



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:52 PM UTC

PDB ID : 1THB / pdb_00001thb
Title : REFINEMENT OF A PARTIALLY OXYGENATED T STATE
HAEMOGLOBIN AT 1.5 ANGSTROMS RESOLUTION
Authors : Waller, D.A.; Liddington, R.C.
Deposited on : 1990-01-23
Resolution : 1.50 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

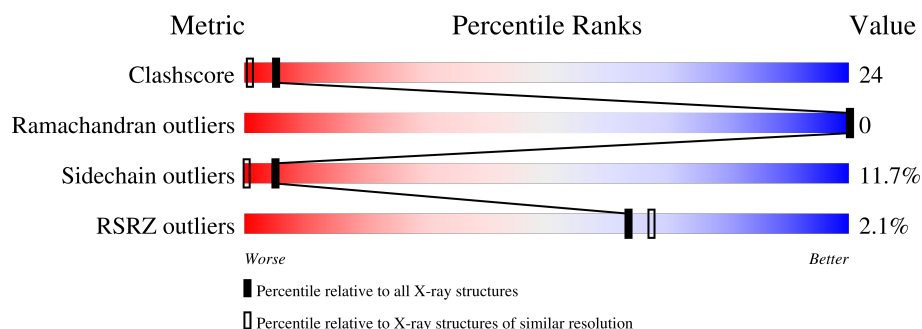
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	% 42% 41% 16% .
1	C	141	3% 24% 45% 26% 6%
2	B	146	% 27% 53% 16% .
2	D	146	3% 21% 40% 32% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4910 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.

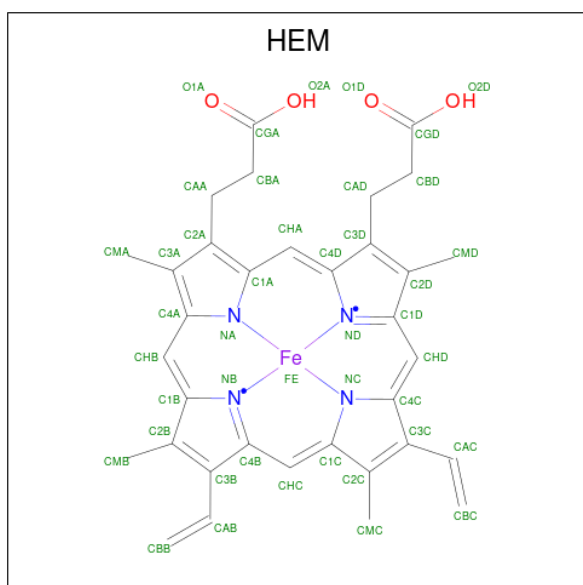
- Molecule 1 is a protein called HEMOGLOBIN A (OXY) (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN A (DEOXY) (BETA CHAIN).

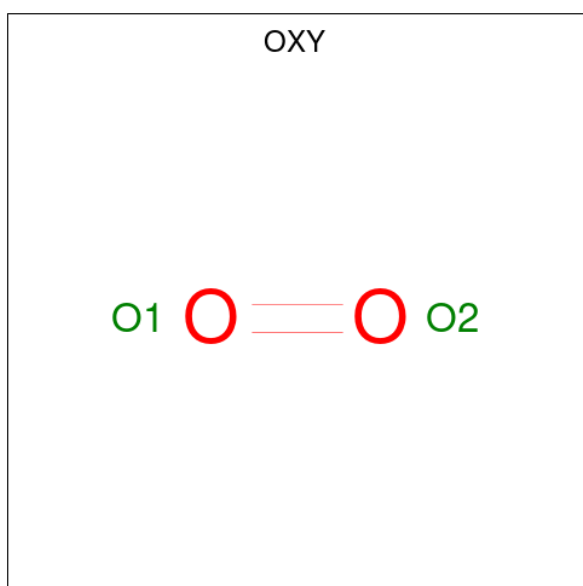
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



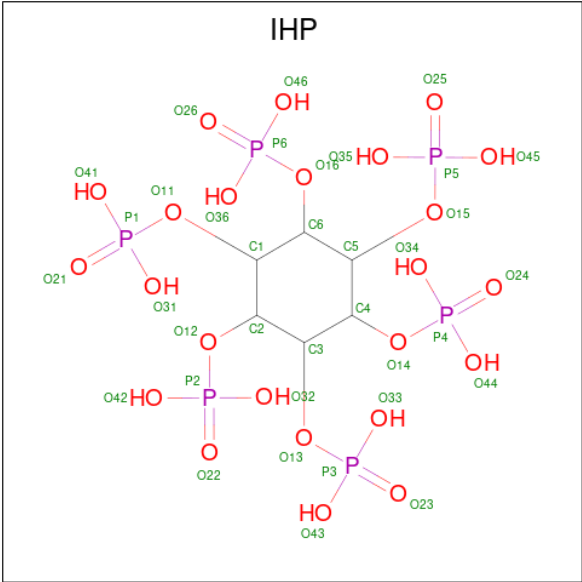
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 5 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			36	6	24	6		

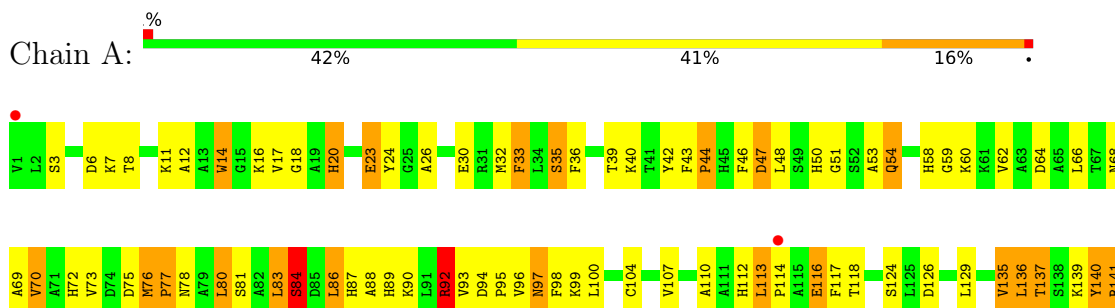
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	0
			91	91		
6	B	91	Total	O	0	0
			91	91		
6	C	76	Total	O	0	0
			76	76		
6	D	56	Total	O	0	0
			56	56		

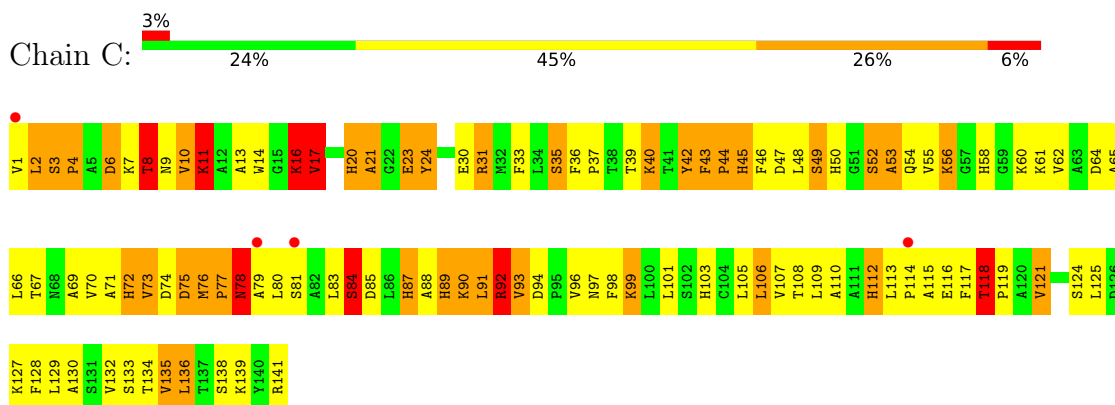
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

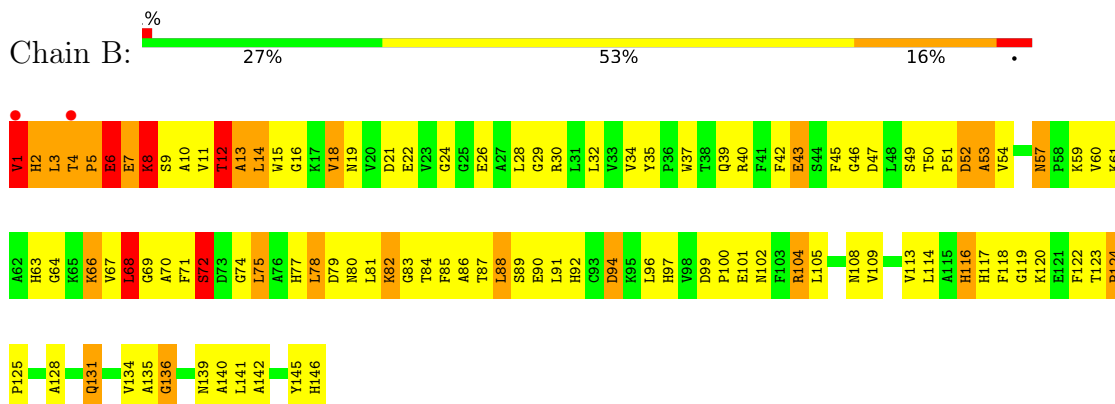
- Molecule 1: HEMOGLOBIN A (OXY) (ALPHA CHAIN)



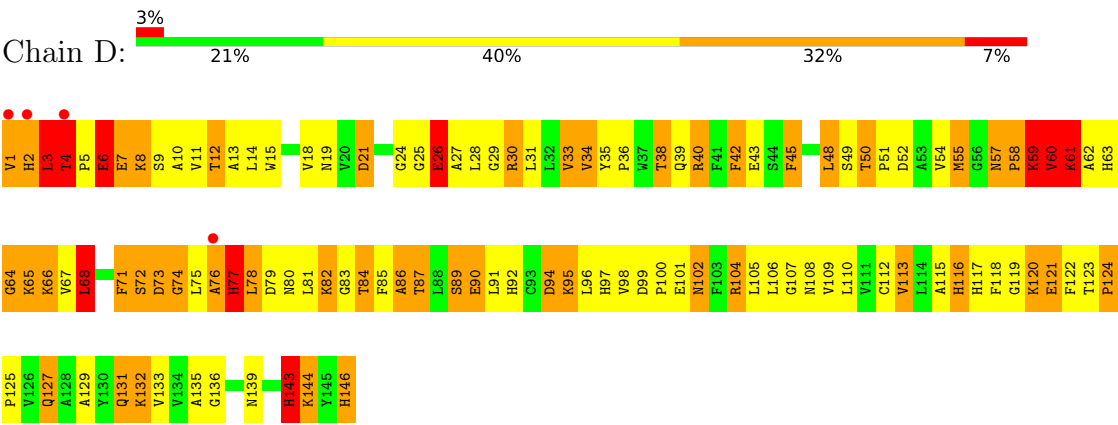
- Molecule 1: HEMOGLOBIN A (OXY) (ALPHA CHAIN)



- Molecule 2: HEMOGLOBIN A (DEOXY) (BETA CHAIN)



● Molecule 2: HEMOGLOBIN A (DEOXY) (BETA CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.80Å 97.80Å 65.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.50 10.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.50) 81.5 (10.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.50Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.196 , (Not available) 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4910	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: OXY, IHP, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.75	11/1097 (1.0%)	2.95	118/1491 (7.9%)
1	C	1.62	7/1097 (0.6%)	3.28	169/1491 (11.3%)
2	B	1.79	12/1153 (1.0%)	3.27	181/1566 (11.6%)
2	D	1.65	6/1153 (0.5%)	3.71	208/1566 (13.3%)
All	All	1.70	36/4500 (0.8%)	3.32	676/6114 (11.1%)

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
1	C	0	1
2	B	0	1
2	D	1	2
All	All	1	5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLY	N-CA	6.79	1.54	1.45
2	B	35	TYR	CA-C	-6.63	1.46	1.52
2	D	112	CYS	CA-C	6.36	1.61	1.52
2	B	100	PRO	N-CD	6.21	1.56	1.47
1	C	89	HIS	CA-CB	6.14	1.62	1.54
1	C	129	LEU	N-CA	6.11	1.54	1.46
1	C	39	THR	CA-CB	6.10	1.64	1.53
2	B	92	HIS	N-CA	6.07	1.53	1.46
1	A	8	THR	CA-CB	5.99	1.62	1.53
2	B	90	GLU	C-N	5.96	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	HIS	N-CA	5.84	1.53	1.46
1	A	137	THR	CA-CB	5.77	1.62	1.53
2	D	38	THR	N-CA	5.76	1.53	1.46
1	C	36	PHE	N-CA	5.75	1.53	1.46
1	A	118	THR	CA-CB	5.74	1.60	1.53
2	B	91	LEU	CA-C	5.73	1.60	1.52
1	C	43	PHE	CA-CB	5.65	1.59	1.53
1	A	75	ASP	N-CA	5.64	1.53	1.46
1	A	11	LYS	N-CA	5.61	1.53	1.46
1	A	70	VAL	CA-C	5.55	1.59	1.52
1	A	47	ASP	CA-C	5.53	1.59	1.52
2	B	34	VAL	N-CA	5.48	1.53	1.46
1	A	64	ASP	N-CA	5.47	1.52	1.46
2	D	50	THR	CA-CB	5.47	1.60	1.54
1	A	94	ASP	CA-C	5.39	1.58	1.53
2	B	102	ASN	N-CA	5.38	1.53	1.46
2	D	109	VAL	CA-C	5.31	1.59	1.52
2	B	109	VAL	N-CA	5.28	1.52	1.46
1	A	70	VAL	N-CA	5.25	1.52	1.46
2	D	67	VAL	C-O	5.25	1.30	1.24
2	B	140	ALA	C-N	5.19	1.41	1.34
1	C	107	VAL	C-O	5.11	1.29	1.24
2	B	39	GLN	N-CA	5.08	1.53	1.46
1	C	93	VAL	CA-CB	5.07	1.60	1.54
2	B	54	VAL	CA-CB	5.05	1.60	1.54
2	D	18	VAL	CA-CB	5.04	1.60	1.54

