



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:16 AM EDT

PDB ID : 1GGK / pdb_00001ggk
Title : CRYSTAL STRUCTURE OF CATALASE HP11 FROM ESCHERICHIA COLI, ASN201HIS VARIANT.
Authors : Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on : 2000-08-21
Resolution : 2.26 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

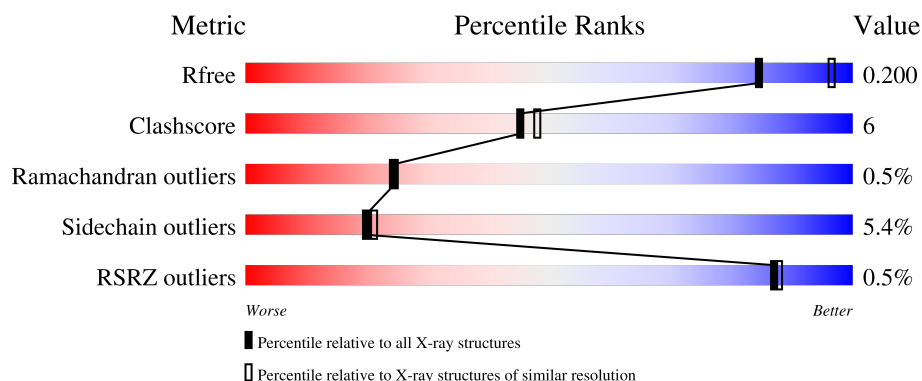
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	% 75% 19%
1	B	753	74% 19%
1	C	753	74% 18%
1	D	753	% 73% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24887 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.

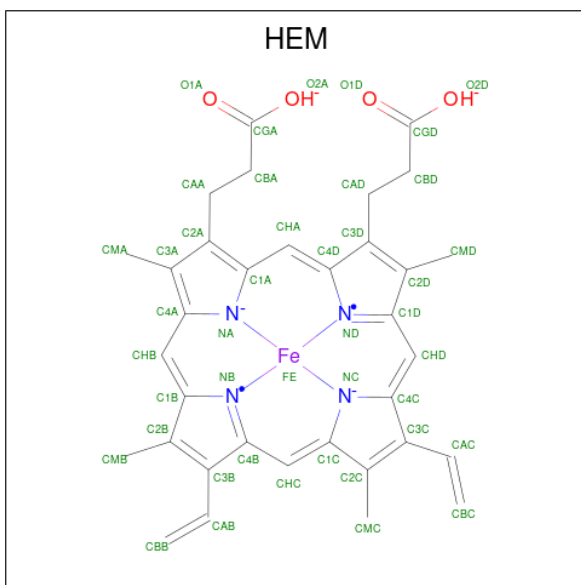
- Molecule 1 is a protein called CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			
1	B	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			
1	C	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			
1	D	727	Total	C	N	O	S	0	0	0
			5748	3649	1006	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	HIS	ASN	engineered mutation	UNP P21179
B	201	HIS	ASN	engineered mutation	UNP P21179
C	201	HIS	ASN	engineered mutation	UNP P21179
D	201	HIS	ASN	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

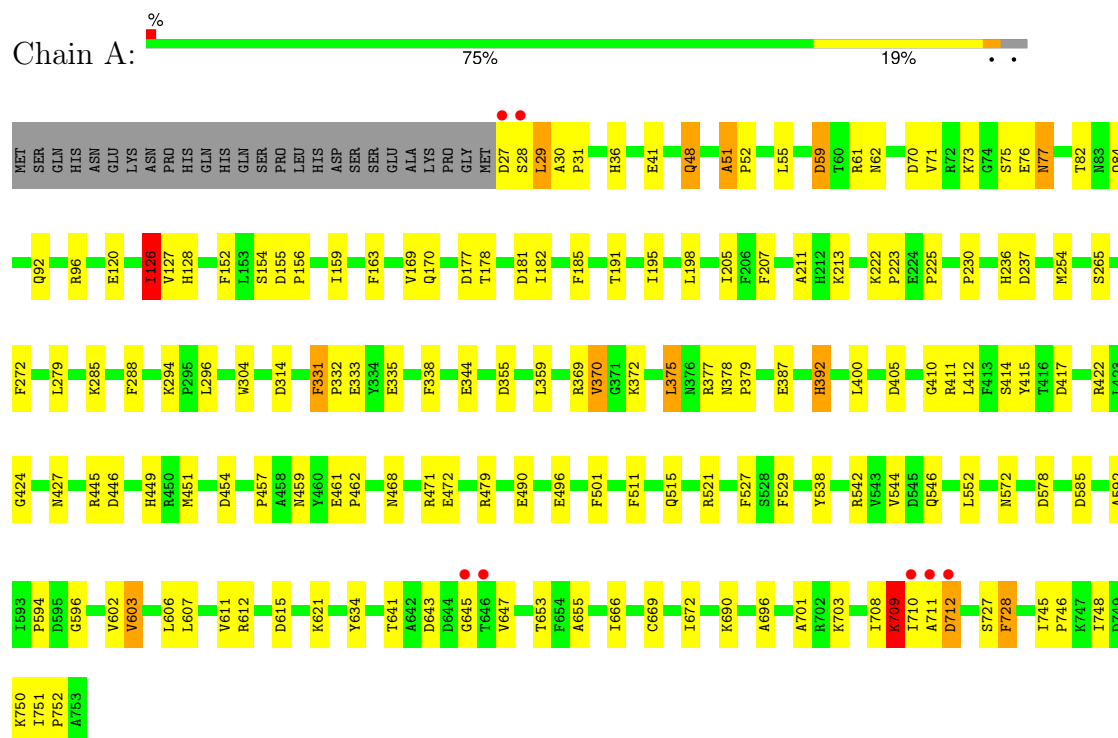
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	460	Total O 460 460	0	0
3	B	409	Total O 409 409	0	0
3	C	404	Total O 404 404	0	0
3	D	450	Total O 450 450	0	0

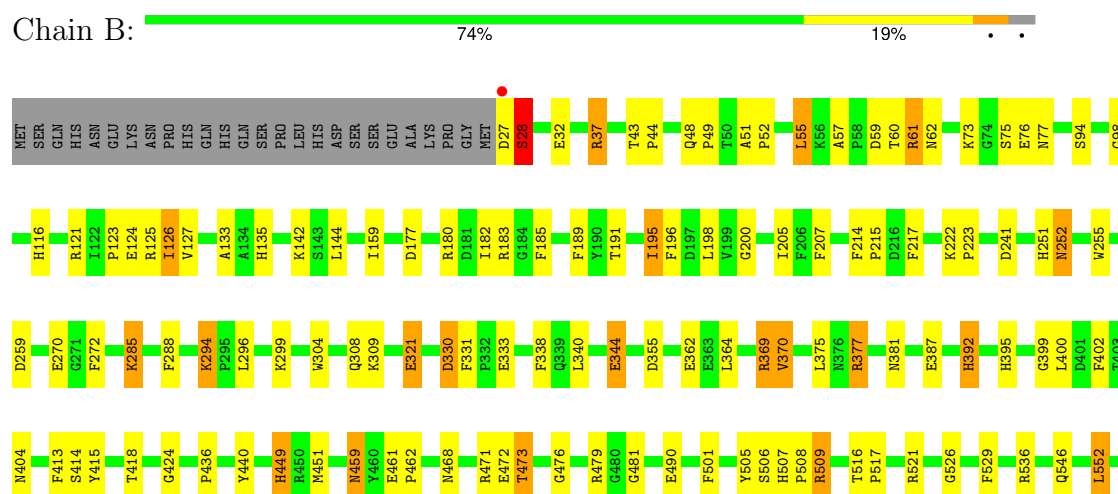
3 Residue-property plots

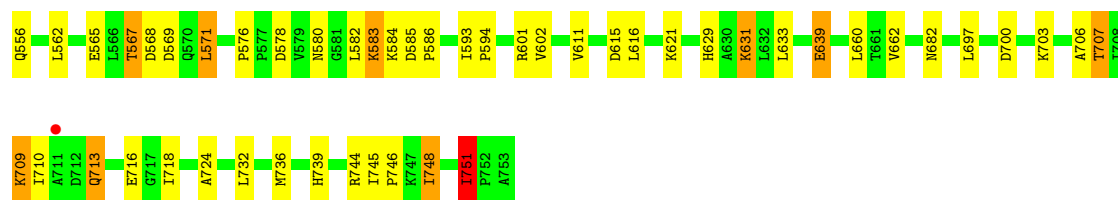
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



