



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:42 PM EDT

PDB ID : 1IPH
Title : STRUCTURE OF CATALASE HPII FROM ESCHERICHIA COLI
Authors : Bravo, J.; Loewen, P.C.; Fita, I.
Deposited on : 1995-12-31
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

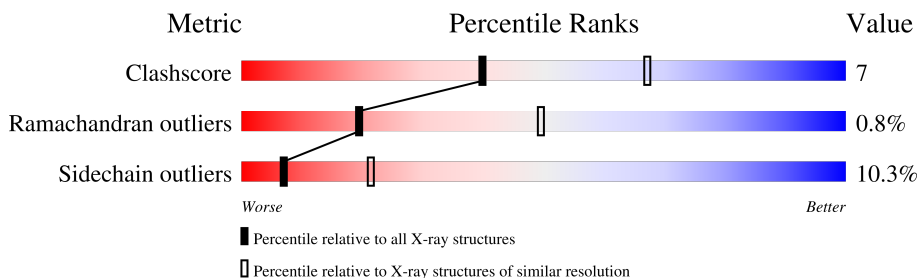
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	753	
1	B	753	
1	C	753	
1	D	753	

2 Entry composition [i](#)

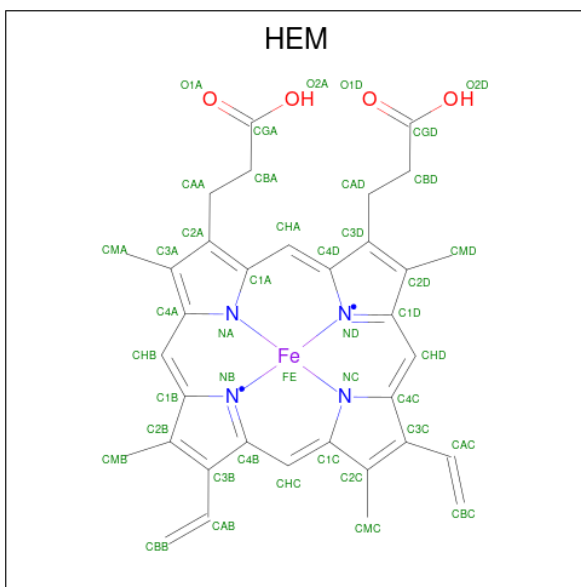
There are 2 unique types of molecules in this entry. The entry contains 23156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	Total 5746	C 3647	N 1005	O 1082	S 12	0	0	0
1	B	727	Total 5746	C 3647	N 1005	O 1082	S 12	0	0	0
1	C	727	Total 5746	C 3647	N 1005	O 1082	S 12	0	0	0
1	D	727	Total 5746	C 3647	N 1005	O 1082	S 12	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
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

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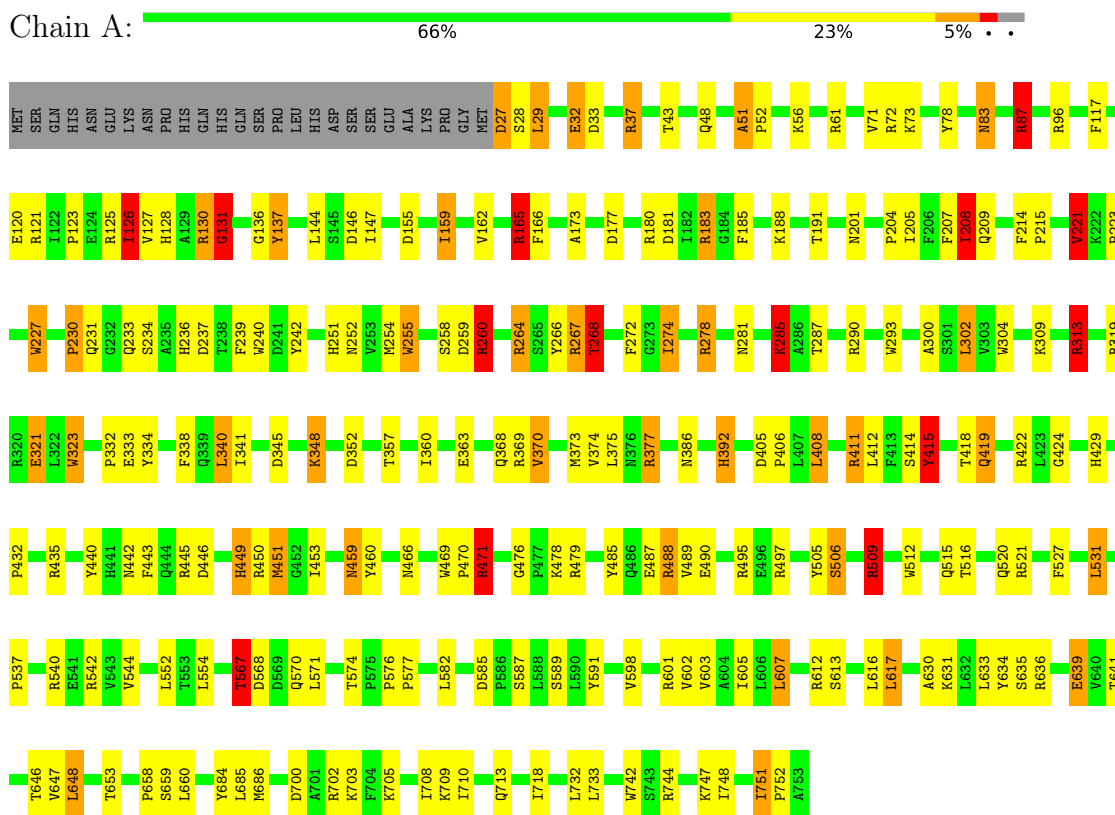
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