All (676) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	HIS	CA-CB-CG	31.68	145.48	113.80
2	D	79	ASP	CA-CB-CG	27.45	140.06	112.60
2	D	78	LEU	CA-C-N	24.68	153.35	120.28
2	D	78	LEU	C-N-CA	24.68	153.35	120.28
2	D	2	HIS	CB-CA-C	24.07	158.31	110.42
1	C	92	ARG	NE-CZ-NH2	16.68	134.21	119.20
2	B	83	GLY	O-C-N	16.14	137.84	122.19
1	C	78	ASN	OD1-CG-ND2	15.94	138.53	122.60
1	A	76	MET	O-C-N	15.90	136.50	120.92
2	D	2	HIS	O-C-N	14.61	142.03	122.59
1	C	9	ASN	O-C-N	14.45	137.44	122.12
2	D	97	HIS	CA-CB-CG	-14.39	99.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	LEU	CA-C-N	14.07	142.07	120.68
2	D	3	LEU	C-N-CA	14.07	142.07	120.68
1	C	118	THR	N-CA-CB	-13.77	90.78	109.78
1	C	49	SER	CA-C-O	13.58	135.94	121.55
2	B	67	VAL	O-C-N	-13.52	108.66	121.91
1	A	72	HIS	CA-CB-CG	-13.19	100.61	113.80
1	C	50	HIS	CA-CB-CG	-12.83	100.97	113.80
1	A	97	ASN	CA-CB-CG	-12.44	100.16	112.60
1	C	78	ASN	CA-CB-CG	-12.37	100.23	112.60
1	C	72	HIS	CA-CB-CG	-12.36	101.44	113.80
2	D	60	VAL	CA-C-O	12.23	133.67	120.95
1	C	94	ASP	CA-CB-CG	-12.11	100.49	112.60
1	A	96	VAL	CA-C-O	-12.05	107.68	120.57
2	D	40	ARG	CD-NE-CZ	12.02	141.23	124.40
2	B	52	ASP	CA-C-O	-12.01	107.69	120.42
2	D	80	ASN	OD1-CG-ND2	11.82	134.42	122.60
1	A	20	HIS	CA-CB-CG	-11.61	102.19	113.80
1	C	116	GLU	CA-CB-CG	11.58	137.27	114.10
2	B	78	LEU	CA-C-N	11.46	137.73	120.31
2	B	78	LEU	C-N-CA	11.46	137.73	120.31
1	C	9	ASN	CA-C-O	-11.44	108.42	120.55
1	A	54	GLN	OE1-CD-NE2	11.38	133.98	122.60
2	D	2	HIS	N-CA-CB	-11.36	91.29	110.49
2	B	131	GLN	CG-CD-NE2	11.33	133.39	116.40
1	C	83	LEU	CA-C-O	-11.29	108.45	120.42
1	A	33	PHE	CA-CB-CG	-11.19	102.61	113.80
2	B	4	THR	CA-CB-OG1	-11.18	92.83	109.60
1	A	96	VAL	O-C-N	11.04	133.02	121.87
1	C	20	HIS	CA-CB-CG	-11.02	102.78	113.80
2	D	34	VAL	O-C-N	11.00	133.16	121.83
2	B	12	THR	OG1-CB-CG2	10.96	131.21	109.30
2	D	117	HIS	CA-C-O	-10.93	109.65	120.90
1	A	68	ASN	CA-CB-CG	-10.85	101.75	112.60
2	B	77	HIS	CA-CB-CG	-10.74	103.06	113.80
1	C	75	ASP	CA-CB-CG	10.67	123.27	112.60
2	B	34	VAL	CA-C-O	-10.65	108.97	120.47
2	B	14	LEU	O-C-N	10.61	134.25	122.15
2	B	46	GLY	O-C-N	10.60	133.58	123.19
2	D	131	GLN	CG-CD-NE2	10.58	132.27	116.40
1	A	78	ASN	OD1-CG-ND2	10.54	133.14	122.60
1	C	121	VAL	O-C-N	10.51	132.65	121.83
1	A	72	HIS	O-C-N	10.50	136.12	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	GLU	OE1-CD-OE2	10.46	148.01	122.90
2	B	91	LEU	O-C-N	10.44	132.82	122.07
1	A	20	HIS	O-C-N	10.42	136.08	122.42
2	D	30	ARG	CD-NE-CZ	10.40	138.95	124.40
2	B	108	ASN	O-C-N	10.39	133.99	122.15
2	D	10	ALA	O-C-N	10.36	136.21	122.33
2	D	85	PHE	CA-CB-CG	-10.31	103.49	113.80
2	D	83	GLY	O-C-N	10.29	134.17	122.34
1	A	76	MET	CA-C-O	-10.28	108.01	117.98
2	B	12	THR	N-CA-CB	-10.27	95.12	110.01
1	C	11	LYS	CA-CB-CG	10.22	134.55	114.10
2	D	21	ASP	O-C-N	10.22	132.72	122.09
2	B	67	VAL	CA-C-O	10.01	131.78	121.17
2	D	107	GLY	O-C-N	-9.98	112.25	122.13
2	B	52	ASP	O-C-N	9.96	133.50	122.15
1	C	54	GLN	OE1-CD-NE2	9.91	132.51	122.60
2	B	108	ASN	CA-CB-CG	-9.91	102.69	112.60
1	A	129	LEU	O-C-N	9.90	133.44	122.15
2	D	45	PHE	CA-CB-CG	-9.87	103.93	113.80
2	D	108	ASN	O-C-N	9.83	133.36	122.15
1	A	112	HIS	CA-C-N	9.83	133.90	122.89
1	A	112	HIS	C-N-CA	9.83	133.90	122.89
2	B	94	ASP	CA-C-N	-9.82	105.30	122.79
2	B	94	ASP	C-N-CA	-9.82	105.30	122.79
1	C	108	THR	CA-CB-OG1	-9.78	94.93	109.60
2	B	68	LEU	CA-C-N	-9.74	109.29	120.00
2	B	68	LEU	C-N-CA	-9.74	109.29	120.00
2	B	26	GLU	CA-CB-CG	9.72	133.55	114.10
2	B	66	LYS	N-CA-CB	9.67	124.61	110.20
2	B	79	ASP	CA-CB-CG	9.60	122.19	112.60
1	C	76	MET	O-C-N	9.54	128.97	120.48
2	B	90	GLU	CB-CG-CD	-9.51	96.44	112.60
2	D	50	THR	O-C-N	9.47	128.94	121.55
2	D	107	GLY	CA-C-O	9.45	130.78	121.05
2	D	146	HIS	CA-CB-CG	-9.33	104.47	113.80
2	B	108	ASN	OD1-CG-ND2	9.31	131.91	122.60
1	A	126	ASP	CA-CB-CG	-9.19	103.41	112.60
1	C	141	ARG	NE-CZ-NH2	-9.14	110.97	119.20
2	D	59	LYS	O-C-N	9.11	135.03	122.46
2	D	58	PRO	CA-C-N	-9.11	105.20	121.14
2	D	58	PRO	C-N-CA	-9.11	105.20	121.14
2	D	71	PHE	CA-C-O	9.10	130.37	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ASP	O-C-N	9.01	131.72	122.08
1	A	89	HIS	CA-CB-CG	-8.99	104.81	113.80
2	D	117	HIS	CA-CB-CG	-8.98	104.82	113.80
2	D	108	ASN	CB-CG-ND2	-8.96	102.96	116.40
2	D	122	PHE	CA-CB-CG	-8.91	104.89	113.80
2	D	3	LEU	N-CA-C	-8.84	94.83	109.24
2	D	52	ASP	O-C-N	8.83	131.63	122.09
2	B	80	ASN	OD1-CG-ND2	8.83	131.43	122.60
2	D	117	HIS	O-C-N	8.82	131.55	122.03
2	D	68	LEU	CA-C-O	8.76	130.04	119.97
2	B	139	ASN	O-C-N	8.72	131.37	122.12
2	B	40	ARG	CD-NE-CZ	8.69	136.56	124.40
1	A	66	LEU	O-C-N	8.65	132.01	122.15
2	D	76	ALA	CA-C-N	8.64	136.87	122.79
2	D	76	ALA	C-N-CA	8.64	136.87	122.79
2	B	108	ASN	CB-CG-ND2	-8.62	103.47	116.40
1	A	50	HIS	CA-CB-CG	8.61	122.41	113.80
1	C	84	SER	N-CA-CB	8.59	122.87	110.16
1	A	83	LEU	CA-C-O	-8.58	110.10	119.97
2	D	104	ARG	NH1-CZ-NH2	8.58	130.45	119.30
2	D	11	VAL	CA-C-N	8.57	132.11	120.54
2	D	11	VAL	C-N-CA	8.57	132.11	120.54
2	B	66	LYS	CB-CG-CD	-8.56	91.61	111.30
2	B	86	ALA	N-CA-C	8.51	120.56	111.28
2	B	118	PHE	CA-CB-CG	-8.50	105.30	113.80
2	D	35	TYR	O-C-N	8.47	128.99	121.37
1	A	92	ARG	CA-CB-CG	-8.46	97.19	114.10
1	C	4	PRO	O-C-N	8.44	131.70	122.17
1	C	78	ASN	O-C-N	8.43	132.37	122.17
2	B	66	LYS	CA-CB-CG	8.43	130.96	114.10
1	C	67	THR	CA-C-O	8.31	129.36	120.55
1	C	132	VAL	O-C-N	8.31	129.93	121.87
2	D	104	ARG	NE-CZ-NH1	-8.30	113.20	121.50
1	A	62	VAL	O-C-N	8.29	130.37	121.83
1	C	61	LYS	CB-CA-C	-8.27	97.06	110.79
1	C	55	VAL	N-CA-C	-8.26	102.49	110.42
2	D	79	ASP	CA-C-O	8.25	129.30	120.55
1	C	21	ALA	CA-C-N	8.24	129.26	120.03
1	C	21	ALA	C-N-CA	8.24	129.26	120.03
2	B	81	LEU	CA-C-N	-8.22	107.81	120.31
2	B	81	LEU	C-N-CA	-8.22	107.81	120.31
2	D	108	ASN	OD1-CG-ND2	8.19	130.79	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	HIS	CA-C-O	-8.16	110.24	118.97
2	D	64	GLY	O-C-N	-8.16	114.35	122.18
1	C	116	GLU	CG-CD-OE2	-8.14	99.68	118.40
1	C	87	HIS	CA-CB-CG	-8.12	105.68	113.80
2	B	30	ARG	CD-NE-CZ	8.11	135.76	124.40
2	B	90	GLU	N-CA-CB	-8.11	97.74	110.22
2	B	32	LEU	O-C-N	8.10	132.23	122.27
1	C	141	ARG	NE-CZ-NH1	8.10	129.60	121.50
1	A	33	PHE	O-C-N	8.07	130.68	122.12
1	C	112	HIS	CA-C-O	-8.07	110.33	118.97
2	B	10	ALA	O-C-N	8.06	130.48	122.09
2	B	69	GLY	O-C-N	8.05	130.00	122.19
1	A	136	LEU	O-C-N	8.04	133.20	122.43
2	D	77	HIS	CA-C-N	8.03	132.10	120.38
2	D	77	HIS	C-N-CA	8.03	132.10	120.38
1	C	17	VAL	CA-C-O	8.00	129.65	121.17
1	C	72	HIS	CA-C-O	-7.98	109.86	120.15
1	A	46	PHE	CA-CB-CG	-7.92	105.88	113.80
1	C	20	HIS	O-C-N	7.91	133.29	122.37
2	B	89	SER	CA-C-O	7.90	129.76	121.07
2	D	30	ARG	NE-CZ-NH2	7.89	126.31	119.20
1	A	23	GLU	OE1-CD-OE2	7.89	141.83	122.90
1	C	84	SER	CA-CB-OG	-7.88	95.33	111.10
2	D	3	LEU	CB-CA-C	7.87	122.74	109.75
2	D	45	PHE	CA-C-O	7.86	129.04	119.38
2	D	84	THR	N-CA-CB	7.83	121.63	110.12
1	A	47	ASP	N-CA-C	-7.83	96.54	108.67
1	C	115	ALA	O-C-N	7.83	130.13	122.07
2	B	119	GLY	CA-C-O	7.82	131.83	121.51
1	C	54	GLN	O-C-N	7.82	131.06	122.15
1	A	64	ASP	CA-C-O	7.80	128.81	120.55
1	C	78	ASN	CB-CG-ND2	-7.79	104.72	116.40
2	D	55	MET	CA-C-N	7.78	128.56	120.00
2	D	55	MET	C-N-CA	7.78	128.56	120.00
2	B	63	HIS	CA-CB-CG	-7.78	106.02	113.80
1	C	21	ALA	O-C-N	-7.78	114.00	122.09
2	D	116	HIS	CA-CB-CG	-7.73	106.07	113.80
1	A	48	LEU	O-C-N	7.72	131.76	122.26
2	B	68	LEU	O-C-N	7.71	131.76	122.27
2	D	136	GLY	CA-C-O	7.70	128.35	120.80
2	D	71	PHE	CA-CB-CG	-7.69	106.11	113.80
1	A	30	GLU	OE1-CD-OE2	7.69	141.35	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	CA-CB-CG	-7.69	98.73	114.10
1	A	113	LEU	CB-CA-C	-7.68	101.14	111.21
2	B	49	SER	CA-C-O	-7.68	111.42	120.10
2	B	97	HIS	CA-CB-CG	-7.67	106.13	113.80
2	B	66	LYS	O-C-N	7.66	132.19	122.23
1	A	140	TYR	O-C-N	7.65	131.17	122.22
1	C	105	LEU	CA-C-O	-7.64	111.76	120.24
2	D	82	LYS	N-CA-C	7.57	120.19	111.11
2	D	117	HIS	N-CA-CB	7.56	120.95	109.98
2	D	31	LEU	O-C-N	7.54	129.84	122.07
1	C	64	ASP	CA-C-O	-7.51	112.59	120.55
2	B	85	PHE	CA-CB-CG	-7.50	106.30	113.80
2	B	60	VAL	CG1-CB-CG2	7.47	127.25	110.80
2	B	92	HIS	CE1-NE2-CD2	7.46	116.46	109.00
2	D	121	GLU	N-CA-C	7.46	121.48	112.38
2	B	6	GLU	CB-CG-CD	7.44	125.26	112.60
2	B	123	THR	O-C-N	7.44	129.48	121.60
2	B	89	SER	O-C-N	-7.43	114.12	122.08
2	D	26	GLU	CB-CG-CD	-7.43	99.97	112.60
1	A	12	ALA	N-CA-C	7.42	119.00	111.07
2	D	119	GLY	CA-C-O	7.41	133.45	120.57
2	B	70	ALA	O-C-N	-7.40	114.28	122.12
1	A	32	MET	CA-CB-CG	-7.38	99.34	114.10
1	C	58	HIS	CA-CB-CG	-7.38	106.42	113.80
2	B	92	HIS	CA-CB-CG	-7.37	106.43	113.80
1	C	97	ASN	CA-CB-CG	-7.37	105.23	112.60
2	B	139	ASN	CA-C-O	-7.36	112.74	120.55
2	D	81	LEU	CA-C-O	7.36	128.22	120.42
2	D	26	GLU	OE1-CD-OE2	7.36	140.55	122.90
1	A	54	GLN	O-C-N	7.34	129.91	122.12
2	B	63	HIS	O-C-N	-7.34	114.51	122.07
1	C	24	TYR	CA-C-O	-7.34	112.77	120.55
1	C	135	VAL	CA-C-O	7.33	128.58	120.95
2	D	14	LEU	O-C-N	7.33	132.16	122.33
2	D	2	HIS	CA-C-N	-7.33	112.60	122.72
2	D	2	HIS	C-N-CA	-7.33	112.60	122.72
1	A	116	GLU	CA-C-N	-7.33	111.36	122.21
1	A	116	GLU	C-N-CA	-7.33	111.36	122.21
1	C	117	PHE	CA-C-O	7.33	132.08	122.63
1	A	6	ASP	O-C-N	7.32	129.61	122.07
1	C	125	LEU	O-C-N	7.32	129.88	122.12
2	D	30	ARG	CA-C-O	-7.30	112.81	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	HIS	CB-CA-C	-7.30	99.75	111.06
1	C	20	HIS	CB-CA-C	-7.28	96.91	110.01
2	B	104	ARG	NE-CZ-NH2	-7.26	112.67	119.20
1	A	116	GLU	CG-CD-OE2	-7.25	101.73	118.40
1	C	136	LEU	O-C-N	7.25	132.14	122.43
2	B	113	VAL	O-C-N	-7.25	114.81	121.91
2	B	7	GLU	CA-CB-CG	-7.24	99.63	114.10