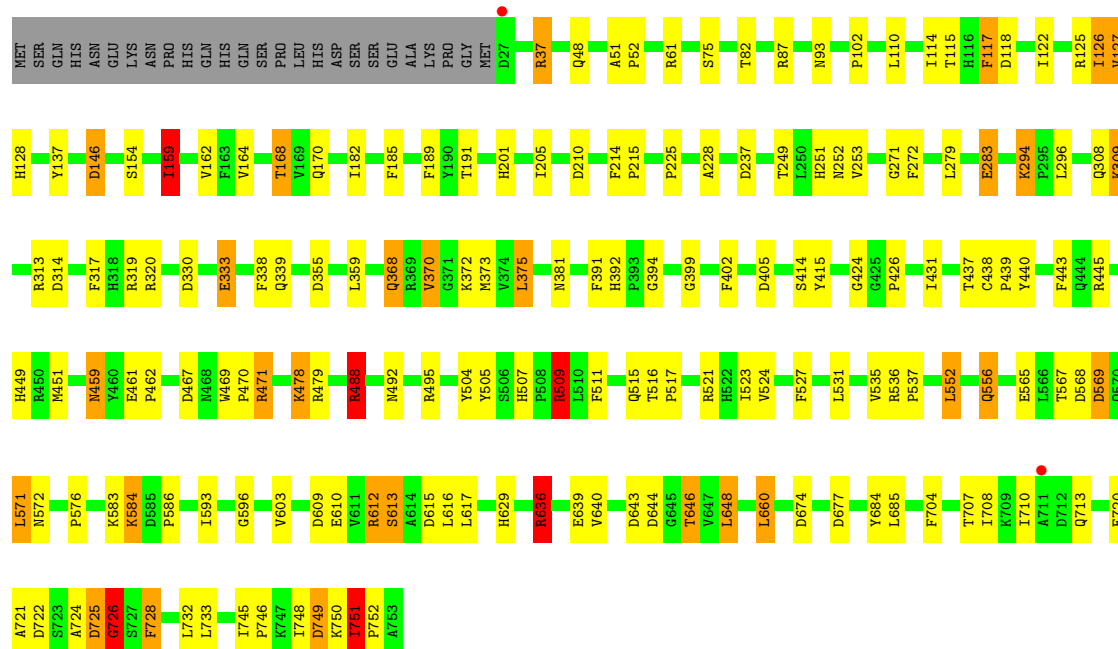
• Molecule 1: CATALASE HPII





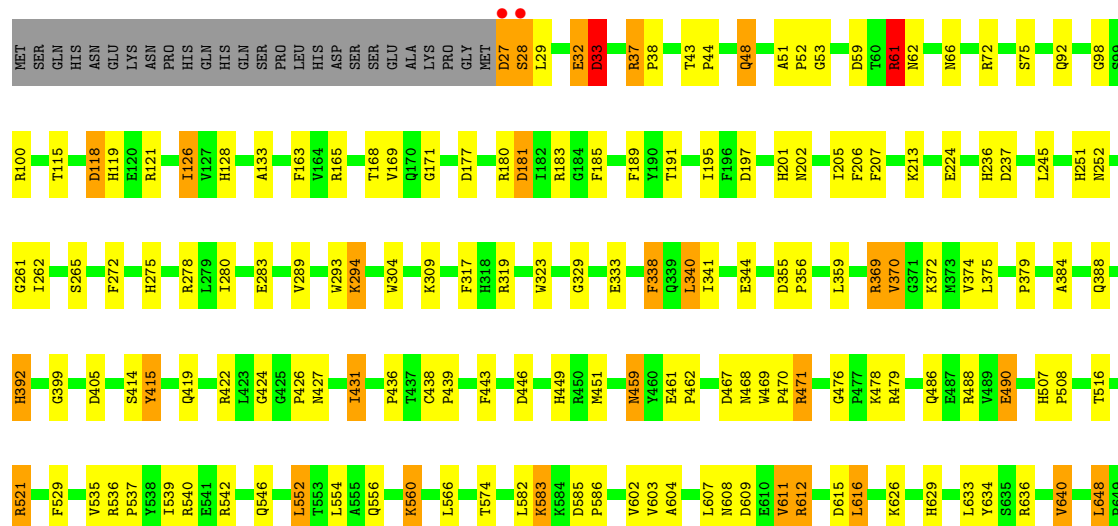
● Molecule 1: CATALASE HP11

Chain C: 74% 18%



● Molecule 1: CATALASE HP11

Chain D: 73% 20%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.23Å 134.70Å 124.45Å 90.00° 109.41° 90.00°	Depositor
Resolution (Å)	117.38 – 2.26 117.38 – 2.26	Depositor EDS
% Data completeness (in resolution range)	87.6 (117.38-2.26) 87.6 (117.38-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.26Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.130 , 0.208 0.138 , 0.200	Depositor DCC
R_{free} test set	6111 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24887	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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	0.63	0/5905	1.66	92/8028 (1.1%)
1	B	0.62	0/5905	1.72	101/8028 (1.3%)
1	C	0.61	0/5905	1.71	97/8028 (1.2%)
1	D	0.63	0/5905	1.74	107/8028 (1.3%)
All	All	0.63	0/23620	1.71	397/32112 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (397) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	521	ARG	CD-NE-CZ	25.68	160.35	124.40
1	D	27	ASP	CA-CB-CG	14.50	127.10	112.60
1	D	369	ARG	CD-NE-CZ	13.45	143.23	124.40
1	D	61	ARG	CD-NE-CZ	11.56	140.59	124.40
1	B	61	ARG	CD-NE-CZ	11.18	140.05	124.40
1	D	72	ARG	CD-NE-CZ	11.15	140.01	124.40
1	B	479	ARG	CD-NE-CZ	11.04	139.86	124.40
1	C	414	SER	N-CA-C	10.83	123.16	111.36
1	A	414	SER	N-CA-C	10.77	122.77	111.14
1	C	355	ASP	CA-C-O	10.71	126.25	119.29
1	A	61	ARG	NE-CZ-NH2	-10.58	109.68	119.20
1	C	636	ARG	CD-NE-CZ	10.53	139.15	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	PHE	CA-CB-CG	10.05	123.85	113.80
1	C	370	VAL	CB-CA-C	9.93	119.96	110.63
1	A	615	ASP	CA-CB-CG	9.90	122.50	112.60
1	A	479	ARG	CD-NE-CZ	9.66	137.93	124.40
1	C	725	ASP	CA-C-N	9.45	139.92	121.41
1	C	725	ASP	C-N-CA	9.45	139.92	121.41
1	B	377	ARG	NE-CZ-NH2	-9.41	110.73	119.20
1	D	33	ASP	CA-CB-CG	9.13	121.73	112.60
1	C	185	PHE	CA-CB-CG	9.12	122.92	113.80
1	C	725	ASP	CA-C-O	9.11	133.54	120.51
1	B	585	ASP	CA-CB-CG	9.08	121.68	112.60
1	B	185	PHE	CA-CB-CG	9.03	122.83	113.80
1	C	317	PHE	CA-C-O	-9.03	111.34	120.82
1	B	125	ARG	NH1-CZ-NH2	8.83	130.77	119.30
1	D	612	ARG	CD-NE-CZ	8.76	136.66	124.40
1	C	170	GLN	N-CA-C	8.67	120.50	111.14
1	A	59	ASP	CA-CB-CG	8.63	121.23	112.60
1	B	43	THR	CA-C-N	8.61	125.86	119.66
1	B	43	THR	C-N-CA	8.61	125.86	119.66
1	A	424	GLY	N-CA-C	8.50	126.67	115.36
1	C	283	GLU	CB-CG-CD	8.43	126.93	112.60
1	D	207	PHE	CA-CB-CG	8.41	122.21	113.80
1	D	414	SER	N-CA-C	8.38	120.19	111.14
1	D	98	GLY	CA-C-O	-8.35	115.37	121.88
1	D	405	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	37	ARG	CA-CB-CG	8.06	130.23	114.10
1	A	155	ASP	CA-CB-CG	8.05	120.65	112.60
1	C	146	ASP	CA-CB-CG	8.02	120.62	112.60
1	D	185	PHE	CA-CB-CG	7.99	121.79	113.80
1	B	259	ASP	CA-CB-CG	7.99	120.59	112.60
1	D	338	PHE	CA-CB-CG	7.96	121.77	113.80
1	D	118	ASP	CA-CB-CG	7.92	120.52	112.60
1	D	449	HIS	CA-CB-CG	7.90	121.70	113.80
1	A	70	ASP	CA-CB-CG	7.85	120.45	112.60
1	D	629	HIS	CA-CB-CG	-7.75	106.06	113.80
1	D	479	ARG	CD-NE-CZ	7.74	135.23	124.40
1	B	414	SER	N-CA-C	7.70	119.68	111.28
1	D	201	HIS	CA-CB-CG	7.65	121.45	113.80
1	D	370	VAL	N-CA-CB	-7.64	101.81	112.35
1	D	317	PHE	CA-C-O	-7.63	112.73	120.90
1	C	424	GLY	N-CA-C	7.58	125.78	115.32
1	A	331	PHE	CA-CB-CG	7.55	121.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	PHE	CA-CB-CG	7.54	121.34	113.80
1	B	125	ARG	NE-CZ-NH2	-7.53	112.42	119.20
1	D	540	ARG	CD-NE-CZ	7.52	134.92	124.40
1	B	189	PHE	CA-CB-CG	7.50	121.30	113.80
1	B	449	HIS	CA-CB-CG	7.49	121.29	113.80
1	D	725	ASP	CA-CB-CG	7.46	120.06	112.60
1	D	100	ARG	CD-NE-CZ	7.42	134.79	124.40
1	C	725	ASP	N-CA-C	7.40	126.57	110.80
1	C	189	PHE	CA-CB-CG	7.39	121.19	113.80
1	B	55	LEU	N-CA-C	-7.34	103.95	113.12
1	D	609	ASP	CA-CB-CG	7.32	119.92	112.60
1	C	728	PHE	CA-CB-CG	7.26	121.06	113.80
1	D	237	ASP	N-CA-C	7.26	119.82	111.11
1	B	44	PRO	N-CA-C	7.21	118.30	110.58
1	D	181	ASP	CA-CB-CG	7.20	119.80	112.60
1	B	304	TRP	N-CA-C	7.19	120.03	111.33
1	C	674	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	236	HIS	CA-CB-CG	7.10	120.90	113.80
1	D	293	TRP	N-CA-CB	7.07	121.69	110.65
1	D	165	ARG	NE-CZ-NH2	7.03	125.53	119.20
1	C	722	ASP	CA-CB-CG	6.99	119.59	112.60
1	A	288	PHE	CA-CB-CG	6.95	120.75	113.80
1	C	308	GLN	O-C-N	-6.94	114.76	122.12
1	C	210	ASP	CA-CB-CG	6.94	119.54	112.60
1	B	501	PHE	CA-CB-CG	6.92	120.72	113.80
1	C	370	VAL	N-CA-CB	-6.89	100.96	111.57
1	B	321	GLU	CA-C-O	-6.88	112.06	119.97
1	C	749	ASP	CA-CB-CG	6.85	119.45	112.60
1	D	43	THR	CA-C-N	6.84	124.65	119.66
1	D	43	THR	C-N-CA	6.84	124.65	119.66
1	C	471	ARG	N-CA-C	6.83	120.73	110.14
1	D	471	ARG	N-CA-C	6.78	120.87	109.76
1	D	415	TYR	CA-C-O	-6.75	113.39	120.55
1	D	542	ARG	CD-NE-CZ	6.74	133.84	124.40
1	C	749	ASP	CB-CA-C	-6.73	99.24	110.68
1	D	189	PHE	CA-CB-CG	6.73	120.53	113.80
1	A	304	TRP	N-CA-C	6.72	119.18	111.11
1	C	726	GLY	N-CA-C	-6.72	97.26	113.18
1	A	712	ASP	N-CA-C	-6.70	105.64	113.88
1	D	37	ARG	N-CA-CB	-6.69	95.54	110.27
1	A	355	ASP	CA-C-O	6.68	123.63	119.29
1	B	509	ARG	NE-CZ-NH2	6.67	125.20	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	355	ASP	CA-CB-CG	6.67	119.27	112.60
1	C	237	ASP	N-CA-C	6.66	119.11	111.11
1	B	567	THR	CA-C-N	6.61	129.37	120.65
1	B	567	THR	C-N-CA	6.61	129.37	120.65
1	B	631	LYS	CB-CA-C	6.60	120.71	110.14
1	C	527	PHE	CA-CB-CG	6.59	120.39	113.80
1	C	271	GLY	O-C-N	-6.56	117.60	123.37
1	D	183	ARG	NE-CZ-NH2	6.56	125.10	119.20
1	B	272	PHE	CA-CB-CG	6.55	120.35	113.80
1	B	471	ARG	N-CA-C	6.54	120.35	109.95
1	D	319	ARG	CD-NE-CZ	6.54	133.56	124.40
1	A	177	ASP	N-CA-C	6.54	118.49	111.36
1	A	728	PHE	CA-CB-CG	6.51	120.31	113.80
1	B	241	ASP	CA-CB-CG	6.50	119.09	112.60
1	A	501	PHE	CA-CB-CG	6.46	120.26	113.80
1	D	272	PHE	CA-CB-CG	6.46	120.26	113.80
1	D	44	PRO	O-C-N	6.45	124.28	121.31
1	B	536	ARG	CD-NE-CZ	6.44	133.41	124.40
1	C	724	ALA	CA-C-O	6.40	128.38	121.02
1	D	329	GLY	CA-C-O	-6.39	111.90	119.06
1	C	115	THR	CA-C-O	-6.38	114.12	120.82
1	D	280	ILE	CA-C-O	-6.37	113.77	120.39
1	B	506	SER	CA-C-O	-6.36	112.66	119.97
1	B	355	ASP	CA-C-O	6.36	123.42	119.29
1	A	314	ASP	O-C-N	-6.34	116.79	121.23
1	B	418	THR	CA-CB-CG2	6.34	121.27	110.50
