



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:40 AM UTC

PDB ID : 1P7Z / pdb_00001p7z
Title : Crystal structure of the D181S variant of catalase HP11 from E. coli
Authors : Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on : 2003-05-06
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

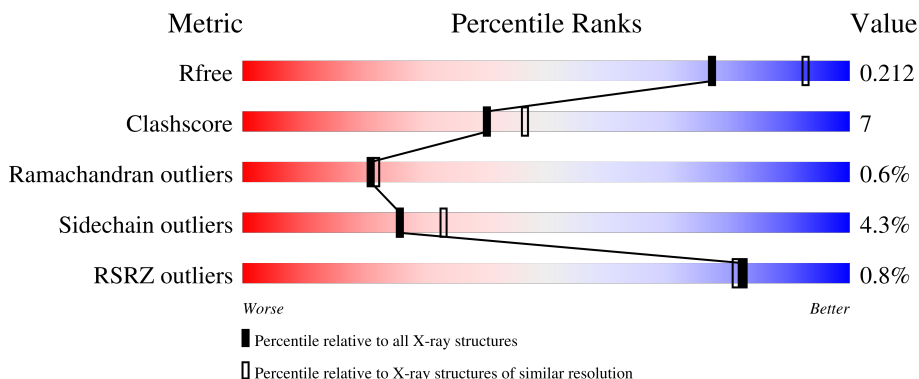
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	753	
1	B	753	
1	C	753	
1	D	753	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25893 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.

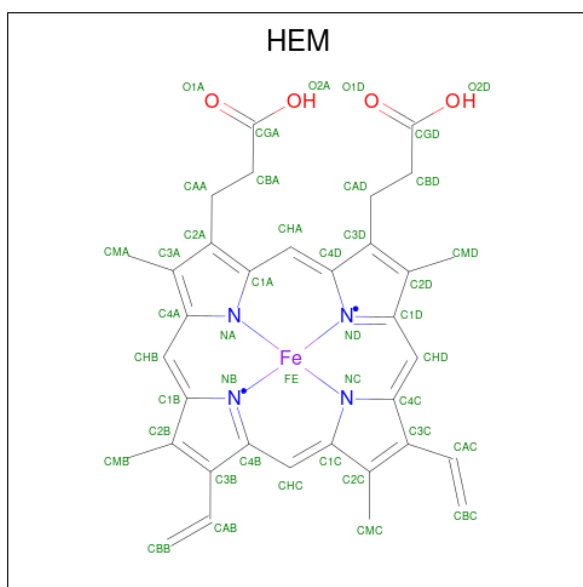
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5747	3649	1005	1081	12			
1	B	727	Total	C	N	O	S	0	1	0
			5747	3649	1005	1081	12			
1	C	727	Total	C	N	O	S	0	1	0
			5747	3649	1005	1081	12			
1	D	727	Total	C	N	O	S	0	1	0
			5747	3649	1005	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	SER	ASP	engineered mutation	UNP P21179
B	181	SER	ASP	engineered mutation	UNP P21179
C	181	SER	ASP	engineered mutation	UNP P21179
D	181	SER	ASP	engineered mutation	UNP P21179

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



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

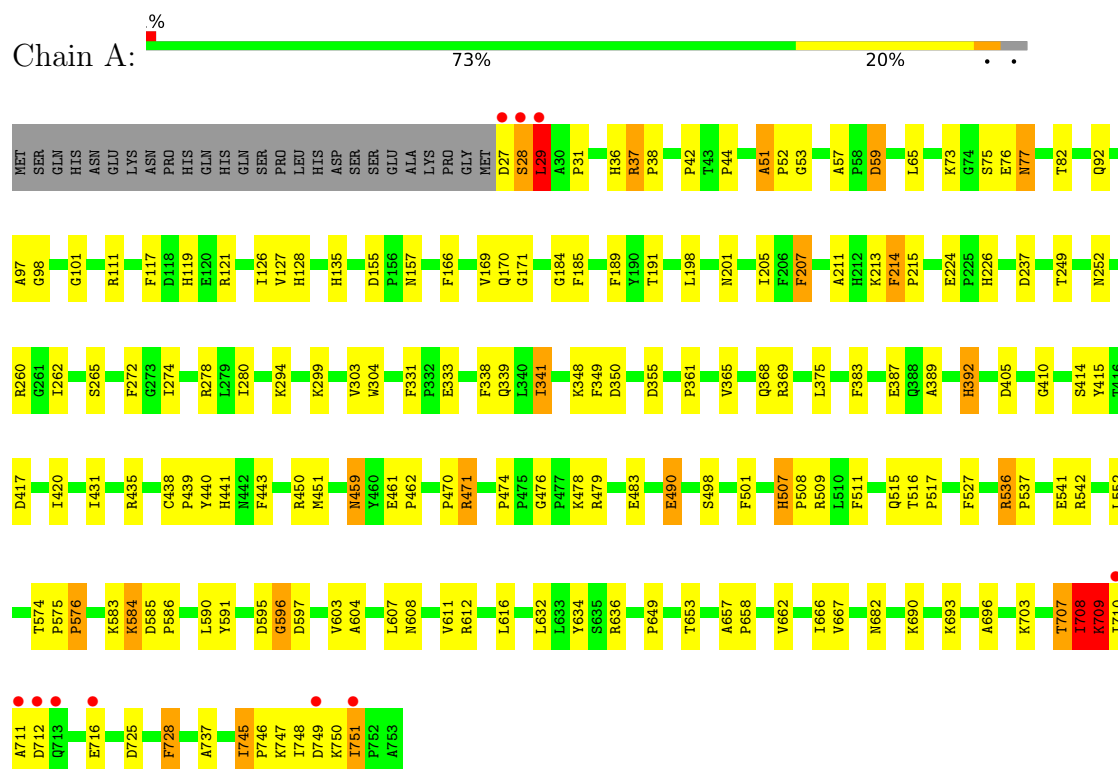
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	739	Total	O	0	0
			739	739		
3	B	610	Total	O	0	0
			610	610		
3	C	674	Total	O	0	0
			674	674		
3	D	710	Total	O	0	0
			710	710		

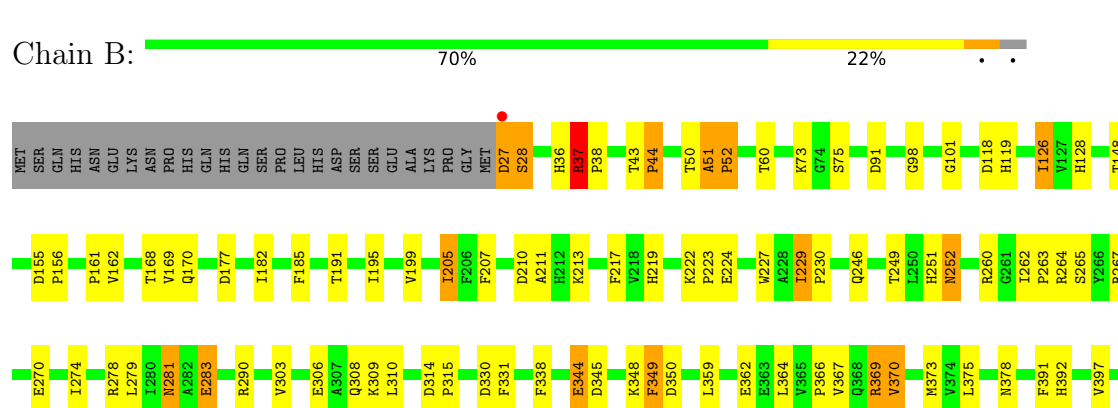
3 Residue-property plots

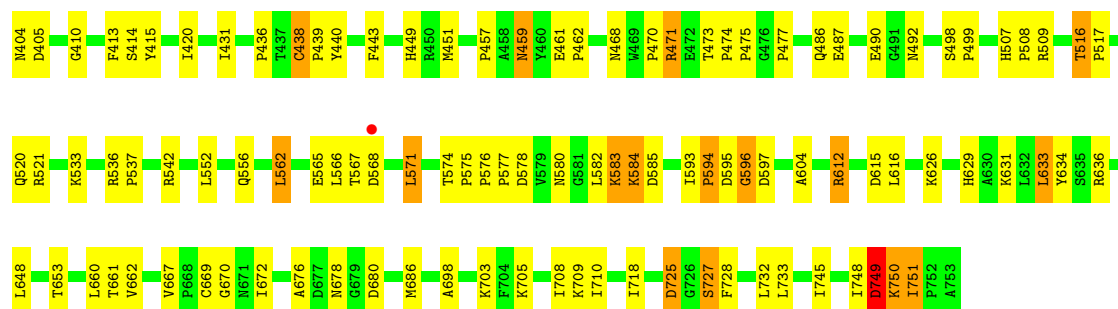
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Catalase HPII

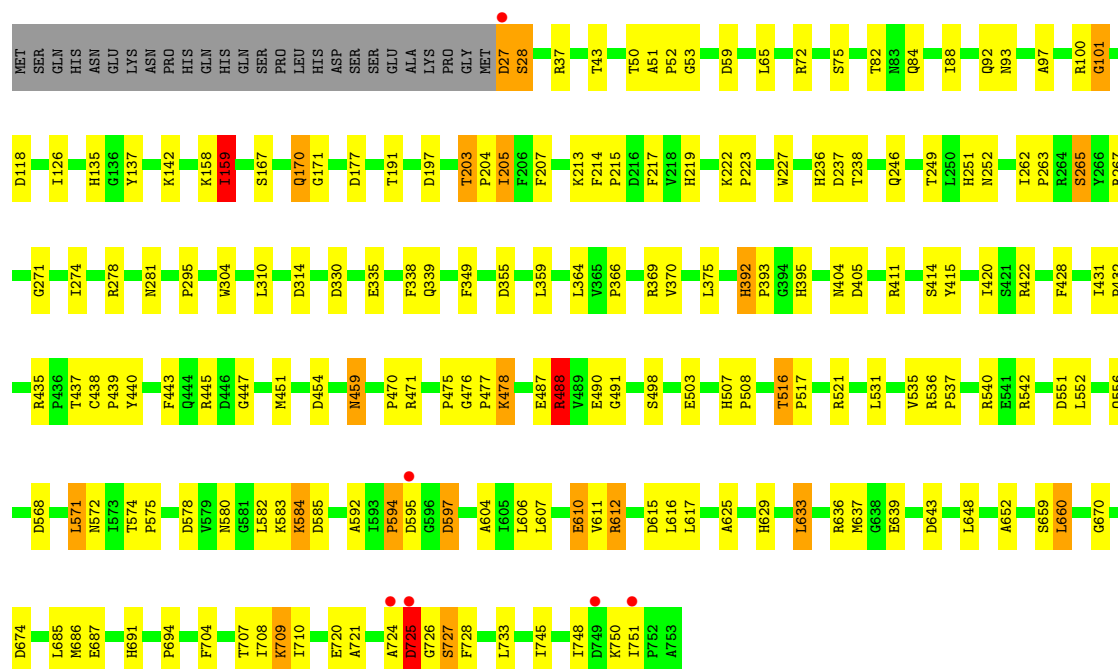
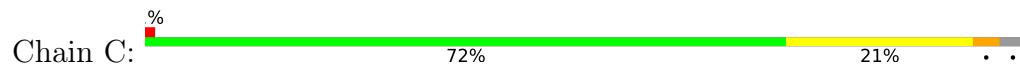