2	B	47	ASP	CA-C-O	7.23	128.77	120.60
2	B	57	ASN	OD1-CG-ND2	-7.23	115.37	122.60
2	B	82	LYS	CA-C-N	-7.19	112.09	120.00
2	B	82	LYS	C-N-CA	-7.19	112.09	120.00
1	C	9	ASN	CA-C-N	-7.19	107.93	120.29
1	C	9	ASN	C-N-CA	-7.19	107.93	120.29
1	A	23	GLU	CG-CD-OE2	-7.18	101.88	118.40
2	D	54	VAL	O-C-N	7.16	129.34	121.90
1	A	7	LYS	CA-C-O	7.12	128.10	120.55
2	D	112	CYS	CA-C-N	-7.11	110.72	120.46
2	D	112	CYS	C-N-CA	-7.11	110.72	120.46
2	D	59	LYS	CA-C-O	-7.11	110.50	119.31
2	B	85	PHE	N-CA-C	7.10	121.66	112.92
2	B	145	TYR	CD1-CG-CD2	7.10	128.75	118.10
2	B	97	HIS	CG-CD2-NE2	-7.06	100.14	107.20
2	D	67	VAL	O-C-N	-7.06	114.99	121.91
2	D	77	HIS	CA-CB-CG	-7.05	106.75	113.80
2	D	1	VAL	N-CA-CB	7.03	123.46	111.50
2	D	61	LYS	CA-CB-CG	-7.03	100.03	114.10
2	B	128	ALA	O-C-N	-7.03	114.67	122.12
2	B	2	HIS	CA-C-O	7.03	128.43	120.84
2	B	77	HIS	N-CA-C	7.01	118.85	110.44
2	B	12	THR	CA-CB-OG1	-6.99	99.12	109.60
1	A	78	ASN	CA-CB-CG	-6.97	105.63	112.60
1	C	116	GLU	OE1-CD-OE2	6.96	139.60	122.90
2	B	105	LEU	O-C-N	6.95	129.23	122.07
2	D	13	ALA	N-CA-C	6.94	118.84	111.28
1	A	116	GLU	CG-CD-OE1	6.93	134.34	118.40
1	C	58	HIS	CA-C-N	6.93	127.68	119.98
1	C	58	HIS	C-N-CA	6.93	127.68	119.98
1	C	55	VAL	CB-CA-C	6.93	120.83	111.97
1	C	71	ALA	CA-C-O	6.92	128.10	120.63
1	A	81	SER	CA-CB-OG	-6.92	97.26	111.10
2	D	6	GLU	O-C-N	6.91	131.69	122.43
2	D	71	PHE	N-CA-CB	-6.89	100.02	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	85	PHE	N-CA-CB	-6.87	100.08	110.73
2	D	72	SER	O-C-N	-6.86	114.95	122.09
2	D	92	HIS	CA-CB-CG	-6.86	106.94	113.80
1	A	87	HIS	CA-C-O	-6.85	113.15	120.42
2	D	26	GLU	CG-CD-OE2	-6.85	102.64	118.40
2	B	94	ASP	O-C-N	6.84	131.49	122.33
1	C	6	ASP	CA-C-N	-6.84	111.12	120.28
1	C	6	ASP	C-N-CA	-6.84	111.12	120.28
2	B	1	VAL	CA-C-N	-6.83	113.35	122.85
2	B	1	VAL	C-N-CA	-6.83	113.35	122.85
2	B	43	GLU	N-CA-CB	-6.83	100.08	110.12
2	B	142	ALA	CA-C-N	6.82	129.75	120.54
2	B	142	ALA	C-N-CA	6.82	129.75	120.54
2	B	60	VAL	CA-CB-CG2	-6.82	98.81	110.40
2	B	105	LEU	CA-C-N	-6.79	111.17	120.28
2	B	105	LEU	C-N-CA	-6.79	111.17	120.28
2	B	66	LYS	CA-C-O	-6.79	112.71	120.24
1	C	60	LYS	CA-CB-CG	-6.79	100.53	114.10
2	B	18	VAL	CA-C-O	6.78	129.18	121.11
1	A	47	ASP	O-C-N	6.77	131.63	122.82
2	D	116	HIS	CA-C-N	6.77	129.83	120.63
2	D	116	HIS	C-N-CA	6.77	129.83	120.63
2	D	12	THR	CA-C-O	-6.75	113.68	120.90
2	B	4	THR	CB-CA-C	6.73	121.59	109.61
2	B	87	THR	O-C-N	6.73	130.54	122.27
1	C	47	ASP	N-CA-C	-6.71	97.60	108.41
1	A	141	ARG	NE-CZ-NH2	-6.69	113.17	119.20
1	C	92	ARG	NH1-CZ-NH2	-6.68	110.61	119.30
1	A	84	SER	N-CA-CB	6.68	119.94	110.12
1	A	80	LEU	N-CA-CB	-6.67	100.82	110.56
2	B	15	TRP	CA-C-O	6.67	127.63	120.10
2	D	85	PHE	O-C-N	6.64	130.15	122.25
1	C	89	HIS	CA-CB-CG	-6.63	107.17	113.80
2	D	9	SER	CA-CB-OG	6.62	124.35	111.10
1	C	139	LYS	N-CA-CB	-6.61	100.85	110.70
1	A	100	LEU	O-C-N	6.59	129.67	122.15
1	A	30	GLU	CG-CD-OE1	-6.58	103.27	118.40
2	D	74	GLY	O-C-N	6.58	129.21	122.24
1	C	91	LEU	O-C-N	6.57	129.19	122.09
2	D	84	THR	N-CA-C	-6.55	104.14	111.28
1	C	30	GLU	CG-CD-OE1	-6.55	103.34	118.40
1	C	98	PHE	CA-CB-CG	-6.55	107.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	THR	OG1-CB-CG2	6.54	122.38	109.30
2	D	131	GLN	CG-CD-OE1	-6.54	107.73	120.80
1	C	47	ASP	O-C-N	6.53	130.76	122.93
2	B	131	GLN	CG-CD-OE1	-6.52	107.76	120.80
1	C	91	LEU	CA-C-O	-6.51	114.00	120.70
2	D	73	ASP	N-CA-CB	6.50	119.78	110.16
1	C	93	VAL	O-C-N	-6.50	115.53	122.61
2	D	77	HIS	CB-CA-C	-6.49	101.03	111.28
2	B	19	ASN	CA-CB-CG	-6.49	106.11	112.60
1	C	30	GLU	CA-C-O	6.49	127.63	120.82
1	C	1	VAL	CA-CB-CG1	6.48	121.42	110.40
2	D	112	CYS	O-C-N	6.48	129.54	122.15
2	D	14	LEU	N-CA-C	-6.48	104.07	112.23
2	B	43	GLU	CB-CG-CD	-6.47	101.60	112.60
2	D	57	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	75	ASP	N-CA-CB	-6.46	104.04	111.79
2	B	136	GLY	N-CA-C	-6.45	105.02	112.50
1	C	80	LEU	CA-C-O	-6.45	111.98	119.59
1	C	110	ALA	CA-C-N	6.44	130.10	120.31
1	C	110	ALA	C-N-CA	6.44	130.10	120.31
1	C	118	THR	CA-C-O	-6.43	113.68	120.88
2	D	94	ASP	N-CA-C	6.43	119.28	111.82
2	D	131	GLN	CA-C-O	6.42	127.36	120.55
2	D	43	GLU	CA-C-N	6.42	130.88	120.60
2	D	43	GLU	C-N-CA	6.42	130.88	120.60
2	D	81	LEU	N-CA-CB	-6.41	100.67	110.16
1	C	84	SER	O-C-N	6.41	129.46	122.15
2	D	105	LEU	CA-C-N	-6.41	111.69	120.28
2	D	105	LEU	C-N-CA	-6.41	111.69	120.28
1	A	18	GLY	CA-C-N	6.40	132.90	120.99
1	A	18	GLY	C-N-CA	6.40	132.90	120.99
2	B	72	SER	CA-CB-OG	-6.40	98.30	111.10
2	B	92	HIS	CG-CD2-NE2	-6.39	100.81	107.20
2	D	115	ALA	N-CA-CB	-6.39	100.72	110.12
2	B	117	HIS	CA-C-O	-6.38	114.13	120.70
2	D	77	HIS	N-CA-C	6.36	120.84	111.87
1	C	74	ASP	CA-C-O	-6.35	111.56	119.38
1	C	92	ARG	NE-CZ-NH1	-6.33	115.17	121.50
2	D	132	LYS	O-C-N	6.33	129.37	122.15
2	B	99	ASP	O-C-N	-6.32	115.67	121.30
2	D	132	LYS	N-CA-CB	6.30	119.49	110.16
2	B	45	PHE	CA-C-N	6.30	127.23	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	PHE	C-N-CA	6.30	127.23	121.31
2	B	34	VAL	O-C-N	6.30	128.92	121.80
1	C	24	TYR	O-C-N	6.30	128.79	122.12
1	A	100	LEU	CA-C-O	-6.29	113.75	120.42
2	B	21	ASP	CA-CB-CG	-6.29	106.31	112.60
1	C	125	LEU	N-CA-CB	-6.29	100.88	110.12
1	C	54	GLN	CG-CD-NE2	-6.28	106.98	116.40
2	D	12	THR	O-C-N	6.26	128.60	122.09
1	A	7	LYS	CB-CG-CD	-6.26	96.91	111.30
2	B	63	HIS	CA-C-N	6.25	127.03	120.03
2	B	63	HIS	C-N-CA	6.25	127.03	120.03
2	D	33	VAL	N-CA-C	-6.25	105.05	110.74
2	D	100	PRO	N-CA-CB	6.24	109.45	103.52
2	B	100	PRO	O-C-N	6.24	130.60	122.24
1	C	127	LYS	CA-C-N	6.24	128.55	120.44
1	C	127	LYS	C-N-CA	6.24	128.55	120.44
1	C	141	ARG	CD-NE-CZ	-6.24	115.67	124.40
2	B	134	VAL	O-C-N	6.23	128.84	121.80
1	C	101	LEU	N-CA-C	-6.23	104.57	111.36
1	A	35	SER	CA-C-O	-6.23	112.44	119.79
2	D	12	THR	CA-CB-OG1	-6.20	100.29	109.60
1	C	21	ALA	CB-CA-C	6.20	120.72	110.81
2	D	4	THR	N-CA-C	-6.19	101.54	110.08
2	D	121	GLU	N-CA-CB	-6.19	99.80	110.32
1	A	107	VAL	O-C-N	6.19	127.87	121.87
1	C	128	PHE	O-C-N	6.17	128.43	122.07
2	B	37	TRP	O-C-N	6.17	130.70	122.43
1	C	46	PHE	CB-CA-C	-6.17	99.08	109.50
2	B	24	GLY	O-C-N	-6.15	116.28	122.19
1	A	124	SER	CA-CB-OG	-6.15	98.80	111.10
1	A	84	SER	CA-CB-OG	-6.14	98.81	111.10
1	A	116	GLU	O-C-N	6.14	130.94	122.46
2	B	91	LEU	CA-C-N	-6.14	111.43	120.28
2	B	91	LEU	C-N-CA	-6.14	111.43	120.28
1	C	53	ALA	CA-C-O	6.14	127.03	119.97
1	A	129	LEU	CA-C-O	-6.13	113.92	120.42
1	C	35	SER	O-C-N	6.13	130.54	122.33
2	B	139	ASN	CA-CB-CG	-6.13	106.47	112.60
2	D	83	GLY	CA-C-O	-6.13	113.53	120.09
2	D	127	GLN	CA-C-N	6.13	128.82	120.54
2	D	127	GLN	C-N-CA	6.13	128.82	120.54
1	A	110	ALA	CA-C-O	-6.12	114.35	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	104	ARG	O-C-N	6.12	129.12	122.15
1	C	44	PRO	CA-C-O	6.10	128.82	119.55
1	A	100	LEU	CA-C-N	-6.09	111.64	120.29
1	A	100	LEU	C-N-CA	-6.09	111.64	120.29
2	D	144	LYS	CB-CG-CD	-6.09	97.29	111.30
2	D	62	ALA	CA-C-O	-6.08	113.97	120.42
2	D	85	PHE	N-CA-C	6.07	120.71	112.88
2	B	100	PRO	CA-C-N	-6.07	111.54	120.28
2	B	100	PRO	C-N-CA	-6.07	111.54	120.28
2	D	4	THR	CA-CB-CG2	6.07	120.82	110.50
2	D	29	GLY	CA-C-N	6.07	128.41	120.28
2	D	29	GLY	C-N-CA	6.07	128.41	120.28
2	D	105	LEU	O-C-N	6.07	128.32	122.07
1	C	90	LYS	CB-CG-CD	6.05	125.23	111.30
1	C	69	ALA	N-CA-C	-6.04	104.78	111.36
2	B	6	GLU	CG-CD-OE2	-6.04	104.51	118.40
2	B	57	ASN	CA-CB-CG	-6.04	106.56	112.60
2	D	90	GLU	OE1-CD-OE2	6.04	137.39	122.90
1	C	112	HIS	CA-C-N	6.03	128.43	122.28
1	C	112	HIS	C-N-CA	6.03	128.43	122.28
2	D	64	GLY	CA-C-O	6.02	127.50	121.00
1	C	109	LEU	O-C-N	6.01	128.26	122.07
2	D	99	ASP	CA-C-N	6.01	125.71	119.82
2	D	99	ASP	C-N-CA	6.01	125.71	119.82
2	D	27	ALA	N-CA-CB	6.00	118.67	109.91
1	A	88	ALA	CA-C-O	5.97	127.09	120.82
1	A	98	PHE	CA-CB-CG	-5.96	107.84	113.80
2	D	34	VAL	CA-C-O	-5.96	114.53	120.85
2	D	15	TRP	CB-CA-C	-5.96	100.90	110.79
2	B	11	VAL	CA-C-O	5.95	127.66	121.29
1	C	94	ASP	OD1-CG-OD2	-5.95	108.62	122.90
1	C	73	VAL	CA-C-O	5.95	128.21	120.78
1	A	20	HIS	CA-C-O	-5.94	112.38	119.15
2	D	18	VAL	O-C-N	5.94	129.40	122.81
1	A	99	LYS	N-CA-CB	5.94	118.85	110.12
2	D	80	ASN	N-CA-CB	-5.93	101.58	111.96
1	A	53	ALA	N-CA-CB	5.93	119.47	110.28
2	D	30	ARG	O-C-N	5.93	128.41	122.12
2	D	98	VAL	N-CA-CB	-5.93	104.26	110.72
1	C	117	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	77	PRO	O-C-N	5.92	129.04	122.24
2	B	141	LEU	CA-C-O	5.92	126.77	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	HIS	CA-C-O	-5.91	114.36	121.34
1	A	7	LYS	N-CA-CB	-5.90	101.45	110.12
2	D	121	GLU	CA-CB-CG	5.89	125.89	114.10
2	D	84	THR	CA-C-O	-5.87	114.33	120.55
1	C	45	HIS	CB-CA-C	-5.86	98.98	110.11
1	A	135	VAL	N-CA-CB	5.85	117.40	110.55
2	B	40	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	89	HIS	N-CA-C	5.84	120.53	113.41
2	D	101	GLU	CA-CB-CG	-5.84	102.42	114.10
1	A	97	ASN	OD1-CG-ND2	5.83	128.43	122.60
2	B	122	PHE	CB-CA-C	5.82	121.11	112.03
1	C	130	ALA	N-CA-CB	5.81	118.43	110.01
1	C	90	LYS	CA-C-N	5.81	128.34	120.44
1	C	90	LYS	C-N-CA	5.81	128.34	120.44
2	D	57	ASN	CA-C-O	5.81	124.64	119.59
2	D	59	LYS	CB-CG-CD	-5.79	97.99	111.30
2	B	18	VAL	CG1-CB-CG2	5.79	123.53	110.80
2	D	28	LEU	CA-C-O	-5.78	114.42	120.55
2	D	78	LEU	CA-C-O	5.77	126.66	120.20
2	D	94	ASP	CA-C-N	-5.77	112.52	122.79
2	D	94	ASP	C-N-CA	-5.77	112.52	122.79
1	A	92	ARG	N-CA-CB	-5.76	103.42	112.13
2	D	87	THR	O-C-N	5.76	130.05	122.33
1	C	24	TYR	CD1-CG-CD2	5.76	126.73	118.10
2	D	86	ALA	CB-CA-C	5.76	120.47	110.68
2	D	42	PHE	N-CA-CB	-5.75	102.91	111.43
2	D	60	VAL	CB-CA-C	5.75	119.90	112.14
2	D	62	ALA	O-C-N	5.75	128.70	122.15