1	A	596	GLY	N-CA-C	6.33	119.20	111.93
1	A	237	ASP	N-CA-C	6.30	118.67	111.11
1	B	402	PHE	CA-C-N	6.29	132.66	122.53
1	B	402	PHE	C-N-CA	6.29	132.66	122.53
1	A	446	ASP	CB-CA-C	-6.25	107.64	115.89
1	D	431	ILE	N-CA-C	-6.25	102.83	108.95
1	B	330	ASP	CA-CB-CG	6.24	118.84	112.60
1	C	225	PRO	N-CA-C	6.21	121.71	113.57
1	C	596	GLY	N-CA-C	6.21	118.62	111.36
1	C	317	PHE	CA-CB-CG	6.20	120.00	113.80
1	D	678	ASN	CA-CB-CG	6.20	118.80	112.60
1	B	369	ARG	CA-C-O	-6.17	113.71	120.81
1	B	472	GLU	CA-C-O	-6.17	115.08	121.87
1	B	255	TRP	O-C-N	6.16	128.41	122.07
1	D	427	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	C	159	ILE	CB-CA-C	6.15	120.00	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	278	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	237	ASP	CA-C-O	-6.14	114.33	120.90
1	B	270	GLU	CA-C-N	6.14	126.34	121.61
1	B	270	GLU	C-N-CA	6.14	126.34	121.61
1	B	57	ALA	CA-C-N	6.14	125.76	119.56
1	B	57	ALA	C-N-CA	6.14	125.76	119.56
1	D	552	LEU	N-CA-C	6.12	117.95	111.28
1	D	691	HIS	CA-C-O	6.10	126.81	119.43
1	C	615	ASP	CA-CB-CG	6.10	118.70	112.60
1	D	261	GLY	N-CA-C	6.10	121.38	114.67
1	C	751	ILE	CB-CA-C	6.07	117.83	110.85
1	D	265	SER	N-CA-CB	-6.06	102.35	111.56
1	A	445	ARG	NE-CZ-NH2	-6.05	113.76	119.20
1	C	228	ALA	CA-C-N	6.04	133.31	122.13
1	C	228	ALA	C-N-CA	6.04	133.31	122.13
1	D	666	ILE	N-CA-CB	6.03	119.73	111.41
1	B	529	PHE	CA-C-O	-6.03	114.49	120.82
1	D	53	GLY	O-C-N	-6.03	116.33	122.17
1	C	338	PHE	CA-CB-CG	5.98	119.78	113.80
1	C	168	THR	CA-C-O	-5.94	113.56	121.46
1	B	127	VAL	CA-C-O	-5.94	115.43	121.67
1	A	578	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	123	PRO	CA-C-O	-5.92	114.59	121.34
1	B	381	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	C	488	ARG	CA-C-O	5.91	127.34	120.49
1	D	369	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	C	459	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	643	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	159	ILE	CA-C-O	-5.89	114.05	120.71
1	C	479	ARG	NE-CZ-NH2	5.89	124.51	119.20
1	C	569	ASP	CA-CB-CG	5.89	118.50	112.60
1	B	62	ASN	CA-CB-CG	5.88	118.48	112.60
1	B	424	GLY	N-CA-C	5.87	123.43	115.32
1	D	98	GLY	N-CA-C	-5.86	104.33	112.18
1	C	82	THR	N-CA-CB	5.85	118.20	110.25
1	C	117	PHE	CA-CB-CG	5.85	119.65	113.80
1	A	392	HIS	CA-C-N	5.84	125.52	119.56
1	A	392	HIS	C-N-CA	5.84	125.52	119.56
1	A	471	ARG	CA-C-O	5.84	127.76	121.16
1	C	279	LEU	CA-C-O	-5.83	114.53	120.71
1	D	206	PHE	CA-CB-CG	-5.83	107.97	113.80
1	C	609	ASP	CA-CB-CG	5.83	118.42	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	VAL	N-CA-CB	-5.82	101.11	112.75
1	B	288	PHE	CA-C-O	-5.82	114.42	121.05
1	B	505	TYR	CA-C-O	-5.82	112.75	118.97
1	C	368	GLN	CB-CG-CD	5.81	122.47	112.60
1	A	126	ILE	N-CA-CB	5.80	116.95	110.51
1	B	716	GLU	CB-CG-CD	5.80	122.47	112.60
1	D	560	LYS	CB-CA-C	5.80	120.41	110.79
1	A	427	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	D	224	GLU	CB-CA-C	5.78	118.66	109.52
1	C	272	PHE	CA-CB-CG	5.78	119.58	113.80
1	C	125	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	D	612	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	B	392	HIS	CA-C-N	5.77	125.45	119.56
1	B	392	HIS	C-N-CA	5.77	125.45	119.56
1	B	639	GLU	CB-CG-CD	-5.77	102.80	112.60
1	D	751	ILE	CA-C-O	5.76	127.67	119.95
1	B	509	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	C	492	ASN	CA-CB-CG	5.74	118.34	112.60
1	B	133	ALA	N-CA-C	5.74	118.42	109.52
1	C	339	GLN	N-CA-CB	5.73	119.82	110.37
1	B	321	GLU	N-CA-CB	5.72	119.14	110.28
1	C	391	PHE	CA-CB-CG	5.71	119.52	113.80
1	B	569	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	612	ARG	CA-C-N	5.71	128.20	120.38
1	C	612	ARG	C-N-CA	5.71	128.20	120.38
1	D	392	HIS	CA-C-N	5.71	125.38	119.56
1	D	392	HIS	C-N-CA	5.71	125.38	119.56
1	B	459	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	C	684	TYR	CA-C-O	5.70	127.00	120.90
1	C	313	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	B	338	PHE	CA-CB-CG	5.68	119.48	113.80
1	D	197	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	55	LEU	N-CA-CB	5.68	119.10	110.42
1	D	369	ARG	CA-C-N	5.67	128.59	121.85
1	D	369	ARG	C-N-CA	5.67	128.59	121.85
1	C	593	ILE	N-CA-CB	5.67	118.00	111.31
1	A	152	PHE	CA-CB-CG	5.66	119.46	113.80
1	D	304	TRP	N-CA-C	5.66	120.71	111.37
1	C	182	ILE	CA-C-O	-5.65	115.85	122.13
1	C	118	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	387	GLU	N-CA-C	5.64	117.43	111.28
1	A	712	ASP	CA-C-O	5.64	125.61	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ILE	N-CA-CB	5.63	115.72	111.83
1	C	405	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	154	SER	N-CA-C	5.63	119.99	113.18
1	C	381	ASN	CA-CB-CG	5.62	118.22	112.60
1	D	636	ARG	CA-C-O	-5.62	115.42	121.38
1	A	48	GLN	CB-CA-C	-5.62	99.11	110.17
1	B	331	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	556	GLN	N-CA-C	5.59	117.38	111.28
1	B	217	PHE	CA-C-O	-5.57	114.97	120.82
1	A	62	ASN	CA-C-O	-5.57	115.45	121.36
1	D	529	PHE	CA-CB-CG	-5.56	108.24	113.80
1	D	37	ARG	CB-CA-C	5.55	118.35	110.02
1	A	181	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	454	ASP	CA-CB-CG	-5.54	107.06	112.60
1	D	546	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	D	275	HIS	CA-CB-CG	5.53	119.33	113.80
1	A	82	THR	N-CA-C	-5.53	102.72	110.35
1	A	708	ILE	CA-C-N	5.51	132.06	121.54
1	A	708	ILE	C-N-CA	5.51	132.06	121.54
1	B	195	ILE	CB-CG1-CD1	5.50	125.34	113.80
1	C	372	LYS	CA-CB-CG	5.49	125.08	114.10
1	D	171	GLY	N-CA-C	5.46	119.53	112.54
1	A	472	GLU	CA-C-O	-5.46	115.76	121.55
1	D	236	HIS	CA-CB-CG	5.46	119.26	113.80
1	D	461	GLU	O-C-N	5.46	125.67	121.85
1	D	163	PHE	N-CA-CB	5.44	119.32	110.77
1	D	608	ASN	CA-C-O	-5.44	115.42	121.51
1	A	377	ARG	CD-NE-CZ	5.44	132.01	124.40
1	C	333	GLU	CA-C-O	5.43	126.35	120.32
1	D	53	GLY	N-CA-C	5.43	119.45	112.83
1	C	565	GLU	CA-C-O	-5.43	114.50	120.36
1	B	294	LYS	N-CA-CB	-5.42	100.72	109.94
1	B	751	ILE	CA-C-O	5.42	122.76	119.94
1	D	677	ASP	CA-CB-CG	-5.42	107.18	112.60
1	C	459	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	B	98	GLY	CA-C-O	-5.42	117.66	121.88
1	D	278	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	A	546	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	D	341	ILE	CA-C-O	5.40	122.75	119.94
1	A	71	VAL	CA-C-O	-5.40	113.68	119.35
1	B	340	LEU	CA-C-N	5.40	127.55	122.85
