37	1.45
1	A	51	GLY	N-CA	6.18	1.54	1.45
2	B	144	LYS	CA-C	6.18	1.61	1.52
2	B	80	ASN	C-O	6.17	1.33	1.23
1	A	33	PHE	CA-C	-6.17	1.44	1.52
2	B	120	LYS	CE-NZ	6.17	1.67	1.49
2	D	18	VAL	C-O	-6.17	1.17	1.24
2	D	26	GLU	CD-OE1	6.16	1.37	1.25
1	C	63	ALA	CA-CB	-6.14	1.43	1.53
1	A	141	ARG	C-O	6.13	1.35	1.23
1	A	1	VAL	CB-CG2	6.13	1.72	1.52
2	B	86	ALA	CA-CB	-6.13	1.43	1.53
1	A	108	THR	C-O	-6.12	1.17	1.24
1	A	26	GLY	N-CA	6.12	1.53	1.45
1	A	65	ALA	CA-CB	6.11	1.62	1.53
2	D	44	SER	C-O	-6.10	1.16	1.24
1	C	11	LYS	CD-CE	6.10	1.70	1.52
2	D	66	LYS	CE-NZ	6.10	1.67	1.49
1	C	119	PRO	CA-C	6.07	1.61	1.52
1	C	23	ASP	N-CA	-6.07	1.38	1.46
1	A	135	VAL	CB-CG1	6.06	1.72	1.52
2	B	58	ALA	C-O	6.06	1.31	1.24
2	B	118	PHE	C-O	6.05	1.32	1.24
1	A	31	ARG	CD-NE	6.05	1.54	1.46
2	B	57	ASN	N-CA	-6.05	1.38	1.46
2	B	103	PHE	N-CA	6.04	1.53	1.46
1	C	27	GLU	CA-CB	-6.03	1.43	1.53
1	C	64	ASP	N-CA	-6.01	1.39	1.46
1	A	16	LYS	C-O	6.00	1.31	1.24
1	C	27	GLU	CA-C	5.98	1.60	1.52
1	A	98	PHE	CD1-CE1	5.97	1.56	1.38
2	D	97	HIS	C-O	5.97	1.31	1.24
1	C	109	LEU	CA-C	-5.97	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	31	LEU	C-N	-5.97	1.25	1.33
2	B	34	VAL	N-CA	5.96	1.53	1.46
2	D	129	ALA	CA-CB	-5.96	1.44	1.53
2	D	140	ALA	CA-CB	-5.96	1.43	1.53
2	D	43	ASP	CG-OD1	5.96	1.36	1.25
1	C	109	LEU	CG-CD2	-5.95	1.32	1.52
2	B	26	GLU	CD-OE2	5.93	1.36	1.25
1	C	60	LYS	CB-CG	5.93	1.70	1.52
1	C	127	LYS	N-CA	-5.93	1.39	1.46
1	A	3	SER	CA-C	5.93	1.60	1.52
1	A	11	LYS	CA-C	-5.93	1.45	1.52
1	A	75	ASP	CG-OD2	5.93	1.36	1.25
2	D	22	GLU	CD-OE1	5.93	1.36	1.25
2	D	47	ASP	CG-OD2	5.92	1.36	1.25
1	A	27	GLU	CG-CD	5.91	1.66	1.52
1	C	90	LYS	C-O	5.89	1.30	1.24
2	B	56	SER	N-CA	-5.89	1.37	1.45
1	A	91	LEU	N-CA	5.89	1.53	1.46
2	D	28	LEU	CA-C	5.89	1.60	1.52
1	C	111	CYS	C-O	5.89	1.31	1.24
2	B	111	VAL	N-CA	5.88	1.53	1.46
1	A	4	PRO	CA-CB	5.88	1.64	1.53
2	B	20	VAL	C-N	5.88	1.41	1.33
1	C	141	ARG	C-OXT	5.88	1.35	1.23
2	B	20	VAL	CA-C	5.87	1.60	1.52
2	D	123	THR	N-CA	5.87	1.54	1.46
1	C	10	ILE	CA-CB	-5.87	1.47	1.54
2	B	62	ALA	C-O	-5.87	1.16	1.24
2	D	93	CYS	N-CA	5.86	1.53	1.46
1	A	105	LEU	C-N	5.86	1.41	1.33
1	A	138	SER	C-O	5.85	1.31	1.24
1	C	24	TYR	N-CA	5.85	1.53	1.46
2	D	15	TRP	CE2-CZ2	5.84	1.52	1.39
1	A	17	ILE	C-O	5.84	1.31	1.24
1	C	117	PHE	CA-CB	-5.83	1.43	1.53
1	A	49	SER	CB-OG	5.83	1.53	1.42
2	D	12	SER	C-O	5.83	1.31	1.24
1	A	63	ALA	N-CA	-5.82	1.38	1.46
1	C	11	LYS	CE-NZ	5.82	1.66	1.49
1	C	92	ARG	CB-CG	5.81	1.69	1.52
2	B	32	LEU	CG-CD1	-5.81	1.33	1.52
2	D	125	GLN	CD-OE1	5.81	1.34	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	GLU	CG-CD	5.80	1.66	1.52
1	A	141	ARG	CB-CG	5.80	1.69	1.52
2	D	81	LEU	C-O	-5.80	1.17	1.24
1	C	45	HIS	CA-C	-5.80	1.44	1.52
1	A	26	GLY	C-O	5.79	1.30	1.23
2	B	85	PHE	N-CA	5.78	1.53	1.46
2	B	143	HIS	CG-ND1	5.78	1.44	1.38
1	A	64	ASP	CG-OD2	5.75	1.36	1.25
1	C	141	ARG	CZ-NH1	5.74	1.40	1.32
2	B	72	SER	C-O	5.74	1.31	1.24
2	B	134	VAL	CA-C	5.74	1.60	1.52
2	B	55	MET	CB-CG	5.74	1.69	1.52
2	B	36	PRO	CA-CB	-5.73	1.45	1.53
2	B	127	GLN	CA-C	5.72	1.60	1.52
2	D	26	GLU	CA-C	-5.71	1.45	1.52
2	D	74	GLY	N-CA	5.71	1.53	1.45
2	D	40	ARG	N-CA	5.71	1.53	1.46
1	C	98	PHE	CE1-CZ	-5.68	1.21	1.38
2	D	125	GLN	CG-CD	5.68	1.66	1.52
1	C	71	ALA	N-CA	5.68	1.53	1.46
2	D	60	VAL	CB-CG1	-5.66	1.33	1.52
2	B	109	VAL	C-O	-5.66	1.16	1.24
2	B	83	GLY	N-CA	5.66	1.53	1.45
2	D	2	HIS	CA-C	-5.65	1.45	1.52
2	D	43	ASP	C-O	5.65	1.30	1.24
1	C	1	VAL	N-CA	5.64	1.56	1.46
2	D	43	ASP	CA-C	5.64	1.59	1.52
1	A	73	LEU	CG-CD1	5.63	1.71	1.52
2	B	27	ALA	CA-C	5.63	1.60	1.52
2	B	1	VAL	CB-CG2	5.62	1.71	1.52
2	D	45	PHE	CD1-CE1	-5.62	1.21	1.38
1	C	92	ARG	NE-CZ	5.62	1.39	1.33
2	B	115	ALA	CA-CB	5.62	1.62	1.53
1	C	27	GLU	C-O	5.62	1.30	1.24
2	B	6	GLU	C-O	5.62	1.30	1.24
1	C	41	THR	CA-C	-5.61	1.45	1.52
1	C	89	TYR	CG-CD2	5.61	1.51	1.39
2	B	88	LEU	CA-C	-5.61	1.45	1.52
2	B	85	PHE	CB-CG	-5.60	1.37	1.50
1	C	18	GLY	N-CA	5.59	1.53	1.45
2	D	57	ASN	CG-ND2	5.59	1.45	1.33
2	B	57	ASN	CG-ND2	5.58	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	LEU	CA-C	-5.58	1.45	1.52
2	D	79	ASP	CA-C	-5.58	1.44	1.52
2	B	28	LEU	CA-C	-5.58	1.45	1.52
2	D	97	HIS	C-N	5.58	1.40	1.33
1	C	17	ILE	CA-CB	-5.57	1.46	1.54
1	A	66	LEU	C-O	5.57	1.30	1.24
1	C	98	PHE	N-CA	-5.57	1.39	1.46
1	A	126	ASP	N-CA	-5.56	1.39	1.46
2	B	6	GLU	N-CA	5.56	1.52	1.46
2	D	123	THR	CA-C	5.56	1.59	1.52
1	A	70	VAL	CA-C	5.55	1.59	1.52
2	B	121	GLU	CD-OE2	5.55	1.35	1.25
2	D	51	PRO	CA-C	5.55	1.60	1.52
1	C	51	GLY	C-O	-5.55	1.16	1.23
1	C	126	ASP	CA-C	-5.55	1.44	1.52
1	C	101	LEU	CA-CB	-5.54	1.44	1.53
2	B	5	ALA	CA-C	-5.53	1.45	1.52
2	B	123	THR	N-CA	5.52	1.53	1.46
1	A	24	TYR	CA-C	-5.50	1.45	1.52
2	B	125	GLN	CD-OE1	5.50	1.34	1.23
1	A	82	ALA	CA-C	5.49	1.60	1.52
2	B	26	GLU	C-O	5.48	1.30	1.24
2	B	45	PHE	C-O	-5.48	1.17	1.23
1	C	65	ALA	CA-CB	-5.48	1.44	1.53
1	C	118	THR	C-O	-5.47	1.16	1.23
2	B	40	ARG	C-O	-5.47	1.17	1.24
1	C	92	ARG	CA-C	5.47	1.60	1.53
2	B	54	VAL	CB-CG1	-5.47	1.34	1.52
2	B	133	VAL	CB-CG2	-5.46	1.34	1.52
2	D	22	GLU	CG-CD	5.44	1.65	1.52
2	D	79	ASP	CG-OD1	5.44	1.35	1.25
1	A	10	ILE	C-O	5.43	1.30	1.24
1	A	121	VAL	CB-CG2	-5.42	1.34	1.52
2	D	102	ASN	CA-C	-5.42	1.45	1.52
2	D	88	LEU	CA-CB	-5.41	1.44	1.53
1	C	31	ARG	NE-CZ	5.41	1.39	1.33
1	A	100	LEU	CA-C	-5.41	1.45	1.52
2	B	21	ASP	CA-C	5.41	1.60	1.52
1	C	117	PHE	CA-C	5.40	1.60	1.52
2	B	27	ALA	C-O	5.40	1.30	1.24
2	B	41	PHE	CE1-CZ	-5.39	1.22	1.38
1	C	42	TYR	CA-C	-5.38	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	105	LEU	N-CA	-5.38	1.39	1.46
1	C	21	ALA	C-O	-5.38	1.17	1.24
1	C	87	HIS	C-O	5.38	1.30	1.24
2	B	145	TYR	CD1-CE1	5.37	1.54	1.38
1	C	118	THR	CB-CG2	-5.37	1.34	1.52
1	C	138	SER	C-O	5.37	1.30	1.24
2	D	133	VAL	N-CA	-5.37	1.40	1.46
1	C	11	LYS	CG-CD	5.35	1.68	1.52
2	B	94	ASP	C-O	-5.34	1.16	1.23
2	D	58	ALA	N-CA	5.34	1.53	1.46
2	D	146	HIS	CA-CB	5.34	1.64	1.53
2	B	55	MET	N-CA	5.34	1.53	1.46
2	B	78	LEU	N-CA	5.34	1.53	1.46
1	A	98	PHE	CD2-CE2	5.33	1.54	1.38
2	B	109	VAL	CA-C	-5.33	1.44	1.52
2	B	107	GLY	CA-C	5.33	1.58	1.51
1	C	22	GLY	C-O	-5.32	1.17	1.23
1	C	74	ASP	CG-OD1	5.32	1.35	1.25
2	D	9	SER	CB-OG	5.31	1.52	1.42
2	D	11	VAL	CA-C	-5.31	1.46	1.52
2	B	94	ASP	CG-OD2	5.30	1.35	1.25
2	B	14	LEU	CA-CB	-5.30	1.44	1.53
1	A	66	LEU	CG-CD1	5.28	1.70	1.52
1	C	121	VAL	CA-CB	5.27	1.60	1.54
2	D	40	ARG	C-O	-5.27	1.17	1.24
1	A	61	LYS	CG-CD	5.26	1.68	1.52
2	D	77	ASN	CA-C	-5.26	1.46	1.53
1	A	11	LYS	CG-CD	5.24	1.68	1.52
1	A	17	ILE	CA-C	5.24	1.61	1.52
1	A	68	THR	C-O	-5.24	1.17	1.24
2	B	2	HIS	CA-CB	5.24	1.60	1.53
1	A	11	LYS	CA-CB	-5.24	1.45	1.53
1	C	56	LYS	CB-CG	5.23	1.68	1.52
1	C	137	THR	CA-C	5.23	1.59	1.52
1	A	137	THR	CB-CG2	-5.22	1.35	1.52
2	B	51	PRO	CA-CB	5.22	1.61	1.53
2	D	13	GLY	CA-C	-5.22	1.46	1.52
2	B	119	GLY	C-O	-5.21	1.16	1.23
1	A	31	ARG	CA-CB	-5.20	1.44	1.53
2	B	54	VAL	C-O	5.19	1.30	1.24
2	B	120	LYS	CD-CE	5.19	1.68	1.52
2	B	61	LYS	C-O	5.18	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	115	ALA	CA-C	-5.18	1.45	1.52
1	A	92	ARG	NE-CZ	5.18	1.38	1.33
1	C	84	SER	CB-OG	5.18	1.52	1.42
1	C	35	SER	CB-OG	5.18	1.52	1.42
1	C	41	THR	CB-CG2	5.17	1.69	1.52
1	A	41	THR	CA-C	-5.16	1.45	1.52
2	B	40	ARG	CD-NE	5.16	1.53	1.46
2	B	40	ARG	CZ-NH2	5.16	1.40	1.33
2	B	55	MET	CG-SD	5.14	1.93	1.80
1	A	117	PHE	N-CA	5.14	1.52	1.46
1	A	74	ASP	CB-CG	5.13	1.64	1.52
2	B	76	LYS	CD-CE	5.13	1.67	1.52
1	A	127	LYS	N-CA	-5.12	1.39	1.46
1	C	45	HIS	C-O	-5.12	1.17	1.24
2	B	120	LYS	CA-C	-5.12	1.45	1.52
2	B	40	ARG	CZ-NH1	5.11	1.40	1.32
1	C	36	PHE	CE2-CZ	-5.11	1.23	1.38
2	D	41	PHE	C-O	5.11	1.30	1.24
1	C	56	LYS	CE-NZ	5.11	1.64	1.49
1	A	77	PRO	CB-CG	5.10	1.75	1.49
1	A	2	LEU	C-N	5.10	1.40	1.33
2	B	15	TRP	N-CA	-5.09	1.39	1.46
2	B	132	LYS	CD-CE	5.09	1.67	1.52
1	C	51	GLY	N-CA	5.09	1.52	1.45
2	B	54	VAL	CA-C	5.09	1.59	1.52
1	A	136	LEU	N-CA	5.08	1.52	1.46
1	A	35	SER	C-O	5.07	1.30	1.24
1	A	20	HIS	CG-ND1	5.07	1.43	1.38
1	C	15	ASP	CG-OD1	5.07	1.34	1.25
1	A	8	THR	CB-CG2	5.07	1.69	1.52
1	A	98	PHE	CA-C	-5.07	1.46	1.52
2	B	123	THR	CB-OG1	5.07	1.51	1.43
2	B	130	TYR	CD2-CE2	5.06	1.53	1.38
2	D	35	TYR	CZ-OH	-5.06	1.27	1.38
1	A	97	ASN	CB-CG	5.05	1.64	1.52
1	A	20	HIS	CA-C	-5.04	1.46	1.52
1	A	21	ALA	N-CA	5.03	1.52	1.46
1	A	20	HIS	CE1-NE2	5.03	1.37	1.32
2	D	26	GLU	CD-OE2	5.03	1.34	1.25
1	A	113	HIS	CA-C	-5.03	1.46	1.52
1	C	23	ASP	CG-OD2	5.03	1.34	1.25
1	A	89	TYR	CZ-OH	5.02	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	LYS	N-CA	-5.02	1.39	1.46
2	B	101	GLU	CA-CB	-5.00	1.45	1.53
1	C	109	LEU	CA-CB	-5.00	1.45	1.53