3 Residue-property plots

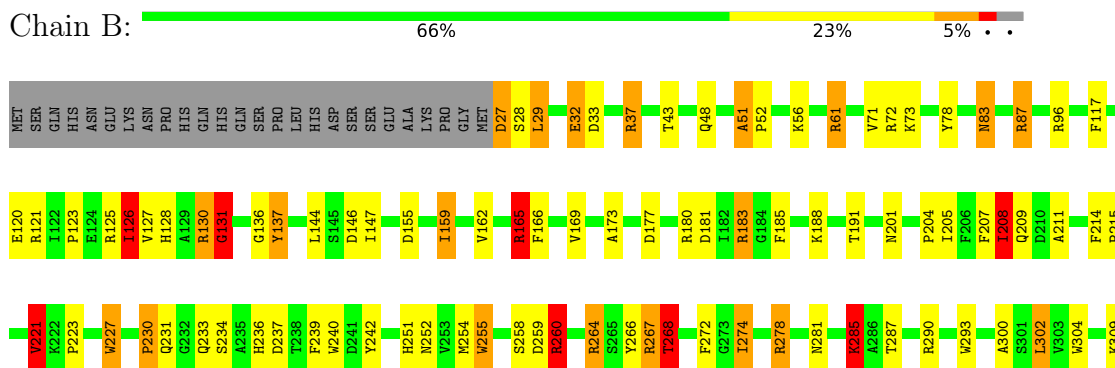
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

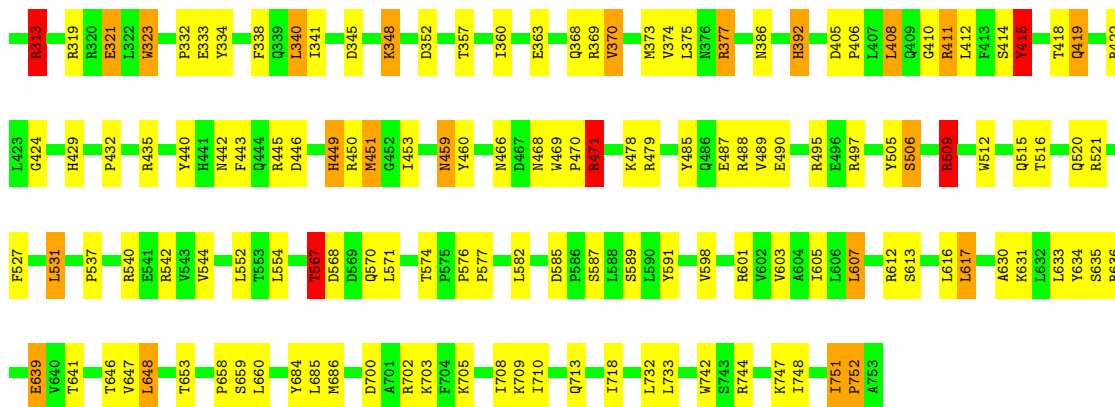
Note EDS was not executed.