1	B	340	LEU	C-N-CA	5.40	127.55	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	28	SER	N-CA-CB	5.39	119.60	110.49
1	A	265	SER	N-CA-CB	-5.39	103.21	111.56
1	C	536	ARG	CA-C-N	5.38	125.46	119.32
1	C	536	ARG	C-N-CA	5.38	125.46	119.32
1	A	527	PHE	CA-CB-CG	5.38	119.18	113.80
1	D	62	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	60	THR	N-CA-CB	5.36	118.74	110.21
1	A	496	GLU	N-CA-CB	-5.36	101.43	111.13
1	A	544	VAL	O-C-N	-5.36	116.67	121.87
1	B	713	GLN	CA-CB-CG	5.36	124.81	114.10
1	A	41	GLU	CA-CB-CG	5.35	124.79	114.10
1	C	677	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	177	ASP	N-CA-C	5.33	116.90	111.14
1	B	476	GLY	CA-C-N	5.33	124.94	119.56
1	B	476	GLY	C-N-CA	5.33	124.94	119.56
1	B	308	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	468	ASN	CA-C-O	-5.32	114.19	120.57
1	A	182	ILE	CA-C-O	-5.32	115.55	121.98
1	A	55	LEU	N-CA-C	-5.31	106.96	113.50
1	B	180	ARG	CA-C-O	-5.31	115.02	120.54
1	D	133	ALA	N-CA-C	5.30	117.73	109.52
1	C	102	PRO	CA-C-O	-5.29	115.21	121.67
1	A	96	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	529	PHE	CA-C-O	-5.29	115.26	120.82
1	D	384	ALA	N-CA-C	5.29	117.13	111.36
1	D	32	GLU	N-CA-CB	5.29	118.49	109.87
1	C	431	ILE	N-CA-C	-5.29	103.77	108.95
1	D	574	THR	CA-C-N	5.29	123.52	119.66
1	D	574	THR	C-N-CA	5.29	123.52	119.66
1	B	473	THR	CA-C-N	5.28	123.52	119.66
1	B	473	THR	C-N-CA	5.28	123.52	119.66
1	A	422	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	399	GLY	N-CA-C	-5.28	107.25	114.64
1	D	419	GLN	CA-C-N	5.27	127.68	120.46
1	D	419	GLN	C-N-CA	5.27	127.68	120.46
1	A	471	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	51	ALA	N-CA-C	5.26	114.19	108.14
1	D	388	GLN	OE1-CD-NE2	-5.26	117.33	122.60
1	A	572	ASN	CA-CB-CG	-5.26	107.34	112.60
1	D	62	ASN	CA-C-O	-5.25	115.81	121.38
1	C	509	ARG	NE-CZ-NH1	-5.25	116.25	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	195	ILE	CB-CA-C	-5.23	103.91	111.34
1	D	32	GLU	N-CA-C	-5.23	101.25	109.25
1	C	314	ASP	CA-C-N	5.23	124.89	119.56
1	C	314	ASP	C-N-CA	5.23	124.89	119.56
1	A	375	LEU	CA-C-O	-5.22	115.11	120.54
1	B	196	PHE	CA-C-O	-5.22	114.71	120.30
1	D	59	ASP	CA-C-O	-5.22	112.97	119.28
1	A	412	LEU	CA-C-O	-5.21	114.21	120.10
1	C	320	ARG	CA-C-N	5.18	127.23	120.28
1	C	320	ARG	C-N-CA	5.18	127.23	120.28
1	D	422	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	A	645	GLY	CA-C-O	-5.18	113.10	119.06
1	B	28	SER	CA-C-O	5.18	127.92	120.51
1	A	655	ALA	CA-C-N	5.18	125.69	120.00
1	A	655	ALA	C-N-CA	5.18	125.69	120.00
1	C	339	GLN	N-CA-C	-5.18	99.35	108.20
1	B	404	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	D	44	PRO	N-CA-C	5.17	115.44	110.47
1	A	170	GLN	CB-CG-CD	5.17	121.39	112.60
1	C	402	PHE	CA-C-N	5.17	130.63	122.36
1	C	402	PHE	C-N-CA	5.17	130.63	122.36
1	B	200	GLY	N-CA-C	5.17	119.94	112.81
1	B	135	HIS	O-C-N	-5.16	117.16	122.94
1	B	748	ILE	CA-C-N	5.16	127.61	120.29
1	B	748	ILE	C-N-CA	5.16	127.61	120.29
1	A	169	VAL	CB-CA-C	-5.16	106.46	111.05
1	B	255	TRP	CA-C-O	-5.15	115.41	120.82
1	D	372	LYS	N-CA-C	5.14	117.80	109.06
1	C	93	ASN	N-CA-C	5.14	117.62	109.50
1	A	446	ASP	N-CA-C	5.13	117.64	109.02
1	A	163	PHE	CA-C-O	-5.13	114.80	120.24
1	B	94	SER	CA-C-O	-5.13	115.20	121.36
1	C	319	ARG	CA-C-N	5.13	127.11	120.44
1	C	319	ARG	C-N-CA	5.13	127.11	120.44
1	B	395	HIS	CA-CB-CG	5.13	118.93	113.80
1	A	585	ASP	CA-C-N	5.12	125.42	119.47
1	A	585	ASP	C-N-CA	5.12	125.42	119.47
1	B	294	LYS	CB-CA-C	5.12	115.52	109.47
1	A	170	GLN	CA-C-N	5.12	126.32	120.53
1	A	170	GLN	C-N-CA	5.12	126.32	120.53
1	D	356	PRO	CB-CA-C	5.12	115.73	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	636	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	D	37	ARG	CA-CB-CG	5.12	124.33	114.10
1	C	646	THR	N-CA-C	5.12	116.52	109.15
1	C	722	ASP	N-CA-CB	5.12	117.43	110.01
1	C	437	THR	N-CA-C	-5.11	106.89	113.23
1	A	272	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	736	MET	CA-C-O	-5.11	115.14	120.55
1	C	445	ARG	CD-NE-CZ	5.11	131.55	124.40
1	D	399	GLY	N-CA-C	-5.10	108.41	114.48
1	B	413	PHE	CA-C-N	5.10	127.11	120.28
1	B	413	PHE	C-N-CA	5.10	127.11	120.28
1	D	317	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	62	ASN	N-CA-C	-5.09	101.71	108.74
1	A	178	THR	N-CA-C	5.09	119.17	112.25
1	B	526	GLY	CA-C-N	5.08	127.09	120.28
1	B	526	GLY	C-N-CA	5.08	127.09	120.28
1	D	738	ALA	CA-C-N	5.08	131.25	121.54
1	D	738	ALA	C-N-CA	5.08	131.25	121.54
1	D	289	VAL	N-CA-C	5.08	115.97	108.45
1	C	613	SER	N-CA-C	5.08	117.48	111.33
1	B	387	GLU	CA-C-O	-5.07	115.17	120.55
1	B	400	LEU	CA-C-O	-5.07	115.53	121.46
1	A	496	GLU	N-CA-C	5.07	117.42	108.75
1	C	495	ARG	NE-CZ-NH2	-5.06	114.64	119.20
1	A	411	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	C	154	SER	N-CA-C	5.06	119.32	113.20
1	A	405	ASP	CA-C-N	5.06	124.72	119.56
1	A	405	ASP	C-N-CA	5.06	124.72	119.56
1	C	644	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	504	TYR	N-CA-C	5.05	121.14	114.12
1	D	424	GLY	N-CA-C	5.05	122.29	115.32
1	A	703	LYS	CA-CB-CG	5.05	124.20	114.10
1	A	77	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	225	PRO	N-CA-C	5.04	120.18	113.57
1	B	198	LEU	CA-C-N	5.04	128.14	122.59
1	B	198	LEU	C-N-CA	5.04	128.14	122.59
1	D	516	THR	CA-C-N	5.04	124.65	119.05
1	D	516	THR	C-N-CA	5.04	124.65	119.05
1	D	446	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	479	ARG	CG-CD-NE	5.03	123.08	112.00
1	A	84	GLN	CB-CA-C	5.03	118.48	110.09
1	D	486	GLN	OE1-CD-NE2	-5.03	117.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	505	TYR	CA-C-O	-5.02	113.52	119.05
1	B	177	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	544	VAL	CA-C-N	5.01	126.99	120.28
1	A	544	VAL	C-N-CA	5.01	126.99	120.28
1	A	712	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	546	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	C	399	GLY	N-CA-C	-5.01	107.63	114.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	726	GLY	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5748	0	5579	61	0
1	B	5748	0	5579	76	0
1	C	5748	0	5579	68	0
1	D	5748	0	5579	79	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
2	C	43	0	30	2	0
2	D	43	0	30	0	0
3	A	460	0	0	10	0
3	B	409	0	0	10	0
3	C	404	0	0	10	0
3	D	450	0	0	7	0
All	All	24887	0	22436	268	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 6.