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	VAL	N-CA-C	-12.20	98.40	110.72
2	B	14	LEU	N-CA-C	11.95	124.39	111.36
2	D	120	LYS	N-CA-C	11.35	124.99	111.82
1	A	85	ASP	N-CA-C	-11.34	98.95	113.12
1	A	3	SER	CA-C-N	-11.19	107.96	120.04
1	A	3	SER	C-N-CA	-11.19	107.96	120.04
1	C	39	THR	N-CA-C	10.69	125.43	111.75
1	C	31	ARG	NE-CZ-NH2	10.52	128.66	119.20
1	C	29	LEU	N-CA-C	10.27	123.76	111.33
2	B	69	ASN	N-CA-C	10.03	123.46	111.33
1	A	121	VAL	N-CA-C	9.98	119.91	110.53
1	C	89	TYR	N-CA-C	9.92	123.89	111.69
2	B	73	ASP	N-CA-C	-9.53	99.20	112.45
2	B	96	LEU	N-CA-C	9.26	124.70	113.12
2	D	32	LEU	CD1-CG-CD2	-9.11	90.76	110.80
1	A	81	SER	CA-C-N	-9.10	106.52	122.26
1	A	81	SER	C-N-CA	-9.10	106.52	122.26
1	A	10	ILE	N-CA-C	9.10	120.99	110.62
2	D	11	VAL	CB-CA-C	-8.83	100.58	111.88
2	D	106	LEU	N-CA-C	8.81	121.98	111.33
1	C	28	ALA	CA-C-O	-8.45	111.86	120.90
2	B	126	VAL	N-CA-C	8.43	120.22	110.62
2	B	2	HIS	N-CA-C	-8.42	94.73	108.12
1	A	11	LYS	O-C-N	8.42	131.75	122.15
2	B	141	LEU	N-CA-C	8.38	121.35	111.71
2	B	9	SER	N-CA-C	-8.32	102.15	111.14
1	A	27	GLU	N-CA-C	8.29	120.09	111.14
2	B	18	VAL	CB-CA-C	-8.28	100.65	110.91
2	D	93	CYS	N-CA-C	8.25	122.62	112.23
1	A	39	THR	N-CA-C	8.24	120.26	111.28
1	A	62	VAL	N-CA-C	-8.18	102.08	111.00
1	A	82	ALA	N-CA-C	-8.08	103.44	113.38
1	C	43	PHE	CA-C-N	-8.08	111.40	119.56
1	C	43	PHE	C-N-CA	-8.08	111.40	119.56
1	C	86	LEU	N-CA-C	-8.04	102.10	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	LYS	N-CA-C	-8.00	103.67	113.50
2	D	32	LEU	N-CA-C	7.92	120.00	111.36
1	C	10	ILE	N-CA-C	7.88	117.83	110.42
2	D	33	ILE	N-CA-C	7.88	117.98	110.42
1	C	109	LEU	CD1-CG-CD2	-7.86	93.50	110.80
1	C	74	ASP	N-CA-C	-7.84	103.94	113.97
1	A	127	LYS	N-CA-C	-7.83	102.74	111.82
1	A	83	LEU	N-CA-C	-7.78	102.70	112.90
2	B	54	VAL	CB-CA-C	-7.78	101.84	112.04
2	D	105	LEU	CA-C-O	-7.73	112.73	120.70
2	D	74	GLY	N-CA-C	7.68	122.20	112.83
2	B	14	LEU	CB-CG-CD2	7.67	133.70	110.70
1	C	128	PHE	CA-C-N	-7.64	109.91	120.38
1	C	128	PHE	C-N-CA	-7.64	109.91	120.38
1	C	61	LYS	N-CA-C	7.63	120.27	111.11
1	C	81	SER	CA-C-N	-7.60	110.09	120.28
1	C	81	SER	C-N-CA	-7.60	110.09	120.28
2	B	28	LEU	CB-CA-C	-7.57	98.94	110.90
1	C	116	GLU	N-CA-C	-7.55	102.72	112.23
2	D	113	VAL	N-CA-C	-7.54	102.78	111.00
2	B	121	GLU	CB-CG-CD	-7.52	99.81	112.60
2	B	45	PHE	N-CA-C	-7.51	104.35	113.97
2	B	105	LEU	N-CA-C	-7.51	102.45	111.69
2	D	130	TYR	N-CA-C	7.50	120.34	111.71
1	C	105	LEU	N-CA-CB	-7.49	98.96	110.42
1	A	31	ARG	NE-CZ-NH2	7.46	125.92	119.20
1	A	92	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	C	32	THR	N-CA-C	-7.41	102.58	111.69
2	D	9	SER	N-CA-C	7.37	119.96	111.11
1	C	5	ALA	N-CA-C	-7.37	103.18	111.14
1	A	31	ARG	NE-CZ-NH1	-7.34	114.16	121.50
1	C	29	LEU	CB-CA-C	-7.33	98.21	110.68
2	D	70	SER	N-CA-C	-7.33	102.67	111.69
1	A	139	LYS	CD-CE-NZ	-7.33	88.45	111.90
1	C	25	GLY	O-C-N	-7.26	114.94	122.13
2	B	20	VAL	N-CA-C	7.24	118.00	110.62
1	C	105	LEU	N-CA-C	-7.23	104.08	113.12
1	A	42	TYR	CA-C-N	7.20	129.62	122.28
1	A	42	TYR	C-N-CA	7.20	129.62	122.28
2	B	110	LEU	CB-CA-C	-7.18	99.31	110.81
1	A	71	ALA	N-CA-C	7.17	119.96	111.71
2	B	58	ALA	N-CA-C	7.17	119.09	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	LEU	CA-C-N	-7.14	110.59	120.38
2	D	105	LEU	C-N-CA	-7.14	110.59	120.38
1	C	89	TYR	N-CA-CB	-7.12	99.59	110.20
1	C	7	LYS	N-CA-C	-7.09	103.29	112.23
2	D	132	LYS	CD-CE-NZ	-7.03	89.41	111.90
1	A	124	SER	N-CA-C	6.99	118.90	111.28
2	B	26	GLU	CB-CG-CD	-6.96	100.77	112.60
2	B	54	VAL	N-CA-CB	-6.94	101.80	110.47
1	A	97	ASN	N-CA-C	6.92	119.71	111.33
2	D	36	PRO	N-CD-CG	-6.91	92.83	103.20
1	A	14	TRP	N-CA-C	-6.91	103.85	112.90
1	A	105	LEU	CA-C-O	-6.90	113.59	120.70
1	A	93	VAL	N-CA-C	6.90	118.78	108.23
2	D	26	GLU	CB-CG-CD	-6.89	100.88	112.60
2	B	112	CYS	N-CA-CB	6.78	120.12	109.82
1	C	57	ALA	N-CA-C	6.76	119.66	111.82
1	A	64	ASP	O-C-N	6.75	129.84	122.15
2	D	63	HIS	CA-C-N	6.71	127.39	119.94
2	D	63	HIS	C-N-CA	6.71	127.39	119.94
2	D	35	TYR	CA-C-N	6.70	126.66	119.28
2	D	35	TYR	C-N-CA	6.70	126.66	119.28
2	D	17	LYS	CD-CE-NZ	-6.65	90.63	111.90
1	C	141	ARG	NE-CZ-NH1	6.58	128.08	121.50
2	D	123	THR	N-CA-C	6.57	124.33	109.81
2	B	133	VAL	CB-CA-C	-6.56	103.57	111.97
1	A	78	GLY	N-CA-C	-6.54	104.58	112.49
1	A	105	LEU	N-CA-C	-6.53	104.09	111.14
1	C	64	ASP	N-CA-C	6.53	118.05	111.07
2	D	67	VAL	N-CA-C	-6.52	103.97	110.62
2	B	99	ASP	N-CA-C	-6.50	101.87	109.93
2	B	108	ASN	N-CA-C	6.50	119.19	111.71
1	A	39	THR	CB-CA-C	-6.49	100.01	110.79
2	B	10	LEU	N-CA-C	6.49	118.36	111.28
2	D	82	LYS	N-CA-C	6.48	121.99	111.37
2	B	1	VAL	CB-CA-C	-6.47	99.10	111.40
1	C	129	PHE	N-CA-C	6.47	119.15	111.33
1	A	116	GLU	N-CA-C	-6.43	104.69	113.30
1	A	82	ALA	CA-C-O	6.41	126.46	119.15
2	B	102	ASN	N-CA-C	6.38	119.22	111.82
1	A	10	ILE	CB-CA-C	-6.38	103.68	112.04
1	A	121	VAL	CB-CA-C	-6.35	103.70	112.02
2	B	11	VAL	N-CA-C	-6.32	104.48	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	24	GLY	N-CA-C	6.32	120.31	112.73
1	C	122	HIS	CA-C-O	-6.31	113.81	120.63
2	D	108	ASN	N-CA-C	6.28	118.93	111.33
1	C	58	HIS	N-CA-C	-6.28	103.72	112.45
2	D	144	LYS	CA-CB-CG	-6.27	101.56	114.10
1	C	94	ASP	N-CA-C	-6.26	100.15	109.42
1	C	32	THR	CA-C-O	-6.25	113.30	120.24
2	D	23	VAL	CA-C-N	-6.25	113.04	119.98
2	D	23	VAL	C-N-CA	-6.25	113.04	119.98
1	A	111	CYS	N-CA-C	6.25	118.09	111.28
1	C	140	TYR	N-CA-C	-6.24	105.79	113.41
2	D	69	ASN	O-C-N	6.24	129.95	122.27
2	B	111	VAL	N-CA-CB	6.22	117.82	110.55
1	A	137	THR	CA-C-O	6.20	126.61	119.35
2	D	54	VAL	N-CA-CB	6.20	117.13	110.62
2	D	31	LEU	CA-C-O	6.19	127.11	120.55
1	C	116	GLU	CA-CB-CG	6.18	126.46	114.10
2	B	85	PHE	CA-C-N	-6.18	111.52	120.29
2	B	85	PHE	C-N-CA	-6.18	111.52	120.29
1	C	21	ALA	N-CA-C	-6.18	103.70	111.11
1	A	50	PRO	CB-CG-CD	-6.18	86.34	106.10
2	D	28	LEU	CD1-CG-CD2	-6.17	97.23	110.80
1	C	16	LYS	CA-CB-CG	-6.16	101.79	114.10
2	B	27	ALA	CA-C-N	6.14	128.80	120.44
2	B	27	ALA	C-N-CA	6.14	128.80	120.44
2	B	120	LYS	CB-CA-C	-6.14	97.47	110.31
2	B	107	GLY	CA-C-O	6.13	127.36	121.05
2	D	22	GLU	N-CA-C	6.12	120.92	111.56
2	D	4	THR	N-CA-C	-6.11	102.89	110.41
1	C	141	ARG	CD-NE-CZ	6.11	132.95	124.40
1	A	120	ALA	CA-C-O	-6.09	114.10	120.92
1	A	4	PRO	N-CD-CG	-6.09	94.06	103.20
1	C	106	LEU	N-CA-C	-6.08	104.66	111.28
1	C	117	PHE	N-CA-C	6.08	123.75	110.80
2	D	126	VAL	CA-C-O	-6.06	114.65	120.95
1	C	23	ASP	CB-CA-C	-6.04	97.69	110.31
1	A	135	VAL	N-CA-CB	6.03	121.18	111.23
1	C	11	LYS	CA-CB-CG	-6.02	102.06	114.10
2	D	132	LYS	N-CA-C	-6.00	104.11	112.45
1	C	82	ALA	N-CA-C	5.99	117.81	111.28
2	B	125	GLN	N-CA-CB	5.97	120.59	110.49
1	C	37	PRO	N-CA-C	5.97	121.71	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	SER	CA-C-N	5.96	127.30	119.84