• Molecule 1: Catalase HPII

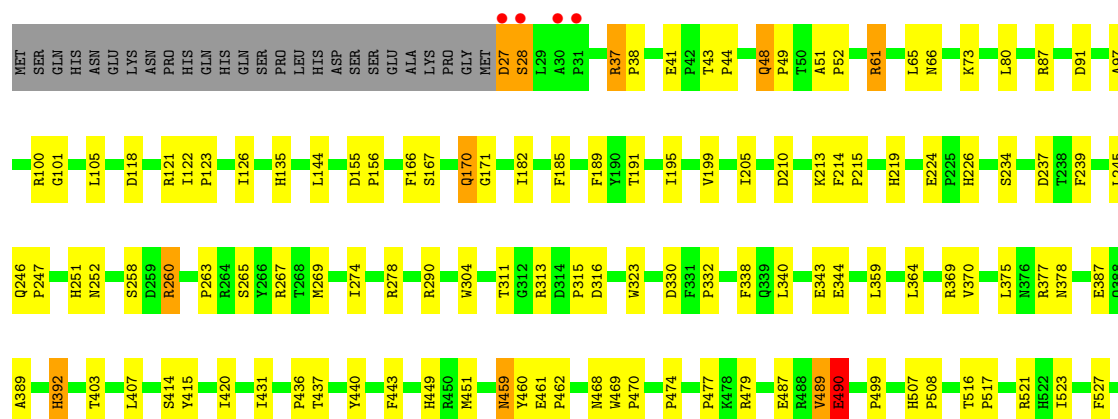


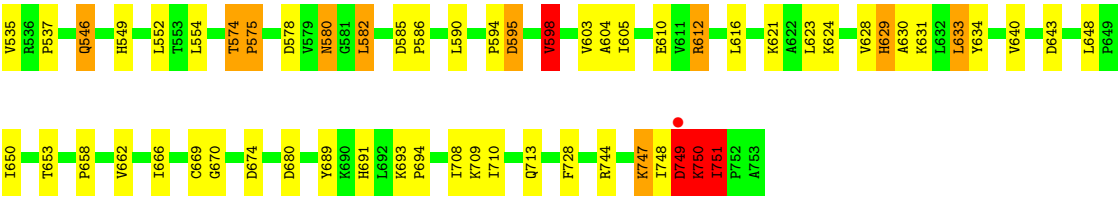


● Molecule 1: Catalase HP11



● Molecule 1: Catalase HP11





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.34Å 132.88Å 121.45Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	29.80 – 2.21 29.80 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.80-2.21) 99.2 (29.80-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.21Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.211 0.161 , 0.212	Depositor DCC
R_{free} test set	6965 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25893	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 3.43% 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	0.70	0/5908	1.71	124/8032 (1.5%)
1	B	0.70	0/5908	1.76	122/8032 (1.5%)
1	C	0.70	0/5908	1.70	104/8032 (1.3%)
1	D	0.71	0/5908	1.74	96/8032 (1.2%)
All	All	0.70	0/23632	1.73	446/32128 (1.4%)

There are no bond length outliers.