All (268) 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:392:HIS:ND1	1:A:415:TYR:HB2	1.13	1.45
1:B:392:HIS:ND1	1:B:415:TYR:HB2	1.20	1.40
1:D:392:HIS:ND1	1:D:415:TYR:HB2	1.11	1.40
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.10	1.39
1:D:392:HIS:ND1	1:D:415:TYR:CB	2.06	1.18
1:A:392:HIS:ND1	1:A:415:TYR:CB	2.07	1.18
1:C:392:HIS:ND1	1:C:415:TYR:CB	2.06	1.17
1:B:392:HIS:ND1	1:B:415:TYR:CB	2.08	1.15
1:C:552:LEU:HD11	1:C:571:LEU:HD12	1.43	1.00
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.03	0.93
1:B:583:LYS:HE2	1:B:583:LYS:H	1.34	0.92
1:B:451:MET:HE2	1:D:451:MET:HE2	1.51	0.91
2:A:760:HEM:HBC2	2:A:760:HEM:HMC2	1.54	0.89
1:A:641:THR:HA	3:A:1219:HOH:O	1.76	0.86
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.08	0.86
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.43	0.84
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.10	0.84
3:B:1162:HOH:O	1:C:126:ILE:HB	1.78	0.83
1:C:392:HIS:CE1	1:C:415:TYR:HB2	2.11	0.83
1:D:611:VAL:HG11	1:D:616:LEU:HD12	1.65	0.78
1:C:438:CYS:HB2	1:C:439:PRO:HD2	1.67	0.77
1:D:640:VAL:HG23	1:D:648:LEU:HD23	1.68	0.76
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.69	0.74
1:A:451:MET:HE2	1:C:451:MET:HE2	1.70	0.72
1:C:751:ILE:HD12	1:C:752:PRO:HD2	1.73	0.71
1:B:682:ASN:OD1	1:B:707:THR:HG21	1.93	0.69
1:B:369:ARG:HB3	3:B:1149:HOH:O	1.92	0.69
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.75	0.69
1:D:27:ASP:O	1:D:28:SER:HB3	1.94	0.67
1:C:552:LEU:HD13	1:C:556:GLN:NE2	2.09	0.67
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.77	0.67
1:A:294:LYS:HB2	3:A:985:HOH:O	1.95	0.67
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.76	0.66
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.78	0.66
1:C:704:PHE:O	1:C:707:THR:HG22	1.96	0.65
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.78	0.65
1:B:611:VAL:HG11	1:B:616:LEU:HG	1.79	0.65
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.79	0.64
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.33	0.64
1:D:603:VAL:HG11	1:D:666:ILE:HD12	1.79	0.63
1:B:567:THR:O	1:B:571:LEU:HD22	1.99	0.63
1:A:672:ILE:HG21	3:A:1216:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.81	0.62
1:B:709:LYS:NZ	1:B:709:LYS:HA	2.15	0.62
1:B:451:MET:CE	1:D:451:MET:HE2	2.27	0.61
1:A:294:LYS:NZ	1:A:369:ARG:HH21	1.98	0.61
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.82	0.61
1:C:478:LYS:HD3	1:C:478:LYS:N	2.16	0.61
1:B:294:LYS:HE2	3:B:1164:HOH:O	2.01	0.61
1:B:294:LYS:HB2	3:B:1006:HOH:O	2.00	0.61
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.35	0.60
1:D:32:GLU:O	1:D:33:ASP:HB3	2.00	0.60
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.82	0.60
1:B:195:ILE:HD11	1:B:436:PRO:HA	1.85	0.59
1:D:648:LEU:HD21	3:D:1205:HOH:O	2.02	0.59
1:D:607:LEU:HD13	1:D:640:VAL:HG21	1.86	0.58
1:C:749:ASP:HB2	1:C:750:LYS:HD3	1.85	0.58
1:B:468:ASN:HD22	1:D:27:ASP:N	2.02	0.58
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.34	0.58
1:C:127:VAL:O	1:C:128:HIS:HB2	2.04	0.57
1:C:535:VAL:O	1:C:537:PRO:HD3	2.03	0.57
1:C:296:LEU:HD12	1:C:333:GLU:HB3	1.86	0.57
2:A:760:HEM:HBC2	2:A:760:HEM:CMC	2.31	0.57
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.35	0.57
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.86	0.57
1:B:700:ASP:HA	1:B:703:LYS:HD3	1.87	0.57
1:D:61:ARG:HG3	1:D:66:ASN:OD1	2.05	0.57
1:B:583:LYS:H	1:B:583:LYS:CE	2.12	0.56
1:C:488:ARG:HD2	3:C:1158:HOH:O	2.04	0.56
1:A:701:ALA:HA	3:A:1216:HOH:O	2.05	0.56
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.19	0.56
1:C:567:THR:O	1:C:571:LEU:HD22	2.04	0.56
1:C:646:THR:O	1:C:648:LEU:HD13	2.06	0.56
1:C:110:LEU:O	1:C:114:ILE:HG12	2.06	0.56
1:C:488:ARG:NH1	3:C:1137:HOH:O	2.38	0.56
1:B:706:ALA:HA	1:B:709:LYS:NZ	2.21	0.55
1:A:607:LEU:HD22	1:A:611:VAL:HG21	1.87	0.55
1:B:48:GLN:HB3	1:B:49:PRO:HD2	1.88	0.55
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.36	0.55
1:A:294:LYS:HZ1	1:A:369:ARG:HH21	1.55	0.54
1:C:516:THR:HB	1:C:517:PRO:CD	2.37	0.54
1:A:213:LYS:HD3	1:D:92:GLN:HA	1.90	0.54
1:A:751:ILE:HD12	1:A:751:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LYS:HB2	3:C:1034:HOH:O	2.08	0.53
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.90	0.53
1:A:369:ARG:HG2	3:A:1209:HOH:O	2.08	0.53
1:D:611:VAL:CG1	1:D:616:LEU:HD12	2.37	0.53
1:C:612:ARG:HA	1:C:643:ASP:OD2	2.08	0.53
1:B:706:ALA:HA	1:B:709:LYS:HZ2	1.73	0.53
1:A:369:ARG:HG3	3:A:1006:HOH:O	2.08	0.52
1:D:469:TRP:CE3	1:D:471:ARG:HG3	2.44	0.52
1:B:552:LEU:HD21	1:B:556:GLN:NE2	2.25	0.52
1:C:478:LYS:HD3	1:C:478:LYS:H	1.73	0.52
1:A:76:GLU:O	1:A:77:ASN:HB2	2.10	0.52
1:B:706:ALA:O	1:B:709:LYS:HD2	2.10	0.52
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.92	0.52
1:D:556:GLN:HG3	1:D:566:LEU:CD1	2.40	0.51
1:B:516:THR:HB	1:B:517:PRO:CD	2.40	0.51
1:C:249:THR:O	1:C:253:VAL:HG23	2.11	0.51
1:B:552:LEU:C	1:B:552:LEU:HD13	2.36	0.51
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.93	0.51
1:D:359:LEU:H	1:D:507:HIS:HD2	1.59	0.51
1:B:344:GLU:CD	1:B:344:GLU:H	2.19	0.51
1:D:626:LYS:HG3	1:D:733:LEU:HD13	1.92	0.51
1:D:603:VAL:CG1	1:D:666:ILE:HD12	2.41	0.51
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.46	0.50
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.46	0.50
1:A:511:PHE:O	1:A:515:GLN:HG2	2.10	0.50
1:A:748:ILE:O	1:A:751:ILE:HG13	2.11	0.50
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.41	0.50
1:D:611:VAL:HB	3:D:1205:HOH:O	2.12	0.50
1:B:748:ILE:O	1:B:751:ILE:HG22	2.12	0.50
1:C:745:ILE:N	1:C:746:PRO:HD2	2.27	0.50
1:C:309:LYS:HD2	1:C:660:LEU:HD21	1.94	0.49
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.94	0.49
1:A:294:LYS:NZ	1:A:369:ARG:NH2	2.60	0.49
1:D:359:LEU:H	1:D:507:HIS:CD2	2.30	0.49
1:B:461:GLU:HA	1:B:462:PRO:C	2.37	0.49
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.95	0.48
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.78	0.48
1:C:359:LEU:C	1:C:359:LEU:HD12	2.37	0.48
1:C:613:SER:O	1:C:617:LEU:HD13	2.13	0.48
1:C:636:ARG:HD3	3:C:1132:HOH:O	2.14	0.48
1:D:323:TRP:CZ3	1:D:379:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASP:HB2	1:D:29:LEU:HG	1.94	0.48
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.95	0.47
1:D:115:THR:O	1:D:119:HIS:HD2	1.97	0.47
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.97	0.47
1:A:461:GLU:HA	1:A:462:PRO:C	2.39	0.47
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.48	0.47
1:B:631:LYS:HE3	1:B:662:VAL:CG1	2.44	0.47
1:C:392:HIS:CD2	1:C:394:GLY:H	2.31	0.47
1:C:461:GLU:HA	1:C:462:PRO:C	2.39	0.47
1:D:536:ARG:HB2	1:D:539:ILE:HD12	1.97	0.47
1:B:586:PRO:HB2	1:B:593:ILE:HD12	1.96	0.47
1:B:615:ASP:HA	1:B:724:ALA:HB3	1.97	0.47
1:A:461:GLU:HB2	1:A:462:PRO:HA	1.97	0.47
1:B:296:LEU:HD12	1:B:333:GLU:HB3	1.95	0.47
1:B:631:LYS:HD3	3:B:1150:HOH:O	2.13	0.47
1:C:720:GLU:O	1:C:721:ALA:HB2	2.15	0.47
1:A:612:ARG:HE	1:A:669:CYS:CB	2.22	0.47
1:B:516:THR:HB	1:B:517:PRO:HD2	1.97	0.47
1:C:572:ASN:HB3	3:C:1139:HOH:O	2.14	0.47
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.96	0.47
1:D:521:ARG:HE	1:D:521:ARG:HA	1.80	0.47
1:B:745:ILE:N	1:B:746:PRO:HD2	2.30	0.47
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.97	0.46
1:A:745:ILE:N	1:A:746:PRO:HD2	2.30	0.46
1:C:523:ILE:O	1:C:524:VAL:C	2.58	0.46
1:A:294:LYS:HZ3	1:A:369:ARG:NH2	2.12	0.46
1:A:538:TYR:O	1:A:542:ARG:HG3	2.15	0.46
1:B:629:HIS:HD2	3:B:1100:HOH:O	1.97	0.46
1:D:27:ASP:O	1:D:28:SER:CB	2.62	0.46
1:A:369:ARG:HH21	1:A:369:ARG:HG2	1.79	0.46
1:B:615:ASP:O	1:B:616:LEU:C	2.59	0.46
1:B:126:ILE:HD13	1:C:117:PHE:O	2.15	0.46
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.98	0.46
1:D:438:CYS:HB2	1:D:439:PRO:HD2	1.97	0.46
1:D:459:ASN:HD22	1:D:459:ASN:H	1.63	0.46
1:D:333:GLU:HG2	1:D:374:VAL:HG22	1.98	0.46
1:D:32:GLU:O	1:D:33:ASP:CB	2.64	0.46
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.98	0.46
1:B:28:SER:HA	1:D:467:ASP:OD1	2.17	0.45
1:B:207:PHE:CD2	1:B:252:ASN:HB3	2.51	0.45
1:D:521:ARG:HE	1:D:521:ARG:CA	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ALA:HB1	1:A:36:HIS:CD2	2.52	0.45
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.52	0.45
1:D:556:GLN:HG3	1:D:566:LEU:HD12	1.98	0.45
1:A:331:PHE:HA	1:A:332:PRO:HD3	1.77	0.45
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.51	0.45
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.98	0.45
1:A:51:ALA:HB1	1:A:52:PRO:CD	2.44	0.45
1:A:127:VAL:O	1:A:128:HIS:HB2	2.16	0.45
1:A:521:ARG:HG3	3:A:1211:HOH:O	2.16	0.45
1:D:180:ARG:O	1:D:181:ASP:HB2	2.17	0.45
1:A:296:LEU:HD21	1:A:335:GLU:HG3	1.98	0.45
1:A:592:ALA:O	1:A:594:PRO:HD3	2.17	0.45
1:D:27:ASP:HB2	1:D:29:LEU:CG	2.47	0.45
1:C:51:ALA:HB1	1:C:52:PRO:CD	2.46	0.44
1:B:59:ASP:HA	1:B:61:ARG:CZ	2.47	0.44
1:B:76:GLU:O	1:B:77:ASN:HB2	2.17	0.44
1:D:61:ARG:NH1	1:D:66:ASN:OD1	2.45	0.44
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.47	0.44
1:C:201:HIS:CG	2:C:760:HEM:HMB2	2.52	0.44
1:C:509:ARG:HD3	1:C:576:PRO:HG2	2.00	0.44
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.77	0.44
1:B:214:PHE:HB3	1:B:215:PRO:HD3	1.98	0.44
1:C:128:HIS:HA	1:C:168:THR:O	2.17	0.44
1:B:59:ASP:OD2	1:B:61:ARG:NH2	2.50	0.44
1:C:87:ARG:NH2	3:C:1130:HOH:O	2.49	0.44
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.52	0.44
3:A:1218:HOH:O	1:C:449:HIS:CE1	2.70	0.44
1:B:507:HIS:N	1:B:508:PRO:CD	2.81	0.44
1:D:294:LYS:NZ	3:D:1181:HOH:O	2.44	0.43
1:D:745:ILE:HB	1:D:746:PRO:HD3	1.99	0.43
1:B:27:ASP:HB3	1:B:28:SER:H	1.61	0.43
1:B:601:ARG:HH12	1:B:739:HIS:CE1	2.36	0.43
1:A:156:PRO:HG2	3:A:1194:HOH:O	2.18	0.43
1:D:727:SER:O	1:D:731:GLU:HG3	2.18	0.43
1:D:748:ILE:O	1:D:751:ILE:HG22	2.18	0.43
1:B:37:ARG:HD3	3:B:1073:HOH:O	2.19	0.43
1:C:751:ILE:HD12	1:C:752:PRO:CD	2.45	0.43
1:D:507:HIS:N	1:D:508:PRO:HD2	2.34	0.43
1:B:182:ILE:HG22	1:B:183:ARG:N	2.34	0.43
1:B:369:ARG:HG2	3:B:768:HOH:O	2.19	0.43
1:C:146:ASP:HB2	3:C:1163:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:TYR:HB3	1:D:650:ILE:HD13	2.00	0.43
1:A:378:ASN:HB3	1:A:379:PRO:HD2	2.01	0.43
1:B:362:GLU:HG3	3:B:988:HOH:O	2.18	0.43
1:B:449:HIS:CE1	1:D:431:ILE:HG13	2.53	0.43
1:D:535:VAL:O	1:D:537:PRO:HD3	2.18	0.43
1:C:201:HIS:CD2	2:C:760:HEM:HMB2	2.54	0.43
1:C:214:PHE:HB3	1:C:215:PRO:HD3	2.01	0.43
1:C:552:LEU:HG	3:C:1142:HOH:O	2.19	0.43
1:A:279:LEU:HD23	1:A:400:LEU:HD23	2.01	0.42
1:B:631:LYS:HE3	1:B:662:VAL:HG12	2.00	0.42
1:C:162:VAL:HG21	1:C:373:MET:SD	2.59	0.42
1:B:583:LYS:O	1:B:584:LYS:HB3	2.18	0.42
1:D:700:ASP:HB2	3:D:1209:HOH:O	2.19	0.42
1:C:748:ILE:O	1:C:751:ILE:HG23	2.19	0.42
1:B:744:ARG:O	1:B:745:ILE:C	2.62	0.42
1:A:359:LEU:C	1:A:359:LEU:HD12	2.44	0.42
1:D:38:PRO:HA	1:D:48:GLN:NE2	2.35	0.42
1:A:285:LYS:HE2	3:A:1106:HOH:O	2.19	0.42
1:B:124:GLU:HG2	3:C:803:HOH:O	2.20	0.42
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.54	0.42
1:D:488:ARG:NH2	1:D:490:GLU:OE1	2.52	0.42
1:A:31:PRO:HD2	1:A:36:HIS:CD2	2.54	0.42
1:A:254:MET:HE3	1:A:254:MET:HB3	1.95	0.42
1:A:449:HIS:CE1	3:C:1152:HOH:O	2.72	0.42
1:B:121:ARG:CZ	1:C:126:ILE:HD12	2.49	0.42
1:B:473:THR:O	1:B:481:GLY:HA3	2.20	0.41
1:C:610:GLU:HG3	1:C:610:GLU:O	2.20	0.41
1:D:612:ARG:HD3	1:D:615:ASP:CG	2.45	0.41
1:B:55:LEU:HD13	3:B:1073:HOH:O	2.20	0.41
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.55	0.41
1:B:285:LYS:NZ	1:B:285:LYS:HB3	2.35	0.41
1:C:725:ASP:HA	1:C:728:PHE:CB	2.50	0.41
1:D:128:HIS:HA	1:D:168:THR:O	2.20	0.41
1:A:36:HIS:CD2	1:A:36:HIS:H	2.38	0.41
1:D:262:ILE:HG13	1:D:262:ILE:O	2.20	0.41
1:B:59:ASP:HA	1:B:61:ARG:NE	2.35	0.41
1:D:195:ILE:HD11	1:D:436:PRO:HA	2.02	0.41
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.83	0.41
1:A:417:ASP:OD2	1:D:118:ASP:OD1	2.38	0.41
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.33	0.41
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASP:HB2	1:D:29:LEU:HD21	2.02	0.41
1:D:283:GLU:HG3	3:D:1136:HOH:O	2.21	0.41
1:D:462:PRO:HA	1:D:468:ASN:OD1	2.21	0.41
1:B:144:LEU:HD11	1:B:370:VAL:HG22	2.01	0.41
1:B:507:HIS:N	1:B:508:PRO:HD2	2.36	0.41
1:A:126:ILE:HD12	1:D:121:ARG:CZ	2.51	0.41
1:D:585:ASP:HA	1:D:586:PRO:HD2	1.92	0.41
1:D:648:LEU:HD22	1:D:648:LEU:N	2.36	0.41
1:C:164:VAL:HG21	1:C:375:LEU:HD11	2.03	0.41
1:D:476:GLY:HA3	3:D:1097:HOH:O	2.21	0.41
1:D:478:LYS:HE2	3:D:1167:HOH:O	2.20	0.41
1:D:640:VAL:HG23	1:D:648:LEU:HB2	2.02	0.41
1:C:584:LYS:HZ2	1:C:586:PRO:HD3	1.86	0.40
1:C:745:ILE:O	1:C:748:ILE:HG12	2.21	0.40
1:D:744:ARG:O	1:D:745:ILE:C	2.63	0.40
1:A:29:LEU:HB2	1:C:467:ASP:OD1	2.21	0.40
1:B:578:ASP:HB3	1:B:582:LEU:O	2.22	0.40
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.40
1:C:137:TYR:CD1	1:C:159:ILE:HD13	2.55	0.40
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.58	0.40
1:C:511:PHE:O	1:C:515:GLN:HG2	2.21	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	725/753 (96%)	701 (97%)	20 (3%)	4 (1%)	21	21
1	B	725/753 (96%)	703 (97%)	20 (3%)	2 (0%)	36	40
1	C	725/753 (96%)	699 (96%)	24 (3%)	2 (0%)	36	40
1	D	725/753 (96%)	700 (97%)	19 (3%)	6 (1%)	16	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2900/3012 (96%)	2803 (97%)	83 (3%)	14 (0%)	24 24