1	C	49	SER	C-N-CA	5.96	127.30	119.84
2	D	138	ALA	N-CA-C	5.96	117.44	111.07
2	B	32	LEU	CD1-CG-CD2	-5.95	97.71	110.80
2	B	108	ASN	CA-C-N	-5.93	110.10	120.29
2	B	108	ASN	C-N-CA	-5.93	110.10	120.29
1	A	77	PRO	CA-C-N	5.92	126.39	119.94
1	A	77	PRO	C-N-CA	5.92	126.39	119.94
2	B	64	GLY	N-CA-C	-5.90	99.21	113.18
1	A	43	PHE	CA-C-N	-5.89	113.61	119.56
1	A	43	PHE	C-N-CA	-5.89	113.61	119.56
2	B	95	LYS	CB-CA-C	5.88	119.99	109.29
2	B	2	HIS	O-C-N	5.86	125.98	120.71
1	C	61	LYS	CA-C-O	-5.80	114.69	120.90
1	C	84	SER	CB-CA-C	5.80	121.18	110.56
1	C	15	ASP	N-CA-C	5.80	117.27	111.07
2	D	144	LYS	CA-C-O	5.79	128.79	120.51
1	A	99	LYS	N-CA-C	-5.78	104.34	111.33
2	B	143	HIS	N-CA-C	5.77	123.09	110.80
2	D	60	VAL	N-CA-C	-5.75	105.24	110.82
1	C	92	ARG	NH1-CZ-NH2	-5.73	111.85	119.30
1	A	94	ASP	CA-C-N	5.73	126.12	119.47
1	A	94	ASP	C-N-CA	5.73	126.12	119.47
2	D	94	ASP	CB-CG-OD2	-5.72	105.24	118.40
2	B	7	GLU	CA-C-N	-5.70	111.64	120.31
2	B	7	GLU	C-N-CA	-5.70	111.64	120.31
2	D	73	ASP	CB-CG-OD2	5.70	131.50	118.40
2	B	101	GLU	N-CA-CB	-5.70	100.86	110.49
2	B	127	GLN	CA-CB-CG	-5.70	102.71	114.10
1	A	69	ALA	N-CA-C	5.69	117.56	111.36
1	A	38	THR	OG1-CB-CG2	-5.69	97.93	109.30
2	B	8	LYS	CA-C-N	5.66	128.14	120.44
2	B	8	LYS	C-N-CA	5.66	128.14	120.44
1	C	31	ARG	NE-CZ-NH1	-5.66	115.84	121.50
2	D	26	GLU	CA-CB-CG	-5.66	102.79	114.10
1	C	69	ALA	N-CA-C	5.64	117.29	111.03
2	B	6	GLU	CA-C-O	5.64	126.71	120.90
1	C	79	ALA	N-CA-C	5.63	118.96	111.75
1	C	61	LYS	CA-C-N	5.63	127.59	120.72
1	C	61	LYS	C-N-CA	5.63	127.59	120.72
2	D	43	ASP	N-CA-CB	-5.63	101.84	110.01
2	B	118	PHE	O-C-N	5.63	129.79	122.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	VAL	CA-C-O	-5.63	115.42	121.27
2	D	136	GLY	O-C-N	-5.62	115.39	122.70
1	C	100	LEU	CB-CA-C	-5.61	99.50	110.11
1	A	54	GLN	CB-CA-C	5.61	119.77	110.90
2	D	88	LEU	CA-CB-CG	-5.61	96.67	116.30
2	B	27	ALA	N-CA-C	5.60	117.83	111.11
2	D	70	SER	CA-C-O	-5.59	114.03	120.24
1	C	24	TYR	N-CA-C	-5.59	104.81	111.69
1	C	139	LYS	CG-CD-CE	-5.59	98.44	111.30
2	B	23	VAL	N-CA-C	5.58	117.49	111.58
1	A	107	VAL	CG1-CB-CG2	-5.55	98.59	110.80
2	B	32	LEU	N-CA-CB	5.54	118.27	110.12
2	D	66	LYS	CA-C-N	5.54	128.06	120.46
2	D	66	LYS	C-N-CA	5.54	128.06	120.46
1	C	87	HIS	CB-CA-C	5.54	120.57	110.11
2	B	19	ASN	CB-CA-C	-5.53	101.70	111.05
2	B	4	THR	N-CA-CB	-5.50	101.94	110.29
2	B	78	LEU	N-CA-C	5.50	122.51	110.80
1	C	106	LEU	CD1-CG-CD2	5.49	122.88	110.80
2	D	48	LEU	CA-C-O	5.48	125.22	119.03
1	C	39	THR	CA-C-O	-5.47	114.07	120.20
1	A	49	SER	N-CA-C	5.45	117.41	109.84
1	C	6	ASP	CA-C-N	-5.43	111.44	120.68
1	C	6	ASP	C-N-CA	-5.43	111.44	120.68
2	B	78	LEU	CA-CB-CG	-5.42	97.31	116.30
2	D	18	VAL	N-CA-C	5.42	116.05	108.89
1	C	7	LYS	CB-CG-CD	-5.42	98.84	111.30
2	D	32	LEU	CB-CG-CD2	-5.41	94.46	110.70
1	C	90	LYS	N-CA-C	5.41	119.83	111.56
2	D	105	LEU	N-CA-C	-5.41	105.30	111.14
1	A	115	THR	CA-C-N	-5.40	114.11	122.49
1	A	115	THR	C-N-CA	-5.40	114.11	122.49
1	A	108	THR	N-CA-C	-5.39	105.40	111.28
2	D	15	TRP	CA-C-O	5.39	125.97	119.61
1	A	138	SER	N-CA-C	5.37	119.09	112.54
2	D	23	VAL	N-CA-CB	-5.37	104.55	110.51
1	C	97	ASN	N-CA-C	5.36	117.88	111.71
1	C	84	SER	CA-CB-OG	-5.36	100.38	111.10
2	D	23	VAL	O-C-N	-5.36	116.58	121.94
1	C	100	LEU	N-CA-C	5.36	119.89	112.45
2	B	4	THR	N-CA-C	-5.35	102.56	110.48
2	D	43	ASP	O-C-N	5.35	127.58	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	57	ASN	N-CA-C	5.35	117.98	109.96
2	D	76	LYS	CA-C-N	-5.35	115.82	123.20
2	D	76	LYS	C-N-CA	-5.35	115.82	123.20
1	C	14	TRP	N-CA-C	-5.35	105.49	112.23
1	C	9	ASN	N-CA-C	-5.34	105.53	111.36
2	B	100	PRO	CB-CA-C	-5.33	103.89	112.21
2	D	78	LEU	O-C-N	-5.33	115.29	122.43
2	B	91	LEU	N-CA-CB	5.32	117.90	110.07
2	B	33	ILE	CB-CA-C	-5.31	105.06	112.02
1	A	50	PRO	CB-CA-C	5.31	120.32	111.56
1	C	128	PHE	N-CA-C	5.31	117.50	111.02
1	A	50	PRO	N-CD-CG	-5.30	95.24	103.20
1	A	111	CYS	CB-CA-C	-5.30	101.99	110.79
2	D	141	LEU	CA-C-O	5.30	125.88	119.31
2	B	56	SER	N-CA-CB	-5.29	102.87	110.65
2	D	79	ASP	N-CA-CB	5.29	118.99	110.42
2	D	52	ASP	CB-CA-C	-5.29	99.90	110.42
2	D	126	VAL	N-CA-CB	5.28	117.73	110.54
1	C	131	ALA	N-CA-C	5.28	117.04	111.28
1	A	134	THR	O-C-N	5.28	128.76	122.27
1	A	16	LYS	CG-CD-CE	-5.27	99.18	111.30
2	B	8	LYS	N-CA-CB	-5.26	102.12	110.28
2	B	91	LEU	CD1-CG-CD2	-5.26	99.22	110.80
2	B	47	ASP	N-CA-CB	5.25	118.44	109.87
1	C	7	LYS	CG-CD-CE	-5.25	99.22	111.30
2	B	84	THR	CA-C-O	-5.25	115.04	120.92
1	C	139	LYS	CA-C-O	5.25	127.31	118.91
1	A	123	ALA	CA-C-O	-5.24	115.32	120.82
2	B	118	PHE	N-CA-C	5.24	119.82	113.38
1	C	141	ARG	CB-CA-C	5.23	120.04	110.10
1	A	95	PRO	CB-CG-CD	-5.21	89.43	106.10
1	A	42	TYR	N-CA-CB	-5.21	102.78	110.49
2	B	127	GLN	CA-C-O	5.21	125.94	119.79
2	D	120	LYS	CA-CB-CG	-5.21	103.68	114.10
2	B	65	LYS	CB-CA-C	5.21	119.14	110.81
1	A	30	ASP	N-CA-CB	5.20	117.73	109.82
2	D	79	ASP	CB-CA-C	5.20	119.98	110.11
2	B	14	LEU	CB-CA-C	-5.19	102.02	110.85
2	B	123	THR	CA-CB-CG2	-5.19	101.67	110.50
1	A	5	ALA	O-C-N	5.18	127.41	122.07
2	B	106	LEU	CB-CG-CD2	-5.17	95.18	110.70
2	B	105	LEU	CA-C-O	-5.16	114.51	120.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	SER	CB-CA-C	-5.14	102.77	110.90
2	B	18	VAL	CA-C-O	-5.14	114.90	120.71
2	D	121	GLU	N-CA-C	5.14	121.75	110.80
1	C	109	LEU	CA-C-O	-5.14	114.97	120.42
1	C	4	PRO	CA-C-N	5.12	127.40	120.44
1	C	4	PRO	C-N-CA	5.12	127.40	120.44
1	C	115	THR	N-CA-CB	-5.12	102.64	110.26
2	B	76	LYS	CA-C-O	5.12	125.92	120.24
2	B	145	TYR	O-C-N	5.11	127.80	122.23
2	D	114	LEU	CA-C-O	-5.10	115.14	120.55
1	A	62	VAL	CA-C-O	-5.09	115.26	120.71
2	B	35	TYR	CE1-CZ-OH	-5.07	104.70	119.90
1	C	4	PRO	N-CA-C	5.07	122.90	112.47
1	C	109	LEU	CB-CG-CD2	-5.06	95.51	110.70
1	A	126	ASP	CB-CA-C	-5.06	102.72	110.81
1	A	128	PHE	N-CA-C	-5.06	105.84	111.36
2	B	110	LEU	CA-C-O	-5.06	115.49	120.90
2	D	11	VAL	CA-CB-CG2	-5.05	101.81	110.40
2	D	11	VAL	N-CA-C	5.05	115.67	110.36
2	D	91	LEU	O-C-N	5.05	127.48	122.03
1	C	87	HIS	N-CA-C	-5.05	105.43	112.45
2	B	33	ILE	CA-CB-CG1	-5.04	101.83	110.40
2	B	59	LYS	CB-CG-CD	-5.03	99.73	111.30
2	D	67	VAL	N-CA-CB	-5.02	103.71	110.54
1	C	26	GLY	CA-C-N	-5.02	113.17	120.29
1	C	26	GLY	C-N-CA	-5.02	113.17	120.29
1	C	2	LEU	CB-CG-CD2	5.01	125.74	110.70
2	B	99	ASP	CB-CA-C	5.01	116.63	109.26
1	A	11	LYS	CA-CB-CG	-5.01	104.08	114.10
2	D	1	VAL	CA-C-N	-5.01	111.97	121.54
2	D	1	VAL	C-N-CA	-5.01	111.97	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	51	GLY	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	1077	0	1069	87	0
1	C	1077	0	1069	39	1
2	B	1131	0	1135	61	1
2	D	1131	0	1135	54	0
3	A	43	0	30	5	0
3	B	43	0	30	6	0
3	C	43	0	30	4	0
3	D	43	0	30	5	0
All	All	4588	0	4528	251	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 28.