- Molecule 1: CATALASE HPII

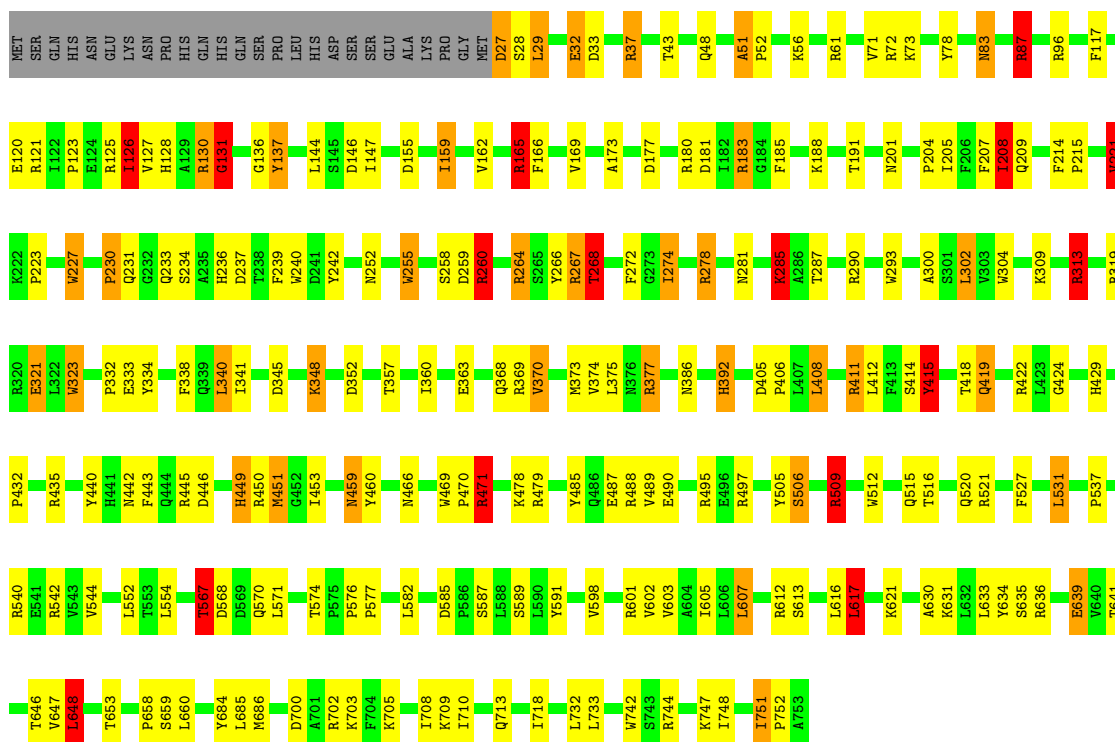


- Molecule 1: CATALASE HPII

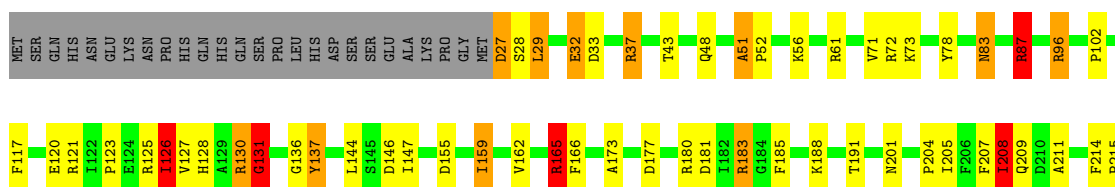


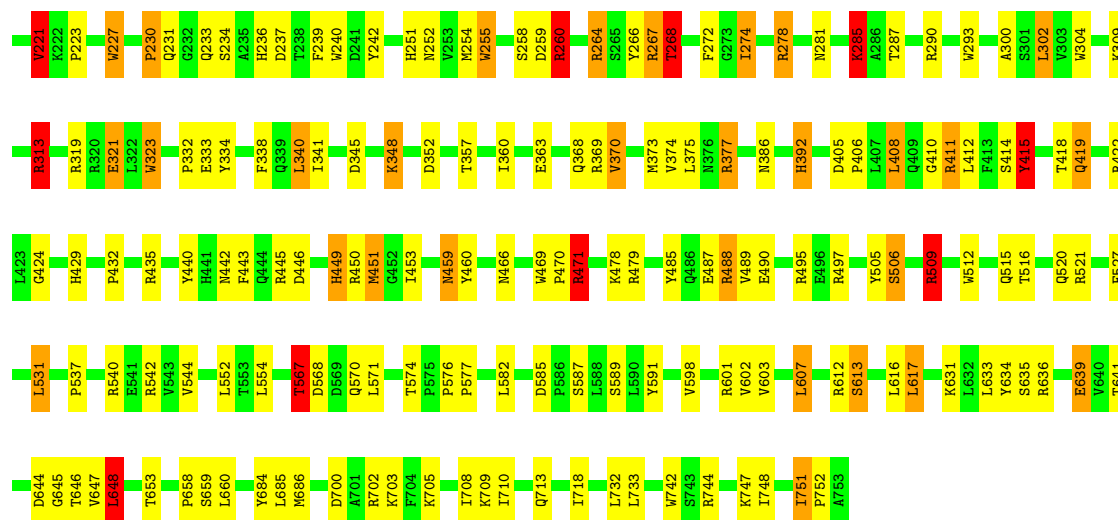


• Molecule 1: CATALASE HPII



• Molecule 1: CATALASE HPII





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.20Å 134.70Å 124.40Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	23156	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.06	7/5902 (0.1%)	1.86	161/8024 (2.0%)
1	B	1.06	8/5902 (0.1%)	1.86	161/8024 (2.0%)
1	C	1.06	7/5902 (0.1%)	1.86	161/8024 (2.0%)
1	D	1.06	7/5902 (0.1%)	1.86	160/8024 (2.0%)
All	All	1.06	29/23608 (0.1%)	1.86	643/32096 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ILE	CA-CB	5.87	1.68	1.54
1	B	208	ILE	CA-CB	5.86	1.68	1.54
1	C	208	ILE	CA-CB	5.86	1.68	1.54
1	D	208	ILE	CA-CB	5.86	1.68	1.54
1	A	449	HIS	CB-CG	5.72	1.60	1.50
1	B	449	HIS	CB-CG	5.71	1.60	1.50
1	D	449	HIS	CB-CG	5.71	1.60	1.50
1	C	449	HIS	CB-CG	5.66	1.60	1.50
1	C	159	ILE	CA-CB	5.54	1.67	1.54
1	D	159	ILE	CA-CB	5.54	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	ILE	CA-CB	5.54	1.67	1.54
1	B	159	ILE	CA-CB	5.52	1.67	1.54
1	C	323	TRP	CD1-NE1	-5.29	1.28	1.38
1	B	323	TRP	CD1-NE1	-5.29	1.28	1.38
1	A	323	TRP	CD1-NE1	-5.28	1.28	1.38
1	D	377	ARG	CZ-NH1	5.27	1.40	1.33
1	D	323	TRP	CD1-NE1	-5.25	1.29	1.38
1	B	377	ARG	CZ-NH1	5.22	1.39	1.33
1	A	377	ARG	CZ-NH1	5.19	1.39	1.33
1	D	126	ILE	CA-CB	5.18	1.66	1.54
1	A	126	ILE	CA-CB	5.18	1.66	1.54
1	C	377	ARG	CZ-NH1	5.17	1.39	1.33
1	C	126	ILE	CA-CB	5.16	1.66	1.54
1	B	126	ILE	CA-CB	5.16	1.66	1.54
1	A	392	HIS	CD2-NE2	-5.10	1.26	1.38
1	B	392	HIS	CD2-NE2	-5.10	1.26	1.38
1	D	392	HIS	CD2-NE2	-5.10	1.26	1.38
1	C	392	HIS	CD2-NE2	-5.07	1.26	1.38
1	B	304	TRP	CD1-NE1	-5.01	1.29	1.38