All (446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	612	ARG	CD-NE-CZ	30.42	166.98	124.40
1	B	37	ARG	CD-NE-CZ	18.24	149.94	124.40
1	D	449	HIS	CA-CB-CG	15.75	129.55	113.80
1	B	283	GLU	CB-CG-CD	12.09	133.15	112.60
1	B	595	ASP	CA-CB-CG	11.33	123.93	112.60
1	D	27	ASP	CA-CB-CG	11.32	123.92	112.60
1	D	61	ARG	CD-NE-CZ	11.26	140.16	124.40
1	C	674	ASP	CA-CB-CG	10.40	123.00	112.60
1	A	414	SER	N-CA-C	10.06	122.32	111.36
1	A	272	PHE	CA-CB-CG	9.90	123.70	113.80
1	A	575	PRO	N-CA-CB	9.69	108.61	103.19
1	A	479	ARG	CD-NE-CZ	9.67	137.94	124.40
1	A	728	PHE	CA-CB-CG	9.59	123.39	113.80
1	B	338	PHE	CA-CB-CG	9.22	123.02	113.80
1	B	749	ASP	CA-CB-CG	9.11	121.71	112.60
1	C	597	ASP	CA-CB-CG	9.10	121.69	112.60
1	B	44	PRO	N-CA-CB	8.96	107.88	103.22
1	B	431	ILE	N-CA-C	-8.86	100.27	108.95
1	C	726	GLY	N-CA-C	-8.86	92.19	113.18
1	D	575	PRO	N-CA-CB	8.85	108.14	103.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	61	ARG	NE-CZ-NH2	8.77	127.09	119.20
1	A	716	GLU	CB-CG-CD	8.76	127.48	112.60
1	D	474	PRO	N-CA-CB	8.75	108.09	103.19
1	C	28	SER	N-CA-C	-8.58	100.63	112.30
1	B	43	THR	CA-C-N	8.50	125.78	119.66
1	B	43	THR	C-N-CA	8.50	125.78	119.66
1	D	189	PHE	CA-CB-CG	8.40	122.20	113.80
1	C	414	SER	N-CA-C	8.28	119.93	111.07
1	D	100	ARG	CD-NE-CZ	8.19	135.87	124.40
1	B	414	SER	N-CA-C	8.19	119.99	111.14
1	A	474	PRO	N-CA-CB	8.16	107.76	103.19
1	A	542	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	B	28	SER	N-CA-CB	8.09	124.16	110.49
1	C	745	ILE	N-CA-CB	8.07	115.93	110.52
1	D	680	ASP	CA-CB-CG	7.90	120.50	112.60
1	B	574	THR	CA-C-N	7.87	125.41	119.66
1	B	574	THR	C-N-CA	7.87	125.41	119.66
1	B	185	PHE	CA-CB-CG	7.87	121.67	113.80
1	D	44	PRO	N-CA-CB	7.85	107.30	103.22
1	A	596	GLY	N-CA-C	7.77	120.45	111.36
1	D	246	GLN	CA-C-N	7.56	127.27	119.56
1	D	246	GLN	C-N-CA	7.56	127.27	119.56
1	C	615	ASP	CA-CB-CG	7.55	120.15	112.60
1	B	224	GLU	CA-C-N	7.51	127.55	119.28
1	B	224	GLU	C-N-CA	7.51	127.55	119.28
1	C	170	GLN	CB-CG-CD	7.50	125.34	112.60
1	D	574	THR	CA-C-O	7.48	126.42	119.76
1	B	474	PRO	N-CA-CB	7.45	107.36	103.19
1	A	595	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	59	ASP	CA-CB-CG	7.39	120.00	112.60
1	D	210	ASP	CA-CB-CG	7.37	119.97	112.60
1	D	431	ILE	N-CA-C	-7.36	101.74	108.95
1	C	72	ARG	CD-NE-CZ	7.36	134.70	124.40
1	A	224	GLU	CA-C-N	7.35	127.36	119.28
1	A	224	GLU	C-N-CA	7.35	127.36	119.28
1	B	575	PRO	N-CA-CB	7.34	107.30	103.19
1	B	155	ASP	CA-CB-CG	7.30	119.90	112.60
1	C	159	ILE	CB-CA-C	7.30	121.91	110.81
1	B	567	THR	CA-C-N	7.28	132.76	121.19
1	B	567	THR	C-N-CA	7.28	132.76	121.19
1	B	210	ASP	CA-CB-CG	7.26	119.86	112.60
1	B	270	GLU	CA-C-N	7.26	126.59	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	GLU	C-N-CA	7.26	126.59	121.65
1	C	728	PHE	CA-CB-CG	7.24	121.04	113.80
1	B	596	GLY	N-CA-C	7.14	120.14	111.93
1	A	77	ASN	CA-CB-CG	-7.14	105.46	112.60
1	D	728	PHE	CA-CB-CG	7.11	120.91	113.80
1	D	414	SER	N-CA-C	7.11	118.81	111.14
1	B	370	VAL	N-CA-CB	-7.09	102.57	112.35
1	C	263	PRO	N-CA-CB	7.07	109.50	103.35
1	B	597	ASP	CA-CB-CG	7.02	119.62	112.60
1	C	725	ASP	N-CA-CB	7.02	122.36	110.49
1	C	171	GLY	N-CA-C	7.02	120.05	112.33
1	D	166	PHE	CA-C-O	-7.01	113.00	121.28
1	C	454	ASP	CA-CB-CG	-6.97	105.63	112.60
1	C	575	PRO	N-CA-CB	6.90	107.06	103.19
1	C	428	PHE	CA-CB-CG	-6.89	106.91	113.80
1	A	51	ALA	N-CA-CB	-6.86	104.22	111.29
1	C	659	SER	CA-C-N	6.84	130.37	120.38
1	C	659	SER	C-N-CA	6.84	130.37	120.38
1	A	37	ARG	CA-C-O	6.84	126.67	119.69
1	A	303	VAL	CA-C-O	-6.84	113.92	121.92
1	B	636	ARG	CA-C-O	-6.83	114.14	121.45
1	B	728	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	314	ASP	CA-C-N	6.82	126.50	119.82
1	B	314	ASP	C-N-CA	6.82	126.50	119.82
1	C	516	THR	CA-C-N	6.80	126.05	118.97
1	C	516	THR	C-N-CA	6.80	126.05	118.97
1	B	331	PHE	CA-C-O	6.76	126.10	119.75
1	C	445	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	A	265	SER	N-CA-CB	-6.75	101.10	111.56
1	D	546	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	B	265	SER	N-CA-CB	-6.70	101.17	111.56
1	B	182	ILE	N-CA-C	-6.70	102.64	110.21
1	D	199	VAL	N-CA-CB	-6.69	104.93	111.89
1	C	177	ASP	CA-C-O	-6.68	113.82	120.70
1	D	43	THR	CA-C-N	6.68	124.47	119.66
1	D	43	THR	C-N-CA	6.68	124.47	119.66
1	D	387	GLU	CA-C-O	-6.67	113.76	120.90
1	D	170	GLN	CA-C-N	6.67	126.44	120.10
1	D	170	GLN	C-N-CA	6.67	126.44	120.10
1	D	338	PHE	CA-CB-CG	6.66	120.46	113.80
1	D	61	ARG	NE-CZ-NH1	-6.65	114.85	121.50
1	A	405	ASP	CA-C-N	6.64	126.27	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	ASP	C-N-CA	6.64	126.27	119.56
1	A	751	ILE	N-CA-CB	6.64	117.55	110.17
1	B	473	THR	CA-C-N	6.61	124.48	119.66
1	B	473	THR	C-N-CA	6.61	124.48	119.66
1	B	486	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	A	708	ILE	CA-C-N	6.57	134.09	121.54
1	A	708	ILE	C-N-CA	6.57	134.09	121.54
1	A	169	VAL	CA-C-N	6.56	129.36	120.44
1	A	169	VAL	C-N-CA	6.56	129.36	120.44
1	B	264	ARG	CA-C-O	6.52	127.34	120.42
1	C	304	TRP	N-CA-C	6.51	118.92	111.11
1	B	405	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	166	PHE	CA-C-O	-6.50	113.82	121.16
1	B	156	PRO	N-CA-CB	6.48	109.73	103.51
1	B	350	ASP	CB-CA-C	6.46	121.61	110.94
1	A	507	HIS	CA-C-N	6.41	125.91	119.24
1	A	507	HIS	C-N-CA	6.41	125.91	119.24
1	B	349	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	749	ASP	CA-CB-CG	-6.36	106.24	112.60
1	B	516	THR	CA-C-N	6.36	125.59	118.97
1	B	516	THR	C-N-CA	6.36	125.59	118.97
1	D	80	LEU	CA-C-O	-6.36	113.44	120.69
1	C	59	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	278	ARG	NE-CZ-NH1	-6.35	115.15	121.50
1	C	551	ASP	CA-CB-CG	-6.35	106.25	112.60
1	C	498	SER	CA-C-N	6.34	126.26	119.28
1	C	498	SER	C-N-CA	6.34	126.26	119.28
1	A	574	THR	CB-CA-C	-6.34	99.50	109.52
1	D	527	PHE	CA-CB-CG	6.33	120.13	113.80
1	A	338	PHE	CA-CB-CG	6.33	120.13	113.80
1	C	725	ASP	CA-CB-CG	-6.32	106.28	112.60
1	B	542	ARG	NE-CZ-NH2	-6.31	113.52	119.20
1	D	595	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	745	ILE	CA-C-N	6.28	126.75	119.47
1	A	745	ILE	C-N-CA	6.28	126.75	119.47
1	C	314	ASP	CA-C-N	6.28	125.97	119.82
1	C	314	ASP	C-N-CA	6.28	125.97	119.82
1	A	636	ARG	CA-C-O	-6.26	114.75	121.45
1	B	309	LYS	CA-C-O	6.26	127.17	119.97
1	D	574	THR	CA-C-N	6.24	124.22	119.66
1	D	574	THR	C-N-CA	6.24	124.22	119.66
1	D	182	ILE	N-CA-C	-6.24	103.16	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	PHE	O-C-N	-6.23	116.12	123.41
1	C	237	ASP	N-CA-C	6.23	118.58	111.11
1	A	658	PRO	N-CA-CB	6.23	109.25	103.39
1	C	585	ASP	CA-C-N	6.22	125.91	119.56
1	C	585	ASP	C-N-CA	6.22	125.91	119.56
1	D	100	ARG	CG-CD-NE	6.21	125.67	112.00
1	D	629	HIS	CA-CB-CG	-6.21	107.59	113.80
1	C	100	ARG	N-CA-C	-6.20	105.03	112.59
1	D	313	ARG	NE-CZ-NH2	6.16	124.75	119.20
1	A	170	GLN	CB-CG-CD	6.16	123.08	112.60
1	B	217	PHE	CA-CB-CG	-6.13	107.67	113.80
1	B	262	ILE	CA-C-N	6.13	126.16	119.90
1	B	262	ILE	C-N-CA	6.13	126.16	119.90
1	B	750	LYS	N-CA-C	6.13	119.47	112.97
1	C	540	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	D	167	SER	CA-C-O	-6.11	114.91	121.38
1	C	295	PRO	N-CA-CB	6.10	107.32	103.23
1	B	161	PRO	N-CA-CB	6.10	108.74	103.31
1	A	392	HIS	CA-C-N	6.09	125.77	119.56
1	A	392	HIS	C-N-CA	6.09	125.77	119.56
1	A	387	GLU	CA-C-O	-6.09	114.10	120.55
1	C	338	PHE	CA-CB-CG	6.08	119.88	113.80
1	C	217	PHE	CA-CB-CG	-6.05	107.75	113.80
1	B	615	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	648	LEU	CA-C-N	6.05	126.25	119.90
1	B	648	LEU	C-N-CA	6.05	126.25	119.90
1	D	436	PRO	N-CA-CB	6.05	108.61	103.35
1	D	170	GLN	CB-CG-CD	6.04	122.87	112.60
1	A	368	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	C	355	ASP	CA-C-O	6.03	123.21	119.29
1	A	420	ILE	CA-C-O	-6.03	114.12	120.57
1	B	52	PRO	CA-C-N	6.03	126.80	119.99
1	B	52	PRO	C-N-CA	6.03	126.80	119.99
1	B	169	VAL	CA-C-N	6.03	128.63	120.44
1	B	169	VAL	C-N-CA	6.03	128.63	120.44
1	A	171	GLY	N-CA-C	6.02	118.95	112.33
1	A	585	ASP	CA-C-N	6.02	125.70	119.56
1	A	585	ASP	C-N-CA	6.02	125.70	119.56
1	B	308	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	C	339	GLN	N-CA-C	-6.01	98.93	108.73
1	A	471	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	B	391	PHE	CA-CB-CG	5.99	119.79	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	ASN	CA-CB-CG	5.97	118.57	112.60
1	C	540	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	A	304	TRP	N-CA-C	5.96	118.26	111.11
1	A	53	GLY	CA-C-O	5.95	126.63	120.80
1	B	60	THR	CA-C-O	-5.95	113.88	120.60
1	D	171	GLY	N-CA-C	5.95	118.77	111.93
1	B	585	ASP	CA-C-N	5.94	125.62	119.56
1	B	585	ASP	C-N-CA	5.94	125.62	119.56
1	D	749	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	649	PRO	N-CA-CB	5.94	108.86	103.34
1	C	438	CYS	CA-C-N	5.92	125.86	119.76
1	C	438	CYS	C-N-CA	5.92	125.86	119.76
1	A	389	ALA	CA-C-O	-5.92	114.67	121.19
1	D	392	HIS	CA-C-N	5.92	125.60	119.56
1	D	392	HIS	C-N-CA	5.92	125.60	119.56
1	C	53	GLY	N-CA-C	5.91	120.04	112.83
1	B	229	ILE	N-CA-C	-5.89	104.36	109.19
1	A	339	GLN	N-CA-C	-5.88	99.14	108.73
1	D	265	SER	N-CA-CB	-5.88	102.44	111.56
1	A	29	LEU	CA-C-O	5.87	128.61	121.68
1	D	226	HIS	CA-C-O	-5.87	114.66	120.70
1	D	215	PRO	N-CA-CB	5.86	109.77	103.33
1	C	82	THR	N-CA-C	-5.85	102.28	110.35
1	D	263	PRO	N-CA-CB	5.85	108.44	103.35
1	C	72	ARG	N-CA-CB	5.84	118.56	109.97
1	D	580	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	383	PHE	CA-CB-CG	-5.84	107.96	113.80
1	C	475	PRO	N-CA-CB	5.83	108.42	103.35
1	C	437	THR	N-CA-C	-5.83	106.33	113.50
1	A	596	GLY	CA-C-O	5.81	126.53	121.41
1	C	370	VAL	O-C-N	-5.80	116.03	122.07
1	A	111	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	D	403	THR	N-CA-CB	5.79	120.99	111.31