All (251) 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:4:PRO:CD	1:A:4:PRO:CG	1.75	1.62
2:D:66:LYS:CE	2:D:66:LYS:CD	1.78	1.60
1:C:56:LYS:CD	1:C:56:LYS:CE	1.80	1.60
2:B:76:LYS:CD	2:B:76:LYS:CG	1.77	1.58
1:A:11:LYS:CE	1:A:11:LYS:CD	1.76	1.57
2:D:66:LYS:CE	2:D:66:LYS:NZ	1.67	1.56
2:B:120:LYS:CE	2:B:120:LYS:NZ	1.67	1.56
1:A:141:ARG:CD	1:A:141:ARG:CG	1.76	1.55
2:D:17:LYS:CE	2:D:17:LYS:CD	1.77	1.54
2:D:120:LYS:CG	2:D:120:LYS:CB	1.79	1.54
2:D:120:LYS:NZ	2:D:120:LYS:CE	1.70	1.54
1:C:60:LYS:NZ	1:C:60:LYS:CE	1.71	1.53
2:B:61:LYS:CD	2:B:61:LYS:CG	1.79	1.53
2:B:59:LYS:CE	2:B:59:LYS:NZ	1.70	1.52
2:D:27:ALA:CB	2:D:27:ALA:CA	1.86	1.52
2:B:132:LYS:NZ	2:B:132:LYS:CE	1.70	1.51
1:A:16:LYS:NZ	1:A:16:LYS:CE	1.70	1.51
1:A:127:LYS:NZ	1:A:127:LYS:CE	1.69	1.49
1:A:139:LYS:CE	1:A:139:LYS:NZ	1.77	1.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:LYS:CE	2:B:66:LYS:NZ	1.78	1.46
1:A:77:PRO:CG	1:A:77:PRO:CB	1.75	1.44
1:A:50:PRO:CG	1:A:50:PRO:CD	1.80	1.43
1:A:11:LYS:CE	1:A:11:LYS:NZ	1.76	1.43
1:C:50:PRO:CB	1:C:50:PRO:CG	1.80	1.43
1:A:3:SER:OG	1:A:3:SER:CB	1.66	1.43
2:D:132:LYS:NZ	2:D:132:LYS:CE	1.81	1.41
2:D:93:CYS:CB	2:D:93:CYS:SG	2.08	1.40
2:B:65:LYS:CE	2:B:65:LYS:NZ	1.87	1.38
2:D:61:LYS:CE	2:D:61:LYS:NZ	1.96	1.27
2:D:93:CYS:SG	2:D:145:TYR:CE2	2.32	1.23
2:D:93:CYS:SG	2:D:145:TYR:CZ	2.35	1.19
1:A:1:VAL:HG12	1:C:141:ARG:O	1.46	1.15
1:A:141:ARG:O	1:C:1:VAL:HG23	1.55	1.06
1:A:58:HIS:O	1:A:61:LYS:N	1.98	0.96
1:A:1:VAL:HG13	1:A:2:LEU:H	1.28	0.96
2:B:63:HIS:O	2:B:66:LYS:N	1.99	0.95
2:D:120:LYS:HD2	2:D:120:LYS:HA	1.50	0.94
1:A:16:LYS:NZ	1:A:16:LYS:HG2	1.87	0.88
1:A:9:ASN:O	1:A:13:THR:HG23	1.74	0.87
1:A:139:LYS:NZ	1:A:139:LYS:CD	2.38	0.86
3:B:147:HEM:HMC1	3:B:147:HEM:HBC2	1.56	0.86
2:D:17:LYS:CD	2:D:17:LYS:NZ	2.38	0.85
2:D:120:LYS:CG	2:D:120:LYS:CA	2.57	0.82
2:D:132:LYS:NZ	2:D:132:LYS:CD	2.42	0.82
2:B:29:GLY:HA3	2:B:55:MET:HE1	1.64	0.80
1:A:58:HIS:HA	1:A:61:LYS:HE3	1.63	0.78
2:D:93:CYS:SG	2:D:145:TYR:CD2	2.77	0.78
1:A:89:TYR:CD1	1:A:139:LYS:HD3	2.19	0.78
2:B:143:HIS:CD2	2:B:144:LYS:HE3	2.19	0.77
2:B:58:ALA:HA	2:B:61:LYS:HE2	1.66	0.77
2:B:87:LYS:HZ3	2:B:87:LYS:HB2	1.49	0.76
1:C:1:VAL:O	1:C:2:LEU:HB2	1.86	0.75
1:A:16:LYS:HG2	1:A:16:LYS:HZ2	1.52	0.74
1:A:46:PHE:HB3	1:A:48:LEU:HD13	1.68	0.74
2:B:87:LYS:HB2	2:B:87:LYS:NZ	2.02	0.73
2:B:63:HIS:ND1	2:B:67:VAL:HG23	2.05	0.71
3:B:147:HEM:HMD1	3:B:147:HEM:HBD1	1.73	0.71
3:B:147:HEM:HBC2	3:B:147:HEM:CMC	2.20	0.70
2:B:2:HIS:O	2:B:3:LEU:HB2	1.91	0.70
3:D:147:HEM:HBC2	3:D:147:HEM:HMC1	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LYS:HA	2:D:120:LYS:CD	2.24	0.68
1:A:141:ARG:CG	1:A:141:ARG:NE	2.56	0.68
2:B:1:VAL:O	2:B:1:VAL:CG2	2.40	0.68
2:B:63:HIS:O	2:B:64:GLY:C	2.37	0.68
1:A:11:LYS:CE	1:A:11:LYS:CG	2.73	0.67
2:D:41:PHE:CD1	3:D:147:HEM:HBC1	2.29	0.67
2:B:120:LYS:HA	2:B:120:LYS:HE3	1.77	0.66
2:D:100:PRO:HG3	2:D:145:TYR:CD2	2.30	0.66
1:A:17:ILE:HD11	1:A:21:ALA:HB2	1.75	0.66
1:A:10:ILE:HD13	1:A:125:LEU:HD12	1.78	0.66
1:A:139:LYS:O	1:A:139:LYS:HG3	1.96	0.65
1:A:89:TYR:CE1	1:A:139:LYS:HE2	2.32	0.65
1:A:127:LYS:NZ	1:A:127:LYS:CD	2.58	0.64
1:C:39:THR:HG22	1:C:97:ASN:ND2	2.12	0.64
1:A:16:LYS:NZ	1:A:16:LYS:CG	2.59	0.64
1:A:58:HIS:HD2	1:A:61:LYS:HE3	1.62	0.64
2:D:17:LYS:CE	2:D:17:LYS:CG	2.76	0.63
2:B:59:LYS:NZ	2:B:59:LYS:CD	2.60	0.63
1:A:66:LEU:O	1:A:70:VAL:HG23	1.99	0.62
2:D:65:LYS:O	2:D:68:LEU:N	2.30	0.62
2:D:37:TRP:HE1	2:D:102:ASN:HD21	1.45	0.61
1:A:1:VAL:CG1	1:A:2:LEU:H	2.05	0.61
1:A:11:LYS:CE	1:A:11:LYS:HB3	2.31	0.60
2:D:93:CYS:SG	2:D:145:TYR:CE1	2.90	0.60
2:D:93:CYS:SG	2:D:93:CYS:CA	2.88	0.60
1:A:38:THR:O	1:A:41:THR:HB	2.02	0.60
1:A:11:LYS:HB3	1:A:11:LYS:HE3	1.84	0.59
1:A:3:SER:CB	1:A:3:SER:HG	2.09	0.59
1:A:6:ASP:O	1:A:10:ILE:HG12	2.04	0.58
1:A:43:PHE:CE2	3:A:142:HEM:HMD3	2.37	0.58
3:B:147:HEM:HBD1	3:B:147:HEM:CMD	2.33	0.58
1:A:113:HIS:N	1:A:114:PRO:CD	2.66	0.58
1:A:14:TRP:HA	1:A:17:ILE:HG23	1.84	0.58
1:A:58:HIS:O	1:A:59:GLY:C	2.46	0.58
1:C:8:THR:O	1:C:12:SER:HB3	2.03	0.57
2:B:127:GLN:O	2:B:131:GLN:HG2	2.04	0.57
2:D:100:PRO:HG3	2:D:145:TYR:CE2	2.38	0.57
1:C:39:THR:HG22	1:C:97:ASN:HD21	1.68	0.57
2:D:66:LYS:CE	2:D:66:LYS:CG	2.82	0.57
2:D:120:LYS:CA	2:D:120:LYS:CD	2.83	0.57
2:D:107:GLY:HA3	2:D:134:VAL:HG13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLY:CA	2:B:55:MET:HE1	2.33	0.56
1:A:43:PHE:N	1:A:44:PRO:CD	2.68	0.56
2:B:33:ILE:HD13	2:B:51:PRO:HB3	1.86	0.56
1:C:60:LYS:NZ	1:C:60:LYS:CD	2.65	0.56
1:A:3:SER:OG	1:A:3:SER:CA	2.50	0.56
1:A:58:HIS:CD2	1:A:61:LYS:HE3	2.40	0.56
1:A:13:THR:O	1:A:17:ILE:CG2	2.54	0.56
2:D:142:ALA:O	2:D:145:TYR:HB2	2.06	0.55
1:A:43:PHE:N	1:A:44:PRO:HD3	2.21	0.55
3:A:142:HEM:CMC	3:A:142:HEM:HBC2	2.36	0.54
2:B:57:ASN:OD1	2:B:57:ASN:C	2.51	0.54
2:D:3:LEU:HA	2:D:7:GLU:OE2	2.07	0.53
1:C:81:SER:O	1:C:82:ALA:C	2.48	0.53
2:B:50:THR:O	2:B:54:VAL:HG23	2.08	0.53
1:C:28:ALA:CB	1:C:105:LEU:HD13	2.38	0.53
1:C:53:ALA:HA	1:C:56:LYS:HE2	1.88	0.53
1:A:76:LEU:N	1:A:77:PRO:CD	2.71	0.53
1:A:58:HIS:HD2	1:A:61:LYS:CE	2.21	0.53
3:D:147:HEM:HBC2	3:D:147:HEM:CMC	2.39	0.53
2:D:110:LEU:C	2:D:110:LEU:HD22	2.34	0.53
1:C:45:HIS:ND1	1:C:45:HIS:N	2.53	0.52
3:B:147:HEM:CMD	3:B:147:HEM:CBD	2.87	0.52
1:A:3:SER:O	1:A:6:ASP:HB2	2.08	0.52
1:A:141:ARG:O	1:C:1:VAL:CG2	2.43	0.52
2:B:143:HIS:C	2:B:145:TYR:H	2.18	0.52
1:A:1:VAL:HG13	1:A:2:LEU:N	2.12	0.52
1:C:57:ALA:HA	1:C:60:LYS:HD2	1.91	0.52
2:B:123:THR:OG1	2:B:126:VAL:HG23	2.11	0.51
1:C:35:SER:HB3	2:D:131:GLN:HG3	1.92	0.51
2:D:64:GLY:O	2:D:65:LYS:C	2.50	0.51
1:C:56:LYS:HE2	1:C:56:LYS:HB2	1.92	0.51
1:A:1:VAL:O	1:A:2:LEU:HB2	2.09	0.51
1:A:42:TYR:C	1:A:44:PRO:HD3	2.35	0.51
1:A:89:TYR:CE1	1:A:139:LYS:CE	2.93	0.50
2:B:1:VAL:O	2:B:1:VAL:HG22	2.11	0.50
3:C:142:HEM:HMB2	3:C:142:HEM:HBB2	1.93	0.50
1:A:28:ALA:CB	1:A:105:LEU:HD13	2.42	0.50
1:A:89:TYR:CZ	1:A:139:LYS:HE2	2.46	0.50
1:A:17:ILE:HD13	1:A:18:GLY:N	2.27	0.50
1:C:66:LEU:O	1:C:69:ALA:HB3	2.12	0.49
2:D:92:HIS:HA	2:D:96:LEU:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:LEU:O	2:D:97:HIS:HB2	2.11	0.49
2:B:122:PHE:CE2	2:B:127:GLN:HB2	2.47	0.49
2:D:90:GLU:O	2:D:94:ASP:HB2	2.13	0.49
1:A:13:THR:O	1:A:17:ILE:HG23	2.13	0.49
2:D:107:GLY:HA3	2:D:134:VAL:CG1	2.43	0.49
2:D:110:LEU:HD22	2:D:110:LEU:O	2.12	0.49
2:D:28:LEU:O	2:D:29:GLY:C	2.55	0.48
1:A:17:ILE:HD13	1:A:17:ILE:C	2.38	0.48
1:A:11:LYS:CE	1:A:11:LYS:CB	2.91	0.48
1:C:135:VAL:O	1:C:138:SER:OG	2.28	0.48
1:A:13:THR:O	1:A:17:ILE:HG22	2.13	0.48
1:A:139:LYS:CD	1:A:139:LYS:HZ2	2.27	0.48
3:A:142:HEM:HMB1	3:A:142:HEM:HBB2	1.94	0.48
1:A:98:PHE:HE1	1:A:136:LEU:HD12	1.78	0.48
2:B:76:LYS:CD	2:B:76:LYS:CB	2.87	0.48
1:A:141:ARG:HB3	1:A:141:ARG:NH1	2.29	0.47
1:A:89:TYR:CZ	1:A:139:LYS:CE	2.98	0.47
2:B:25:GLY:N	2:B:64:GLY:HA3	2.30	0.47
2:B:65:LYS:HE3	2:B:65:LYS:HB3	1.56	0.47
2:B:108:ASN:HD21	2:B:131:GLN:HE22	1.62	0.47
3:D:147:HEM:HHC	3:D:147:HEM:HBB2	1.97	0.47
1:C:85:ASP:O	1:C:89:TYR:HB2	2.14	0.46
2:D:28:LEU:C	2:D:28:LEU:CD2	2.86	0.46
1:A:6:ASP:O	1:A:7:LYS:C	2.57	0.46
1:A:11:LYS:CD	1:A:11:LYS:NZ	2.77	0.46
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.72	0.46
2:B:63:HIS:O	2:B:65:LYS:N	2.48	0.46
1:A:89:TYR:CZ	1:A:139:LYS:NZ	2.83	0.46
1:A:7:LYS:O	1:A:11:LYS:HG3	2.16	0.46
2:B:63:HIS:C	2:B:65:LYS:N	2.73	0.46
1:A:103:HIS:HE1	2:B:131:GLN:OE1	1.98	0.46
2:B:88:LEU:HD23	2:B:88:LEU:HA	1.56	0.46
2:B:26:GLU:OE2	2:B:117:HIS:HE1	1.99	0.45
2:D:28:LEU:HA	2:D:28:LEU:HD23	1.51	0.45
2:D:143:HIS:C	2:D:145:TYR:H	2.23	0.45
1:C:89:TYR:CD1	1:C:139:LYS:CD	2.99	0.45
2:D:95:LYS:HA	2:D:95:LYS:HD3	1.67	0.45
1:A:16:LYS:NZ	1:A:16:LYS:CD	2.71	0.45
2:B:132:LYS:NZ	2:B:132:LYS:CD	2.75	0.45
1:C:49:SER:HA	1:C:50:PRO:HD2	1.71	0.45
1:C:99:LYS:HZ2	1:C:99:LYS:HG2	1.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:ALA:HA	2:D:61:LYS:NZ	2.31	0.45
2:D:120:LYS:NZ	2:D:120:LYS:CD	2.71	0.45
2:B:14:LEU:HD12	2:B:126:VAL:HG11	1.99	0.45
2:B:87:LYS:NZ	2:B:87:LYS:CB	2.76	0.45
3:C:142:HEM:HHC	3:C:142:HEM:HAB	1.57	0.45
2:B:110:LEU:O	2:B:110:LEU:HD22	2.16	0.44
1:C:89:TYR:CD1	1:C:139:LYS:NZ	2.82	0.44
3:A:142:HEM:CMC	3:A:142:HEM:CBC	2.95	0.44
3:A:142:HEM:CBC	3:A:142:HEM:HMC1	2.47	0.44
2:B:125:GLN:CD	2:B:125:GLN:H	2.24	0.44
2:D:27:ALA:CB	2:D:27:ALA:N	2.71	0.44
1:A:1:VAL:CG1	1:A:2:LEU:N	2.78	0.44
2:B:63:HIS:CE1	2:B:67:VAL:HG23	2.51	0.44
1:A:46:PHE:CB	1:A:48:LEU:HD13	2.43	0.44
2:D:78:LEU:HD23	2:D:78:LEU:HA	1.79	0.44
2:B:19:ASN:OD1	2:B:19:ASN:C	2.60	0.44
2:B:66:LYS:HE3	2:B:66:LYS:HB3	1.39	0.43
2:B:63:HIS:ND1	2:B:67:VAL:CG2	2.80	0.43
1:C:7:LYS:HB3	1:C:73:LEU:HD13	1.99	0.43
2:D:127:GLN:O	2:D:131:GLN:HG2	2.18	0.43
2:B:26:GLU:O	2:B:30:ARG:HB2	2.18	0.43
2:B:143:HIS:CD2	2:B:144:LYS:CE	2.97	0.43
2:B:2:HIS:HB2	2:B:3:LEU:H	1.69	0.43
2:B:82:LYS:N	2:B:82:LYS:HD2	2.34	0.43
1:A:103:HIS:O	1:A:107:VAL:HG23	2.19	0.43
1:C:97:ASN:HB3	3:C:142:HEM:HMC1	2.01	0.42
1:C:118:THR:OG1	1:C:121:VAL:HG23	2.19	0.42
1:A:6:ASP:O	1:A:9:ASN:N	2.53	0.42
1:A:58:HIS:HA	1:A:61:LYS:CE	2.42	0.42
1:A:76:LEU:N	1:A:77:PRO:HD3	2.34	0.42
2:B:32:LEU:H	2:B:32:LEU:HG	1.73	0.42
1:A:27:GLU:CD	1:A:108:THR:HG23	2.44	0.42
1:A:141:ARG:C	1:C:1:VAL:H3	2.28	0.42
1:A:88:ALA:CB	1:A:139:LYS:HB3	2.49	0.42
3:B:147:HEM:HMC1	3:B:147:HEM:CBC	2.40	0.42
1:C:87:HIS:HE1	3:C:142:HEM:NA	2.08	0.42
2:D:19:ASN:ND2	2:D:22:GLU:HB2	2.35	0.42
1:C:24:TYR:OH	1:C:113:HIS:HE1	2.01	0.42
2:D:100:PRO:O	2:D:102:ASN:N	2.53	0.42
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.85	0.42
2:B:57:ASN:OD1	2:B:60:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:HIS:CE1	2:B:67:VAL:CG2	3.03	0.42
2:B:96:LEU:HA	2:B:96:LEU:HD23	1.86	0.42
1:C:56:LYS:HE2	1:C:56:LYS:CB	2.49	0.42
1:A:1:VAL:O	1:A:2:LEU:CB	2.68	0.42
1:C:39:THR:C	1:C:41:THR:H	2.26	0.41
1:C:89:TYR:CD1	1:C:139:LYS:HD3	2.55	0.41
2:D:28:LEU:C	2:D:28:LEU:HD22	2.45	0.41
2:B:33:ILE:HD13	2:B:33:ILE:HG21	1.72	0.41
2:D:1:VAL:HG23	2:D:3:LEU:CD1	2.50	0.41
2:D:120:LYS:HD2	2:D:120:LYS:CA	2.31	0.41
1:A:3:SER:OG	1:A:3:SER:C	2.63	0.41
1:A:91:LEU:HB2	1:A:93:VAL:HG23	2.02	0.41
1:C:88:ALA:CB	1:C:139:LYS:HB3	2.51	0.41
1:C:106:LEU:HD21	1:C:125:LEU:HB3	2.03	0.41
2:B:24:GLY:HA3	2:B:64:GLY:C	2.46	0.41
2:B:68:LEU:HD22	2:B:68:LEU:HA	1.90	0.41
2:B:79:ASP:HB3	2:B:80:ASN:H	1.48	0.41
2:B:129:ALA:O	2:B:132:LYS:HB2	2.21	0.41
1:C:58:HIS:O	1:C:62:VAL:HG23	2.21	0.41
2:D:123:THR:OG1	2:D:126:VAL:HG23	2.21	0.41
1:A:141:ARG:NH1	1:A:141:ARG:CB	2.84	0.41
1:C:56:LYS:CE	1:C:56:LYS:CB	2.98	0.41
2:B:43:ASP:C	2:B:45:PHE:H	2.29	0.40
3:D:147:HEM:HMC1	3:D:147:HEM:CBC	2.48	0.40
1:A:77:PRO:O	1:A:81:SER:HB3	2.22	0.40
1:C:128:PHE:O	1:C:129:PHE:C	2.57	0.40
2:B:81:LEU:N	2:B:82:LYS:HD2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ASP:OD1	1:C:75:ASP:OD1[2_645]	2.00	0.20