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	28	SER
1	D	28	SER
1	D	33	ASP
1	A	709	LYS
1	C	75	SER
1	D	726	GLY
1	D	750	LYS
1	D	751	ILE
1	A	75	SER
1	D	75	SER
1	A	647	VAL
1	B	75	SER
1	C	726	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	612/636 (96%)	585 (96%)	27 (4%)	25 29
1	B	612/636 (96%)	580 (95%)	32 (5%)	21 22
1	C	612/636 (96%)	571 (93%)	41 (7%)	15 14
1	D	612/636 (96%)	580 (95%)	32 (5%)	21 22
All	All	2448/2544 (96%)	2316 (95%)	132 (5%)	20 21

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP

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Mol	Chain	Res	Type
1	A	29	LEU
1	A	48	GLN
1	A	59	ASP
1	A	73	LYS
1	A	126	ILE
1	A	159	ILE
1	A	191	THR
1	A	198	LEU
1	A	205	ILE
1	A	230	PRO
1	A	333	GLU
1	A	344	GLU
1	A	370	VAL
1	A	372	LYS
1	A	375	LEU
1	A	459	ASN
1	A	552	LEU
1	A	602	VAL
1	A	603	VAL
1	A	606	LEU
1	A	621	LYS
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	A	727	SER
1	A	750	LYS
1	B	32	GLU
1	B	73	LYS
1	B	126	ILE
1	B	142	LYS
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	285	LYS
1	B	299	LYS
1	B	321	GLU
1	B	344	GLU
1	B	370	VAL
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN

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Mol	Chain	Res	Type
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	602	VAL
1	B	621	LYS
1	B	633	LEU
1	B	639	GLU
1	B	697	LEU
1	B	707	THR
1	B	709	LYS
1	B	713	GLN
1	B	732	LEU
1	B	751	ILE
1	C	37	ARG
1	C	48	GLN
1	C	61	ARG
1	C	126	ILE
1	C	127	VAL
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	252	ASN
1	C	283	GLU
1	C	294	LYS
1	C	309	LYS
1	C	368	GLN
1	C	370	VAL
1	C	375	LEU
1	C	426	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	509	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	568	ASP
1	C	569	ASP

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Mol	Chain	Res	Type
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	603	VAL
1	C	616	LEU
1	C	636	ARG
1	C	639	GLU
1	C	640	VAL
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	713	GLN
1	C	732	LEU
1	C	733	LEU
1	C	751	ILE
1	D	37	ARG
1	D	48	GLN
1	D	61	ARG
1	D	126	ILE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	294	LYS
1	D	309	LYS
1	D	340	LEU
1	D	344	GLU
1	D	369	ARG
1	D	370	VAL
1	D	375	LEU
1	D	459	ASN
1	D	490	GLU
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	560	LYS
1	D	582	LEU
1	D	583	LYS
1	D	602	VAL
1	D	611	VAL
1	D	616	LEU
1	D	633	LEU
1	D	640	VAL

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Mol	Chain	Res	Type
1	D	648	LEU
1	D	716	GLU
1	D	727	SER
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	48	GLN
1	A	66	ASN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	546	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	546	GLN
1	B	556	GLN
1	B	629	HIS
1	C	252	ASN
1	C	449	HIS
1	C	459	ASN
1	C	492	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	682	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	486	GLN
1	D	492	ASN
1	D	507	HIS
1	D	546	GLN
1	D	561	ASN
1	D	629	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	HEM	C	760	1	50,50,50	1.29	8 (16%)	67,82,82	1.01	4 (5%)
2	HEM	B	760	1	50,50,50	1.41	11 (22%)	67,82,82	1.01	4 (5%)
2	HEM	A	760	1	50,50,50	1.36	11 (22%)	67,82,82	0.96	3 (4%)
2	HEM	D	760	1	50,50,50	1.40	8 (16%)	67,82,82	1.05	2 (2%)

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	-	4/14/54/54	-
2	HEM	B	760	1	-	2/14/54/54	-
2	HEM	A	760	1	-	2/14/54/54	-
2	HEM	D	760	1	-	2/14/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HEM	FE-NC	3.33	2.06	1.95
2	D	760	HEM	CAC-C3C	3.12	1.55	1.47
2	A	760	HEM	CAC-C3C	3.05	1.55	1.47
2	C	760	HEM	CAC-C3C	2.98	1.55	1.47
2	D	760	HEM	CAB-C3B	2.94	1.55	1.47
2	B	760	HEM	CAB-C3B	2.88	1.55	1.47
2	A	760	HEM	FE-NC	2.75	2.04	1.95
2	B	760	HEM	CAC-C3C	2.73	1.54	1.47
2	A	760	HEM	CAB-C3B	2.70	1.54	1.47
2	B	760	HEM	CMB-C2B	2.67	1.56	1.50
2	C	760	HEM	CAB-C3B	2.66	1.54	1.47
2	D	760	HEM	CMA-C3A	2.55	1.56	1.50
2	C	760	HEM	FE-NB	2.50	2.02	1.94
2	D	760	HEM	FE-NA	2.46	2.03	1.95
2	B	760	HEM	CMC-C2C	2.44	1.55	1.50
2	A	760	HEM	FE-ND	2.40	2.02	1.94
2	A	760	HEM	FE-NB	2.37	2.02	1.94
2	B	760	HEM	FE-NC	2.36	2.03	1.95
2	B	760	HEM	FE-NB	2.36	2.02	1.94
2	A	760	HEM	CMC-C2C	2.35	1.55	1.50
2	D	760	HEM	CMD-C2D	2.33	1.55	1.50
2	B	760	HEM	CMA-C3A	2.33	1.55	1.50
2	D	760	HEM	CMC-C2C	2.32	1.55	1.50
2	C	760	HEM	FE-ND	2.26	2.01	1.94
2	B	760	HEM	FE-NA	2.26	2.02	1.95
2	B	760	HEM	FE-ND	2.23	2.01	1.94
2	C	760	HEM	FE-NC	2.20	2.02	1.95
2	A	760	HEM	CMA-C3A	2.17	1.55	1.50
2	C	760	HEM	CMC-C2C	2.17	1.55	1.50
2	A	760	HEM	C2A-C3A	-2.16	1.33	1.38
2	D	760	HEM	C3C-C2C	-2.13	1.32	1.37
2	B	760	HEM	C3C-C2C	-2.08	1.32	1.37
2	A	760	HEM	FE-NA	2.08	2.02	1.95
2	C	760	HEM	CMD-C2D	2.07	1.55	1.50
2	B	760	HEM	C3B-C2B	-2.05	1.33	1.37
2	A	760	HEM	CMD-C2D	2.04	1.55	1.50
2	C	760	HEM	CMA-C3A	2.03	1.54	1.50
2	A	760	HEM	CMB-C2B	2.03	1.54	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	C3B-C2B-C1B	2.79	108.50	106.41
2	C	760	HEM	O1A-CGA-CBA	-2.34	115.67	123.09
2	D	760	HEM	CHD-C1D-ND	2.32	126.92	124.42
2	D	760	HEM	CHB-C1B-NB	2.29	127.20	124.37
2	B	760	HEM	CAA-CBA-CGA	-2.23	107.75	113.67
2	C	760	HEM	O2A-CGA-O1A	2.21	129.02	123.33
2	A	760	HEM	CMA-C3A-C4A	-2.14	122.15	125.42
2	B	760	HEM	CBD-CAD-C3D	-2.12	106.67	112.53
2	C	760	HEM	CBC-CAC-C3C	-2.11	116.96	127.53
2	A	760	HEM	CBC-CAC-C3C	-2.08	117.13	127.53
2	B	760	HEM	O1D-CGD-CBD	-2.08	116.50	123.09
2	A	760	HEM	CBA-CAA-C2A	2.08	118.28	112.53
2	C	760	HEM	CBA-CAA-C2A	2.04	118.18	112.53

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	760	HEM	C2B-C3B-CAB-CBB
2	C	760	HEM	C4B-C3B-CAB-CBB
2	D	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O2A

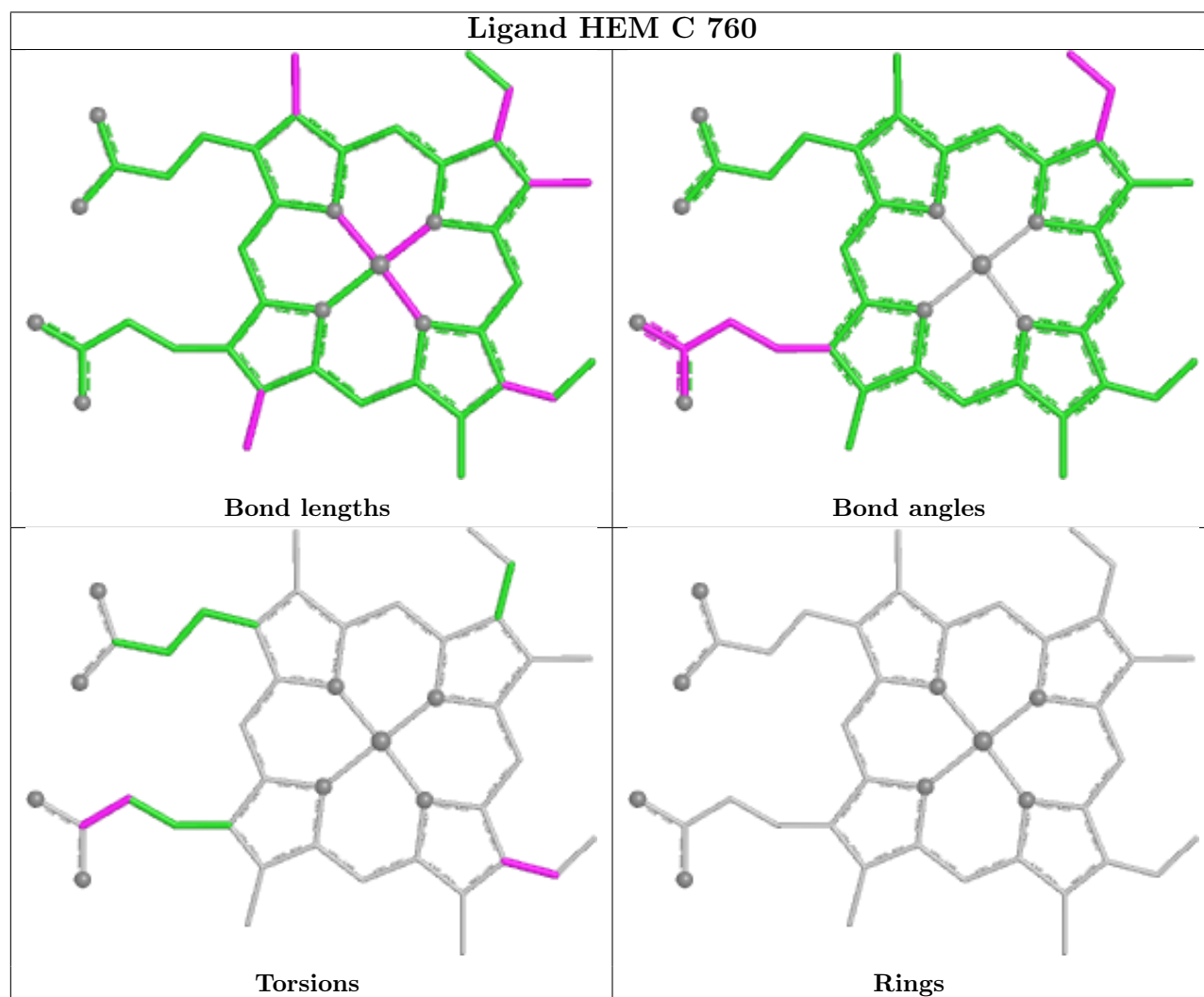
There are no ring outliers.