1	C	1	VAL	CB-CA-C	5.74	122.31	111.40
2	B	5	PRO	N-CA-C	-5.74	106.05	113.57
1	C	13	ALA	N-CA-CB	-5.74	101.10	109.82
2	D	104	ARG	CD-NE-CZ	-5.74	116.37	124.40
1	C	87	HIS	CA-C-O	-5.72	114.35	120.42
2	D	133	VAL	O-C-N	5.72	127.85	121.90
1	A	66	LEU	CA-C-O	-5.71	114.37	120.42
2	D	49	SER	CA-C-N	-5.69	112.95	123.65
2	D	49	SER	C-N-CA	-5.69	112.95	123.65
1	A	73	VAL	CA-C-O	5.69	126.91	120.03
1	A	51	GLY	O-C-N	5.68	129.51	122.41
2	D	123	THR	O-C-N	5.67	127.95	121.31
2	D	110	LEU	CB-CA-C	5.67	119.79	110.88
1	A	51	GLY	CA-C-O	-5.67	112.21	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	THR	CA-CB-CG2	5.67	120.13	110.50
1	A	3	SER	N-CA-CB	-5.66	102.20	109.55
1	C	8	THR	O-C-N	5.65	128.59	122.15
2	D	115	ALA	CA-C-N	5.65	128.17	120.54
2	D	115	ALA	C-N-CA	5.65	128.17	120.54
2	B	61	LYS	O-C-N	5.65	127.89	122.07
2	B	4	THR	N-CA-C	-5.64	101.83	110.01
1	C	124	SER	CA-CB-OG	-5.64	99.82	111.10
2	B	40	ARG	NH1-CZ-NH2	-5.64	111.97	119.30
2	D	26	GLU	CA-C-N	5.63	128.09	120.65
2	D	26	GLU	C-N-CA	5.63	128.09	120.65
1	C	99	LYS	CG-CD-CE	5.63	124.25	111.30
1	A	7	LYS	N-CA-C	5.63	117.41	111.28
1	C	130	ALA	N-CA-C	-5.62	105.05	111.07
1	C	36	PHE	O-C-N	5.62	126.43	121.37
2	B	28	LEU	CA-C-N	-5.61	113.75	119.98
2	B	28	LEU	C-N-CA	-5.61	113.75	119.98
1	C	43	PHE	CB-CA-C	-5.61	103.93	111.11
2	B	135	ALA	N-CA-C	-5.60	105.25	111.36
2	D	91	LEU	O-C-N	5.60	127.83	122.07
2	B	29	GLY	CA-C-O	-5.59	114.99	120.75
1	C	75	ASP	N-CA-CB	-5.59	100.73	111.53
1	C	138	SER	O-C-N	5.59	128.76	122.22
1	C	134	THR	O-C-N	5.59	127.82	122.07
1	A	69	ALA	N-CA-C	-5.58	105.27	111.36
1	A	62	VAL	CA-C-O	-5.58	114.93	120.85
1	C	76	MET	CA-CB-CG	-5.58	102.95	114.10
1	C	81	SER	CA-C-O	-5.58	114.61	120.63
1	A	54	GLN	CG-CD-NE2	-5.57	108.05	116.40
1	C	94	ASP	CA-C-O	-5.56	114.53	119.75
1	A	14	TRP	CA-C-N	5.55	126.11	119.94
1	A	14	TRP	C-N-CA	5.55	126.11	119.94
1	A	77	PRO	CA-C-N	-5.55	111.44	120.71
1	A	77	PRO	C-N-CA	-5.55	111.44	120.71
2	B	57	ASN	O-C-N	-5.54	114.94	121.32
2	B	92	HIS	ND1-CE1-NE2	-5.54	102.86	108.40
2	D	109	VAL	O-C-N	5.54	127.34	121.91
2	B	1	VAL	O-C-N	5.54	131.86	123.00
1	C	62	VAL	N-CA-CB	-5.54	102.28	110.58
1	A	3	SER	CA-CB-OG	-5.53	100.03	111.10
2	B	64	GLY	CA-C-O	5.53	126.22	120.80
2	D	87	THR	CB-CA-C	5.52	121.64	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	69	ALA	CB-CA-C	5.52	120.24	110.85
2	D	14	LEU	CA-C-N	-5.51	112.89	120.28
2	D	14	LEU	C-N-CA	-5.51	112.89	120.28
2	D	73	ASP	O-C-N	5.51	128.43	122.15
2	B	64	GLY	O-C-N	-5.51	116.83	122.17
1	C	16	LYS	N-CA-CB	-5.49	101.28	110.39
2	B	87	THR	CA-C-O	-5.49	113.66	119.97
2	D	129	ALA	O-C-N	5.49	128.40	122.15
2	B	52	ASP	N-CA-CB	5.48	118.27	110.16
1	C	23	GLU	OE1-CD-OE2	5.48	136.04	122.90
1	A	136	LEU	CA-C-N	-5.47	114.06	122.60
1	A	136	LEU	C-N-CA	-5.47	114.06	122.60
2	D	96	LEU	O-C-N	5.47	129.95	122.46
1	A	23	GLU	CB-CG-CD	-5.47	103.31	112.60
1	C	20	HIS	CE1-NE2-CD2	5.46	114.46	109.00
2	D	135	ALA	N-CA-CB	-5.46	102.08	110.16
2	B	145	TYR	CG-CD1-CE1	-5.46	113.02	121.20
1	C	40	LYS	CA-CB-CG	-5.45	103.21	114.10
2	D	43	GLU	CB-CA-C	5.45	120.11	110.85
2	B	96	LEU	CA-C-N	-5.43	114.53	122.19
2	B	96	LEU	C-N-CA	-5.43	114.53	122.19
2	B	50	THR	OG1-CB-CG2	-5.43	98.44	109.30
2	B	88	LEU	N-CA-C	-5.43	105.44	111.36
1	C	14	TRP	O-C-N	5.42	127.87	122.12
1	A	87	HIS	CA-CB-CG	-5.42	108.38	113.80
1	C	84	SER	N-CA-C	-5.42	105.46	111.36
2	B	116	HIS	ND1-CG-CD2	5.41	111.51	106.10
2	B	42	PHE	N-CA-CB	-5.41	103.50	111.51
1	A	11	LYS	N-CA-CB	-5.41	102.17	110.12
2	B	117	HIS	CB-CA-C	-5.40	102.36	110.90
2	B	97	HIS	ND1-CG-CD2	5.40	111.50	106.10
1	A	141	ARG	CG-CD-NE	-5.40	100.12	112.00
2	B	32	LEU	N-CA-CB	-5.40	101.91	110.28
1	A	36	PHE	O-C-N	5.39	126.22	121.37
2	D	86	ALA	N-CA-CB	-5.39	101.97	110.06
2	D	90	GLU	CA-CB-CG	-5.39	103.32	114.10
2	B	28	LEU	O-C-N	5.39	128.29	122.15
2	D	48	LEU	N-CA-CB	-5.38	103.20	110.95
1	C	119	PRO	O-C-N	-5.38	116.05	122.24
2	D	91	LEU	N-CA-CB	-5.38	102.21	110.01
1	C	133	SER	CA-CB-OG	-5.38	100.34	111.10
2	B	66	LYS	CA-C-N	-5.37	113.79	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	LYS	C-N-CA	-5.37	113.79	120.56
1	C	139	LYS	CB-CG-CD	-5.37	98.95	111.30
2	D	7	GLU	CA-C-O	-5.37	115.17	120.80
2	D	143	HIS	CB-CA-C	5.35	119.68	110.79
2	D	68	LEU	CB-CA-C	5.35	120.95	110.67
2	D	35	TYR	CA-CB-CG	-5.35	104.27	113.90
2	B	109	VAL	O-C-N	5.34	127.05	121.87
1	C	31	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	44	PRO	CA-C-O	5.33	127.17	119.34
2	D	38	THR	O-C-N	5.32	129.81	122.46
2	D	59	LYS	N-CA-CB	5.32	119.08	110.40
2	B	96	LEU	N-CA-CB	-5.32	102.14	110.44
2	B	3	LEU	CA-CB-CG	5.32	134.91	116.30
1	C	103	HIS	CA-CB-CG	-5.32	108.48	113.80
1	C	75	ASP	OD1-CG-OD2	5.31	135.64	122.90
2	D	127	GLN	CA-CB-CG	-5.31	103.48	114.10
2	D	7	GLU	CA-C-N	5.30	127.64	120.38
2	D	7	GLU	C-N-CA	5.30	127.64	120.38
2	B	19	ASN	CA-C-N	5.29	127.99	120.53
2	B	19	ASN	C-N-CA	5.29	127.99	120.53
2	B	75	LEU	O-C-N	5.29	129.27	122.39
1	C	119	PRO	CA-C-N	5.29	127.80	120.29
1	C	119	PRO	C-N-CA	5.29	127.80	120.29
1	C	81	SER	O-C-N	5.28	127.72	122.12
1	C	89	HIS	CA-C-O	5.28	124.62	118.97
2	D	60	VAL	N-CA-C	-5.28	105.23	110.62
1	C	85	ASP	CA-C-O	5.28	126.37	120.82
1	A	110	ALA	O-C-N	5.28	127.58	122.09
1	C	107	VAL	CA-C-N	5.27	127.66	120.54
1	C	107	VAL	C-N-CA	5.27	127.66	120.54
2	D	72	SER	CA-C-N	5.26	127.77	120.29
2	D	72	SER	C-N-CA	5.26	127.77	120.29
1	A	60	LYS	CA-CB-CG	5.26	124.62	114.10
1	C	64	ASP	CB-CG-OD1	-5.26	106.30	118.40
1	A	50	HIS	N-CA-CB	5.26	117.73	109.69
1	A	140	TYR	CA-C-O	-5.25	114.16	120.10
1	C	39	THR	CA-CB-OG1	-5.25	101.72	109.60
2	B	97	HIS	CE1-NE2-CD2	5.25	114.25	109.00
1	A	47	ASP	CA-C-O	-5.24	114.68	120.60
2	D	120	LYS	O-C-N	5.24	128.55	122.20
2	B	102	ASN	CB-CG-ND2	-5.24	108.54	116.40
1	C	132	VAL	N-CA-C	-5.24	105.28	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	VAL	N-CA-C	-5.24	105.39	110.42
2	D	67	VAL	N-CA-CB	-5.24	104.42	110.55
1	C	2	LEU	N-CA-CB	5.23	117.77	109.71
1	C	24	TYR	CA-CB-CG	-5.22	104.50	113.90
1	C	88	ALA	CA-C-O	5.22	125.96	120.42
2	D	42	PHE	CE1-CZ-CE2	5.22	129.40	120.00
2	B	69	GLY	CA-C-O	-5.21	115.14	120.66
1	A	58	HIS	CB-CA-C	5.21	119.70	110.85
2	B	139	ASN	CB-CG-ND2	-5.20	108.59	116.40
1	C	42	TYR	CG-CD2-CE2	5.20	129.00	121.20
1	A	26	ALA	O-C-N	-5.19	116.62	122.12
2	B	101	GLU	OE1-CD-OE2	5.19	135.36	122.90
1	C	9	ASN	CB-CG-ND2	5.19	124.19	116.40
2	D	89	SER	CA-CB-OG	-5.19	100.72	111.10
1	C	80	LEU	N-CA-CB	-5.18	102.70	110.73
2	D	7	GLU	N-CA-CB	5.18	117.69	110.07
2	B	97	HIS	CB-CA-C	-5.17	104.38	111.73
2	D	10	ALA	CA-C-O	-5.17	113.68	119.79
1	C	24	TYR	CB-CG-CD1	-5.17	113.04	120.80
2	D	113	VAL	O-C-N	-5.16	116.86	121.87
1	C	4	PRO	CA-C-O	-5.16	112.55	120.03
2	B	100	PRO	N-CA-CB	5.16	108.64	103.48
2	B	51	PRO	O-C-N	-5.15	116.05	122.23
1	C	3	SER	CA-C-O	5.13	128.66	121.27
1	A	59	GLY	O-C-N	5.13	127.11	122.18
2	B	71	PHE	CA-C-O	5.12	125.85	120.42
2	B	8	LYS	CB-CG-CD	-5.12	99.52	111.30
2	B	30	ARG	NE-CZ-NH1	5.12	126.62	121.50
2	B	67	VAL	CB-CA-C	5.11	118.52	111.97
2	D	83	GLY	N-CA-C	-5.11	106.19	113.86
1	A	104	CYS	O-C-N	5.11	128.56	122.27
2	D	1	VAL	CA-C-O	5.11	129.49	120.80
2	D	97	HIS	ND1-CG-CD2	5.10	111.20	106.10
1	A	33	PHE	CA-C-O	-5.10	115.14	120.55
1	C	39	THR	OG1-CB-CG2	5.09	119.49	109.30
2	B	79	ASP	CA-C-N	-5.09	115.19	122.67
2	B	79	ASP	C-N-CA	-5.09	115.19	122.67
1	A	86	LEU	CA-C-O	5.08	126.66	121.07
1	A	7	LYS	CG-CD-CE	5.08	122.98	111.30
2	D	102	ASN	CB-CG-ND2	-5.08	108.78	116.40
1	C	65	ALA	CA-C-O	-5.08	115.17	120.55
2	D	133	VAL	CA-C-N	-5.08	112.45	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	133	VAL	C-N-CA	-5.08	112.45	120.47
1	C	35	SER	CA-C-N	-5.07	116.92	123.16
1	C	35	SER	C-N-CA	-5.07	116.92	123.16
2	B	122	PHE	CA-CB-CG	-5.07	108.73	113.80
2	B	43	GLU	N-CA-C	5.07	116.80	111.28
2	B	13	ALA	CA-C-O	5.06	126.32	120.90
1	C	134	THR	CA-CB-OG1	-5.06	102.01	109.60
2	D	73	ASP	CB-CA-C	-5.06	102.24	110.85
2	D	139	ASN	CA-CB-CG	-5.06	107.54	112.60
2	B	67	VAL	N-CA-CB	-5.06	104.63	110.55
1	A	14	TRP	CB-CA-C	5.06	119.98	110.63
1	A	97	ASN	CB-CG-OD1	-5.06	110.68	120.80
1	C	54	GLN	CA-CB-CG	-5.05	104.00	114.10
2	B	54	VAL	N-CA-CB	-5.05	104.95	110.65
2	B	53	ALA	N-CA-CB	5.04	117.52	110.12
1	C	14	TRP	N-CA-CB	5.03	117.52	110.12
1	C	97	ASN	CB-CG-ND2	-5.03	108.85	116.40
1	C	2	LEU	O-C-N	5.03	129.30	122.96
2	D	50	THR	CA-CB-OG1	-5.03	102.06	109.60
2	D	7	GLU	OE1-CD-OE2	5.03	134.97	122.90
2	B	2	HIS	N-CA-CB	5.02	118.68	110.39
1	A	7	LYS	CD-CE-NZ	-5.02	95.84	111.90
1	C	77	PRO	O-C-N	5.02	128.01	122.24
1	C	9	ASN	OD1-CG-ND2	-5.02	117.58	122.60
2	B	63	HIS	CA-C-O	5.02	126.09	120.82
2	B	79	ASP	O-C-N	5.02	128.44	122.27
1	C	80	LEU	N-CA-C	5.01	119.35	112.88
2	D	39	GLN	CA-CB-CG	-5.01	104.07	114.10
2	B	124	PRO	O-C-N	-5.01	115.55	121.46
1	A	17	VAL	N-CA-C	-5.01	105.10	110.36
2	B	43	GLU	CA-C-O	5.01	125.86	120.55
2	B	80	ASN	CA-CB-CG	-5.01	107.59	112.60
2	D	48	LEU	CB-CA-C	5.01	118.36	109.75
2	B	28	LEU	CA-C-O	-5.00	115.12	120.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2	HIS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	ARG	Sidechain
2	B	104	ARG	Sidechain
1	C	92	ARG	Sidechain
2	D	104	ARG	Sidechain
2	D	40	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	35	0
1	C	1069	0	1073	49	0
2	B	1123	0	1118	35	0
2	D	1123	0	1117	110	0
3	A	43	0	30	3	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	8	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	B	36	0	6	2	0
6	A	91	0	0	1	1
6	B	91	0	0	1	0
6	C	76	0	0	2	0
6	D	56	0	0	7	0
All	All	4910	0	4507	222	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 24.