All (643) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	NE-CZ-NH1	17.64	129.12	120.30
1	D	183	ARG	NE-CZ-NH1	17.51	129.06	120.30
1	A	183	ARG	NE-CZ-NH1	17.50	129.05	120.30
1	B	183	ARG	NE-CZ-NH1	17.49	129.04	120.30
1	D	183	ARG	NE-CZ-NH2	-16.94	111.83	120.30
1	C	183	ARG	NE-CZ-NH2	-16.93	111.84	120.30
1	A	183	ARG	NE-CZ-NH2	-16.80	111.90	120.30
1	B	183	ARG	NE-CZ-NH2	-16.79	111.90	120.30
1	B	165	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	C	377	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	A	165	ARG	NE-CZ-NH1	14.59	127.59	120.30
1	C	165	ARG	NE-CZ-NH1	14.52	127.56	120.30
1	B	377	ARG	NE-CZ-NH2	-14.49	113.06	120.30
1	D	165	ARG	NE-CZ-NH1	14.48	127.54	120.30
1	D	377	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	377	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	96	ARG	NE-CZ-NH1	14.03	127.31	120.30
1	C	96	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	B	96	ARG	NE-CZ-NH1	13.92	127.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ARG	NE-CZ-NH1	13.92	127.26	120.30
1	C	471	ARG	NE-CZ-NH2	-13.87	113.36	120.30
1	D	471	ARG	NE-CZ-NH2	-13.86	113.37	120.30
1	A	471	ARG	NE-CZ-NH2	-13.81	113.39	120.30
1	B	471	ARG	NE-CZ-NH2	-13.77	113.42	120.30
1	B	165	ARG	NE-CZ-NH2	-13.19	113.71	120.30
1	A	165	ARG	NE-CZ-NH2	-13.14	113.73	120.30
1	C	165	ARG	NE-CZ-NH2	-13.08	113.76	120.30
1	D	165	ARG	NE-CZ-NH2	-13.03	113.78	120.30
1	C	37	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	D	37	ARG	NE-CZ-NH1	12.79	126.70	120.30
1	B	37	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	A	37	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	A	479	ARG	NE-CZ-NH1	12.68	126.64	120.30
1	D	471	ARG	NE-CZ-NH1	12.67	126.63	120.30
1	B	471	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	A	471	ARG	NE-CZ-NH1	12.63	126.62	120.30
1	C	471	ARG	NE-CZ-NH1	12.63	126.62	120.30
1	C	479	ARG	NE-CZ-NH1	12.61	126.61	120.30
1	D	479	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	B	479	ARG	NE-CZ-NH1	12.53	126.57	120.30
1	C	96	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	A	96	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	B	96	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	D	96	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	D	415	TYR	CB-CG-CD2	-11.35	114.19	121.00
1	C	415	TYR	CB-CG-CD2	-11.33	114.20	121.00
1	B	415	TYR	CB-CG-CD2	-11.30	114.22	121.00
1	A	415	TYR	CB-CG-CD2	-11.29	114.23	121.00
1	B	278	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	278	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	D	278	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	C	278	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	B	72	ARG	NE-CZ-NH1	10.31	125.46	120.30
1	C	72	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	D	72	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	A	72	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	B	591	TYR	CB-CG-CD2	-9.93	115.04	121.00
1	D	591	TYR	CB-CG-CD2	-9.90	115.06	121.00
1	C	591	TYR	CB-CG-CD2	-9.89	115.06	121.00
1	A	411	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	591	TYR	CB-CG-CD2	-9.88	115.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	419	GLN	CA-CB-CG	-9.82	91.80	113.40
1	C	411	ARG	NE-CZ-NH1	9.81	125.21	120.30
1	D	419	GLN	CA-CB-CG	-9.81	91.83	113.40
1	B	419	GLN	CA-CB-CG	-9.80	91.85	113.40
1	C	419	GLN	CA-CB-CG	-9.79	91.86	113.40
1	B	293	TRP	CD1-CG-CD2	9.75	114.10	106.30
1	C	293	TRP	CD1-CG-CD2	9.72	114.07	106.30
1	A	293	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	D	411	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	D	293	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	D	469	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	A	469	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	B	469	TRP	CD1-CG-CD2	9.64	114.01	106.30
1	C	469	TRP	CD1-CG-CD2	9.61	113.99	106.30
1	A	313	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	C	313	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	D	313	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	278	ARG	NE-CZ-NH2	-9.45	115.57	120.30
1	B	313	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	B	278	ARG	NE-CZ-NH2	-9.42	115.59	120.30
1	A	278	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	D	278	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	C	208	ILE	CA-CB-CG2	9.38	129.66	110.90
1	B	208	ILE	CA-CB-CG2	9.37	129.64	110.90
1	D	208	ILE	CA-CB-CG2	9.37	129.64	110.90
1	A	208	ILE	CA-CB-CG2	9.35	129.60	110.90
1	B	304	TRP	CD1-CG-CD2	9.17	113.63	106.30
1	C	304	TRP	CD1-CG-CD2	9.17	113.63	106.30
1	A	304	TRP	CD1-CG-CD2	9.14	113.61	106.30
1	D	304	TRP	CD1-CG-CD2	9.13	113.60	106.30
1	B	612	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	C	612	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	D	612	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	612	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	C	208	ILE	CA-CB-CG1	-8.83	94.22	111.00
1	A	208	ILE	CA-CB-CG1	-8.82	94.24	111.00
1	B	512	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	D	208	ILE	CA-CB-CG1	-8.82	94.24	111.00
1	B	208	ILE	CA-CB-CG1	-8.81	94.25	111.00
1	A	512	TRP	CD1-CG-CD2	8.81	113.35	106.30
1	D	512	TRP	CD1-CG-CD2	8.80	113.34	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	512	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	A	542	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	C	61	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	542	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	A	61	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	D	542	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	542	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	A	313	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	D	61	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	D	313	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	B	313	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	C	313	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	61	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	509	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	B	509	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	C	32	GLU	CA-C-N	-8.37	98.78	117.20
1	B	32	GLU	CA-C-N	-8.37	98.80	117.20
1	D	32	GLU	CA-C-N	-8.35	98.83	117.20
1	A	32	GLU	CA-C-N	-8.35	98.83	117.20
1	B	227	TRP	CD1-CG-CD2	8.34	112.97	106.30