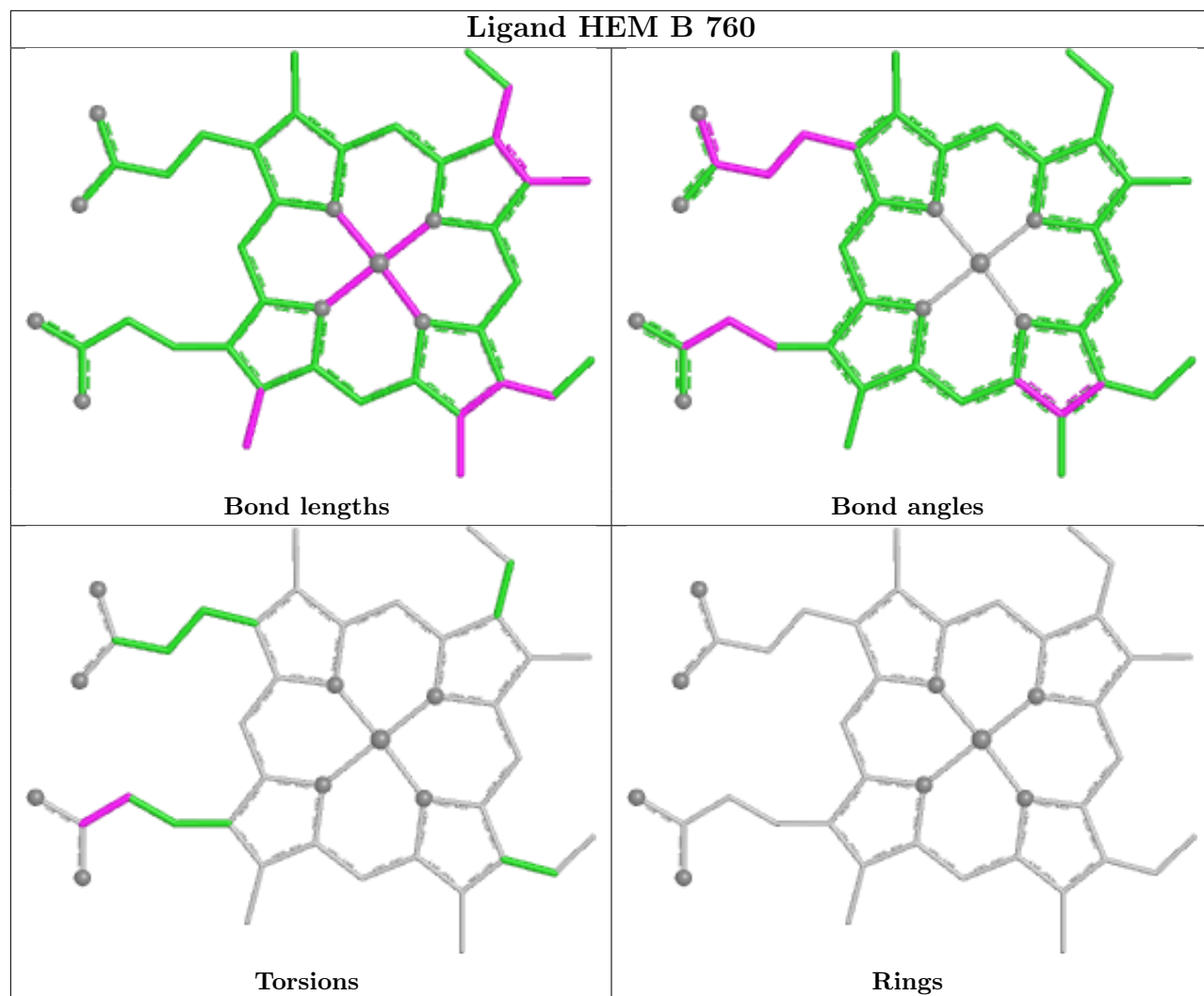
2 monomers are involved in 4 short contacts:

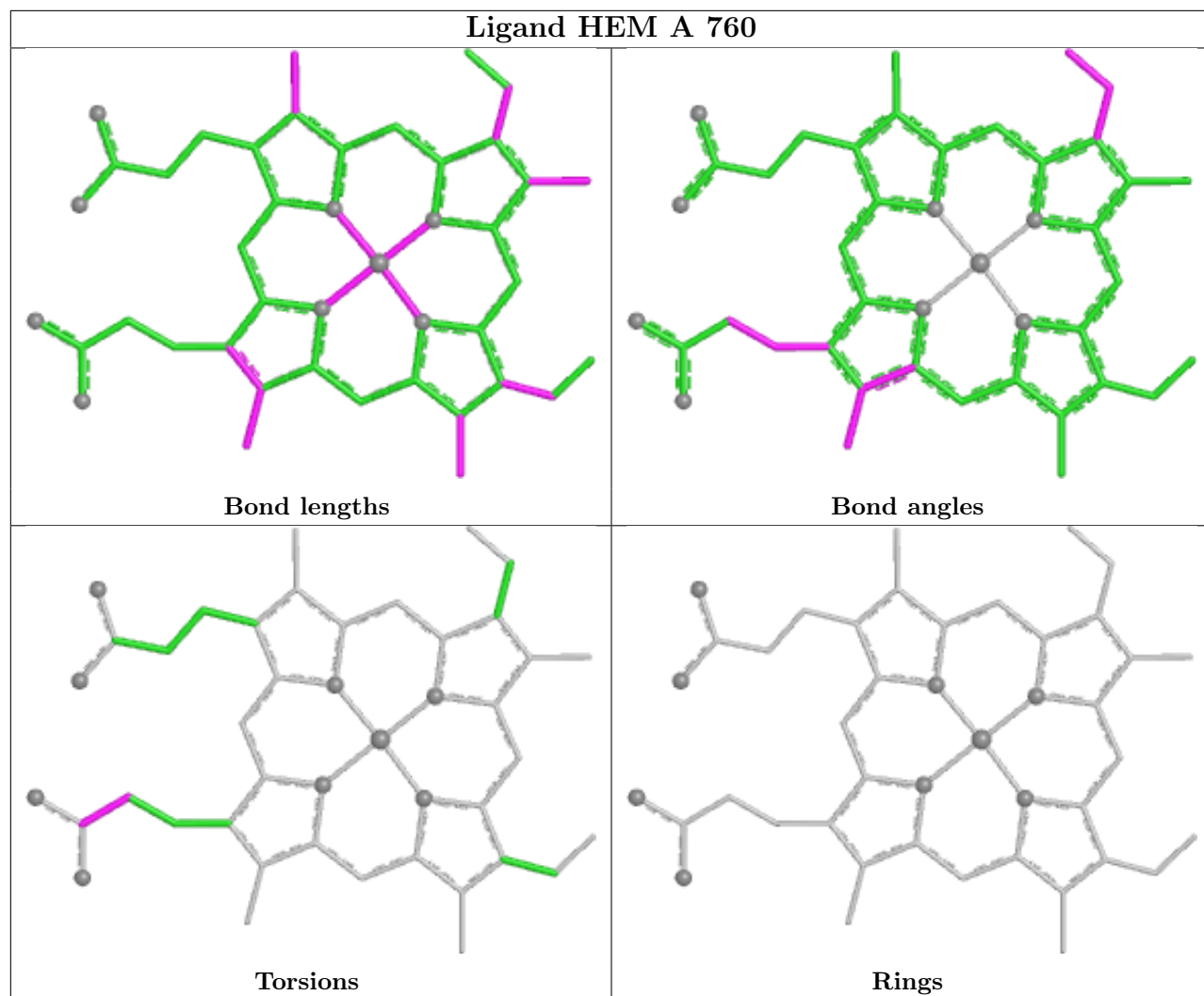
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	2	0
2	A	760	HEM	2	0

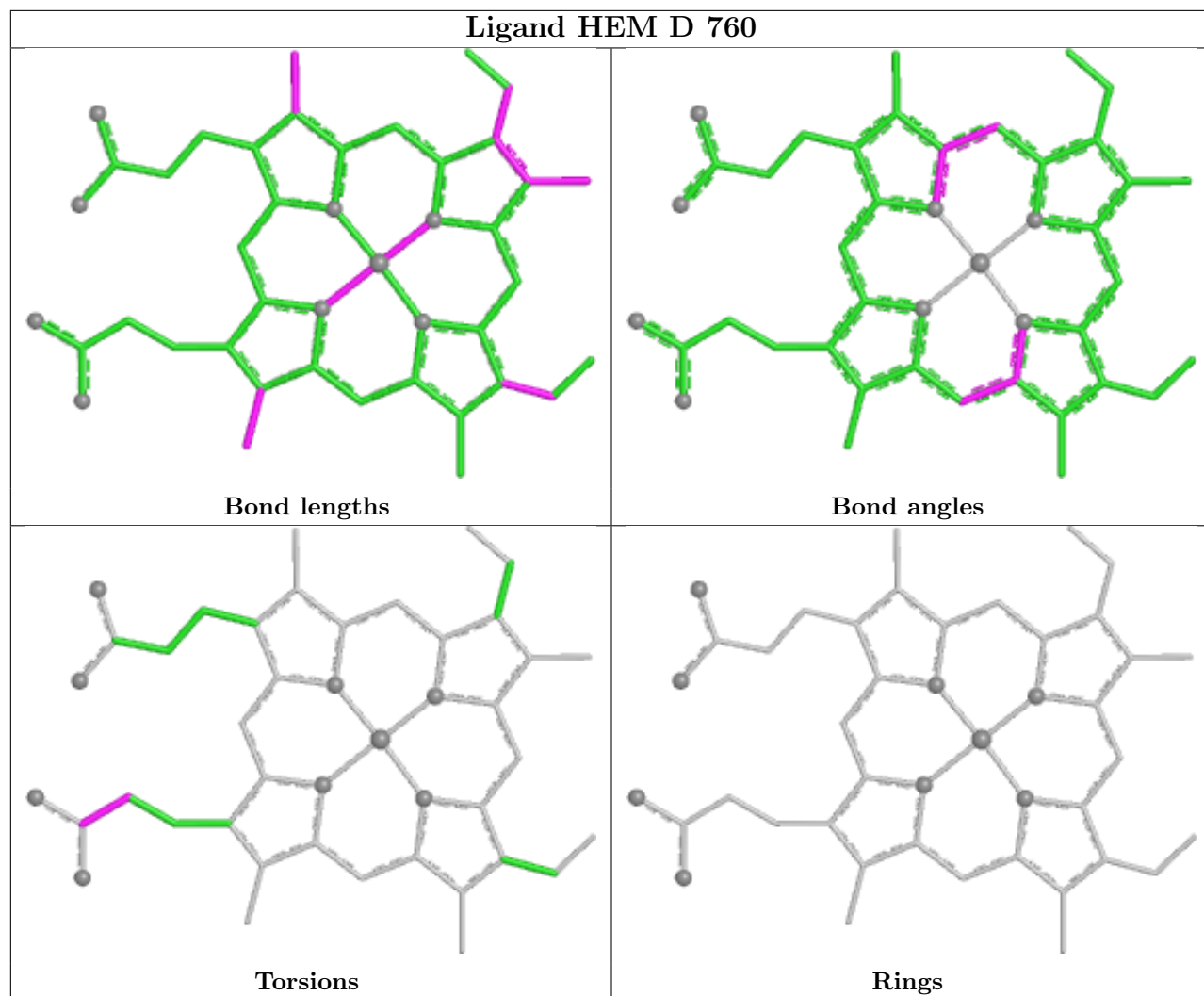
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/753 (96%)	-0.76	7 (0%) 79 81	5, 14, 42, 82	1 (0%)
1	B	727/753 (96%)	-0.73	2 (0%) 90 90	5, 16, 44, 84	1 (0%)
1	C	727/753 (96%)	-0.73	2 (0%) 90 90	6, 17, 44, 82	1 (0%)
1	D	727/753 (96%)	-0.77	4 (0%) 85 86	5, 15, 42, 82	1 (0%)
All	All	2908/3012 (96%)	-0.75	15 (0%) 87 88	5, 15, 44, 84	4 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	5.0
1	A	27	ASP	2.9
1	D	28	SER	2.9
1	A	28	SER	2.8
1	A	712	ASP	2.8
1	A	646	THR	2.6
1	D	710	ILE	2.6
1	A	710	ILE	2.4
1	C	711	ALA	2.3
1	D	27	ASP	2.2
1	A	645	GLY	2.2
1	C	27	ASP	2.1
1	B	27	ASP	2.1
1	B	711	ALA	2.0
1	D	711	ALA	2.0