All (222) 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)
2:D:1:VAL:CG2	2:D:3:LEU:HD12	1.57	1.33
2:D:60:VAL:HG12	6:D:191:HOH:O	0.95	1.12
2:D:4:THR:HG23	2:D:6:GLU:OE2	1.52	1.08
2:D:3:LEU:HD23	2:D:7:GLU:HB3	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:VAL:HG21	2:D:3:LEU:HD12	1.03	1.02
2:D:4:THR:CG2	2:D:6:GLU:HG2	1.88	1.01
3:D:147:HEM:HHC	3:D:147:HEM:HBB2	1.43	1.01
2:D:1:VAL:HG21	2:D:3:LEU:CD1	1.94	0.95
2:D:3:LEU:HD23	2:D:7:GLU:CB	1.99	0.93
2:B:1:VAL:CG1	2:B:3:LEU:HD13	1.99	0.92
2:B:5:PRO:HA	2:B:8:LYS:HD2	1.51	0.92
2:B:8:LYS:O	2:B:12:THR:HB	1.70	0.91
1:A:114:PRO:O	2:B:116:HIS:HE1	1.51	0.90
2:B:1:VAL:HG13	2:B:3:LEU:HD13	1.53	0.90
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.55	0.89
2:D:1:VAL:CG2	2:D:3:LEU:CD1	2.50	0.88
2:D:5:PRO:HD2	2:D:6:GLU:OE2	1.75	0.87
2:D:124:PRO:HB2	2:D:125:PRO:HD3	1.57	0.87
2:D:3:LEU:CD2	2:D:7:GLU:HB3	2.04	0.86
2:B:9:SER:O	2:B:12:THR:HG22	1.76	0.85
1:A:16:LYS:HE2	1:A:16:LYS:HA	1.59	0.84
2:D:1:VAL:HG23	2:D:3:LEU:HD12	1.62	0.82
2:D:95:LYS:HD3	2:D:95:LYS:N	1.95	0.81
1:C:118:THR:HG22	1:C:121:VAL:H	1.46	0.81
1:C:7:LYS:O	1:C:11:LYS:HG2	1.81	0.80
1:A:114:PRO:HA	2:B:116:HIS:CE1	2.16	0.80
2:D:1:VAL:HG23	2:D:3:LEU:HB2	1.64	0.80
2:D:106:LEU:HD23	3:D:147:HEM:CBB	2.14	0.77
2:D:73:ASP:HB3	6:D:203:HOH:O	1.86	0.74
1:C:17:VAL:HG12	1:C:21:ALA:HB2	1.68	0.74
2:D:73:ASP:O	2:D:77:HIS:CD2	2.40	0.74
2:D:4:THR:O	2:D:8:LYS:HG2	1.87	0.74
2:D:4:THR:HB	2:D:7:GLU:HG3	1.70	0.73
2:D:86:ALA:HB1	2:D:144:LYS:HE2	1.71	0.71
2:D:4:THR:HG22	2:D:6:GLU:HG2	1.72	0.70
1:C:4:PRO:O	1:C:8:THR:HG23	1.93	0.69
1:C:114:PRO:HB3	6:D:178:HOH:O	1.91	0.69
2:D:4:THR:HB	2:D:7:GLU:CG	2.22	0.69
2:B:5:PRO:HA	2:B:8:LYS:CD	2.24	0.68
1:A:114:PRO:O	2:B:116:HIS:CE1	2.42	0.67
2:D:1:VAL:C	2:D:3:LEU:H	2.03	0.67
2:D:4:THR:CG2	2:D:7:GLU:HG3	2.26	0.66
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.78	0.65
2:D:73:ASP:O	2:D:77:HIS:HD2	1.77	0.65
2:D:106:LEU:HD23	3:D:147:HEM:HBB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:PRO:O	2:D:55:MET:HG2	1.96	0.65
2:B:1:VAL:CG2	2:B:136:GLY:HA3	2.27	0.65
2:D:60:VAL:CG1	6:D:191:HOH:O	1.77	0.65
2:D:4:THR:CG2	2:D:6:GLU:CG	2.71	0.65
2:D:3:LEU:O	2:D:8:LYS:HE3	1.96	0.64
1:C:17:VAL:CG1	1:C:21:ALA:HB2	2.27	0.64
2:D:4:THR:HG21	2:D:6:GLU:HG2	1.76	0.64
2:D:124:PRO:N	2:D:125:PRO:CD	2.61	0.64
2:D:1:VAL:O	2:D:3:LEU:N	2.23	0.64
2:D:68:LEU:O	2:D:72:SER:HB2	1.97	0.64
1:C:114:PRO:HA	2:D:116:HIS:CD2	2.33	0.63
1:C:76:MET:N	1:C:77:PRO:CD	2.61	0.63
2:B:1:VAL:HG13	2:B:3:LEU:CD1	2.25	0.63
2:D:3:LEU:HB3	2:D:8:LYS:HD3	1.81	0.63
1:C:6:ASP:O	1:C:10:VAL:HG13	1.98	0.63
2:D:6:GLU:CD	2:D:6:GLU:H	2.06	0.63
1:C:56:LYS:NZ	1:C:56:LYS:CB	2.63	0.62
1:A:47:ASP:N	1:A:54:GLN:OE1	2.28	0.62
2:D:57:ASN:OD1	2:D:59:LYS:HG2	2.00	0.62
2:D:4:THR:HG23	2:D:6:GLU:CD	2.22	0.62
2:B:5:PRO:HG2	2:B:6:GLU:N	2.14	0.61
2:D:124:PRO:CB	2:D:125:PRO:HD3	2.25	0.61
1:C:24:TYR:N	1:C:24:TYR:CD2	2.69	0.61
2:D:26:GLU:HG2	2:D:113:VAL:CG1	2.32	0.60
2:D:4:THR:HG22	2:D:7:GLU:H	1.66	0.60
1:A:16:LYS:HZ3	1:A:16:LYS:HB3	1.66	0.60
2:D:89:SER:HB3	2:D:144:LYS:HG3	1.84	0.59
2:D:1:VAL:C	2:D:3:LEU:N	2.59	0.59
1:A:16:LYS:HE2	1:A:16:LYS:CA	2.32	0.59
1:C:3:SER:O	1:C:7:LYS:HG3	2.03	0.59
1:C:76:MET:HB2	1:C:77:PRO:HD3	1.85	0.59
1:C:89:HIS:C	1:C:92:ARG:HD2	2.28	0.58
2:D:4:THR:O	2:D:8:LYS:CG	2.50	0.58
1:C:31:ARG:HD3	2:D:127:GLN:OE1	2.03	0.58
2:D:45:PHE:HD2	2:D:45:PHE:N	2.00	0.58
1:C:113:LEU:N	1:C:114:PRO:CD	2.66	0.58
2:D:3:LEU:HD23	2:D:7:GLU:HB2	1.84	0.58
2:D:45:PHE:N	2:D:45:PHE:CD2	2.72	0.57
1:A:16:LYS:HA	1:A:16:LYS:CE	2.25	0.57
1:C:56:LYS:NZ	1:C:56:LYS:HB3	2.19	0.57
2:D:38:THR:HG22	2:D:102:ASN:ND2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:O	1:C:70:VAL:HG23	2.04	0.57
5:B:315:IHP:O36	2:D:82:LYS:NZ	2.38	0.56
2:D:45:PHE:CG	2:D:59:LYS:HG3	2.40	0.56
1:C:53:ALA:HA	1:C:56:LYS:HD3	1.87	0.56
2:D:21:ASP:HA	2:D:65:LYS:HG3	1.88	0.56
1:C:99:LYS:HG2	6:C:198:HOH:O	2.06	0.55
2:D:30:ARG:O	2:D:34:VAL:HG23	2.06	0.55
2:D:2:HIS:O	2:D:132:LYS:NZ	2.37	0.55
1:A:43:PHE:N	1:A:44:PRO:CD	2.69	0.55
1:C:49:SER:O	1:C:52:SER:HB3	2.06	0.55
2:D:73:ASP:CB	6:D:203:HOH:O	2.51	0.54
2:D:45:PHE:O	2:D:59:LYS:HE3	2.08	0.54
1:A:16:LYS:HB3	1:A:16:LYS:NZ	2.22	0.54
2:B:1:VAL:HG21	2:B:136:GLY:HA3	1.89	0.54
2:B:1:VAL:HG23	2:B:136:GLY:HA3	1.89	0.54
1:C:40:LYS:HG2	1:C:48:LEU:HD13	1.90	0.54
2:D:124:PRO:HD2	2:D:125:PRO:HD3	1.90	0.53
2:D:94:ASP:C	2:D:95:LYS:HD3	2.33	0.53
2:B:53:ALA:O	2:B:57:ASN:HB2	2.07	0.53
2:B:124:PRO:HB2	2:B:125:PRO:HD3	1.90	0.53
2:B:5:PRO:CA	2:B:8:LYS:HD2	2.34	0.52
3:B:147:HEM:HBC2	3:B:147:HEM:HMC2	1.91	0.52
2:D:1:VAL:CG2	2:D:3:LEU:HB2	2.39	0.52
2:D:124:PRO:CD	2:D:125:PRO:HD3	2.39	0.52
2:B:5:PRO:CG	2:B:6:GLU:N	2.72	0.52
1:C:56:LYS:HB3	1:C:56:LYS:HZ3	1.74	0.52
2:D:124:PRO:HB2	2:D:125:PRO:CD	2.36	0.52
2:D:4:THR:O	2:D:7:GLU:HB2	2.10	0.51
1:A:20:HIS:HB3	1:A:24:TYR:CE2	2.46	0.51
1:A:43:PHE:N	1:A:44:PRO:HD3	2.25	0.51
1:A:114:PRO:HA	2:B:116:HIS:HE1	1.71	0.51
2:D:1:VAL:HG23	2:D:3:LEU:CB	2.38	0.51
2:D:26:GLU:HG2	2:D:113:VAL:HG13	1.91	0.51
2:B:12:THR:HG22	2:B:13:ALA:N	2.26	0.51
2:D:19:ASN:OD1	2:D:21:ASP:HB2	2.11	0.51
2:D:34:VAL:C	2:D:36:PRO:HD3	2.36	0.51
5:B:315:IHP:O21	2:D:2:HIS:NE2	2.44	0.50
2:D:4:THR:CB	2:D:7:GLU:HG3	2.38	0.50
2:B:68:LEU:O	2:B:72:SER:HB2	2.10	0.50
1:C:75:ASP:OD1	1:C:78:ASN:HB2	2.12	0.50
2:D:63:HIS:HE1	3:D:147:HEM:CHA	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:TYR:C	1:A:44:PRO:HD3	2.37	0.49
1:A:39:THR:HG22	1:A:97:ASN:HD22	1.77	0.49
1:C:16:LYS:NZ	1:C:16:LYS:HB3	2.27	0.49
2:D:89:SER:HB3	2:D:144:LYS:CG	2.41	0.49
2:D:63:HIS:CE1	3:D:147:HEM:C4D	3.01	0.49
1:C:43:PHE:N	1:C:44:PRO:CD	2.75	0.49
2:D:82:LYS:HB2	6:D:168:HOH:O	2.12	0.49
2:B:43:GLU:HG3	6:B:351:HOH:O	2.13	0.49
2:D:74:GLY:HA2	2:D:84:THR:HG21	1.94	0.49
2:D:86:ALA:O	2:D:90:GLU:HG3	2.12	0.49
2:D:24:GLY:HA2	2:D:68:LEU:HG	1.95	0.48
2:D:50:THR:HB	6:D:181:HOH:O	2.13	0.48
2:D:143:HIS:CE1	2:D:144:LYS:HD3	2.49	0.48
2:D:66:LYS:HD3	3:D:147:HEM:HAA2	1.95	0.48
1:A:16:LYS:CA	1:A:16:LYS:CE	2.87	0.48
1:C:72:HIS:CB	1:C:79:ALA:HB2	2.43	0.48
1:C:17:VAL:HG23	1:C:113:LEU:HD11	1.96	0.48
2:D:71:PHE:CE2	2:D:75:LEU:HD11	2.49	0.48
1:A:33:PHE:CD1	1:A:40:LYS:HG2	2.48	0.48
2:D:63:HIS:HE1	3:D:147:HEM:C4D	2.32	0.47
1:A:86:LEU:HD21	3:A:142:HEM:HBA2	1.96	0.47
1:C:87:HIS:HA	1:C:91:LEU:HB2	1.97	0.47
1:C:84:SER:HB3	1:C:135:VAL:O	2.15	0.47
1:C:76:MET:N	1:C:77:PRO:HD2	2.28	0.47
2:B:74:GLY:HA2	2:B:84:THR:HG21	1.97	0.46
1:A:42:TYR:CE1	1:A:93:VAL:HA	2.50	0.46
1:C:3:SER:HB2	1:C:4:PRO:HD2	1.98	0.46
2:D:60:VAL:O	2:D:64:GLY:N	2.40	0.46
1:C:56:LYS:CB	1:C:56:LYS:HZ2	2.29	0.46
1:C:114:PRO:HA	2:D:116:HIS:NE2	2.31	0.46
2:D:82:LYS:HD3	2:D:143:HIS:CG	2.51	0.46
1:A:113:LEU:HB3	1:A:116:GLU:HB2	1.97	0.45
1:C:3:SER:CB	1:C:4:PRO:CD	2.94	0.45
2:B:14:LEU:C	2:B:16:GLY:N	2.73	0.45
2:B:5:PRO:CD	2:B:6:GLU:H	2.28	0.45
2:B:94:ASP:OD2	2:B:146:HIS:NE2	2.45	0.45
1:C:106:LEU:HA	1:C:106:LEU:HD12	1.62	0.45
1:C:76:MET:CB	1:C:77:PRO:HD3	2.46	0.45
1:A:92:ARG:HD2	6:A:186:HOH:O	2.17	0.45
2:D:82:LYS:HD3	2:D:143:HIS:CD2	2.52	0.45
2:D:57:ASN:HA	2:D:58:PRO:HD2	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:THR:CG2	2:D:6:GLU:OE2	2.44	0.44
1:C:96:VAL:HG12	6:C:190:HOH:O	2.17	0.44
1:A:137:THR:HA	1:A:140:TYR:CD2	2.52	0.44
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.45	0.44
2:B:12:THR:CG2	2:B:13:ALA:N	2.80	0.44
2:D:25:GLY:HA3	2:D:61:LYS:HG3	1.99	0.44
2:B:88:LEU:HD23	2:B:88:LEU:HA	1.88	0.43
2:D:38:THR:HG22	2:D:102:ASN:HD21	1.83	0.43
1:A:113:LEU:N	1:A:114:PRO:CD	2.81	0.43
2:D:45:PHE:O	2:D:57:ASN:ND2	2.43	0.43
1:C:3:SER:HB2	1:C:4:PRO:CD	2.48	0.43
1:C:20:HIS:HB3	1:C:24:TYR:CE2	2.54	0.43
2:D:124:PRO:CD	2:D:125:PRO:CD	2.96	0.43
1:A:16:LYS:NZ	1:A:16:LYS:CB	2.77	0.43
1:A:33:PHE:HD1	1:A:33:PHE:HA	1.63	0.42
2:D:4:THR:HG22	2:D:7:GLU:N	2.34	0.42
2:D:77:HIS:CD2	2:D:77:HIS:N	2.84	0.42
1:A:113:LEU:O	1:A:117:PHE:N	2.52	0.42
1:C:112:HIS:C	1:C:114:PRO:HD3	2.44	0.42
1:A:141:ARG:HB3	2:D:36:PRO:HG2	2.01	0.42
2:B:3:LEU:HG	2:B:7:GLU:HB3	2.01	0.42
1:C:42:TYR:CE1	1:C:93:VAL:HA	2.55	0.42
2:D:76:ALA:HB3	2:D:77:HIS:NE2	2.34	0.42
2:D:146:HIS:CD2	2:D:146:HIS:N	2.87	0.42
1:A:80:LEU:HB2	1:A:135:VAL:HG11	2.02	0.42
2:D:4:THR:HB	2:D:7:GLU:OE2	2.19	0.42
1:A:136:LEU:HD12	3:A:142:HEM:HBB2	2.00	0.42
1:C:2:LEU:HD22	1:C:6:ASP:HB3	2.02	0.41
1:C:20:HIS:O	1:C:23:GLU:HB2	2.20	0.41
2:D:42:PHE:O	2:D:48:LEU:HD11	2.20	0.41
2:D:71:PHE:HE2	2:D:75:LEU:HD11	1.85	0.41
2:D:77:HIS:CB	2:D:84:THR:OG1	2.68	0.41
2:B:5:PRO:CG	2:B:6:GLU:H	2.34	0.41
1:A:35:SER:HB3	2:B:131:GLN:HG3	2.01	0.41
2:D:3:LEU:HA	2:D:7:GLU:OE2	2.20	0.41
1:C:35:SER:HB3	2:D:131:GLN:HG3	2.03	0.41
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.82	0.41
2:D:118:PHE:O	2:D:121:GLU:HB3	2.21	0.41
1:A:83:LEU:HD21	3:A:142:HEM:HBB	2.02	0.41
1:C:37:PRO:HA	1:C:40:LYS:HD3	2.03	0.41
2:D:33:VAL:HG22	2:D:51:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:THR:HA	2:D:51:PRO:HD3	1.93	0.41
1:A:14:TRP:CG	1:A:70:VAL:HG21	2.56	0.41
1:A:76:MET:N	1:A:77:PRO:CD	2.84	0.41
2:B:8:LYS:HE2	2:B:8:LYS:HB3	1.40	0.41
1:C:24:TYR:N	1:C:24:TYR:HD2	2.19	0.41
1:A:92:ARG:HE	1:A:92:ARG:HB2	1.53	0.40
1:C:33:PHE:CD1	1:C:40:LYS:HG3	2.56	0.40
3:D:147:HEM:HHC	3:D:147:HEM:CBB	2.29	0.40
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.91	0.40
2:D:30:ARG:HD2	2:D:113:VAL:CG2	2.51	0.40
2:D:66:LYS:HB2	2:D:66:LYS:HE3	1.15	0.40
2:D:68:LEU:HA	2:D:68:LEU:HD22	1.70	0.40
2:D:4:THR:HG23	2:D:6:GLU:CG	2.48	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)
6:A:234:HOH:O	6:A:234:HOH:O[2_665]	1.76	0.44