1	D	509	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	D	227	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	D	445	ARG	NE-CZ-NH2	8.27	124.44	120.30
1	B	445	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	C	505	TYR	CB-CG-CD2	-8.25	116.05	121.00
1	C	304	TRP	CE2-CD2-CG	-8.25	100.70	107.30
1	A	505	TYR	CB-CG-CD2	-8.24	116.05	121.00
1	A	227	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	A	509	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	304	TRP	CE2-CD2-CG	-8.23	100.71	107.30
1	C	445	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	D	505	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	B	505	TYR	CB-CG-CD2	-8.21	116.07	121.00
1	C	227	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	D	304	TRP	CE2-CD2-CG	-8.21	100.73	107.30
1	B	323	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	A	304	TRP	CE2-CD2-CG	-8.19	100.75	107.30
1	A	87	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	A	323	TRP	CE2-CD2-CG	-8.16	100.77	107.30
1	D	742	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	A	445	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	C	87	ARG	NE-CZ-NH1	8.16	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	323	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	C	323	TRP	CE2-CD2-CG	-8.12	100.81	107.30
1	C	742	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	D	87	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	742	TRP	CD1-CG-CD2	8.11	112.79	106.30
1	A	255	TRP	CD1-CG-CD2	8.11	112.78	106.30
1	B	321	GLU	CA-CB-CG	8.11	131.24	113.40
1	A	321	GLU	CA-CB-CG	8.10	131.22	113.40
1	D	255	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	D	321	GLU	CA-CB-CG	8.10	131.22	113.40
1	A	742	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	C	321	GLU	CA-CB-CG	8.09	131.20	113.40
1	B	255	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	A	131	GLY	N-CA-C	8.07	133.28	113.10
1	A	435	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	B	87	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	C	131	GLY	N-CA-C	8.07	133.27	113.10
1	B	131	GLY	N-CA-C	8.06	133.25	113.10
1	C	435	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	D	131	GLY	N-CA-C	8.05	133.22	113.10
1	C	255	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A	78	TYR	CB-CG-CD1	-8.02	116.19	121.00
1	B	591	TYR	CB-CG-CD1	8.01	125.81	121.00
1	C	78	TYR	CB-CG-CD1	-8.00	116.20	121.00
1	C	591	TYR	CB-CG-CD1	8.00	125.80	121.00
1	B	435	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	D	435	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	B	78	TYR	CB-CG-CD1	-7.97	116.22	121.00
1	D	255	TRP	CE2-CD2-CG	-7.97	100.92	107.30
1	D	78	TYR	CB-CG-CD1	-7.97	116.22	121.00
1	A	591	TYR	CB-CG-CD1	7.96	125.78	121.00
1	A	255	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	D	591	TYR	CB-CG-CD1	7.94	125.76	121.00
1	B	512	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	C	255	TRP	CE2-CD2-CG	-7.93	100.96	107.30
1	A	29	LEU	N-CA-C	-7.92	89.61	111.00
1	B	255	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	C	29	LEU	N-CA-C	-7.92	89.62	111.00
1	D	29	LEU	N-CA-C	-7.91	89.63	111.00
1	B	29	LEU	N-CA-C	-7.90	89.67	111.00
1	A	512	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	C	512	TRP	CE2-CD2-CG	-7.89	100.99	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	512	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	293	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	B	293	TRP	CE2-CD2-CG	-7.86	101.02	107.30
1	B	323	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	D	72	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	293	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	485	TYR	CB-CG-CD1	-7.81	116.31	121.00
1	A	323	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	B	485	TYR	CB-CG-CD1	-7.79	116.33	121.00
1	D	293	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	C	323	TRP	CG-CD2-CE3	7.78	140.90	133.90
1	D	485	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	D	323	TRP	CG-CD2-CE3	7.76	140.88	133.90
1	B	72	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	B	319	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	319	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	C	485	TYR	CB-CG-CD1	-7.72	116.37	121.00
1	D	319	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	C	72	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	268	THR	N-CA-CB	-7.65	95.76	110.30
1	C	268	THR	N-CA-CB	-7.64	95.78	110.30
1	C	319	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	268	THR	N-CA-CB	-7.63	95.80	110.30
1	D	268	THR	N-CA-CB	-7.62	95.82	110.30
1	C	422	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	422	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	B	422	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	742	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	72	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	469	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B	742	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B	603	VAL	CG1-CB-CG2	-7.54	98.84	110.90
1	D	603	VAL	CG1-CB-CG2	-7.52	98.86	110.90
1	C	469	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	603	VAL	CG1-CB-CG2	-7.51	98.88	110.90
1	C	603	VAL	CG1-CB-CG2	-7.51	98.88	110.90
1	B	469	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	D	469	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	D	422	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	A	742	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	C	742	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	D	415	TYR	CB-CG-CD1	7.42	125.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	TYR	CB-CG-CD1	7.42	125.45	121.00
1	B	415	TYR	CB-CG-CD1	7.35	125.41	121.00
1	A	415	TYR	CB-CG-CD1	7.32	125.39	121.00
1	C	497	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	D	497	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	497	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	D	617	LEU	CA-CB-CG	7.26	132.00	115.30
1	A	617	LEU	CA-CB-CG	7.26	131.99	115.30
1	B	617	LEU	CA-CB-CG	7.25	131.98	115.30
1	C	617	LEU	CA-CB-CG	7.25	131.97	115.30
1	B	497	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	D	227	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	A	290	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	290	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	227	TRP	CE2-CD2-CG	-7.04	101.66	107.30