1	A	750	LYS	N-CA-C	-5.79	106.34	113.41
1	B	593	ILE	CA-C-N	5.79	127.08	119.84
1	B	593	ILE	C-N-CA	5.79	127.08	119.84
1	C	93	ASN	N-CA-C	5.79	118.20	109.23
1	D	437	THR	N-CA-C	-5.78	106.23	113.28
1	B	37	ARG	CA-C-N	5.77	125.68	119.85
1	B	37	ARG	C-N-CA	5.77	125.68	119.85
1	B	749	ASP	CA-C-N	5.76	132.06	122.66
1	B	749	ASP	C-N-CA	5.76	132.06	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ASP	CA-C-N	5.76	125.38	119.56
1	B	155	ASP	C-N-CA	5.76	125.38	119.56
1	C	445	ARG	CD-NE-CZ	5.75	132.46	124.40
1	D	658	PRO	N-CA-CB	5.74	108.79	103.39
1	C	503	GLU	CA-C-O	-5.74	113.22	120.28
1	D	612	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	C	158	LYS	CA-C-N	-5.73	115.71	123.10
1	C	158	LYS	C-N-CA	-5.73	115.71	123.10
1	B	431	ILE	CA-C-N	5.72	125.19	119.24
1	B	431	ILE	C-N-CA	5.72	125.19	119.24
1	A	44	PRO	N-CA-CB	5.71	108.62	103.08
1	D	369	ARG	CD-NE-CZ	5.71	132.40	124.40
1	C	395	HIS	CA-CB-CG	5.71	119.51	113.80
1	A	226	HIS	CA-C-O	-5.71	114.82	120.70
1	A	155	ASP	CA-CB-CG	5.70	118.30	112.60
1	D	311	THR	N-CA-CB	5.69	118.99	110.22
1	B	290	ARG	N-CA-CB	5.69	120.64	110.80
1	D	479	ARG	CD-NE-CZ	5.69	132.37	124.40
1	C	439	PRO	CB-CA-C	-5.68	104.13	111.46
1	A	476	GLY	CA-C-N	5.68	125.35	119.05
1	A	476	GLY	C-N-CA	5.68	125.35	119.05
1	A	527	PHE	CA-C-O	-5.68	114.50	120.63
1	C	101	GLY	CA-C-N	5.68	125.44	119.76
1	C	101	GLY	C-N-CA	5.68	125.44	119.76
1	D	224	GLU	CA-C-N	5.68	125.52	119.28
1	D	224	GLU	C-N-CA	5.68	125.52	119.28
1	D	290	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	B	438	CYS	CA-C-N	5.67	125.60	119.76
1	B	438	CYS	C-N-CA	5.67	125.60	119.76
1	A	224	GLU	CB-CA-C	5.66	118.31	109.42
1	C	339	GLN	N-CA-CB	5.66	119.65	110.42
1	A	541	GLU	CA-CB-CG	-5.66	102.78	114.10
1	B	366	PRO	N-CA-CB	5.65	108.59	103.33
1	A	42	PRO	N-CA-CB	5.62	107.80	103.30
1	D	586	PRO	N-CA-CB	5.62	109.09	103.48
1	A	237	ASP	N-CA-C	5.61	117.85	111.11
1	D	643	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	37	ARG	CA-C-N	5.61	125.53	119.76
1	A	37	ARG	C-N-CA	5.61	125.53	119.76
1	A	214	PHE	CA-C-N	5.60	125.26	119.05
1	A	214	PHE	C-N-CA	5.60	125.26	119.05
1	B	38	PRO	N-CA-CB	5.60	108.54	103.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	GLN	N-CA-C	5.58	117.16	111.14
1	C	610	GLU	CA-CB-CG	5.57	125.25	114.10
1	A	280	ILE	CA-C-O	-5.57	114.60	120.39
1	C	639	GLU	CA-C-O	-5.57	115.31	121.33
1	B	405	ASP	CA-C-N	5.56	125.18	119.56
1	B	405	ASP	C-N-CA	5.56	125.18	119.56
1	A	608	ASN	CA-C-O	-5.56	115.13	121.58
1	C	572	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	441	HIS	CA-CB-CG	-5.56	108.24	113.80
1	B	169	VAL	N-CA-C	5.56	116.70	111.48
1	C	670	GLY	N-CA-C	-5.55	105.95	111.56
1	D	214	PHE	CA-C-N	5.55	125.21	119.05
1	D	214	PHE	C-N-CA	5.55	125.21	119.05
1	A	657	ALA	CA-C-N	5.54	125.85	119.92
1	A	657	ALA	C-N-CA	5.54	125.85	119.92
1	A	597	ASP	N-CA-CB	-5.54	102.07	110.77
1	B	177	ASP	CA-C-O	-5.53	114.10	120.24
1	C	595	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	435	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	A	667	VAL	CA-C-N	5.50	125.49	120.21
1	A	667	VAL	C-N-CA	5.50	125.49	120.21
1	C	366	PRO	N-CA-CB	5.50	108.13	103.35
1	D	247	PRO	N-CA-CB	5.48	108.96	103.48
1	C	246	GLN	CA-C-N	5.47	125.82	119.47
1	C	246	GLN	C-N-CA	5.47	125.82	119.47
1	D	517	PRO	N-CA-CB	5.47	109.35	103.33
1	D	344	GLU	CB-CA-C	-5.47	98.78	110.32
1	B	349	PHE	CA-C-N	-5.46	113.94	122.73
1	B	349	PHE	C-N-CA	-5.46	113.94	122.73
1	A	262	ILE	CA-C-N	5.46	125.36	119.85
1	A	262	ILE	C-N-CA	5.46	125.36	119.85
1	C	271	GLY	O-C-N	-5.46	118.50	123.36
1	C	43	THR	CA-C-N	5.45	126.00	120.38
1	C	43	THR	C-N-CA	5.45	126.00	120.38
1	B	182	ILE	CA-C-O	-5.45	116.08	122.13
1	C	488	ARG	CD-NE-CZ	5.44	132.01	124.40
1	C	594	PRO	N-CA-CB	5.43	108.08	103.19
1	D	237	ASP	CA-C-O	-5.42	115.10	120.90
1	A	501	PHE	CA-CB-CG	5.41	119.21	113.80
1	C	476	GLY	CA-C-N	5.41	125.23	119.28
1	C	476	GLY	C-N-CA	5.41	125.23	119.28
1	D	304	TRP	N-CA-C	5.41	117.61	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	369	ARG	NE-CZ-NH2	5.41	124.06	119.20
1	A	693	LYS	CA-C-N	5.40	125.66	119.83
1	A	693	LYS	C-N-CA	5.40	125.66	119.83
1	B	27	ASP	CA-C-N	5.39	131.84	121.54
1	B	27	ASP	C-N-CA	5.39	131.84	121.54
1	D	167	SER	O-C-N	5.39	128.93	123.26
1	A	612	ARG	CD-NE-CZ	5.39	131.95	124.40
1	C	422	ARG	CD-NE-CZ	5.38	131.94	124.40
1	D	156	PRO	N-CA-CB	5.38	108.63	103.52
1	B	126[A]	ILE	N-CA-CB	5.37	117.85	110.54
1	B	126[B]	ILE	N-CA-CB	5.37	117.85	110.54
1	B	369	ARG	CA-C-O	-5.36	114.25	120.62
1	D	343	GLU	CA-C-N	5.36	129.17	120.60
1	D	343	GLU	C-N-CA	5.36	129.17	120.60
1	A	576	PRO	N-CA-CB	5.35	108.27	103.08
1	C	471	ARG	N-CA-C	5.35	118.78	110.17
1	A	57	ALA	CA-C-N	5.34	125.15	119.28
1	A	57	ALA	C-N-CA	5.34	125.15	119.28
1	C	727	SER	N-CA-CB	-5.34	102.77	110.56
1	D	549	HIS	CA-CB-CG	-5.34	108.46	113.80
1	C	205	ILE	CA-C-O	-5.34	116.23	121.67
1	C	236	HIS	CA-C-N	5.34	127.74	120.54
1	C	236	HIS	C-N-CA	5.34	127.74	120.54
1	B	246	GLN	CA-C-N	5.33	125.00	119.56
1	B	246	GLN	C-N-CA	5.33	125.00	119.56
1	B	404	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	98	GLY	N-CA-C	-5.33	106.03	112.48
1	D	489	VAL	CA-C-O	5.33	126.13	120.48
1	A	361	PRO	N-CA-CB	5.33	108.06	103.27
1	C	84	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	A	536	ARG	CA-C-N	5.30	124.94	119.05
1	A	536	ARG	C-N-CA	5.30	124.94	119.05
1	B	492	ASN	CA-CB-CG	-5.30	107.30	112.60
1	A	348	LYS	N-CA-C	5.29	119.72	113.16
1	B	471	ARG	N-CA-C	5.29	118.36	109.95
1	D	185	PHE	CA-CB-CG	5.29	119.09	113.80
1	D	585	ASP	CA-C-N	5.29	124.95	119.56
1	D	585	ASP	C-N-CA	5.29	124.95	119.56
1	B	205	ILE	CA-C-O	-5.29	116.46	121.64
1	C	392	HIS	CA-C-N	5.27	124.94	119.56
1	C	392	HIS	C-N-CA	5.27	124.94	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	536	ARG	CA-C-O	5.27	122.71	119.29
1	A	350	ASP	CB-CA-C	5.26	119.73	110.37
1	D	674	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	490	GLU	N-CA-C	5.26	116.61	107.93
1	B	101	GLY	CA-C-N	5.25	125.01	119.76
1	B	101	GLY	C-N-CA	5.25	125.01	119.76
1	D	499	PRO	N-CA-CB	5.25	109.06	103.39
1	D	377	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	C	88	ILE	CA-C-O	-5.24	114.96	120.57
1	D	691	HIS	CA-C-O	5.24	126.04	119.59
1	B	378	ASN	CA-CB-CG	-5.24	107.36	112.60
1	C	349	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	349	PHE	CA-CB-CG	-5.23	108.57	113.80
1	C	694	PRO	N-CA-CB	5.22	107.89	103.19
1	D	598	VAL	N-CA-CB	-5.22	100.69	111.76
1	C	447	GLY	CA-C-O	-5.22	117.81	121.88
1	B	661	THR	CA-C-O	-5.21	112.97	119.18
1	A	751	ILE	CA-C-O	5.21	124.82	119.82
1	B	397	VAL	CA-C-N	5.21	125.50	119.93
1	B	397	VAL	C-N-CA	5.21	125.50	119.93
1	A	574	THR	CA-C-N	5.19	123.45	119.66
1	A	574	THR	C-N-CA	5.19	123.45	119.66
1	A	471	ARG	N-CA-C	5.19	118.52	110.17
1	B	577	PRO	N-CA-CB	5.19	108.83	103.38
1	D	269	MET	CA-C-O	-5.18	115.54	121.40
1	C	542	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	B	263	PRO	N-CA-CB	5.18	107.81	103.25
1	C	265	SER	N-CA-CB	-5.18	103.54	111.56
1	C	197	ASP	CA-C-O	-5.17	114.83	120.36
1	A	483	GLU	CA-C-O	-5.16	114.59	120.32
1	C	262	ILE	CA-C-N	5.16	125.10	119.78
1	C	262	ILE	C-N-CA	5.16	125.10	119.78
1	D	260	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	B	51	ALA	CA-C-N	5.16	125.16	119.90
1	B	51	ALA	C-N-CA	5.16	125.16	119.90
1	D	316	ASP	CA-C-O	-5.16	114.31	120.55
1	C	491	GLY	CA-C-O	-5.15	116.58	121.83
1	A	355	ASP	CA-C-O	5.14	123.13	119.32
1	B	667	VAL	CA-C-N	5.14	125.35	120.31
1	B	667	VAL	C-N-CA	5.14	125.35	120.31
1	D	516	THR	CA-C-N	5.14	124.76	119.05
1	D	516	THR	C-N-CA	5.14	124.76	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	GLU	CB-CG-CD	5.13	121.33	112.60
1	A	431	ILE	N-CA-C	-5.13	103.92	108.95
1	A	31	PRO	N-CA-CB	5.12	107.80	103.35
1	C	203	THR	N-CA-CB	5.10	119.70	110.72
1	A	591	TYR	N-CA-C	5.10	121.26	113.61
1	A	576	PRO	CA-C-N	5.10	125.08	120.03
1	A	576	PRO	C-N-CA	5.10	125.08	120.03
1	A	450	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	167	SER	N-CA-C	5.09	116.04	108.60
1	B	475	PRO	N-CA-CB	5.09	107.78	103.35
1	A	207	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	498	SER	CA-C-N	5.09	124.88	119.28
1	A	498	SER	C-N-CA	5.09	124.88	119.28
1	B	73	LYS	O-C-N	-5.09	117.24	123.30
1	A	616	LEU	CA-C-N	5.09	127.41	120.54
1	A	616	LEU	C-N-CA	5.09	127.41	120.54
1	D	389	ALA	CA-C-O	-5.08	115.60	121.19
1	C	170	GLN	N-CA-C	5.08	116.63	111.14
1	A	189	PHE	CA-C-O	-5.08	114.93	120.36
1	A	82	THR	N-CA-C	-5.08	103.34	110.35
1	A	586	PRO	N-CA-CB	5.08	108.56	103.48
1	A	707	THR	N-CA-CB	5.08	117.58	110.12
1	B	520	GLN	CA-C-N	5.06	127.47	120.29
1	B	520	GLN	C-N-CA	5.06	127.47	120.29
1	C	652	ALA	CA-C-O	-5.05	115.90	121.31
1	D	37	ARG	N-CA-CB	-5.05	101.46	110.05
1	A	341	ILE	CB-CG1-CD1	5.05	124.40	113.80
1	B	303	VAL	CA-C-O	-5.05	114.99	121.40
1	A	53	GLY	O-C-N	-5.04	117.28	122.17
1	B	370	VAL	CA-C-O	5.04	123.33	118.90
1	C	281	ASN	CA-CB-CG	5.04	117.64	112.60
1	D	477	PRO	N-CA-CB	5.04	108.83	103.39
1	A	350	ASP	CA-CB-CG	5.03	117.63	112.60
1	D	155	ASP	CA-C-N	5.03	124.75	119.82
1	D	155	ASP	C-N-CA	5.03	124.75	119.82
1	B	457	PRO	N-CA-CB	5.02	108.81	103.39
1	B	698	ALA	CA-C-O	5.02	125.91	120.43
1	D	37	ARG	CA-C-O	5.02	124.21	119.59
1	C	691	HIS	CA-C-O	5.02	125.51	119.43
1	B	98	GLY	CA-C-O	-5.02	117.87	122.24
1	B	199	VAL	N-CA-CB	-5.02	106.67	111.89
1	D	521	ARG	NE-CZ-NH2	5.02	123.72	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	ASP	N-CA-C	5.02	117.13	111.11
1	A	747	LYS	N-CA-C	5.01	119.11	112.89
1	C	625	ALA	CA-C-O	-5.01	114.44	120.10
1	C	281	ASN	CA-C-N	5.01	127.49	120.28
1	C	281	ASN	C-N-CA	5.01	127.49	120.28
1	B	260	ARG	CA-C-O	-5.00	114.45	120.10