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%)	136 (98%)	3 (2%)	0	100	100
1	C	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
2	B	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	D	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
All	All	566/574 (99%)	550 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	113/113 (100%)	109 (96%)	4 (4%)	32	7
1	C	113/113 (100%)	98 (87%)	15 (13%)	4	0
2	B	118/118 (100%)	102 (86%)	16 (14%)	3	0
2	D	118/118 (100%)	99 (84%)	19 (16%)	2	0
All	All	462/462 (100%)	408 (88%)	54 (12%)	5	0

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	84	SER
1	A	90	LYS
1	A	95	PRO
2	B	1	VAL
2	B	2	HIS
2	B	6	GLU
2	B	8	LYS
2	B	12	THR
2	B	18	VAL
2	B	22	GLU
2	B	52	ASP
2	B	59	LYS
2	B	66	LYS
2	B	68	LEU
2	B	72	SER
2	B	75	LEU
2	B	78	LEU
2	B	82	LYS
2	B	120	LYS
1	C	8	THR
1	C	10	VAL
1	C	11	LYS
1	C	16	LYS

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Mol	Chain	Res	Type
1	C	17	VAL
1	C	45	HIS
1	C	52	SER
1	C	56	LYS
1	C	73	VAL
1	C	78	ASN
1	C	84	SER
1	C	90	LYS
1	C	106	LEU
1	C	118	THR
1	C	136	LEU
2	D	3	LEU
2	D	4	THR
2	D	6	GLU
2	D	8	LYS
2	D	12	THR
2	D	26	GLU
2	D	59	LYS
2	D	60	VAL
2	D	61	LYS
2	D	65	LYS
2	D	66	LYS
2	D	68	LEU
2	D	77	HIS
2	D	78	LEU
2	D	87	THR
2	D	95	LYS
2	D	120	LYS
2	D	124	PRO
2	D	143	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	97	ASN
2	B	80	ASN
2	B	102	ASN
2	B	116	HIS
2	B	117	HIS
1	C	68	ASN
2	D	63	HIS

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Mol	Chain	Res	Type
2	D	77	HIS
2	D	80	ASN
2	D	102	ASN

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](#)

7 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	C	142	1,4	50,50,50	1.61	9 (18%)	67,82,82	1.86	14 (20%)
5	IHP	B	315	-	36,36,36	1.28	6 (16%)	60,60,60	1.15	4 (6%)
4	OXY	C	143	3	1,1,1	0.44	0	-		
4	OXY	A	143	3	1,1,1	0.31	0	-		
3	HEM	D	147	2	50,50,50	1.64	11 (22%)	67,82,82	2.53	24 (35%)
3	HEM	A	142	1,4	50,50,50	1.93	12 (24%)	67,82,82	2.13	27 (40%)
3	HEM	B	147	2	50,50,50	1.70	12 (24%)	67,82,82	2.75	28 (41%)

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	C	142	1,4	-	6/14/54/54	-
5	IHP	B	315	-	-	2/30/54/54	0/1/1/1
3	HEM	D	147	2	-	5/14/54/54	-
3	HEM	A	142	1,4	-	6/14/54/54	-
3	HEM	B	147	2	-	2/14/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	142	HEM	FE-NC	4.85	2.11	1.95
3	A	142	HEM	FE-ND	4.49	2.08	1.94
3	B	147	HEM	FE-NA	4.09	2.08	1.95
3	C	142	HEM	FE-NB	4.07	2.07	1.94
3	A	142	HEM	CAC-C3C	3.96	1.58	1.47
3	C	142	HEM	FE-NC	3.89	2.08	1.95
3	B	147	HEM	FE-NC	3.88	2.08	1.95
3	A	142	HEM	CAB-C3B	3.76	1.57	1.47
3	A	142	HEM	FE-NB	3.71	2.06	1.94
3	D	147	HEM	FE-NC	3.71	2.07	1.95
3	D	147	HEM	CAC-C3C	3.65	1.57	1.47
3	C	142	HEM	FE-ND	3.60	2.06	1.94
3	D	147	HEM	FE-NA	3.45	2.06	1.95
3	D	147	HEM	CAB-C3B	3.44	1.56	1.47
3	B	147	HEM	CAB-C3B	3.32	1.56	1.47
3	A	142	HEM	CMB-C2B	3.24	1.57	1.50
3	B	147	HEM	C4A-C3A	3.24	1.50	1.43
5	B	315	IHP	P4-O14	3.23	1.65	1.59
3	D	147	HEM	CMB-C2B	3.23	1.57	1.50
3	B	147	HEM	C1C-C2C	3.18	1.51	1.45
3	C	142	HEM	CAB-C3B	3.05	1.55	1.47
3	D	147	HEM	C2A-C3A	-2.93	1.31	1.38
3	C	142	HEM	CMB-C2B	2.84	1.56	1.50
3	B	147	HEM	C1A-C2A	2.79	1.50	1.44
5	B	315	IHP	C6-C1	2.78	1.58	1.52
3	A	142	HEM	CMD-C2D	2.72	1.56	1.50
3	B	147	HEM	CAC-C3C	2.69	1.54	1.47
3	A	142	HEM	FE-NA	2.68	2.04	1.95
3	C	142	HEM	C1B-NB	-2.57	1.35	1.40
3	A	142	HEM	C2A-C3A	-2.52	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	C3C-C4C	2.51	1.50	1.46
3	A	142	HEM	CHD-C4C	2.45	1.43	1.38
3	C	142	HEM	CMD-C2D	2.42	1.55	1.50
5	B	315	IHP	P2-O12	2.41	1.63	1.59
3	B	147	HEM	CMB-C2B	2.39	1.55	1.50
3	D	147	HEM	FE-NB	2.35	2.02	1.94
3	C	142	HEM	FE-NA	2.34	2.02	1.95
3	B	147	HEM	O2A-CGA	-2.32	1.23	1.30
5	B	315	IHP	P3-O13	2.25	1.63	1.59
3	A	142	HEM	CHC-C1C	2.25	1.42	1.38
3	C	142	HEM	C2A-C3A	-2.24	1.33	1.38
3	D	147	HEM	CHB-C4A	-2.15	1.34	1.39
3	D	147	HEM	CBA-CAA	2.11	1.59	1.51
3	D	147	HEM	CBD-CAD	2.06	1.59	1.51
5	B	315	IHP	P5-O15	2.05	1.63	1.59
3	B	147	HEM	C4C-NC	-2.04	1.35	1.39
3	A	142	HEM	CBA-CGA	2.04	1.55	1.50
3	D	147	HEM	CBD-CGD	2.02	1.55	1.50
3	B	147	HEM	CAD-C3D	2.02	1.56	1.51
5	B	315	IHP	C6-C5	2.01	1.56	1.52

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	C3B-C4B-NB	10.40	116.94	109.47
3	B	147	HEM	C1B-NB-C4B	-7.05	96.86	105.21
3	B	147	HEM	CHC-C4B-NB	-6.59	117.33	124.42
3	D	147	HEM	CHB-C1B-NB	6.00	131.79	124.37
3	B	147	HEM	C2B-C1B-NB	5.78	116.49	109.84
3	D	147	HEM	CHB-C4A-NA	5.20	133.29	123.86
3	D	147	HEM	C4A-CHB-C1B	-5.16	114.11	126.25
3	C	142	HEM	O2D-CGD-O1D	4.91	135.96	123.33
3	D	147	HEM	CMA-C3A-C4A	-4.85	118.03	125.42
3	D	147	HEM	CMA-C3A-C2A	4.82	135.85	125.62
3	C	142	HEM	CMB-C2B-C1B	-4.81	117.53	125.03
3	D	147	HEM	C2A-C1A-NA	-4.74	104.89	110.15
3	D	147	HEM	O1D-CGD-CBD	-4.73	108.08	123.09
3	C	142	HEM	C3B-C2B-C1B	4.73	109.96	106.41
3	D	147	HEM	O2D-CGD-O1D	4.69	135.39	123.33
3	D	147	HEM	CBA-CAA-C2A	-4.67	99.61	112.53
3	A	142	HEM	CAD-C3D-C4D	-4.66	116.58	124.70
3	B	147	HEM	CHD-C4C-NC	4.59	129.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	142	HEM	CHB-C1B-NB	4.55	129.99	124.37
3	B	147	HEM	C2A-C1A-NA	-4.49	105.17	110.15
3	D	147	HEM	O2A-CGA-O1A	4.44	134.75	123.33
3	B	147	HEM	C4C-C3C-C2C	4.44	110.66	106.81
3	A	142	HEM	CHB-C1B-NB	4.40	129.81	124.37
3	D	147	HEM	CAA-CBA-CGA	-4.19	102.56	113.67
3	D	147	HEM	CAD-CBD-CGD	-4.00	103.06	113.67
3	A	142	HEM	O1D-CGD-CBD	-3.99	110.43	123.09
3	A	142	HEM	C4D-C3D-C2D	3.97	112.68	106.89
3	C	142	HEM	C1B-NB-C4B	3.95	109.89	105.21
3	A	142	HEM	C2A-C1A-NA	-3.92	105.80	110.15
3	C	142	HEM	CHC-C4B-NB	3.90	128.62	124.42
3	B	147	HEM	C4B-C3B-C2B	-3.82	103.77	107.28
3	A	142	HEM	CAA-CBA-CGA	-3.81	103.55	113.67
3	B	147	HEM	O2A-CGA-CBA	3.81	126.05	114.00
3	B	147	HEM	C4A-NA-C1A	3.81	112.03	105.82
3	B	147	HEM	CAA-C2A-C1A	-3.77	117.58	124.94
3	D	147	HEM	CAA-C2A-C1A	-3.75	117.62	124.94
3	B	147	HEM	C4C-NC-C1C	3.71	111.86	105.82
3	A	142	HEM	C3B-C4B-NB	-3.69	106.82	109.47
3	A	142	HEM	C3D-C4D-ND	-3.64	106.18	110.17
3	A	142	HEM	CHC-C4B-NB	3.50	128.19	124.42
3	D	147	HEM	C3D-C4D-ND	-3.46	106.37	110.17
3	D	147	HEM	CMD-C2D-C1D	-3.34	119.81	125.03
3	D	147	HEM	CHB-C1B-C2B	-3.34	117.46	126.95
3	A	142	HEM	CAA-C2A-C1A	-3.17	118.75	124.94
3	D	147	HEM	C1A-C2A-C3A	3.14	111.72	106.87
3	B	147	HEM	C4C-CHD-C1D	-3.05	119.55	126.02
3	A	142	HEM	C1A-C2A-C3A	3.04	111.58	106.87
3	D	147	HEM	CMD-C2D-C3D	3.03	134.35	126.15
3	B	147	HEM	CHD-C1D-C2D	-2.99	120.31	125.03
3	D	147	HEM	CHB-C4A-C3A	-2.99	118.74	127.43
3	A	142	HEM	C1B-NB-C4B	2.99	108.74	105.21
3	A	142	HEM	C1D-C2D-C3D	-2.98	103.84	106.98
3	D	147	HEM	C4D-C3D-C2D	2.98	111.23	106.89
3	C	142	HEM	O1D-CGD-CBD	-2.98	113.65	123.09
3	A	142	HEM	CHB-C4A-NA	2.91	129.14	123.86
5	B	315	IHP	C5-C4-C3	2.88	116.75	110.43
3	C	142	HEM	C3B-C4B-NB	-2.85	107.42	109.47
3	B	147	HEM	C2D-C1D-ND	2.85	113.20	109.90
3	A	142	HEM	CHA-C1A-NA	2.83	129.00	123.86
3	C	142	HEM	CHA-C4D-C3D	2.76	130.32	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	147	HEM	CHB-C4A-NA	2.73	128.80	123.86
3	B	147	HEM	CHA-C1A-NA	2.69	128.73	123.86
3	C	142	HEM	C2B-C1B-NB	-2.61	106.84	109.84
3	C	142	HEM	CHA-C4D-ND	-2.60	121.15	124.37
3	B	147	HEM	C3C-C2C-C1C	-2.58	104.61	107.05
3	A	142	HEM	CMB-C2B-C1B	-2.58	121.01	125.03
3	B	147	HEM	CAA-C2A-C3A	2.57	132.83	127.07
3	D	147	HEM	CBD-CAD-C3D	-2.54	105.52	112.53
3	D	147	HEM	C4A-NA-C1A	2.53	109.95	105.82
3	D	147	HEM	CHA-C4D-C3D	2.50	129.84	125.23
3	D	147	HEM	O1A-CGA-CBA	-2.47	115.26	123.09
5	B	315	IHP	P2-O12-C2	-2.47	116.84	123.43
3	B	147	HEM	C4D-ND-C1D	-2.45	102.31	105.21
3	A	142	HEM	C4A-CHB-C1B	-2.44	120.51	126.25
3	C	142	HEM	C4C-C3C-C2C	2.41	108.90	106.81
3	B	147	HEM	C3A-C4A-NA	-2.40	106.29	110.14
3	B	147	HEM	CBA-CAA-C2A	-2.39	105.92	112.53
3	B	147	HEM	C1C-CHC-C4B	2.38	131.08	126.02
3	B	147	HEM	CBC-CAC-C3C	-2.36	115.73	127.53
3	C	142	HEM	C1C-CHC-C4B	-2.36	121.00	126.02
3	A	142	HEM	O2D-CGD-O1D	2.30	129.24	123.33
3	B	147	HEM	O1A-CGA-CBA	-2.26	115.92	123.09
3	A	142	HEM	CBD-CAD-C3D	-2.26	106.29	112.53
3	A	142	HEM	CAD-CBD-CGD	-2.24	107.73	113.67
5	B	315	IHP	O14-C4-C5	-2.18	104.12	108.76
3	C	142	HEM	CHC-C1C-NC	2.16	126.80	124.45
3	A	142	HEM	CHB-C1B-C2B	-2.15	120.84	126.95
5	B	315	IHP	C3-C2-C1	2.14	115.11	110.43
3	A	142	HEM	CMD-C2D-C3D	2.11	131.87	126.15
3	A	142	HEM	CBC-CAC-C3C	-2.11	117.01	127.53
3	A	142	HEM	C4A-NA-C1A	2.08	109.22	105.82
3	A	142	HEM	C4C-C3C-C2C	2.07	108.61	106.81
3	B	147	HEM	O2A-CGA-O1A	-2.07	118.00	123.33
3	A	142	HEM	CHA-C4D-ND	2.06	126.92	124.37
3	B	147	HEM	CMC-C2C-C3C	2.06	133.42	128.43
3	A	142	HEM	O2A-CGA-O1A	2.03	128.55	123.33
3	B	147	HEM	CHB-C1B-C2B	-2.00	121.25	126.95

There are no chirality outliers.