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](#)

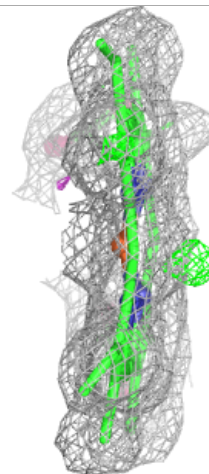
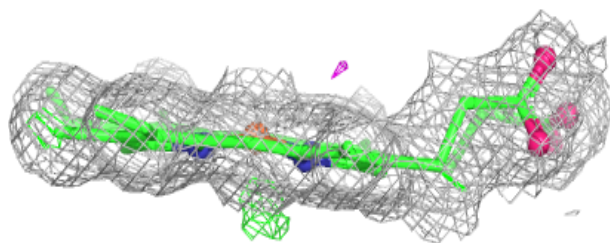
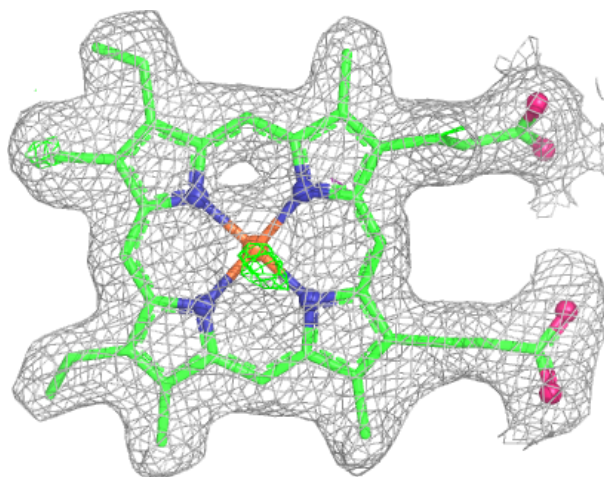
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	760	43/43	0.98	0.05	5,9,12,14	0
2	HEM	B	760	43/43	0.98	0.05	6,8,10,11	0
2	HEM	C	760	43/43	0.98	0.05	10,11,15,17	0
2	HEM	D	760	43/43	0.98	0.04	5,9,12,15	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

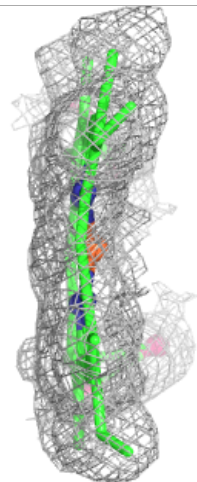
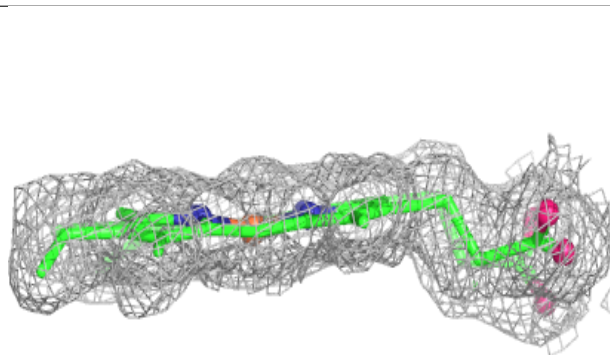
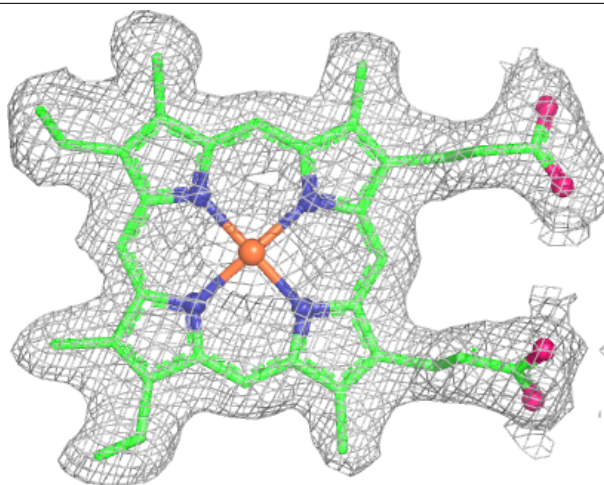
Electron density around HEM A 760:

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



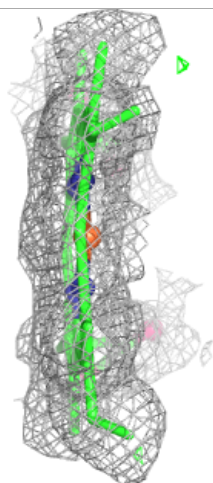
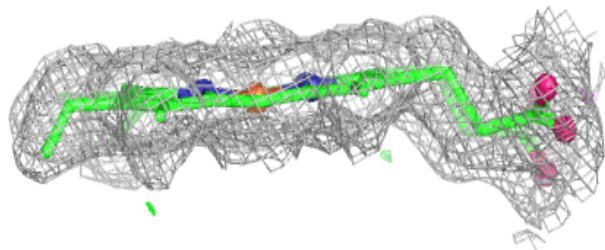
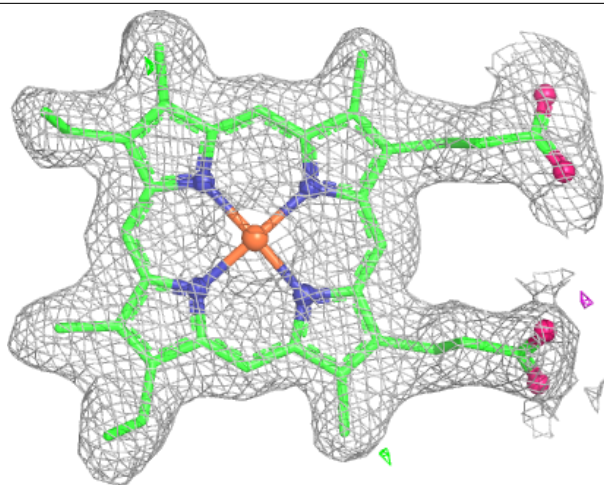
Electron density around HEM B 760:

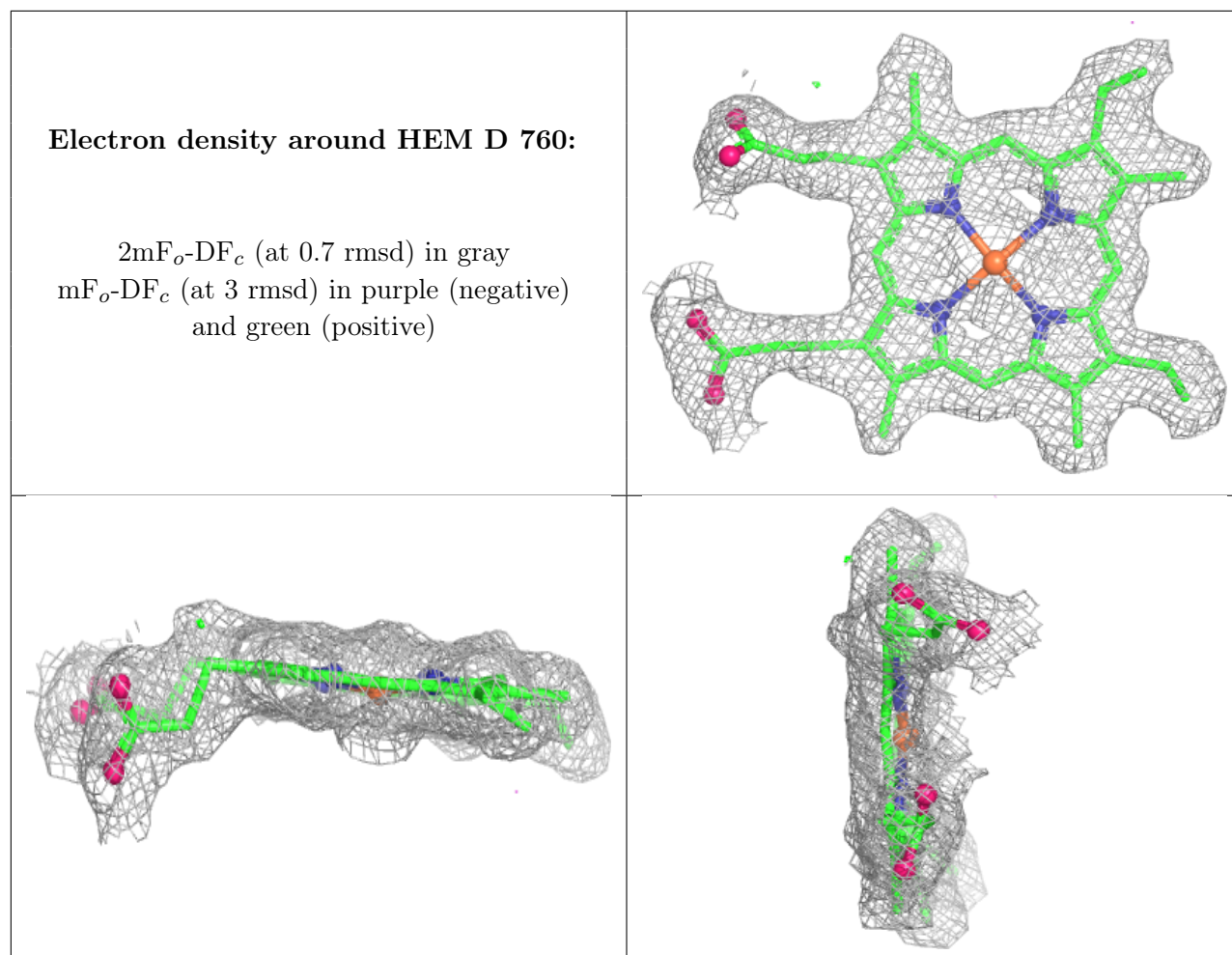
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.