1	B	240	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	D	240	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	A	240	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	C	240	TRP	CD1-CG-CD2	7.01	111.91	106.30
1	B	290	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	227	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	C	227	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	D	290	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	240	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	D	240	TRP	CE2-CD2-CG	-6.93	101.75	107.30
1	C	240	TRP	CE2-CD2-CG	-6.92	101.76	107.30
1	A	221	VAL	CB-CA-C	-6.91	98.27	111.40
1	A	240	TRP	CE2-CD2-CG	-6.90	101.78	107.30
1	D	260	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	221	VAL	CB-CA-C	-6.88	98.33	111.40
1	C	221	VAL	CB-CA-C	-6.88	98.33	111.40
1	C	260	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	125	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	221	VAL	CB-CA-C	-6.86	98.37	111.40
1	B	125	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	260	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	125	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	260	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	125	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	221	VAL	CG1-CB-CG2	6.73	121.67	110.90
1	A	221	VAL	CG1-CB-CG2	6.72	121.66	110.90
1	B	221	VAL	CG1-CB-CG2	6.72	121.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	221	VAL	CG1-CB-CG2	6.72	121.65	110.90
1	A	369	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	369	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	369	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	180	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	180	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	449	HIS	CA-C-N	-6.60	102.69	117.20
1	B	449	HIS	CA-C-N	-6.58	102.72	117.20
1	D	449	HIS	CA-C-N	-6.58	102.72	117.20
1	D	180	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	449	HIS	CA-C-N	-6.56	102.77	117.20
1	D	255	TRP	CG-CD2-CE3	6.55	139.80	133.90
1	B	227	TRP	CG-CD1-NE1	-6.55	103.55	110.10
1	C	512	TRP	CG-CD2-CE3	6.54	139.79	133.90
1	A	607	LEU	CA-CB-CG	6.53	130.31	115.30
1	B	512	TRP	CG-CD2-CE3	6.53	139.78	133.90
1	B	607	LEU	CA-CB-CG	6.53	130.31	115.30
1	A	440	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	C	440	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	D	607	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	293	TRP	CG-CD1-NE1	-6.51	103.59	110.10
1	A	255	TRP	CG-CD2-CE3	6.51	139.76	133.90
1	B	293	TRP	CG-CD1-NE1	-6.51	103.59	110.10
1	D	512	TRP	CG-CD2-CE3	6.51	139.76	133.90
1	D	440	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	A	227	TRP	CG-CD1-NE1	-6.51	103.59	110.10
1	B	180	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	293	TRP	CG-CD1-NE1	-6.51	103.59	110.10
1	D	227	TRP	CG-CD1-NE1	-6.50	103.60	110.10
1	C	607	LEU	CA-CB-CG	6.50	130.25	115.30
1	D	293	TRP	CG-CD1-NE1	-6.49	103.61	110.10
1	A	512	TRP	CG-CD2-CE3	6.48	139.74	133.90
1	C	255	TRP	CG-CD2-CE3	6.48	139.73	133.90
1	B	255	TRP	CG-CD2-CE3	6.47	139.73	133.90
1	B	323	TRP	CD1-CG-CD2	6.47	111.48	106.30
1	C	227	TRP	CG-CD1-NE1	-6.47	103.63	110.10
1	C	352	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	424	GLY	CA-C-N	6.46	129.12	116.20
1	D	352	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	440	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	B	352	ASP	CB-CG-OD1	6.45	124.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	VAL	CA-CB-CG1	-6.45	101.23	110.90
1	A	424	GLY	CA-C-N	6.45	129.09	116.20
1	B	450	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	450	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	C	424	GLY	CA-C-N	6.44	129.09	116.20
1	D	612	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	450	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	612	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	424	GLY	CA-C-N	6.42	129.05	116.20
1	C	285	LYS	CG-CD-CE	6.42	131.17	111.90
1	D	221	VAL	CA-CB-CG1	-6.42	101.27	110.90
1	A	323	TRP	CD1-CG-CD2	6.42	111.44	106.30
1	C	323	TRP	CD1-CG-CD2	6.42	111.44	106.30
1	B	285	LYS	CG-CD-CE	6.42	131.15	111.90
1	D	285	LYS	CG-CD-CE	6.41	131.14	111.90
1	A	285	LYS	CG-CD-CE	6.41	131.14	111.90
1	B	221	VAL	CA-CB-CG1	-6.41	101.28	110.90
1	C	221	VAL	CA-CB-CG1	-6.41	101.28	110.90
1	D	323	TRP	CD1-CG-CD2	6.40	111.42	106.30
1	A	352	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	32	GLU	O-C-N	6.38	132.90	122.70
1	D	450	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	C	32	GLU	O-C-N	6.36	132.87	122.70
1	D	488	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	488	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	32	GLU	O-C-N	6.33	132.83	122.70
1	D	32	GLU	O-C-N	6.31	132.80	122.70
1	B	488	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	612	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	488	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	274	ILE	O-C-N	-6.28	112.66	122.70
1	A	274	ILE	CA-C-N	6.27	131.00	117.20
1	B	274	ILE	CA-C-N	6.27	131.00	117.20
1	A	612	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	274	ILE	CA-C-N	6.26	130.96	117.20
1	C	274	ILE	O-C-N	-6.25	112.70	122.70
1	C	377	ARG	CA-CB-CG	-6.25	99.66	113.40
1	D	274	ILE	CA-C-N	6.24	130.94	117.20
1	D	377	ARG	CA-CB-CG	-6.24	99.68	113.40
1	D	274	ILE	O-C-N	-6.24	112.72	122.70
1	B	274	ILE	O-C-N	-6.23	112.73	122.70
1	B	377	ARG	CA-CB-CG	-6.23	99.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	CA-CB-CG	-6.22	99.71	113.40
1	A	512	TRP	CB-CG-CD1	-6.22	118.92	127.00
1	D	512	TRP	CB-CG-CD1	-6.21	118.92	127.00
1	B	512	TRP	CB-CG-CD1	-6.21	118.93	127.00
1	D	201	ASN	CB-CG-ND2	-6.21	101.81	116.70
1	C	201	ASN	CB-CG-ND2	-6.19	101.83	116.70
1	B	201	ASN	CB-CG-ND2	-6.19	101.84	116.70
1	A	201	ASN	CB-CG-ND2	-6.19	101.85	116.70
1	B	495	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	A	126	ILE	CB-CG1-CD1	-6.17	96.62	113.90
1	C	126	ILE	CB-CG1-CD1	-6.17	96.64	113.90
1	D	126	ILE	CB-CG1-CD1	-6.16	96.64	113.90
1	B	126	ILE	CB-CG1-CD1	-6.16	96.65	113.90
1	C	512	TRP	CB-CG-CD1	-6.16	119.00	127.00
1	D	264	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	469	TRP	CG-CD1-NE1	-6.14	103.96	110.10
1	A	469	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	B	469	TRP	CG-CD1-NE1	-6.13	103.97	110.10