There are no chirality outliers.

There are no planarity outliers.

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	5747	0	5586	65	0
1	B	5747	0	5586	103	0
1	C	5747	0	5586	78	0
1	D	5747	0	5586	84	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
3	A	739	0	0	3	0
3	B	610	0	0	14	0
3	C	674	0	0	10	0
3	D	710	0	0	8	0
All	All	25893	0	22464	300	0

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 7.

All (300) 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:451:MET:HE2	1:C:451:MET:HE2	1.26	1.09
1:B:451:MET:HE2	1:D:451:MET:HE2	1.36	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:760:HEM:HMC2	2:C:760:HEM:HBC2	1.63	0.81
1:D:750:LYS:HD3	1:D:751:ILE:H	1.49	0.78
1:B:583:LYS:NZ	1:B:583:LYS:H	1.84	0.75
1:D:267:ARG:HG2	1:D:332:PRO:HB3	1.69	0.74
1:C:267:ARG:HG3	3:C:3862:HOH:O	1.89	0.72
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.70	0.72
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.71	0.71
1:B:468:ASN:HD22	1:D:27:ASP:N	1.88	0.71
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.73	0.70
1:B:37:ARG:HD2	3:B:3832:HOH:O	1.91	0.69
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.74	0.69
1:D:748:ILE:O	1:D:751:ILE:HG22	1.95	0.66
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.78	0.66
1:C:748:ILE:O	1:C:751:ILE:HG22	1.96	0.66
1:B:310:LEU:HD13	1:B:660:LEU:HB3	1.77	0.65
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.79	0.65
1:B:267:ARG:HG3	3:B:2872:HOH:O	1.96	0.64
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.78	0.64
1:D:546:GLN:HG3	3:D:3688:HOH:O	1.97	0.64
1:C:578:ASP:HB2	1:C:582:LEU:O	1.97	0.63
1:B:705:LYS:HE3	1:B:710:ILE:HG22	1.81	0.62
1:B:748:ILE:O	1:B:751:ILE:HG22	2.00	0.61
3:A:1161:HOH:O	1:D:126[B]:ILE:HD11	2.01	0.60
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.02	0.60
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.60
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.84	0.59
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.17	0.59
1:A:121:ARG:HG2	1:D:126[B]:ILE:HD13	1.85	0.59
1:B:27:ASP:HB3	3:B:3519:HOH:O	2.02	0.59
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.86	0.58
1:B:281:ASN:OD1	1:B:283:GLU:HG2	2.03	0.58
1:B:267:ARG:HD2	3:B:1632:HOH:O	2.03	0.58
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.50	0.57
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.35	0.57
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.70	0.57
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.86	0.57
1:A:126[B]:ILE:HD11	3:D:4171:HOH:O	2.05	0.57
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.35	0.56
1:D:750:LYS:CD	1:D:751:ILE:H	2.15	0.56
1:B:36:HIS:HD1	1:B:36:HIS:H	1.54	0.56
1:D:594:PRO:HA	3:D:3812:HOH:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:PHE:O	1:C:707:THR:HG22	2.05	0.56
1:D:629:HIS:HD2	3:D:2510:HOH:O	1.88	0.56
1:B:634:TYR:O	1:B:653:THR:HA	2.06	0.56
1:C:516:THR:HB	1:C:517:PRO:HD2	1.88	0.56
1:A:748:ILE:O	1:A:751:ILE:HG13	2.05	0.56
1:D:507:HIS:N	1:D:508:PRO:HD2	2.21	0.56
1:A:27:ASP:O	1:A:28:SER:C	2.50	0.55
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.89	0.55
1:C:214:PHE:HB3	1:C:215:PRO:HD3	1.88	0.55
3:B:3419:HOH:O	1:C:126[B]:ILE:HD11	2.07	0.55
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.87	0.55
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.89	0.55
1:A:583:LYS:O	1:A:584:LYS:HB3	2.07	0.55
1:D:315:PRO:HB2	3:D:2309:HOH:O	2.06	0.55
1:D:535:VAL:O	1:D:537:PRO:HD3	2.06	0.55
1:D:392:HIS:ND1	1:D:415:TYR:HB2	2.22	0.54
1:D:634:TYR:O	1:D:653:THR:HA	2.08	0.54
1:C:535:VAL:O	1:C:537:PRO:HD3	2.07	0.54
1:D:624:LYS:HD3	1:D:624:LYS:C	2.33	0.54
1:B:369:ARG:HG3	3:B:1254:HOH:O	2.07	0.54
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.90	0.54
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.89	0.53
1:C:612:ARG:HB2	1:C:612:ARG:CZ	2.38	0.53
1:A:751:ILE:HD12	1:A:751:ILE:O	2.07	0.53
1:C:392:HIS:ND1	1:C:415:TYR:HB2	2.24	0.53
1:D:267:ARG:HG3	3:D:2871:HOH:O	2.09	0.53
1:D:48:GLN:HB3	1:D:49:PRO:HD2	1.91	0.53
1:C:592:ALA:O	1:C:594:PRO:HD3	2.09	0.53
1:A:28:SER:CB	1:D:245:LEU:HD22	2.40	0.52
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.90	0.52
1:D:359:LEU:H	1:D:507:HIS:HD2	1.58	0.52
1:A:471:ARG:CZ	1:C:27:ASP:HA	2.40	0.52
1:A:596:GLY:HA3	1:A:737:ALA:O	2.09	0.52
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.75	0.52
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.91	0.51
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.31	0.51
1:B:533:LYS:NZ	3:B:4179:HOH:O	2.43	0.51
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.93	0.51
1:B:359:LEU:HD12	1:B:359:LEU:C	2.36	0.51
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.93	0.51
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:THR:HB	1:C:517:PRO:CD	2.41	0.51
1:B:516:THR:HB	1:B:517:PRO:CD	2.41	0.51
1:A:478:LYS:HE2	3:A:3725:HOH:O	2.10	0.51
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.91	0.51
1:B:596:GLY:HA3	3:B:3145:HOH:O	2.10	0.51
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.94	0.50
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.94	0.50
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.27	0.50
1:B:583:LYS:HE2	1:B:584:LYS:HG2	1.94	0.50
1:B:344:GLU:CD	1:B:344:GLU:H	2.19	0.49
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.47	0.49
1:B:126[B]:ILE:HD11	1:C:118:ASP:O	2.12	0.49
1:B:315:PRO:HB2	3:B:1492:HOH:O	2.12	0.49
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.41	0.49
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.47	0.49
1:A:708:ILE:O	1:A:710:ILE:HG22	2.12	0.49
1:B:669:CYS:SG	1:B:670:GLY:N	2.81	0.49
1:D:27:ASP:O	1:D:28:SER:HB2	2.12	0.49
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.77	0.49
1:C:435:ARG:HD3	3:C:2150:HOH:O	2.13	0.49
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.28	0.49
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.93	0.49
1:B:310:LEU:HD13	1:B:660:LEU:CB	2.42	0.49
1:B:471:ARG:NH1	1:D:28:SER:HA	2.28	0.49
1:D:748:ILE:O	1:D:749:ASP:C	2.56	0.49
1:A:725:ASP:H	1:A:728:PHE:HB3	1.78	0.48
1:D:631:LYS:HG3	1:D:633:LEU:HD13	1.95	0.48
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.95	0.48
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.94	0.48
1:A:509:ARG:HD2	1:A:576:PRO:HD2	1.95	0.48
1:B:170:GLN:HB2	3:B:4166:HOH:O	2.14	0.48
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.97	0.48
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.95	0.48
1:A:52:PRO:HG3	3:C:1996:HOH:O	2.14	0.48
1:A:299:LYS:HE2	3:A:2744:HOH:O	2.13	0.48
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.95	0.48
1:D:359:LEU:H	1:D:507:HIS:CD2	2.32	0.48
1:A:207:PHE:O	1:A:249:THR:HA	2.13	0.48
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.96	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.29	0.47
1:B:459:ASN:HD22	1:B:459:ASN:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.45	0.47
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.50	0.47
1:A:126[A]:ILE:HD12	1:D:121:ARG:CZ	2.45	0.47
1:B:556:GLN:HA	1:B:566:LEU:HD21	1.97	0.47
1:B:626:LYS:NZ	3:B:3404:HOH:O	2.47	0.47
1:C:459:ASN:H	1:C:459:ASN:HD22	1.62	0.47
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.79	0.47
1:B:612:ARG:HD3	1:B:670:GLY:HA2	1.96	0.47
1:B:678:ASN:OD1	1:B:680:ASP:HB2	2.15	0.47
1:C:507:HIS:N	1:C:508:PRO:HD2	2.29	0.47
1:D:87:ARG:NE	3:D:2163:HOH:O	2.48	0.47
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.50	0.47
1:C:203:THR:HB	1:C:204:PRO:HD2	1.97	0.47
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.96	0.47
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.97	0.46
1:D:669:CYS:SG	1:D:670:GLY:N	2.88	0.46
1:A:392:HIS:ND1	1:A:415:TYR:HB2	2.29	0.46
1:C:709:LYS:HD3	1:C:709:LYS:N	2.30	0.46
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.84	0.46
1:A:461:GLU:HB2	1:A:462:PRO:HA	1.96	0.46
1:B:745:ILE:O	1:B:748:ILE:HG12	2.15	0.46
1:A:28:SER:HB2	1:D:245:LEU:HD22	1.98	0.46
1:D:407:LEU:HD11	2:D:760:HEM:HMC2	1.97	0.46
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.33	0.46
1:D:507:HIS:N	1:D:508:PRO:CD	2.78	0.46
1:A:37:ARG:HG3	1:A:38:PRO:HD2	1.97	0.46
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.50	0.46
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.98	0.46
1:D:623:LEU:HD22	1:D:628:VAL:HG11	1.97	0.46
1:B:207:PHE:O	1:B:249:THR:HA	2.16	0.46
1:B:359:LEU:H	1:B:507:HIS:HD2	1.64	0.46
1:C:137:TYR:HB2	1:C:159:ILE:HD12	1.98	0.46
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.97	0.46
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.98	0.46
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.51	0.45
1:D:461:GLU:HA	1:D:462:PRO:C	2.40	0.45
1:A:76:GLU:O	1:A:77:ASN:HB2	2.16	0.45
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.24	0.45
1:B:594:PRO:HA	3:B:2927:HOH:O	2.16	0.45
1:C:583:LYS:O	1:C:584:LYS:HB3	2.17	0.45
1:D:640:VAL:HG13	1:D:650:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLU:HA	1:A:462:PRO:C	2.41	0.45
1:B:369:ARG:HG2	3:B:2593:HOH:O	2.16	0.45
1:C:660:LEU:HD13	1:C:687:GLU:CD	2.41	0.45
1:C:686:MET:CB	1:C:751:ILE:HD11	2.46	0.45
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.52	0.45
1:B:578:ASP:HB3	1:B:582:LEU:O	2.17	0.45
1:B:118:ASP:O	1:C:126[B]:ILE:HD11	2.16	0.45
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.52	0.45
1:A:745:ILE:N	1:A:746:PRO:HD2	2.32	0.45
1:C:404:ASN:O	1:C:405:ASP:C	2.60	0.45
1:D:603:VAL:HG11	1:D:666:ILE:HG13	1.97	0.45
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.99	0.45
1:A:260:ARG:HD3	1:A:590:LEU:HD21	1.99	0.45
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.35	0.45
1:C:28:SER:HA	3:C:3596:HOH:O	2.16	0.45
1:C:335:GLU:OE2	1:C:369:ARG:NH2	2.50	0.45
1:B:413:PHE:HB2	1:D:105:LEU:HD11	1.99	0.44
1:C:359:LEU:H	1:C:507:HIS:HD2	1.66	0.44
1:D:574:THR:HG22	3:D:2568:HOH:O	2.16	0.44
1:B:708:ILE:HG13	1:B:710:ILE:HD12	1.98	0.44
1:C:751:ILE:HB	3:C:3317:HOH:O	2.16	0.44
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.99	0.44
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.82	0.44
1:D:364:LEU:HD11	1:D:580:ASN:HB2	2.00	0.44
1:B:362:GLU:HG2	1:B:367:VAL:HG23	2.00	0.44
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.47	0.44
1:A:331:PHE:O	1:A:333:GLU:HG3	2.17	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.18	0.44
1:B:516:THR:HB	1:B:517:PRO:HD2	1.98	0.44
1:C:720:GLU:O	1:C:721:ALA:HB2	2.17	0.44
1:D:97:ALA:O	1:D:101:GLY:HA3	2.18	0.44
1:D:574:THR:HA	1:D:575:PRO:HD3	1.83	0.44
1:C:411:ARG:HG2	2:C:760:HEM:C2C	2.53	0.44
1:D:122:ILE:HB	1:D:123:PRO:HD2	2.00	0.44
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.99	0.43
1:C:238:THR:HB	1:D:460:TYR:CE2	2.53	0.43
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.53	0.43
1:C:604:ALA:HB1	1:C:633:LEU:HD22	1.99	0.43
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.53	0.43
2:B:760:HEM:HBC2	2:B:760:HEM:CMC	2.47	0.43
1:C:607:LEU:HD22	1:C:611:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.26	0.43
1:A:127:VAL:O	1:A:128:HIS:HB2	2.18	0.43
1:A:511:PHE:O	1:A:515:GLN:HG2	2.18	0.43
1:B:461:GLU:HA	1:B:462:PRO:C	2.44	0.43
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.54	0.43
1:C:490:GLU:HG3	1:D:490:GLU:CG	2.46	0.43
1:A:36:HIS:CD2	1:A:36:HIS:H	2.36	0.43
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	2.00	0.43
1:B:195:ILE:HD11	1:B:436:PRO:HA	2.00	0.43
1:B:556:GLN:HG2	1:B:566:LEU:HD23	2.01	0.43
1:B:562:LEU:HA	1:C:637:MET:HB2	2.01	0.43
1:C:170:GLN:HB2	3:C:4198:HOH:O	2.18	0.43
1:C:724:ALA:O	1:C:725:ASP:HB2	2.18	0.43
1:D:260:ARG:HD3	1:D:590:LEU:HD21	2.01	0.43
1:D:469:TRP:HA	1:D:470:PRO:C	2.43	0.43
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.49	0.43
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.43
1:B:507:HIS:N	1:B:508:PRO:HD2	2.33	0.43
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.43
1:C:392:HIS:HA	1:C:393:PRO:HD2	1.87	0.43
1:A:29:LEU:HB2	3:C:3355:HOH:O	2.18	0.43
1:A:603:VAL:HG11	1:A:666:ILE:HD12	2.01	0.43
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.43
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.53	0.43
1:B:725:ASP:OD2	1:B:727:SER:N	2.51	0.43
1:C:126[B]:ILE:HG12	3:C:1937:HOH:O	2.18	0.43
1:C:490:GLU:HA	1:D:489:VAL:O	2.19	0.42
1:C:727:SER:HA	3:C:3660:HOH:O	2.18	0.42
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.88	0.42
1:B:612:ARG:CD	1:B:670:GLY:HA2	2.49	0.42
1:D:234:SER:HB2	1:D:239:PHE:CD2	2.55	0.42
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.75	0.42
1:D:603:VAL:CG1	1:D:666:ILE:HG13	2.49	0.42
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.37	0.42
1:B:229:ILE:HG23	1:B:230:PRO:HA	2.00	0.42
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.54	0.42
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.54	0.42
1:A:607:LEU:HD11	1:A:632:LEU:HB3	2.01	0.42
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.28	0.42
1:C:686:MET:HB3	1:C:751:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.55	0.42
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.55	0.42
1:A:117:PHE:CZ	1:D:126[A]:ILE:HG12	2.55	0.42
1:C:310:LEU:HD13	1:C:660:LEU:HB3	2.01	0.42
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.50	0.42
1:A:536:ARG:HA	1:A:537:PRO:HD3	1.84	0.42
1:C:477:PRO:HB2	1:C:478:LYS:HD3	2.02	0.42
1:D:258:SER:HA	1:D:523:ILE:HG12	2.02	0.42
1:A:604:ALA:HB2	1:A:662:VAL:HG11	2.02	0.42
1:A:703:LYS:HA	1:A:703:LYS:HD3	1.89	0.42
1:C:267:ARG:HH11	1:C:267:ARG:HD2	1.65	0.42
1:C:507:HIS:N	1:C:508:PRO:CD	2.82	0.42
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.56	0.42
1:B:306:GLU:O	1:B:310:LEU:HB2	2.20	0.41
2:B:760:HEM:CMB	2:B:760:HEM:HBB2	2.50	0.41
1:C:65:LEU:HD21	1:C:135:HIS:CG	2.55	0.41
1:C:359:LEU:H	1:C:507:HIS:CD2	2.38	0.41
1:B:162:VAL:HG21	1:B:373:MET:SD	2.60	0.41
1:B:213:LYS:HD3	1:C:92:GLN:HA	2.03	0.41
1:B:507:HIS:N	1:B:508:PRO:CD	2.83	0.41
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.46	0.41
1:D:323:TRP:CH2	1:D:378:ASN:HB3	2.55	0.41
1:D:751:ILE:C	1:D:751:ILE:HD13	2.45	0.41
1:A:184:GLY:HA2	1:A:201:ASN:OD1	2.20	0.41
1:A:516:THR:HB	1:A:517:PRO:HD2	2.01	0.41
1:B:749:ASP:HB3	1:B:750:LYS:HG2	2.02	0.41
1:B:207:PHE:CD2	1:B:252:ASN:HB3	2.55	0.41
1:B:349:PHE:CD1	1:B:349:PHE:N	2.88	0.41
1:B:438:CYS:HB2	1:B:439:PRO:HD2	2.01	0.41
1:A:708:ILE:O	1:A:709:LYS:C	2.63	0.41
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.02	0.41
1:C:431:ILE:HA	1:C:432:PRO:HD3	1.91	0.41
1:A:341:ILE:HD11	1:A:365:VAL:HG21	2.02	0.41
1:B:148:THR:HB	1:B:279:LEU:HB3	2.03	0.41
1:B:227:TRP:CZ3	1:C:50:THR:HG21	2.56	0.41
1:B:345:ASP:HA	1:B:348:LYS:HD2	2.02	0.41
1:B:392:HIS:ND1	1:B:415:TYR:HB2	2.35	0.41
1:B:477:PRO:HD2	3:B:1263:HOH:O	2.20	0.41
1:B:536:ARG:HA	1:B:537:PRO:HD3	1.89	0.41
1:B:631:LYS:HG3	1:B:633:LEU:HD13	2.02	0.41
1:C:97:ALA:O	1:C:101:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126[A]:ILE:CG2	2:D:760:HEM:HMD1	2.50	0.41
1:B:498:SER:HA	1:B:499:PRO:HD3	1.79	0.41
1:B:626:LYS:HG3	1:B:733:LEU:HD13	2.03	0.41
1:C:142:LYS:HE2	3:C:3019:HOH:O	2.20	0.41
1:A:507:HIS:N	1:A:508:PRO:CD	2.84	0.40
1:C:552:LEU:HD13	1:C:556:GLN:HE21	1.86	0.40
1:D:578:ASP:HB3	1:D:582:LEU:O	2.21	0.40
1:A:97:ALA:O	1:A:101:GLY:HA3	2.21	0.40
1:B:672:ILE:HG22	1:B:676:ALA:HB2	2.03	0.40
1:A:708:ILE:O	1:A:710:ILE:N	2.53	0.40
1:A:438:CYS:HB2	1:A:439:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