All (21) torsion outliers are listed below:

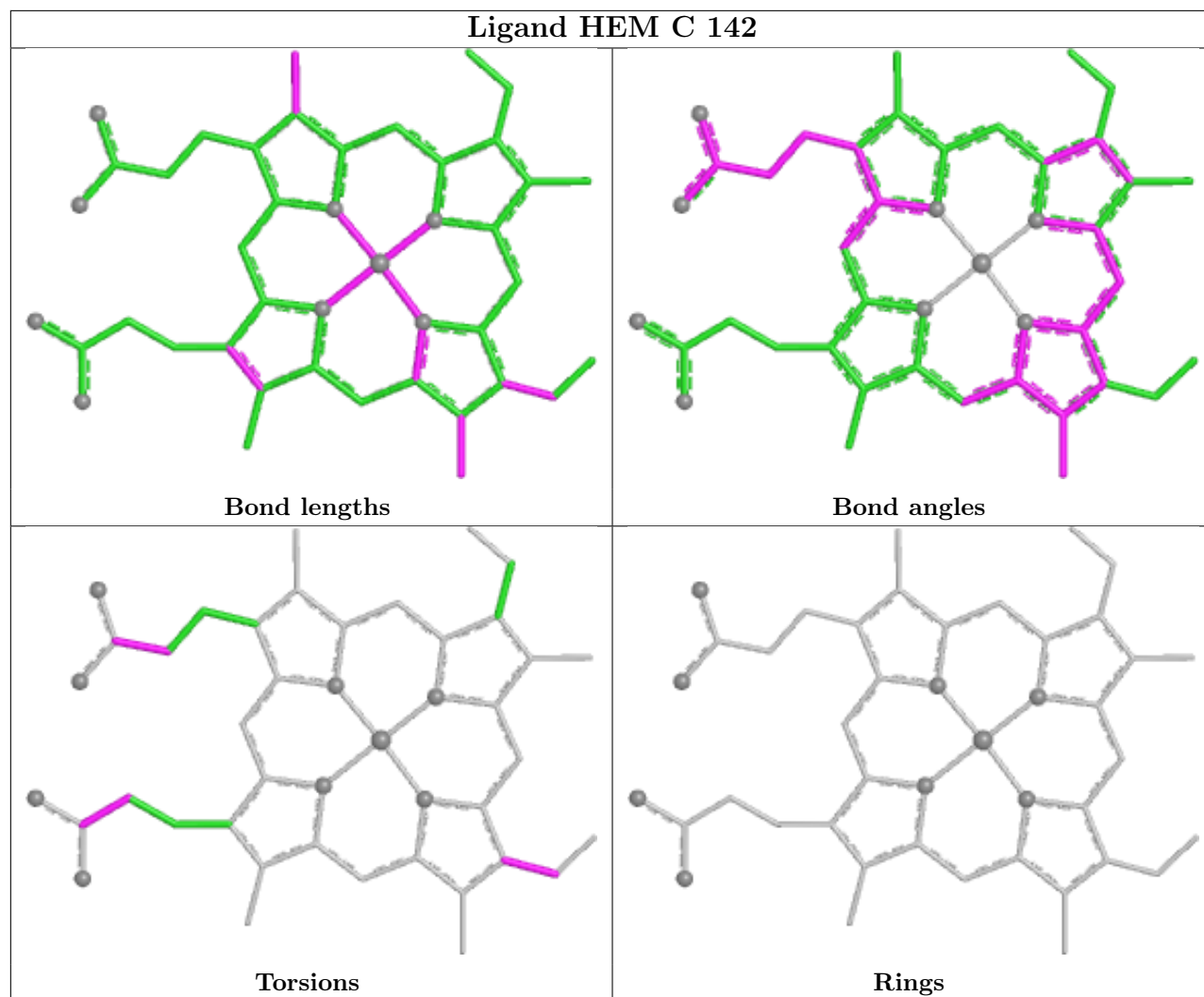
Mol	Chain	Res	Type	Atoms
3	C	142	HEM	C2B-C3B-CAB-CBB
3	C	142	HEM	C4B-C3B-CAB-CBB
5	B	315	IHP	C1-O11-P1-O21
3	A	142	HEM	C2B-C3B-CAB-CBB
3	D	147	HEM	C4B-C3B-CAB-CBB
3	C	142	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAA-CBA-CGA-O1A
3	D	147	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O1D
3	C	142	HEM	CAD-CBD-CGD-O1D
3	D	147	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O2D
3	C	142	HEM	CAD-CBD-CGD-O2D
3	D	147	HEM	CAA-CBA-CGA-O2A
3	B	147	HEM	CAD-CBD-CGD-O1D
3	B	147	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	C4B-C3B-CAB-CBB
3	D	147	HEM	CAD-CBD-CGD-O2D
5	B	315	IHP	C6-O16-P6-O46

There are no ring outliers.

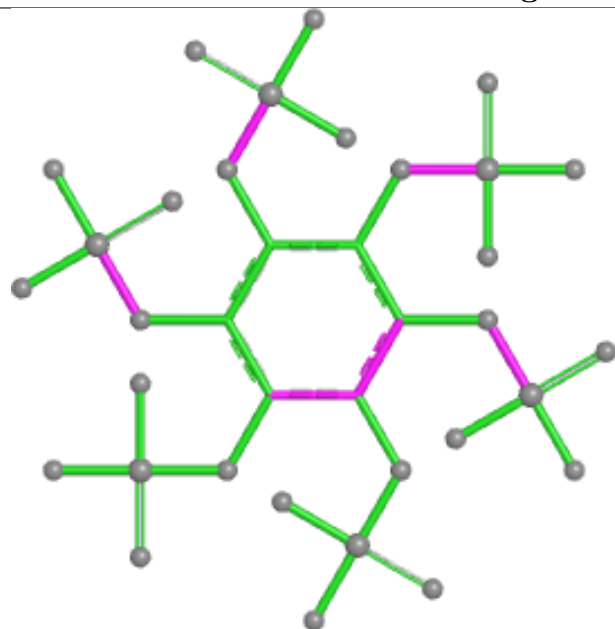
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	315	IHP	2	0
3	D	147	HEM	8	0
3	A	142	HEM	3	0
3	B	147	HEM	1	0

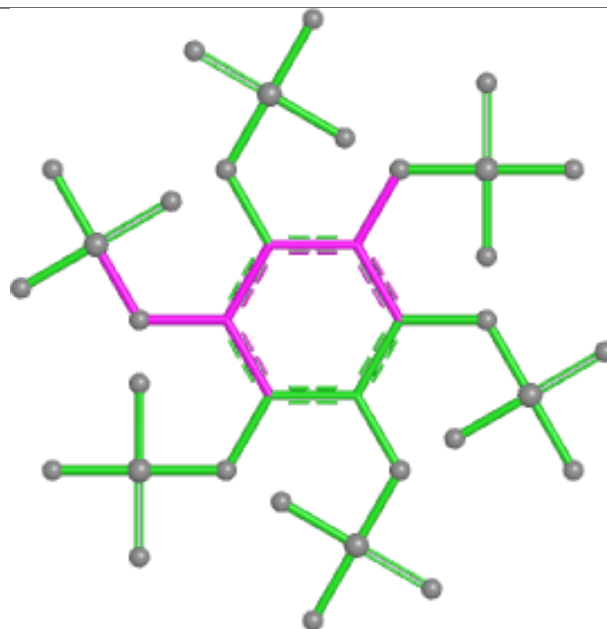
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