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	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	2	22
1	C	139/141 (99%)	124 (89%)	12 (9%)	3 (2%)	5	30
2	B	144/146 (99%)	121 (84%)	13 (9%)	10 (7%)	1	10
2	D	144/146 (99%)	121 (84%)	18 (12%)	5 (4%)	3	23
All	All	566/574 (99%)	483 (85%)	60 (11%)	23 (4%)	2	19

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	78	LEU
2	B	144	LYS
1	C	50	PRO
1	A	2	LEU
1	A	18	GLY
1	A	59	GLY
1	A	136	LEU
2	B	3	LEU
2	B	5	ALA
2	B	25	GLY
2	B	82	LYS
2	B	125	GLN
1	C	18	GLY
2	D	44	SER
2	D	101	GLU
2	D	144	LYS
1	A	21	ALA
2	B	79	ASP
2	B	44	SER
2	D	3	LEU
2	D	139	ASN
2	B	143	HIS
1	C	2	LEU

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	116/116 (100%)	95 (82%)	21 (18%)	2	10
1	C	116/116 (100%)	99 (85%)	17 (15%)	3	17
2	B	121/121 (100%)	92 (76%)	29 (24%)	1	4
2	D	121/121 (100%)	101 (84%)	20 (16%)	2	13
All	All	474/474 (100%)	387 (82%)	87 (18%)	1	9

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	11	LYS
1	A	16	LYS
1	A	17	ILE
1	A	38	THR
1	A	41	THR
1	A	48	LEU
1	A	49	SER
1	A	50	PRO
1	A	62	VAL
1	A	84	SER
1	A	86	LEU
1	A	89	TYR
1	A	95	PRO
1	A	105	LEU
1	A	109	LEU
1	A	115	THR
1	A	116	GLU
1	A	125	LEU
1	A	127	LYS
1	A	139	LYS
2	B	2	HIS
2	B	6	GLU
2	B	8	LYS
2	B	9	SER
2	B	20	VAL
2	B	22	GLU
2	B	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	32	LEU
2	B	44	SER
2	B	48	LEU
2	B	57	ASN
2	B	61	LYS
2	B	65	LYS
2	B	66	LYS
2	B	68	LEU
2	B	72	SER
2	B	76	LYS
2	B	79	ASP
2	B	81	LEU
2	B	82	LYS
2	B	87	LYS
2	B	91	LEU
2	B	109	VAL
2	B	110	LEU
2	B	113	VAL
2	B	117	HIS
2	B	120	LYS
2	B	127	GLN
2	B	144	LYS
1	C	1	VAL
1	C	2	LEU
1	C	17	ILE
1	C	35	SER
1	C	38	THR
1	C	41	THR
1	C	45	HIS
1	C	50	PRO
1	C	56	LYS
1	C	68	THR
1	C	81	SER
1	C	86	LEU
1	C	89	TYR
1	C	92	ARG
1	C	116	GLU
1	C	125	LEU
1	C	141	ARG
2	D	9	SER
2	D	10	LEU
2	D	14	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	20	VAL
2	D	28	LEU
2	D	42	PHE
2	D	50	THR
2	D	59	LYS
2	D	61	LYS
2	D	65	LYS
2	D	66	LYS
2	D	68	LEU
2	D	70	SER
2	D	75	LEU
2	D	81	LEU
2	D	96	LEU
2	D	109	VAL
2	D	110	LEU
2	D	120	LYS
2	D	141	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	58	HIS
1	A	103	HIS
2	B	2	HIS
2	B	69	ASN
2	B	102	ASN
2	B	108	ASN
2	B	117	HIS
2	B	143	HIS
1	C	9	ASN
1	C	34	GLN
1	C	97	ASN
1	C	103	HIS
1	C	112	HIS
1	C	113	HIS
2	D	102	ASN
2	D	108	ASN
2	D	131	GLN
2	D	146	HIS

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	$\# Z > 2$
3	HEM	B	147	2	50,50,50	2.29	21 (42%)	67,82,82	3.00	22 (32%)
3	HEM	A	142	1	50,50,50	2.77	21 (42%)	67,82,82	2.97	35 (52%)
3	HEM	D	147	2	50,50,50	2.05	16 (32%)	67,82,82	2.44	30 (44%)
3	HEM	C	142	1	50,50,50	2.16	23 (46%)	67,82,82	4.12	43 (64%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	147	2	-	4/14/54/54	-
3	HEM	A	142	1	-	5/14/54/54	-
3	HEM	D	147	2	-	7/14/54/54	-
3	HEM	C	142	1	-	7/14/54/54	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	O1A-CGA	7.04	1.45	1.22
3	D	147	HEM	C3C-C2C	-6.50	1.24	1.37
3	A	142	HEM	CHC-C1C	-6.27	1.26	1.38
3	B	147	HEM	C4D-C3D	-5.37	1.35	1.45
3	B	147	HEM	O1D-CGD	4.97	1.38	1.22
3	A	142	HEM	CBA-CGA	4.90	1.61	1.50
3	A	142	HEM	C1A-C2A	-4.85	1.34	1.44
3	A	142	HEM	C1C-C2C	-4.80	1.35	1.45
3	A	142	HEM	C3C-C2C	-4.73	1.27	1.37
3	B	147	HEM	CBD-CGD	4.61	1.61	1.50
3	C	142	HEM	CBD-CAD	4.34	1.67	1.51
3	A	142	HEM	CBD-CAD	4.30	1.66	1.51
3	A	142	HEM	C1C-NC	-4.17	1.31	1.39
3	A	142	HEM	C3D-C2D	4.09	1.45	1.36
3	D	147	HEM	C3D-C2D	4.07	1.45	1.36
3	D	147	HEM	C3B-C2B	-3.98	1.29	1.37
3	B	147	HEM	CMB-C2B	3.93	1.58	1.50
3	A	142	HEM	C4C-NC	-3.91	1.32	1.39
3	A	142	HEM	C2A-C3A	-3.83	1.28	1.38
3	A	142	HEM	C3C-C4C	-3.76	1.39	1.46
3	B	147	HEM	FE-NB	3.73	2.06	1.94
3	C	142	HEM	C3D-C2D	3.57	1.44	1.36
3	B	147	HEM	C4A-C3A	3.55	1.51	1.43
3	C	142	HEM	C2A-C3A	-3.44	1.29	1.38
3	C	142	HEM	C4C-NC	-3.41	1.33	1.39
3	D	147	HEM	C2A-C3A	-3.37	1.30	1.38
3	C	142	HEM	CBC-CAC	3.33	1.46	1.30
3	A	142	HEM	CAA-C2A	-3.32	1.42	1.51
3	C	142	HEM	FE-NC	-3.31	1.84	1.95
3	D	147	HEM	C4D-C3D	3.31	1.50	1.45
3	A	142	HEM	CBD-CGD	3.28	1.58	1.50
3	C	142	HEM	CMC-C2C	3.26	1.57	1.50
3	C	142	HEM	CAC-C3C	3.26	1.56	1.47
3	D	147	HEM	CMB-C2B	-3.20	1.44	1.50
3	A	142	HEM	O2A-CGA	3.18	1.41	1.30
3	C	142	HEM	O1A-CGA	3.15	1.32	1.22
3	B	147	HEM	C3D-C2D	3.10	1.43	1.36
3	B	147	HEM	C3C-C2C	-3.10	1.30	1.37
3	C	142	HEM	C4B-NB	3.07	1.44	1.38
3	C	142	HEM	CHD-C1D	-3.06	1.32	1.39
3	C	142	HEM	CMB-C2B	-2.97	1.44	1.50
3	B	147	HEM	C4B-NB	-2.96	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	CBD-CAD	2.95	1.62	1.51
3	A	142	HEM	CHB-C4A	-2.95	1.32	1.39
3	A	142	HEM	C4D-C3D	-2.93	1.40	1.45
3	C	142	HEM	C1A-C2A	-2.90	1.38	1.44
3	B	147	HEM	C1C-NC	2.89	1.45	1.39
3	B	147	HEM	CHA-C4D	-2.88	1.32	1.38
3	D	147	HEM	O1A-CGA	2.88	1.31	1.22
3	B	147	HEM	C4A-NA	2.85	1.45	1.39
3	D	147	HEM	CHD-C4C	2.79	1.43	1.38
3	C	142	HEM	CBD-CGD	2.75	1.56	1.50
3	D	147	HEM	CAD-C3D	2.72	1.58	1.51
3	C	142	HEM	C1D-C2D	2.68	1.50	1.44
3	D	147	HEM	FE-NC	-2.67	1.86	1.95
3	C	142	HEM	CHC-C1C	-2.66	1.33	1.38
3	D	147	HEM	CAC-C3C	-2.65	1.40	1.47
3	C	142	HEM	C1B-C2B	-2.60	1.39	1.44
3	C	142	HEM	CHB-C1B	-2.60	1.33	1.38
3	B	147	HEM	CAC-C3C	-2.59	1.40	1.47
3	D	147	HEM	CMA-C3A	2.59	1.56	1.50
3	B	147	HEM	FE-NA	-2.54	1.86	1.95
3	B	147	HEM	CHC-C4B	-2.53	1.33	1.39
3	B	147	HEM	CBA-CGA	2.42	1.56	1.50
3	A	142	HEM	C4D-ND	-2.39	1.36	1.40
3	B	147	HEM	C1D-C2D	-2.35	1.39	1.44
3	C	142	HEM	O1D-CGD	2.33	1.29	1.22
3	C	142	HEM	CHD-C4C	-2.31	1.33	1.38
3	D	147	HEM	C1B-NB	2.31	1.44	1.40
3	B	147	HEM	CAA-C2A	2.23	1.57	1.51
3	D	147	HEM	CBA-CGA	2.23	1.55	1.50
3	C	142	HEM	C3B-C4B	-2.21	1.40	1.44
3	C	142	HEM	C3C-C4C	-2.20	1.42	1.46
3	D	147	HEM	C1B-C2B	-2.19	1.40	1.44
3	B	147	HEM	CMA-C3A	2.16	1.55	1.50
3	D	147	HEM	C1D-C2D	2.14	1.48	1.44
3	A	142	HEM	CHA-C1A	-2.13	1.34	1.39
3	B	147	HEM	CHD-C1D	-2.12	1.34	1.39
3	C	142	HEM	O2A-CGA	-2.08	1.23	1.30
3	A	142	HEM	C1A-NA	-2.03	1.35	1.39
3	A	142	HEM	FE-NB	-2.03	1.88	1.94