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	726/753 (96%)	699 (96%)	21 (3%)	6 (1%)	16	15
1	B	726/753 (96%)	703 (97%)	18 (2%)	5 (1%)	18	18
1	C	726/753 (96%)	705 (97%)	19 (3%)	2 (0%)	36	41
1	D	726/753 (96%)	698 (96%)	24 (3%)	4 (1%)	21	22
All	All	2904/3012 (96%)	2805 (97%)	82 (3%)	17 (1%)	21	22

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	709	LYS
1	B	28	SER
1	D	28	SER

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Mol	Chain	Res	Type
1	D	750	LYS
1	D	751	ILE
1	A	711	ALA
1	C	725	ASP
1	A	75	SER
1	B	725	ASP
1	C	75	SER
1	B	75	SER
1	B	584	LYS
1	A	584	LYS
1	D	595	ASP
1	A	708	ILE
1	B	594	PRO

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	613/636 (96%)	595 (97%)	18 (3%)	37	49
1	B	613/636 (96%)	588 (96%)	25 (4%)	27	35
1	C	613/636 (96%)	580 (95%)	33 (5%)	20	23
1	D	613/636 (96%)	584 (95%)	29 (5%)	23	29
All	All	2452/2544 (96%)	2347 (96%)	105 (4%)	26	33

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	59	ASP
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	198	LEU
1	A	205	ILE
1	A	213	LYS

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	294	LYS
1	A	369	ARG
1	A	375	LEU
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	611	VAL
1	A	709	LYS
1	A	712	ASP
1	B	37	ARG
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	344	GLU
1	B	370	VAL
1	B	375	LEU
1	B	420	ILE
1	B	440	TYR
1	B	449	HIS
1	B	459	ASN
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	709	LYS
1	B	727	SER
1	B	732	LEU
1	B	749	ASP
1	B	751	ILE
1	C	27	ASP
1	C	37	ARG
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	265	SER
1	C	375	LEU
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	568	ASP
1	C	571	LEU
1	C	574	THR
1	C	584	LYS
1	C	597	ASP
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	41	GLU
1	D	48	GLN
1	D	73	LYS
1	D	170	GLN
1	D	191	THR
1	D	195	ILE
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU

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Mol	Chain	Res	Type
1	D	598	VAL
1	D	610	GLU
1	D	612	ARG
1	D	616	LEU
1	D	621	LYS
1	D	633	LEU
1	D	648	LEU
1	D	709	LYS
1	D	713	GLN
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	139	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	556	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	449	HIS
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	139	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN

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Mol	Chain	Res	Type
1	D	572	ASN
1	D	629	HIS
1	D	671	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	C	760	1	50,50,50	1.38	6 (12%)	67,82,82	1.04	4 (5%)
2	HEM	B	760	1	50,50,50	1.40	10 (20%)	67,82,82	1.19	7 (10%)
2	HEM	D	760	1	50,50,50	1.40	10 (20%)	67,82,82	1.04	5 (7%)
2	HEM	A	760	1	50,50,50	1.37	9 (18%)	67,82,82	1.01	4 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	760	1	-	3/14/54/54	-
2	HEM	B	760	1	-	2/14/54/54	-
2	HEM	D	760	1	-	2/14/54/54	-
2	HEM	A	760	1	-	2/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	FE-ND	3.20	2.04	1.94
2	B	760	HEM	CAC-C3C	3.16	1.55	1.47
2	D	760	HEM	CAC-C3C	3.02	1.55	1.47
2	A	760	HEM	CAC-C3C	2.99	1.55	1.47
2	D	760	HEM	CAB-C3B	2.98	1.55	1.47
2	D	760	HEM	FE-NB	2.97	2.04	1.94
2	D	760	HEM	CMD-C2D	2.96	1.56	1.50
2	C	760	HEM	FE-NB	2.93	2.03	1.94
2	A	760	HEM	FE-NB	2.90	2.03	1.94
2	C	760	HEM	CAC-C3C	2.85	1.55	1.47
2	B	760	HEM	CAB-C3B	2.78	1.54	1.47
2	C	760	HEM	CAB-C3B	2.71	1.54	1.47
2	C	760	HEM	CMB-C2B	2.68	1.56	1.50
2	B	760	HEM	C3B-C2B	-2.65	1.31	1.37
2	A	760	HEM	FE-NA	2.57	2.03	1.95
2	B	760	HEM	CMB-C2B	2.53	1.56	1.50
2	B	760	HEM	CMA-C3A	2.53	1.56	1.50
2	B	760	HEM	CMC-C2C	2.49	1.55	1.50
2	C	760	HEM	C3B-C2B	-2.43	1.32	1.37
2	A	760	HEM	CMD-C2D	2.37	1.55	1.50
2	A	760	HEM	CMB-C2B	2.36	1.55	1.50
2	D	760	HEM	CMC-C2C	2.35	1.55	1.50
2	A	760	HEM	FE-NC	2.35	2.02	1.95
2	B	760	HEM	C2A-C3A	-2.31	1.32	1.38
2	D	760	HEM	CAD-C3D	2.29	1.57	1.51
2	D	760	HEM	C3B-C2B	-2.26	1.32	1.37
2	B	760	HEM	FE-ND	2.26	2.01	1.94
2	A	760	HEM	CAB-C3B	2.24	1.53	1.47
2	B	760	HEM	C3C-C2C	-2.17	1.32	1.37
2	D	760	HEM	FE-ND	2.11	2.01	1.94
2	A	760	HEM	C2A-C3A	-2.08	1.33	1.38
2	D	760	HEM	C2A-C3A	-2.08	1.33	1.38
2	B	760	HEM	CMD-C2D	2.07	1.55	1.50
2	D	760	HEM	FE-NC	2.01	2.01	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C2D	-2.01	1.32	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	O1A-CGA-CBA	-3.02	113.51	123.09
2	A	760	HEM	CHD-C4C-NC	2.73	127.43	124.45
2	D	760	HEM	CHD-C4C-NC	2.67	127.36	124.45
2	C	760	HEM	O2A-CGA-O1A	2.66	130.17	123.33
2	D	760	HEM	O1A-CGA-CBA	-2.63	114.73	123.09
2	C	760	HEM	O1D-CGD-CBD	-2.62	114.78	123.09
2	B	760	HEM	O2A-CGA-O1A	2.62	130.06	123.33
2	A	760	HEM	O1A-CGA-CBA	-2.59	114.88	123.09
2	D	760	HEM	CAD-CBD-CGD	2.47	120.22	113.67
2	B	760	HEM	CBC-CAC-C3C	-2.31	115.97	127.53
2	A	760	HEM	O2A-CGA-O1A	2.30	129.25	123.33
2	B	760	HEM	CHC-C1C-NC	2.17	126.82	124.45
2	B	760	HEM	C1A-CHA-C4D	-2.17	121.14	126.25
2	B	760	HEM	O1A-CGA-CBA	-2.13	116.33	123.09
2	B	760	HEM	CHD-C1D-ND	2.11	126.69	124.42
2	D	760	HEM	CHC-C4B-NB	2.11	126.69	124.42
2	D	760	HEM	C1C-CHC-C4B	-2.06	121.65	126.02
2	B	760	HEM	CHA-C4D-ND	2.06	126.91	124.37
2	C	760	HEM	CMA-C3A-C2A	2.04	129.96	125.62
2	A	760	HEM	C1C-CHC-C4B	-2.02	121.72	126.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

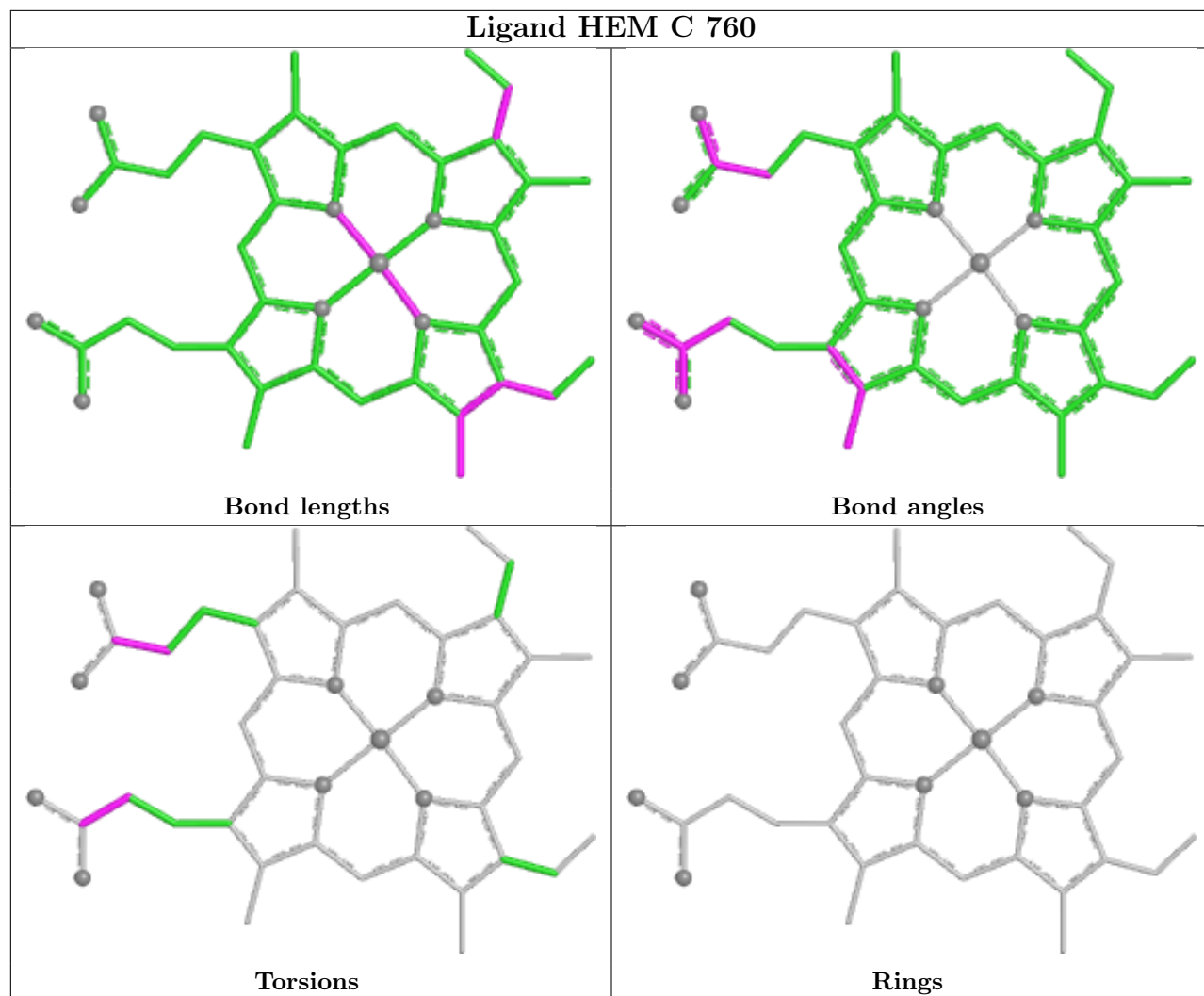
Mol	Chain	Res	Type	Atoms
2	D	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAD-CBD-CGD-O2D