1	C	495	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	D	495	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	C	521	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	469	TRP	CG-CD1-NE1	-6.09	104.01	110.10
1	C	264	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	264	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	A	521	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	495	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	C	29	LEU	CA-C-N	6.07	130.55	117.20
1	A	601	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	264	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	521	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	442	ASN	CA-C-N	6.05	130.51	117.20
1	A	29	LEU	CA-C-N	6.04	130.50	117.20
1	B	521	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	29	LEU	CA-C-N	6.04	130.48	117.20
1	C	442	ASN	CA-C-N	6.03	130.47	117.20
1	D	29	LEU	CA-C-N	6.03	130.46	117.20
1	D	208	ILE	CB-CA-C	6.02	123.65	111.60
1	B	240	TRP	CG-CD2-CE3	6.02	139.32	133.90
1	D	240	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	A	208	ILE	CB-CA-C	6.01	123.62	111.60
1	A	442	ASN	CA-C-N	6.01	130.42	117.20
1	B	442	ASN	CA-C-N	6.01	130.42	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	ILE	CB-CA-C	6.00	123.61	111.60
1	B	601	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	208	ILE	CB-CA-C	5.99	123.58	111.60
1	C	742	TRP	CB-CG-CD1	-5.99	119.22	127.00
1	A	742	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	D	137	TYR	CB-CG-CD1	-5.97	117.42	121.00
1	B	742	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	D	742	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	A	240	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	C	137	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	C	240	TRP	CG-CD2-CE3	5.93	139.24	133.90
1	C	601	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	C	497	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	C	567	THR	CA-CB-CG2	5.90	120.66	112.40
1	B	567	THR	CA-CB-CG2	5.89	120.65	112.40
1	A	567	THR	CA-CB-CG2	5.89	120.65	112.40
1	D	567	THR	CA-CB-CG2	5.88	120.63	112.40
1	D	601	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	405	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	137	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	497	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	137	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	D	242	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	A	415	TYR	CA-CB-CG	5.82	124.45	113.40
1	D	405	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	405	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	370	VAL	N-CA-CB	-5.80	98.75	111.50
1	C	370	VAL	N-CA-CB	-5.80	98.75	111.50
1	A	125	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	B	497	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	C	125	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	B	405	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	415	TYR	CA-CB-CG	5.79	124.40	113.40
1	D	497	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	370	VAL	N-CA-CB	-5.79	98.77	111.50
1	B	242	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	D	370	VAL	N-CA-CB	-5.79	98.77	111.50
1	C	415	TYR	CA-CB-CG	5.78	124.39	113.40
1	D	267	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	686	MET	CG-SD-CE	-5.77	90.96	100.20
1	D	686	MET	CG-SD-CE	-5.77	90.97	100.20
1	B	686	MET	CG-SD-CE	-5.77	90.97	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	ARG	NH1-CZ-NH2	-5.77	113.05	119.40
1	D	415	TYR	CA-CB-CG	5.77	124.36	113.40
1	A	686	MET	CG-SD-CE	-5.76	90.99	100.20
1	B	125	ARG	NH1-CZ-NH2	-5.76	113.07	119.40
1	B	702	ARG	CG-CD-NE	5.75	123.87	111.80
1	C	267	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	702	ARG	CG-CD-NE	5.74	123.86	111.80
1	D	702	ARG	CG-CD-NE	5.73	123.84	111.80
1	A	702	ARG	CG-CD-NE	5.73	123.84	111.80
1	C	242	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	C	183	ARG	CB-CG-CD	5.71	126.44	111.60
1	A	242	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	D	183	ARG	CB-CG-CD	5.70	126.42	111.60
1	B	183	ARG	CB-CG-CD	5.70	126.41	111.60
1	A	183	ARG	CB-CG-CD	5.69	126.39	111.60
1	B	445	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
1	B	267	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	236	HIS	CA-CB-CG	5.67	123.25	113.60
1	C	309	LYS	CB-CG-CD	-5.67	96.85	111.60
1	A	236	HIS	CA-CB-CG	5.67	123.24	113.60
1	A	267	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	309	LYS	CB-CG-CD	-5.67	96.86	111.60
1	D	309	LYS	CB-CG-CD	-5.67	96.87	111.60
1	B	309	LYS	CB-CG-CD	-5.66	96.88	111.60
1	B	236	HIS	CA-CB-CG	5.64	123.20	113.60
1	D	236	HIS	CA-CB-CG	5.64	123.19	113.60
1	D	445	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
1	C	285	LYS	CA-CB-CG	5.64	125.80	113.40
1	D	285	LYS	CA-CB-CG	5.62	125.78	113.40
1	A	285	LYS	CA-CB-CG	5.62	125.76	113.40
1	C	445	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
1	B	285	LYS	CA-CB-CG	5.61	125.74	113.40
1	A	445	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
1	C	544	VAL	CA-CB-CG2	-5.59	102.51	110.90
1	D	544	VAL	CA-CB-CG2	-5.59	102.52	110.90
1	A	512	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	B	544	VAL	CA-CB-CG2	-5.58	102.52	110.90
1	A	544	VAL	CA-CB-CG2	-5.58	102.53	110.90
1	A	377	ARG	NH1-CZ-NH2	5.58	125.53	119.40
1	C	377	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	D	512	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	C	505	TYR	CB-CG-CD1	5.56	124.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	N-CA-C	-5.55	96.01	111.00
1	D	183	ARG	CA-CB-CG	5.55	125.60	113.40
1	B	27	ASP	N-CA-C	-5.54	96.03	111.00
1	B	183	ARG	CA-CB-CG	5.54	125.59	113.40
1	C	183	ARG	CA-CB-CG	5.54	125.59	113.40
1	D	27	ASP	N-CA-C	-5.54	96.03	111.00
1	A	183	ARG	CA-CB-CG	5.54	125.59	113.40
1	C	27	ASP	N-CA-C	-5.54	96.04	111.00
1	B	377	ARG	NH1-CZ-NH2	5.54	125.49	119.40
1	D	377	ARG	NH1-CZ-NH2	5.53	125.48	119.40
1	C	177	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	177	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	512	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	B	432	PRO	O-C-N	-5.52	113.87	122.70
1	B	471	ARG	CB-CG-CD	5.52	125.94	111.60
1	A	177	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	177	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	460	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	C	432	PRO	O-C-N	-5.51	113.89	122.70
1	C	471	ARG	CB-CG-CD	5.51	125.92	111.60