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	CHC-C4B-NB	12.02	137.36	124.42
3	B	147	HEM	C3B-C2B-C1B	-11.93	97.45	106.41
3	C	142	HEM	C3B-C4B-NB	-11.47	101.23	109.47
3	B	147	HEM	C4C-C3C-C2C	11.38	116.68	106.81
3	C	142	HEM	CMD-C2D-C1D	8.94	139.01	125.03
3	C	142	HEM	CHD-C4C-NC	7.94	133.10	124.45
3	C	142	HEM	C4A-C3A-C2A	7.88	115.85	106.82
3	C	142	HEM	C4B-C3B-C2B	7.40	114.08	107.28
3	A	142	HEM	CHD-C4C-NC	7.08	132.17	124.45
3	C	142	HEM	C3C-C2C-C1C	-7.08	100.35	107.05
3	A	142	HEM	CHB-C1B-NB	6.90	132.90	124.37
3	C	142	HEM	CHD-C4C-C3C	-6.76	113.80	125.21
3	C	142	HEM	O1D-CGD-CBD	-6.27	103.20	123.09
3	B	147	HEM	C2B-C1B-NB	6.26	117.04	109.84
3	C	142	HEM	C1C-CHC-C4B	-6.23	112.77	126.02
3	A	142	HEM	CHC-C4B-NB	6.17	131.06	124.42
3	A	142	HEM	C3C-C2C-C1C	-6.13	101.24	107.05
3	C	142	HEM	CBA-CAA-C2A	5.99	129.11	112.53
3	B	147	HEM	C4B-C3B-C2B	5.91	112.71	107.28
3	C	142	HEM	CHD-C1D-ND	-5.85	118.12	124.42
3	C	142	HEM	C1D-C2D-C3D	-5.54	101.16	106.98
3	A	142	HEM	C4C-C3C-C2C	5.36	111.46	106.81
3	A	142	HEM	C4A-CHB-C1B	-5.30	113.79	126.25
3	A	142	HEM	CMC-C2C-C1C	5.30	134.06	124.73
3	B	147	HEM	CAC-C3C-C4C	-5.28	112.20	124.82
3	B	147	HEM	CHA-C4D-C3D	-5.01	115.99	125.23
3	D	147	HEM	C3D-C4D-ND	4.92	115.56	110.17
3	D	147	HEM	CHD-C1D-ND	-4.89	119.16	124.42
3	D	147	HEM	CBD-CAD-C3D	-4.89	99.02	112.53
3	D	147	HEM	CAA-C2A-C1A	4.80	134.31	124.94
3	A	142	HEM	O2D-CGD-CBD	4.67	128.76	114.00
3	B	147	HEM	CHA-C4D-ND	4.66	130.14	124.37
3	D	147	HEM	C4C-C3C-C2C	4.50	110.72	106.81
3	C	142	HEM	C2D-C1D-ND	4.41	115.00	109.90
3	D	147	HEM	CHC-C1C-NC	-4.38	119.68	124.45
3	C	142	HEM	CMC-C2C-C1C	4.38	132.44	124.73
3	B	147	HEM	C3C-C2C-C1C	-4.36	102.92	107.05
3	D	147	HEM	C4C-NC-C1C	-4.34	98.75	105.82
3	A	142	HEM	CMD-C2D-C1D	4.33	131.80	125.03
3	A	142	HEM	C1C-CHC-C4B	-4.30	116.88	126.02
3	A	142	HEM	CAA-CBA-CGA	-4.28	102.31	113.67
3	C	142	HEM	C3A-C4A-NA	-4.20	103.42	110.14
3	C	142	HEM	C1B-NB-C4B	4.12	110.08	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	142	HEM	CHC-C1C-NC	-4.11	119.98	124.45
3	D	147	HEM	C2D-C1D-ND	4.05	114.59	109.90
3	A	142	HEM	C1A-C2A-C3A	3.97	113.02	106.87
3	C	142	HEM	C4C-C3C-C2C	3.96	110.25	106.81
3	A	142	HEM	C2C-C1C-NC	3.92	116.89	109.64
3	C	142	HEM	C4A-CHB-C1B	-3.91	117.04	126.25
3	D	147	HEM	CAA-C2A-C3A	-3.90	118.32	127.07
3	D	147	HEM	CAC-C3C-C4C	-3.89	115.54	124.82
3	D	147	HEM	CHA-C4D-ND	-3.76	119.72	124.37
3	A	142	HEM	CHD-C1D-ND	-3.76	120.38	124.42
3	A	142	HEM	CBD-CAD-C3D	-3.76	102.15	112.53
3	D	147	HEM	C4B-C3B-C2B	3.75	110.73	107.28
3	C	142	HEM	CHB-C4A-NA	3.75	130.65	123.86
3	D	147	HEM	CMD-C2D-C1D	3.74	130.87	125.03
3	A	142	HEM	O2D-CGD-O1D	-3.68	113.86	123.33
3	C	142	HEM	CAC-C3C-C4C	-3.65	116.11	124.82
3	B	147	HEM	C1B-NB-C4B	-3.60	100.94	105.21
3	C	142	HEM	CAB-C3B-C4B	-3.60	108.48	124.39
3	A	142	HEM	CHD-C4C-C3C	-3.50	119.30	125.21
3	C	142	HEM	O2D-CGD-O1D	3.47	132.25	123.33
3	B	147	HEM	CMD-C2D-C1D	3.45	130.43	125.03
3	C	142	HEM	CAA-C2A-C1A	3.45	131.68	124.94
3	A	142	HEM	C1D-C2D-C3D	-3.44	103.37	106.98
3	B	147	HEM	CBD-CAD-C3D	-3.43	103.05	112.53
3	A	142	HEM	CHB-C4A-NA	3.42	130.06	123.86
3	C	142	HEM	CHA-C1A-NA	3.41	130.04	123.86
3	B	147	HEM	C3D-C4D-ND	3.37	113.87	110.17
3	C	142	HEM	O2D-CGD-CBD	3.34	124.54	114.00
3	D	147	HEM	CHB-C4A-NA	3.23	129.72	123.86
3	B	147	HEM	C3B-C4B-NB	3.23	111.79	109.47
3	C	142	HEM	C2B-C1B-NB	-3.20	106.17	109.84
3	A	142	HEM	CMB-C2B-C1B	-3.19	120.05	125.03
3	D	147	HEM	O1D-CGD-CBD	-3.13	113.17	123.09
3	B	147	HEM	C2A-C1A-NA	3.10	113.59	110.15
3	B	147	HEM	CMB-C2B-C3B	3.08	135.88	128.43
3	A	142	HEM	C2A-C1A-NA	-3.06	106.76	110.15
3	C	142	HEM	CMA-C3A-C2A	-2.96	119.35	125.62
3	D	147	HEM	C4A-CHB-C1B	-2.93	119.36	126.25
3	D	147	HEM	CAD-C3D-C4D	2.93	129.80	124.70
3	C	142	HEM	C2C-C1C-NC	2.88	114.96	109.64
3	D	147	HEM	C4D-ND-C1D	-2.87	101.81	105.21
3	D	147	HEM	CBA-CAA-C2A	2.86	120.45	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	147	HEM	C4D-C3D-C2D	-2.80	102.81	106.89
3	A	142	HEM	CHB-C1B-C2B	-2.79	119.02	126.95
3	A	142	HEM	CAC-C3C-C4C	-2.77	118.20	124.82
3	C	142	HEM	CHA-C1A-C2A	-2.76	119.26	125.30
3	C	142	HEM	CAB-C3B-C2B	2.74	137.33	128.43
3	C	142	HEM	C1A-CHA-C4D	-2.71	119.89	126.25
3	C	142	HEM	CAD-C3D-C2D	-2.70	122.81	127.87
3	C	142	HEM	CAA-CBA-CGA	-2.66	106.60	113.67
3	A	142	HEM	CHD-C1D-C2D	2.64	129.20	125.03
3	B	147	HEM	C4C-CHD-C1D	-2.62	120.44	126.02
3	D	147	HEM	C1B-NB-C4B	-2.55	102.19	105.21
3	A	142	HEM	C1A-CHA-C4D	-2.52	120.31	126.25
3	A	142	HEM	C3B-C2B-C1B	2.52	108.30	106.41
3	D	147	HEM	C1C-CHC-C4B	-2.51	120.68	126.02
3	D	147	HEM	O2A-CGA-O1A	2.51	129.79	123.33
3	A	142	HEM	C4B-C3B-C2B	2.50	109.58	107.28
3	C	142	HEM	C4C-NC-C1C	-2.47	101.80	105.82
3	C	142	HEM	C3B-C2B-C1B	2.46	108.26	106.41
3	C	142	HEM	C1A-C2A-C3A	-2.46	103.07	106.87
3	D	147	HEM	C4A-NA-C1A	-2.44	101.85	105.82
3	D	147	HEM	CHB-C4A-C3A	-2.40	120.46	127.43
3	A	142	HEM	C4C-NC-C1C	-2.38	101.94	105.82
3	C	142	HEM	CMD-C2D-C3D	-2.33	119.83	126.15
3	D	147	HEM	C2A-C1A-NA	2.32	112.73	110.15
3	B	147	HEM	CHB-C1B-C2B	-2.32	120.35	126.95
3	B	147	HEM	CBA-CAA-C2A	2.29	118.86	112.53
3	A	142	HEM	C3B-C4B-NB	-2.28	107.83	109.47
3	A	142	HEM	CBC-CAC-C3C	-2.27	116.17	127.53
3	B	147	HEM	CHD-C4C-NC	2.22	126.87	124.45
3	A	142	HEM	CAD-C3D-C4D	-2.21	120.85	124.70
3	C	142	HEM	CAD-C3D-C4D	2.20	128.53	124.70
3	C	142	HEM	C3D-C4D-ND	2.18	112.56	110.17
3	D	147	HEM	O1A-CGA-CBA	-2.18	116.19	123.09
3	C	142	HEM	O2A-CGA-CBA	-2.15	107.22	114.00
3	C	142	HEM	CMB-C2B-C1B	-2.13	121.70	125.03
3	D	147	HEM	O2D-CGD-CBD	2.13	120.72	114.00
3	B	147	HEM	CAD-C3D-C2D	2.11	131.82	127.87
3	D	147	HEM	CAB-C3B-C2B	-2.10	121.60	128.43
3	B	147	HEM	CHD-C4C-C3C	2.08	128.72	125.21
3	A	142	HEM	C4D-ND-C1D	2.08	107.67	105.21
3	C	142	HEM	CHC-C1C-NC	-2.08	122.19	124.45
3	B	147	HEM	CAB-C3B-C4B	-2.07	115.24	124.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	147	HEM	CHB-C1B-NB	2.07	126.93	124.37
3	A	142	HEM	CHC-C4B-C3B	-2.05	120.98	125.07
3	A	142	HEM	CHA-C1A-NA	2.01	127.51	123.86

There are no chirality outliers.