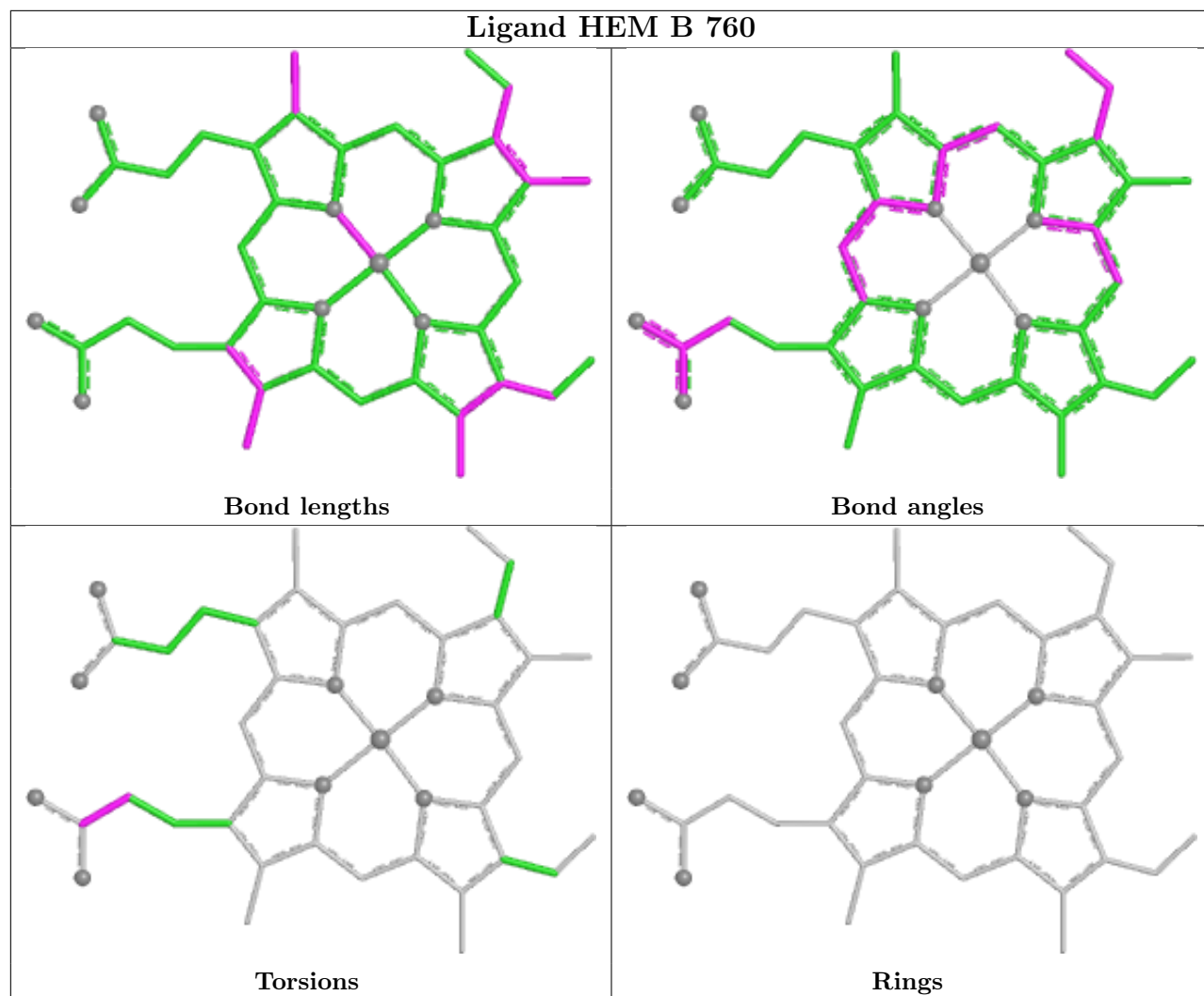
There are no ring outliers.

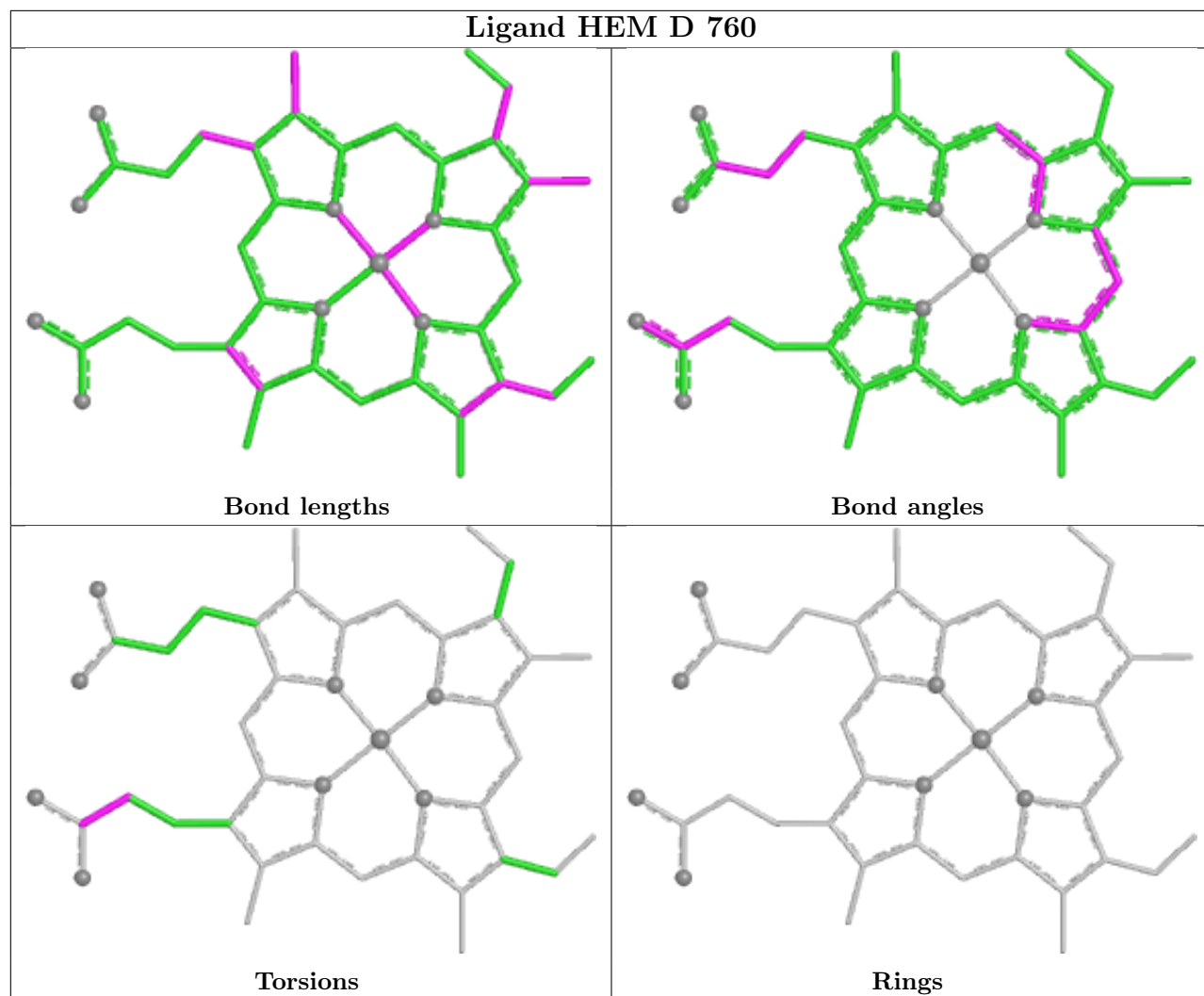
4 monomers are involved in 10 short contacts:

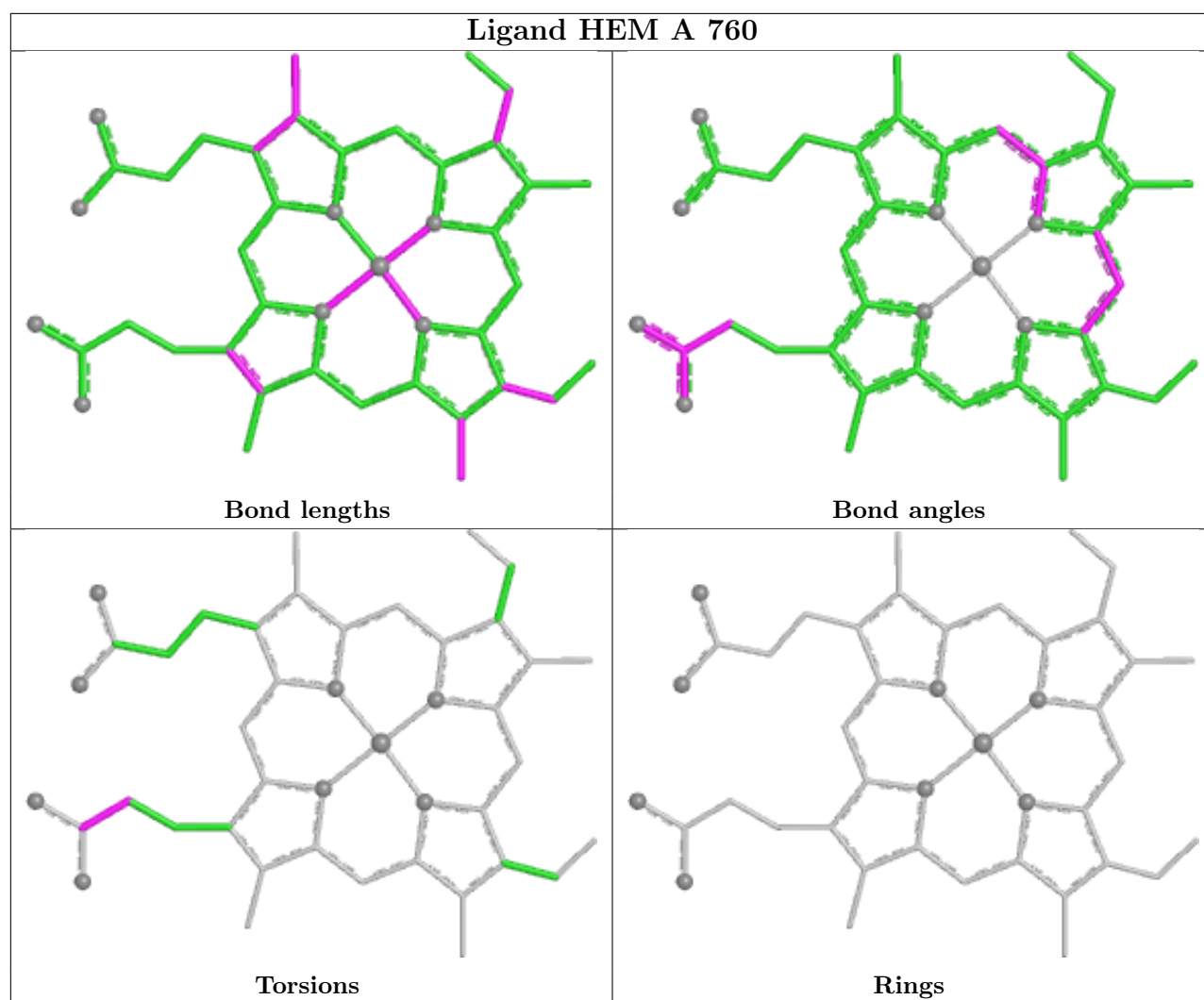
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	3	0
2	B	760	HEM	3	0
2	D	760	HEM	3	0
2	A	760	HEM	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	727/753 (96%)	-0.38	10 (1%) 73 72	10, 19, 41, 73	2 (0%)
1	B	727/753 (96%)	-0.40	2 (0%) 90 89	11, 20, 47, 65	2 (0%)
1	C	727/753 (96%)	-0.43	6 (0%) 82 81	11, 20, 44, 64	2 (0%)
1	D	727/753 (96%)	-0.15	5 (0%) 84 83	10, 19, 42, 65	2 (0%)
All	All	2908/3012 (96%)	-0.34	23 (0%) 82 81	10, 19, 44, 73	8 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	4.8
1	C	27	ASP	4.0
1	A	27	ASP	3.6
1	A	749	ASP	3.4
1	D	27	ASP	3.3
1	B	27	ASP	3.3
1	A	712	ASP	3.2
1	A	710	ILE	3.0
1	A	711	ALA	2.9
1	C	724	ALA	2.8
1	D	28	SER	2.8
1	D	30	ALA	2.6
1	C	751	ILE	2.6
1	D	31	PRO	2.5
1	A	716	GLU	2.4
1	D	749	ASP	2.4
1	A	713	GLN	2.3
1	C	725	ASP	2.3
1	B	568	ASP	2.2
1	C	595	ASP	2.1
1	A	751	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	749	ASP	2.1
1	A	29	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