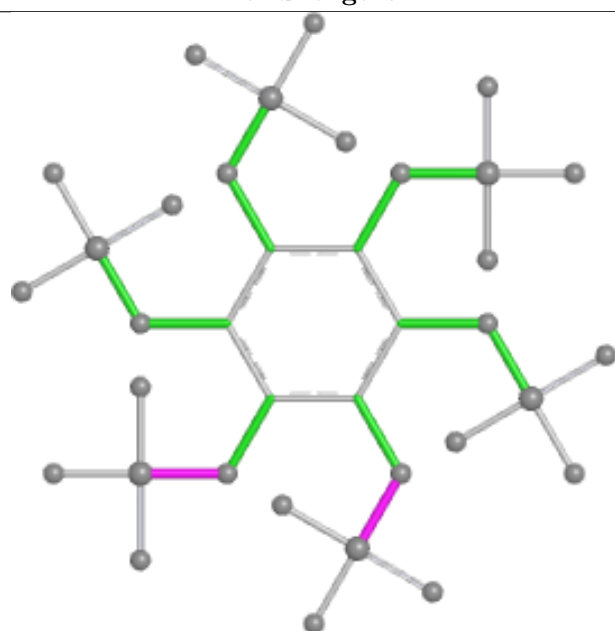
Ligand IHP B 315



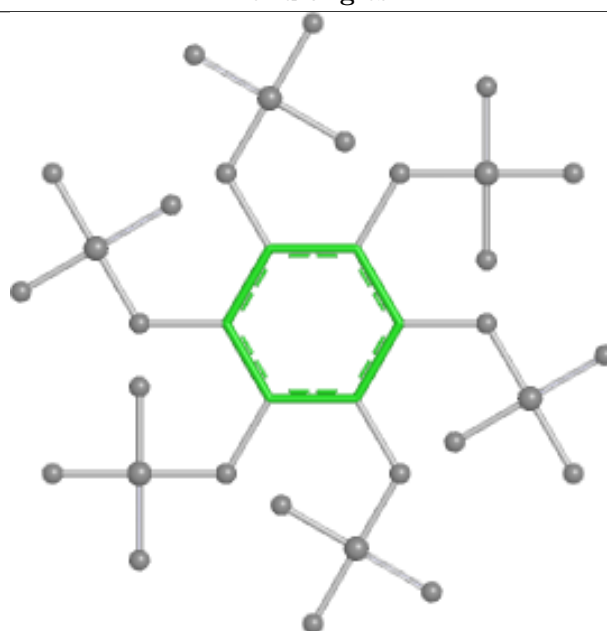
Bond lengths



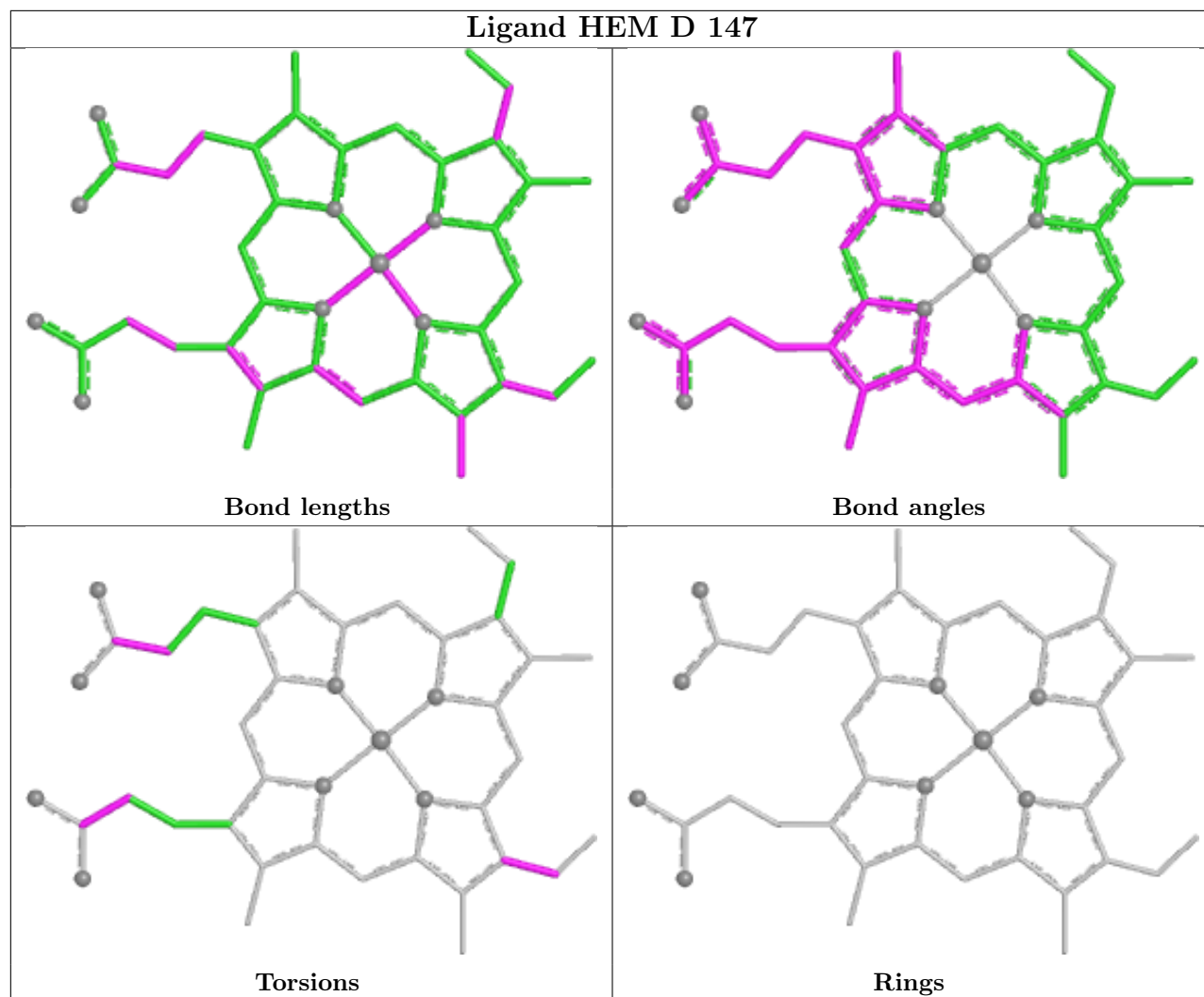
Bond angles

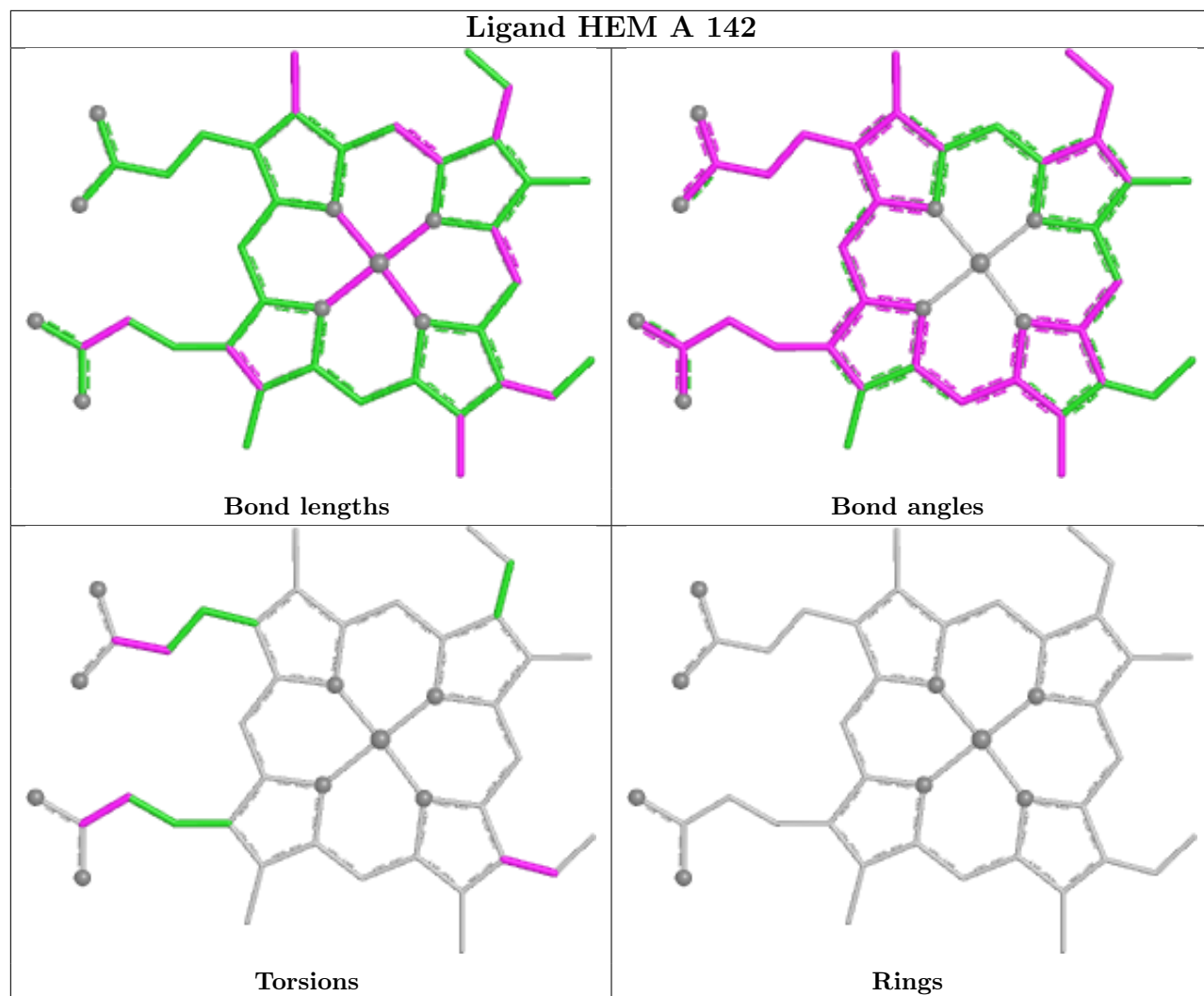


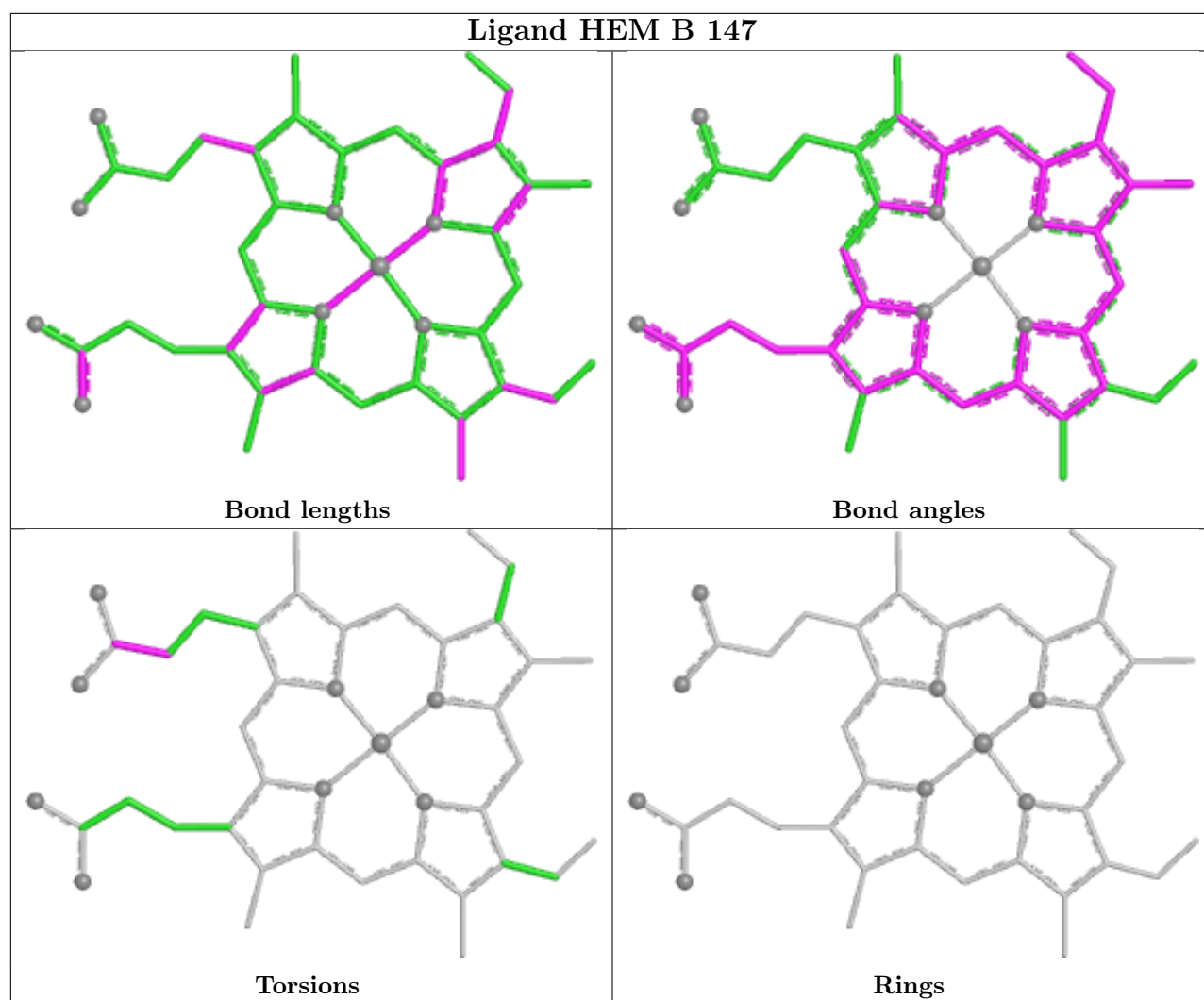
Torsions



Rings







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.27	2 (1%) 73 77	15, 23, 46, 114	0
1	C	141/141 (100%)	0.02	4 (2%) 55 59	16, 29, 51, 72	0
2	B	146/146 (100%)	-0.20	2 (1%) 73 77	14, 23, 53, 75	0
2	D	146/146 (100%)	0.20	4 (2%) 56 60	18, 32, 61, 75	0
All	All	574/574 (100%)	-0.06	12 (2%) 63 67	14, 27, 54, 114	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	VAL	5.2
2	B	1	VAL	3.8
2	D	2	HIS	3.6
1	C	1	VAL	2.9
2	B	4	THR	2.9
1	A	114	PRO	2.6
1	C	114	PRO	2.3
1	A	1	VAL	2.2
2	D	4	THR	2.2
1	C	79	ALA	2.1
2	D	76	ALA	2.1
1	C	81	SER	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

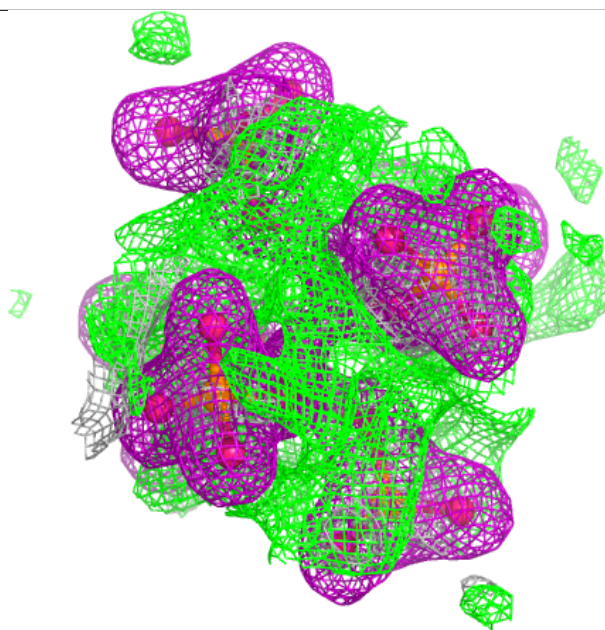
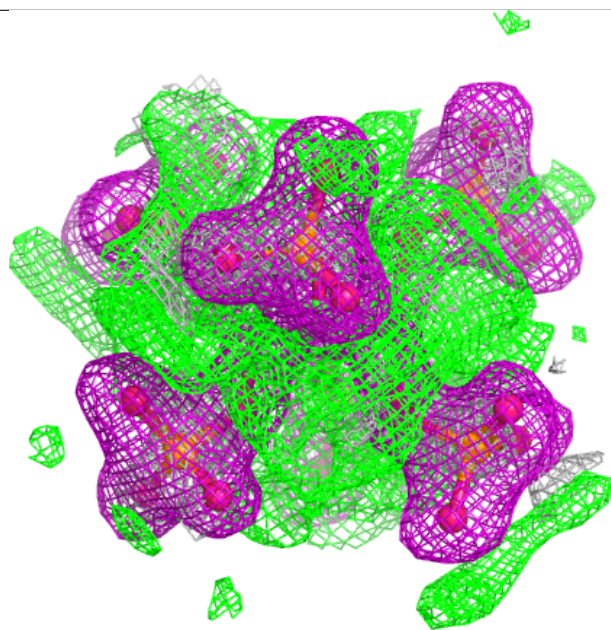
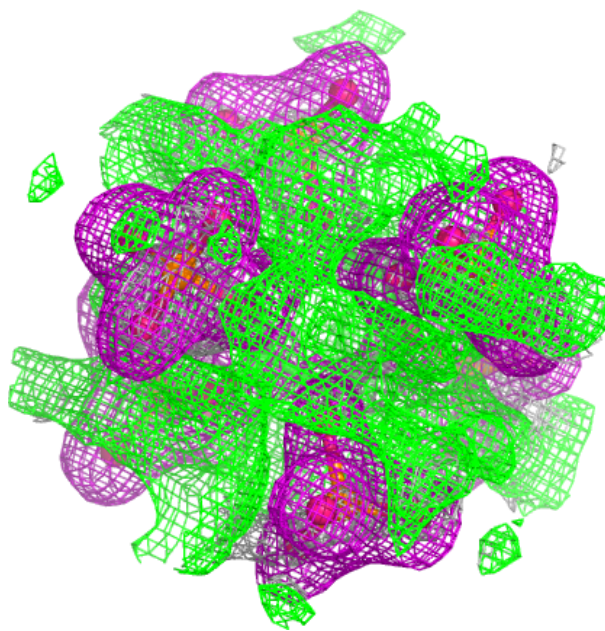
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IHP	B	315	36/36	0.42	0.21	20,20,20,20	0
4	OXY	A	143	2/2	0.86	0.20	25,25,25,36	1
4	OXY	C	143	2/2	0.92	0.10	21,21,21,32	1
3	HEM	D	147	43/43	0.97	0.07	17,27,76,77	0
3	HEM	A	142	43/43	0.97	0.06	17,23,49,77	0
3	HEM	C	142	43/43	0.98	0.05	15,20,41,71	0
3	HEM	B	147	43/43	0.99	0.04	11,16,33,53	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.

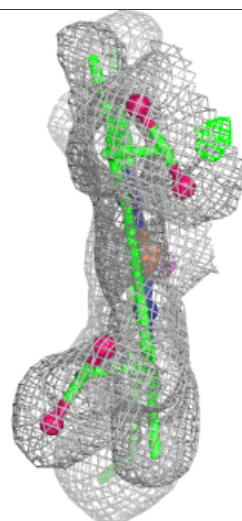
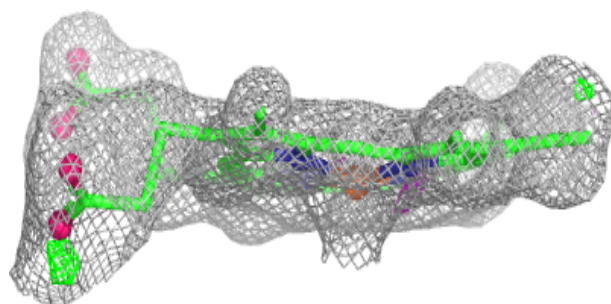
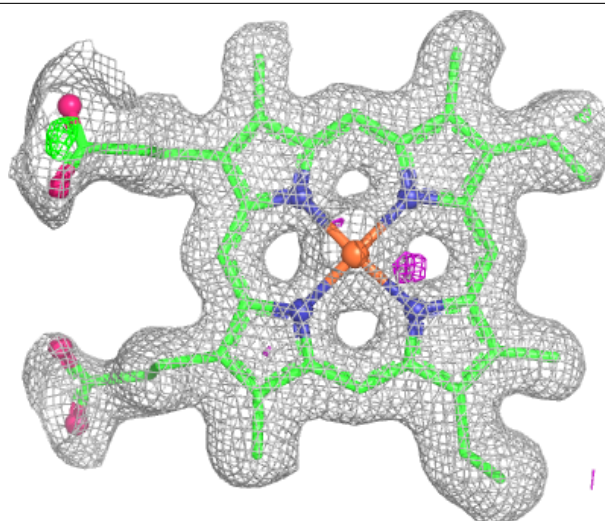
Electron density around IHP B 315:

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



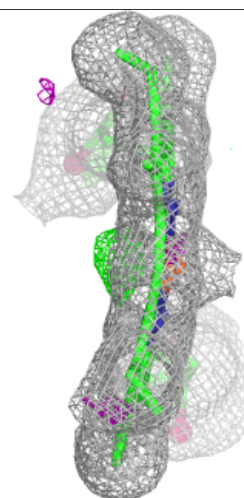
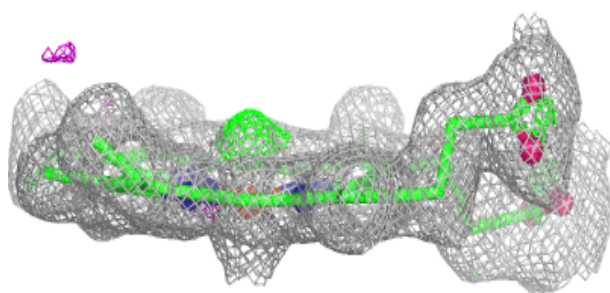
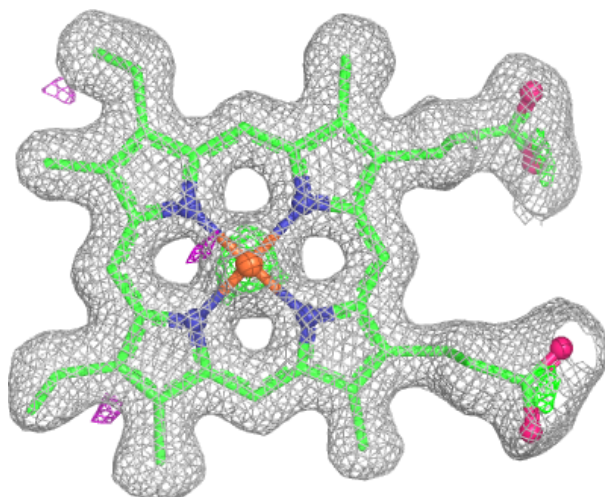
Electron density around HEM D 147:

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



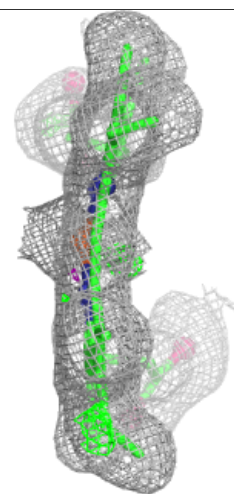
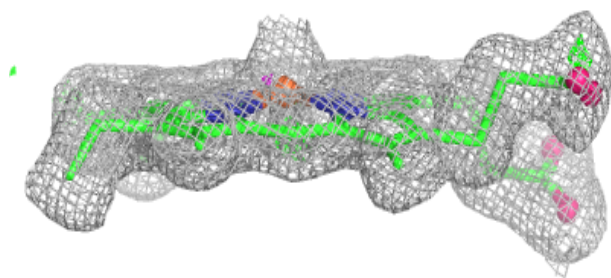
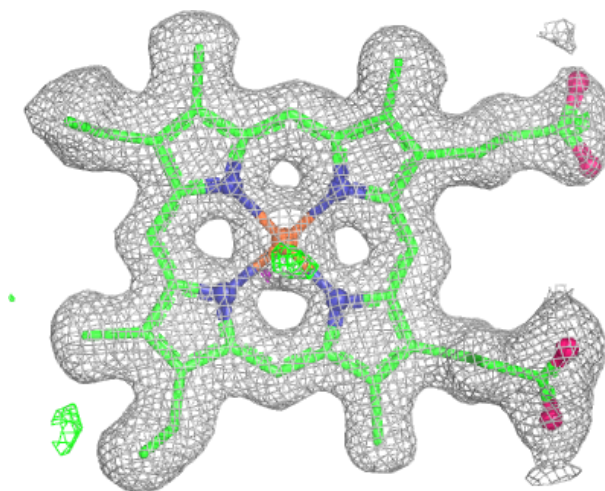
Electron density around HEM A 142:

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



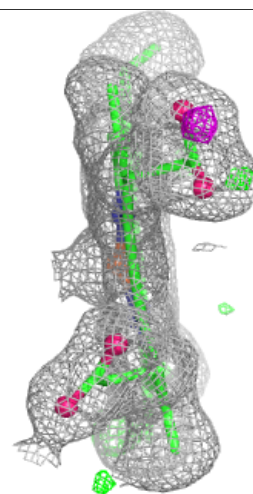
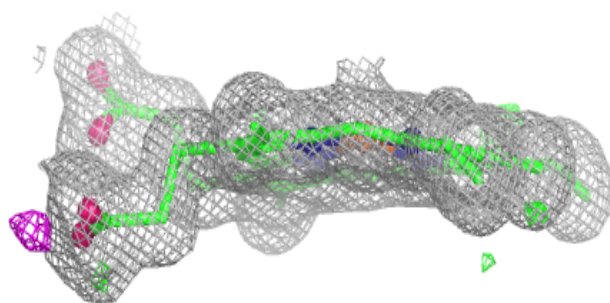
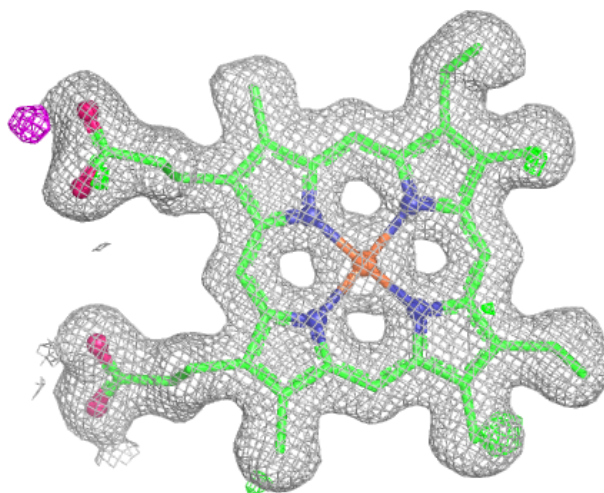
Electron density around HEM C 142:

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



Electron density around HEM B 147:

$2mF_o-DF_c$ (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.