All (23) torsion outliers are listed below:

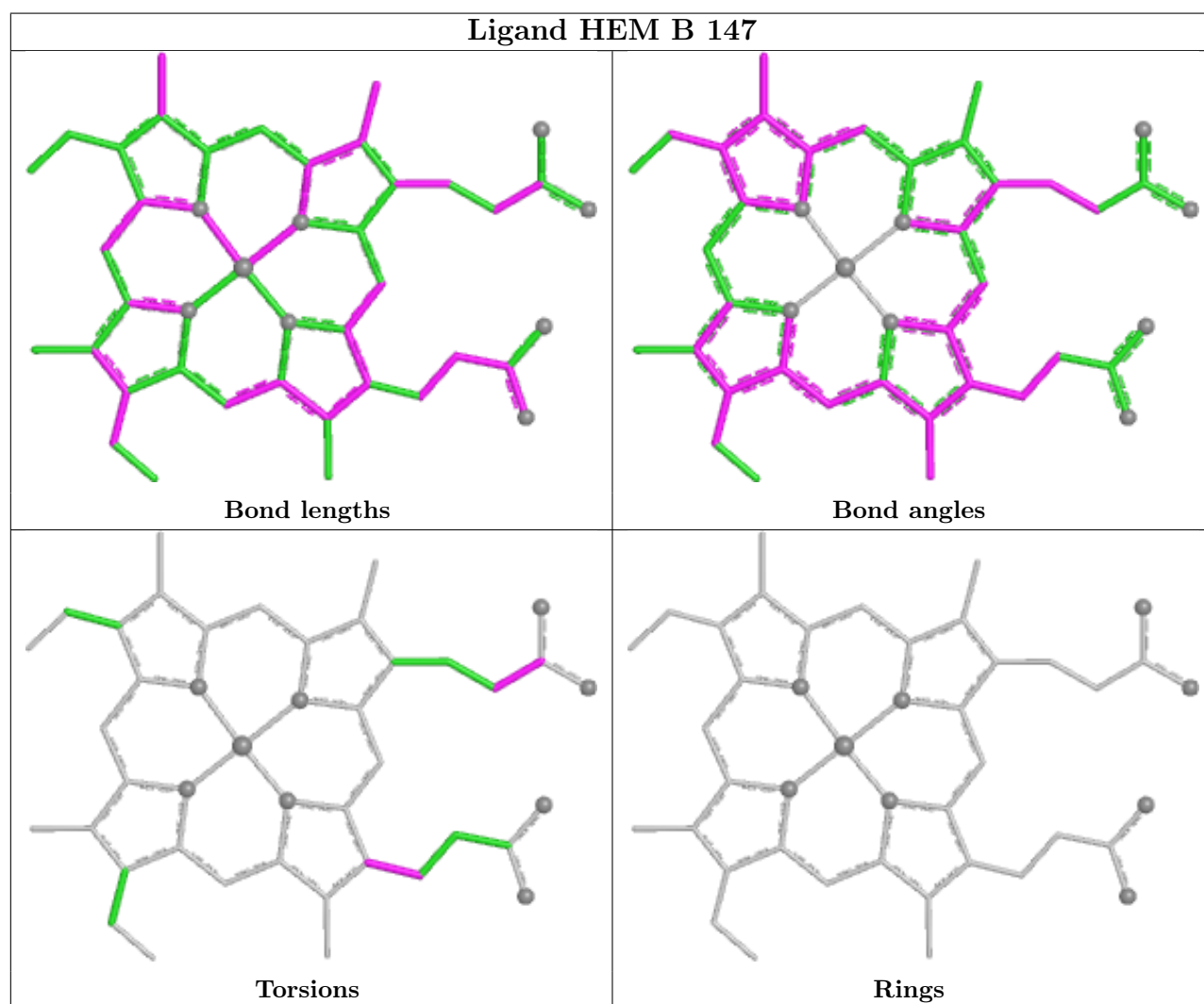
Mol	Chain	Res	Type	Atoms
3	B	147	HEM	C2D-C3D-CAD-CBD
3	B	147	HEM	C4D-C3D-CAD-CBD
3	D	147	HEM	C2A-CAA-CBA-CGA
3	C	142	HEM	C3A-C2A-CAA-CBA
3	C	142	HEM	C1A-C2A-CAA-CBA
3	A	142	HEM	C2D-C3D-CAD-CBD
3	D	147	HEM	C3A-C2A-CAA-CBA
3	C	142	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	C3D-CAD-CBD-CGD
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAA-CBA-CGA-O1A
3	C	142	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAA-CBA-CGA-O2A
3	D	147	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	C1A-C2A-CAA-CBA

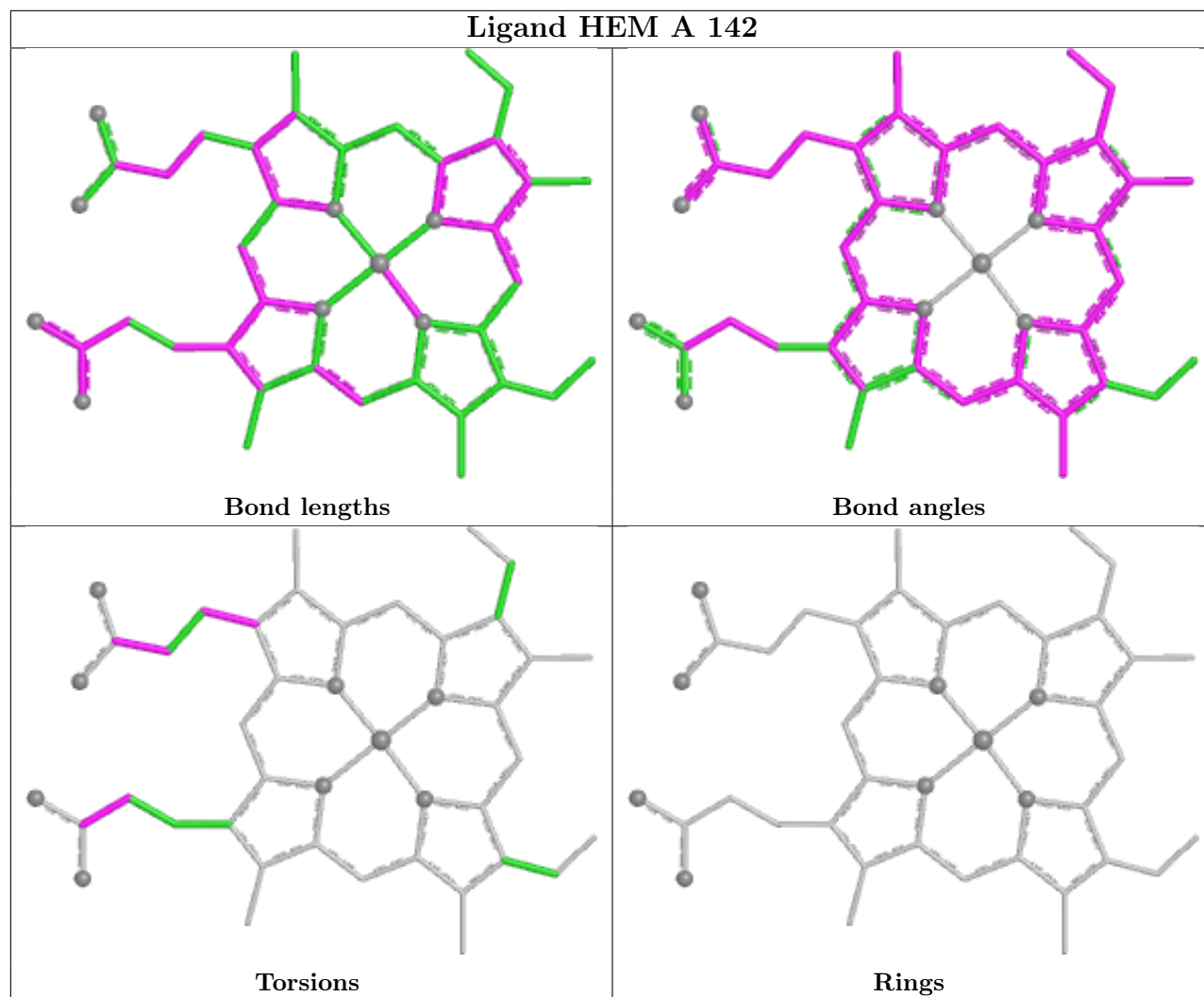
There are no ring outliers.

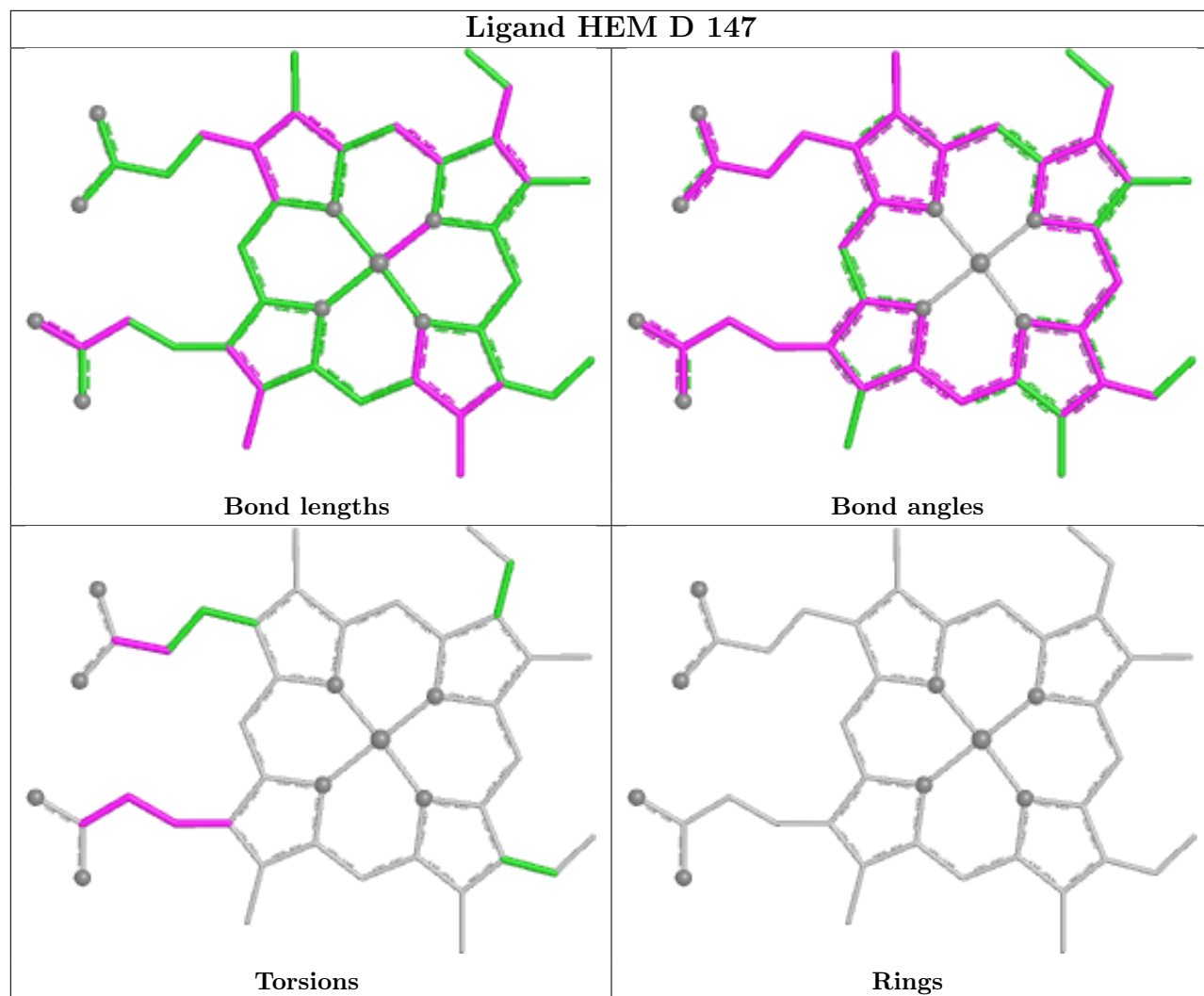
4 monomers are involved in 20 short contacts:

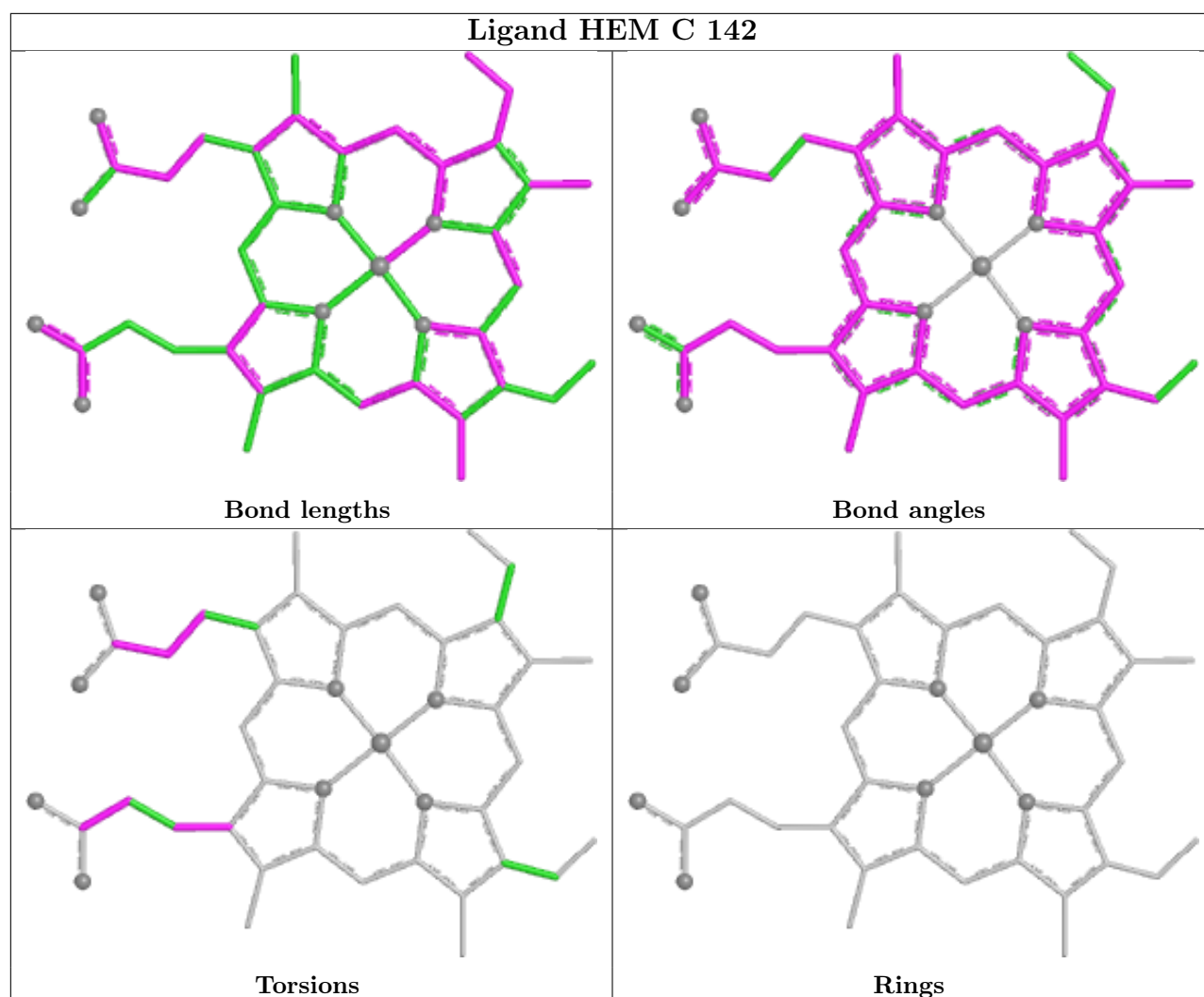
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	HEM	6	0
3	A	142	HEM	5	0
3	D	147	HEM	5	0
3	C	142	HEM	4	0