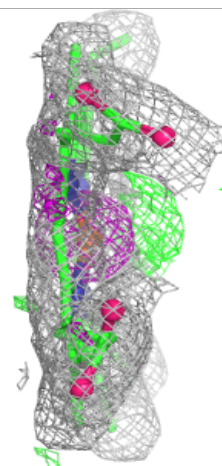
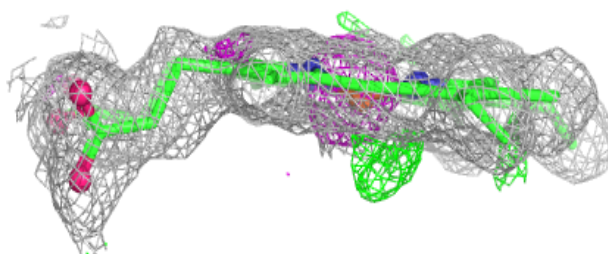
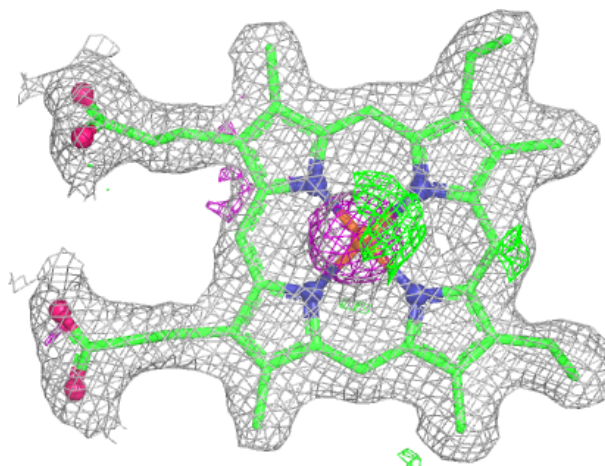
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	760	43/43	0.96	0.08	2,12,15,17	0
2	HEM	B	760	43/43	0.97	0.07	2,12,14,15	0
2	HEM	C	760	43/43	0.98	0.05	11,14,17,19	0
2	HEM	A	760	43/43	0.98	0.05	9,13,15,17	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.

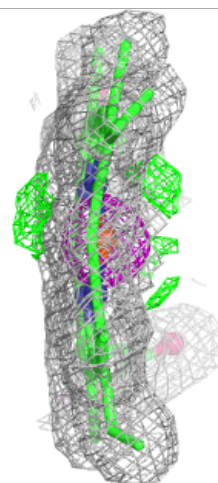
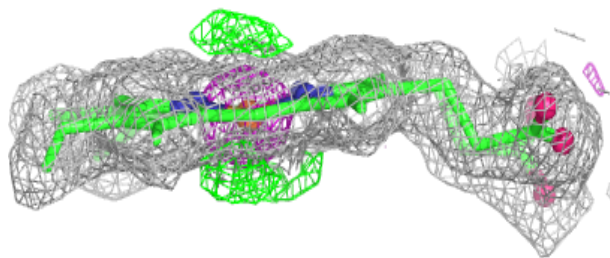
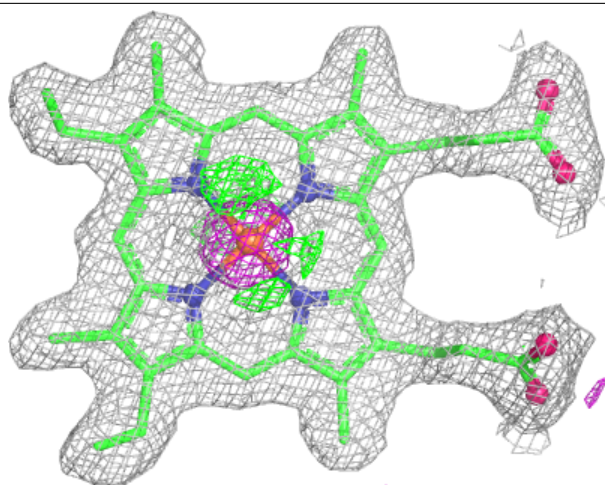
Electron density around HEM D 760:

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



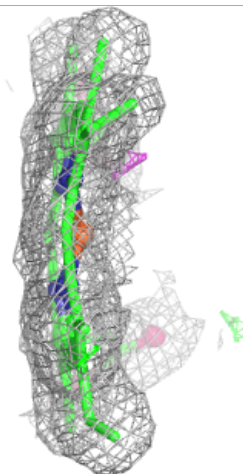
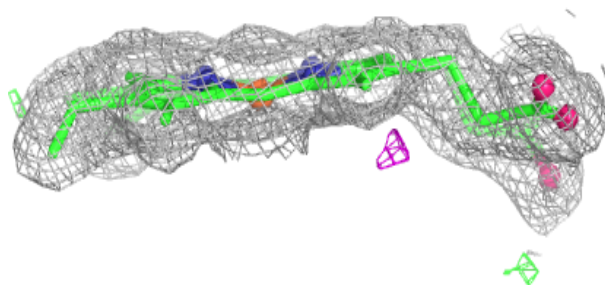
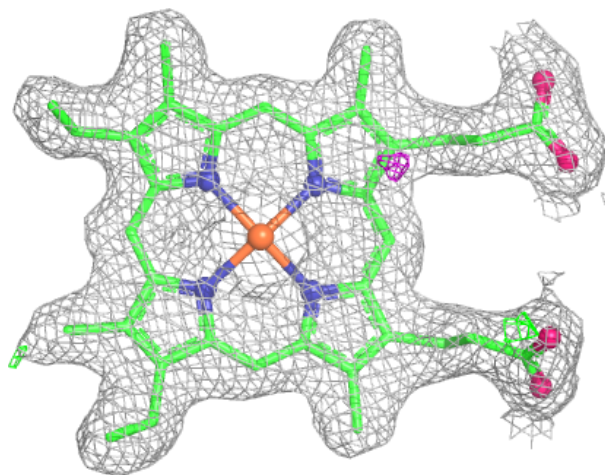
Electron density around HEM B 760:

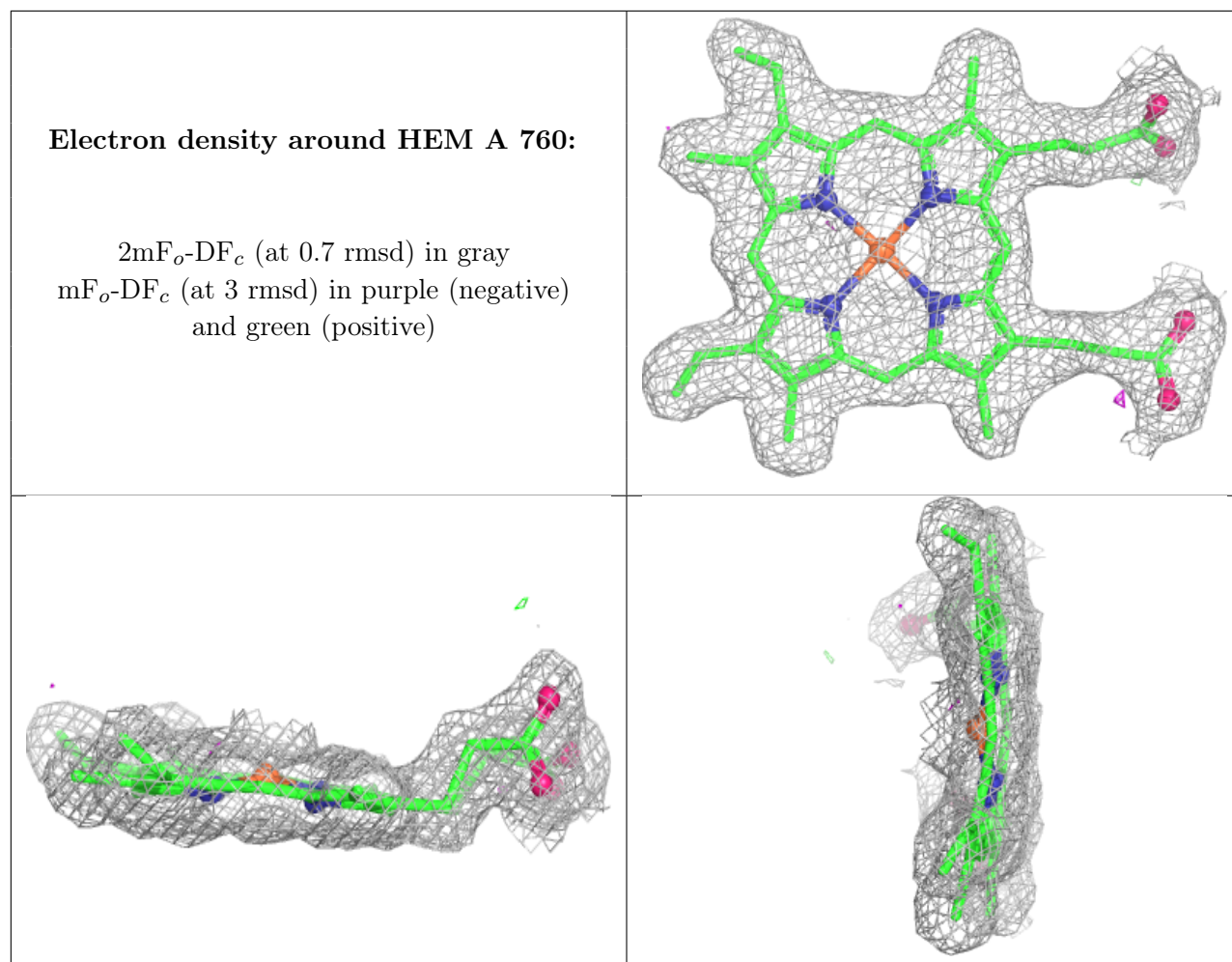
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 760:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.