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	141/141 (100%)	-0.46	0 100 100	2, 19, 42, 56	0
1	C	141/141 (100%)	-0.49	0 100 100	3, 16, 40, 59	0
2	B	146/146 (100%)	-0.32	0 100 100	2, 30, 53, 62	0
2	D	146/146 (100%)	-0.50	0 100 100	2, 21, 47, 71	0
All	All	574/574 (100%)	-0.44	0 100 100	2, 21, 49, 71	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](#)

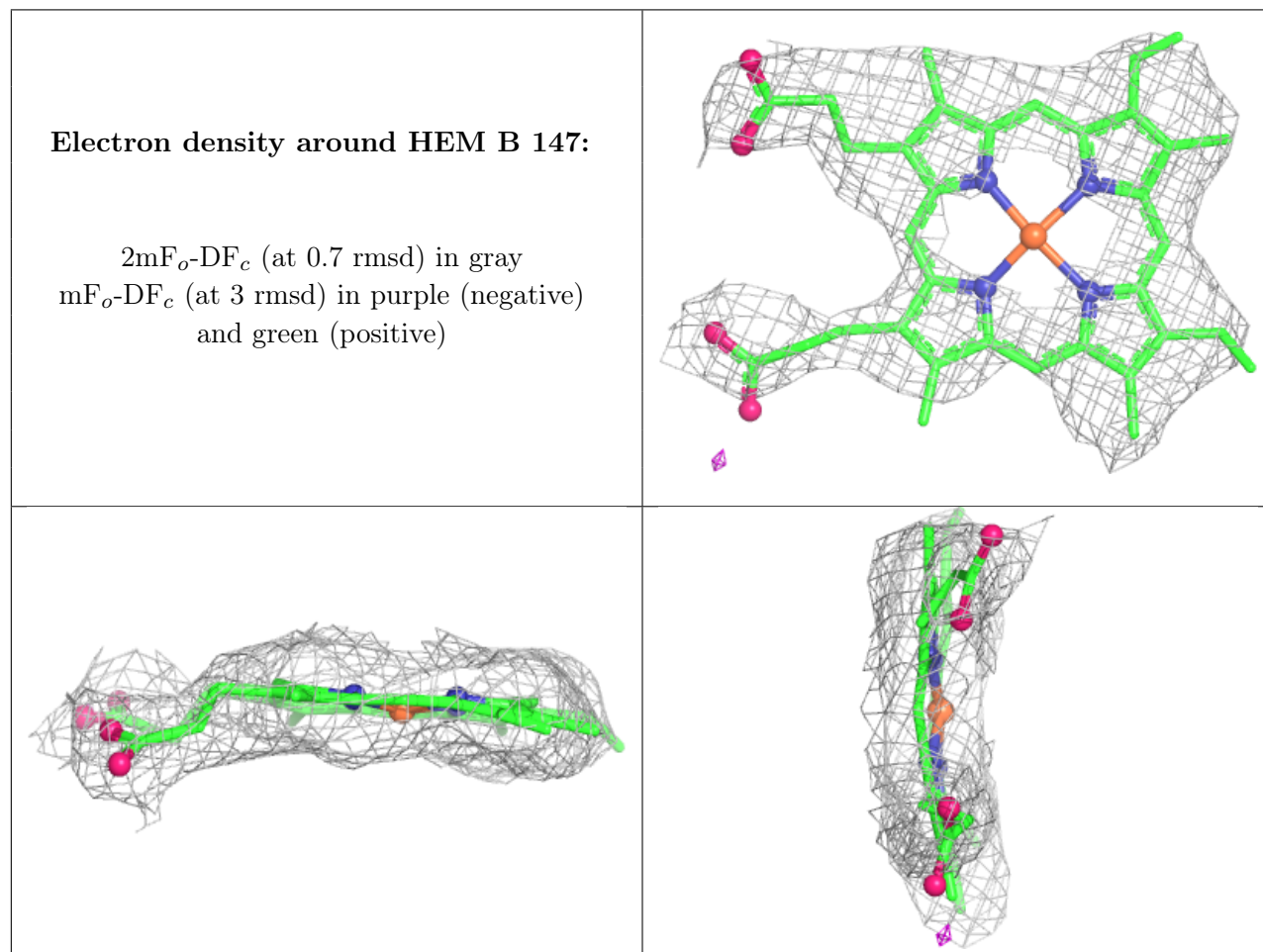
There are no oligosaccharides in this entry.

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.

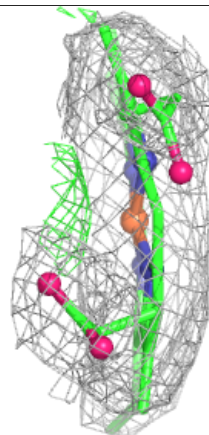
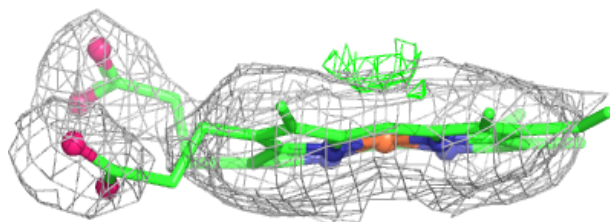
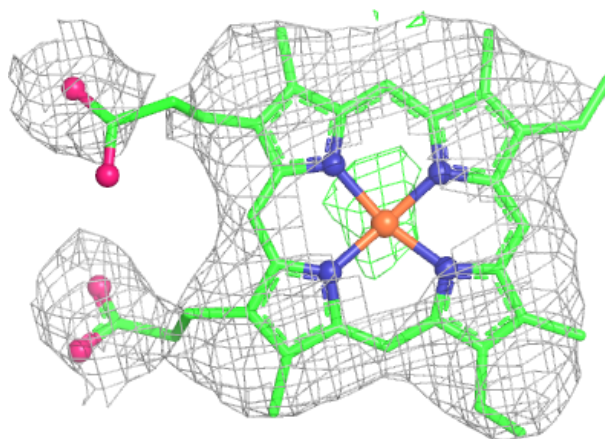
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HEM	B	147	43/43	0.94	0.10	3,21,51,68	0
3	HEM	A	142	43/43	0.97	0.08	2,10,34,57	0
3	HEM	C	142	43/43	0.97	0.07	2,14,30,31	0
3	HEM	D	147	43/43	0.98	0.07	5,20,46,53	0

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.



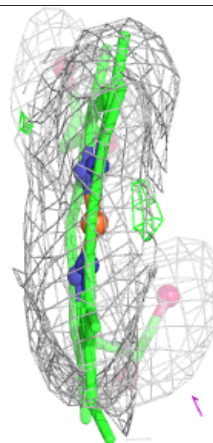
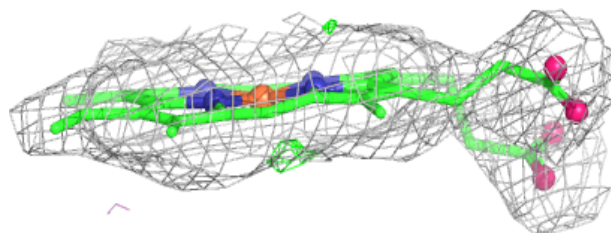
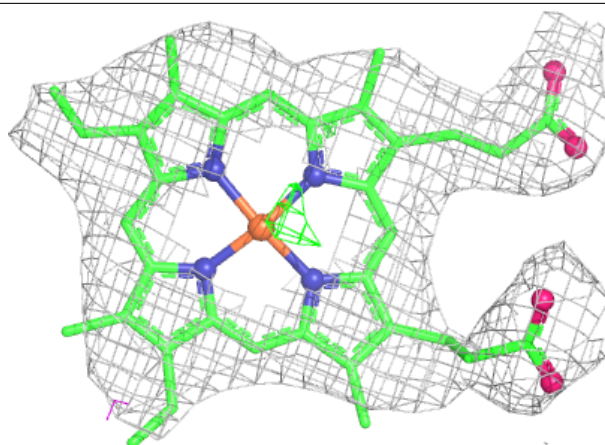
Electron density around HEM A 142:

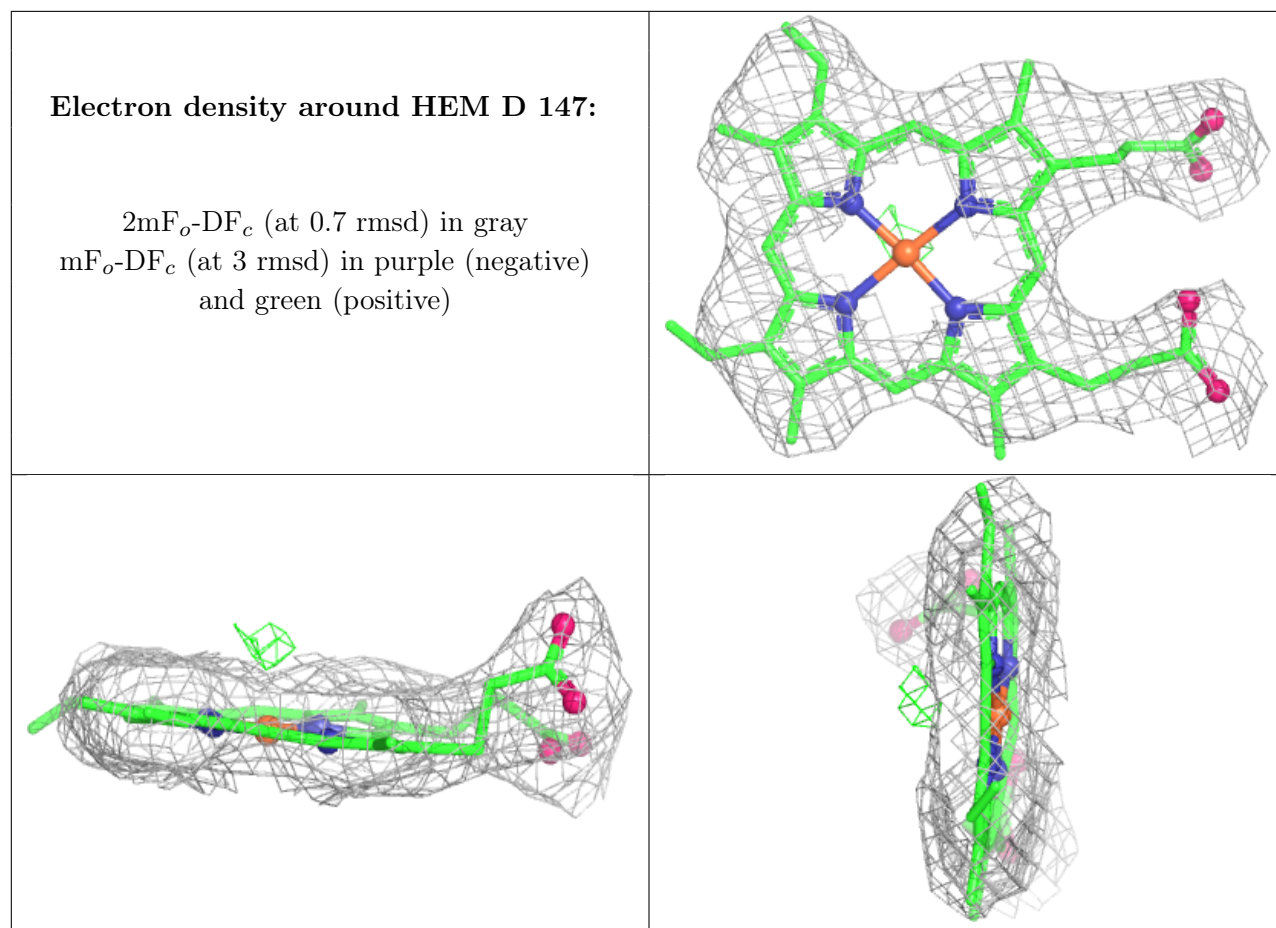
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 142:

$2mF_o-DF_c$ (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.