1	C	512	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	A	471	ARG	CB-CG-CD	5.50	125.91	111.60
1	D	471	ARG	CB-CG-CD	5.50	125.90	111.60
1	B	181	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	505	TYR	CB-CG-CD1	5.49	124.29	121.00
1	A	505	TYR	CB-CG-CD1	5.48	124.29	121.00
1	D	432	PRO	O-C-N	-5.47	113.95	122.70
1	D	587	SER	CA-CB-OG	5.47	125.96	111.20
1	A	587	SER	CA-CB-OG	5.46	125.95	111.20
1	B	505	TYR	CB-CG-CD1	5.46	124.28	121.00
1	B	587	SER	CA-CB-OG	5.46	125.94	111.20
1	A	83	ASN	CB-CG-ND2	5.46	129.80	116.70
1	A	460	TYR	CB-CG-CD1	-5.46	117.73	121.00
1	C	460	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	C	587	SER	CA-CB-OG	5.45	125.92	111.20
1	A	432	PRO	O-C-N	-5.45	113.98	122.70
1	B	83	ASN	CB-CG-ND2	5.44	129.76	116.70
1	C	83	ASN	CB-CG-ND2	5.44	129.75	116.70
1	B	460	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	A	181	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	181	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	83	ASN	CB-CG-ND2	5.42	129.72	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	648	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	648	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	201	ASN	CA-CB-CG	5.40	125.28	113.40
1	B	648	LEU	CA-CB-CG	5.39	127.70	115.30
1	C	201	ASN	CA-CB-CG	5.39	125.25	113.40
1	C	648	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	201	ASN	CA-CB-CG	5.39	125.25	113.40
1	D	181	ASP	CB-CG-OD1	5.38	123.15	118.30
1	B	201	ASN	CA-CB-CG	5.38	125.23	113.40
1	D	155	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	255	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	D	255	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	B	255	TRP	CB-CG-CD1	-5.36	120.04	127.00
1	B	422	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	422	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	255	TRP	CB-CG-CD1	-5.35	120.05	127.00
1	C	636	ARG	CA-CB-CG	5.35	125.17	113.40
1	C	155	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	414	SER	N-CA-C	5.33	125.40	111.00
1	B	636	ARG	CA-CB-CG	5.33	125.13	113.40
1	A	37	ARG	CG-CD-NE	5.33	122.99	111.80
1	A	414	SER	N-CA-C	5.32	125.37	111.00
1	A	636	ARG	CA-CB-CG	5.32	125.11	113.40
1	D	37	ARG	CG-CD-NE	5.32	122.98	111.80
1	B	155	ASP	CB-CG-OD1	5.32	123.08	118.30
1	D	636	ARG	CA-CB-CG	5.32	125.10	113.40
1	B	37	ARG	CG-CD-NE	5.32	122.96	111.80
1	B	414	SER	N-CA-C	5.31	125.34	111.00
1	C	37	ARG	CG-CD-NE	5.31	122.96	111.80
1	D	422	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	422	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	208	ILE	N-CA-CB	-5.31	98.59	110.80
1	C	414	SER	N-CA-C	5.31	125.33	111.00
1	D	208	ILE	N-CA-CB	-5.31	98.60	110.80
1	A	208	ILE	N-CA-CB	-5.30	98.60	110.80
1	C	208	ILE	N-CA-CB	-5.30	98.60	110.80
1	A	155	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	255	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	255	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	C	408	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	408	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	255	TRP	CG-CD1-NE1	-5.25	104.86	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	LEU	CA-CB-CG	5.24	127.34	115.30
1	D	408	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	334	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	B	432	PRO	CA-C-N	5.22	128.69	117.20
1	C	411	ARG	NH1-CZ-NH2	-5.22	113.65	119.40
1	C	432	PRO	CA-C-N	5.22	128.69	117.20
1	B	751	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	C	255	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	D	751	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	D	466	ASN	CB-CG-ND2	5.22	129.22	116.70
1	D	432	PRO	CA-C-N	5.21	128.67	117.20
1	A	466	ASN	CB-CG-ND2	5.21	129.21	116.70
1	C	751	ILE	CG1-CB-CG2	-5.21	99.94	111.40
1	C	125	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	751	ILE	CG1-CB-CG2	-5.20	99.95	111.40
1	D	585	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	432	PRO	CA-C-N	5.20	128.63	117.20
1	D	466	ASN	OD1-CG-ND2	-5.20	109.95	121.90
1	C	466	ASN	CB-CG-ND2	5.19	129.16	116.70
1	D	742	TRP	CG-CD2-CE3	5.19	138.57	133.90
1	B	466	ASN	CB-CG-ND2	5.18	129.14	116.70
1	B	466	ASN	OD1-CG-ND2	-5.18	109.98	121.90
1	D	125	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	466	ASN	OD1-CG-ND2	-5.18	109.99	121.90
1	C	466	ASN	OD1-CG-ND2	-5.18	109.99	121.90
1	B	411	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
1	C	334	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	D	334	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	C	266	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	B	266	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	B	742	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	A	334	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	C	702	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	C	742	TRP	CG-CD2-CE3	5.15	138.53	133.90
1	D	411	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
1	B	585	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	411	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	D	567	THR	N-CA-CB	-5.14	100.54	110.30
1	B	567	THR	N-CA-CB	-5.13	100.55	110.30
1	D	702	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	567	THR	N-CA-CB	-5.12	100.57	110.30
1	A	125	ARG	NE-CZ-NH2	5.12	122.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	585	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	266	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	C	319	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	319	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	567	THR	N-CA-CB	-5.11	100.58	110.30
1	A	742	TRP	CG-CD2-CE3	5.11	138.50	133.90
1	D	684	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	A	319	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	357	THR	CA-CB-CG2	5.10	119.54	112.40
1	A	266	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	B	125	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	D	357	THR	CA-CB-CG2	5.09	119.52	112.40
1	C	451	MET	CA-C-N	5.08	126.37	116.20
1	C	357	THR	CA-CB-CG2	5.08	119.51	112.40
1	A	585	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	D	451	MET	CA-C-N	5.07	126.34	116.20
1	A	451	MET	CA-C-N	5.06	126.32	116.20
1	B	451	MET	CA-C-N	5.06	126.32	116.20
1	A	357	THR	CA-CB-CG2	5.06	119.48	112.40
1	C	684	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	D	319	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	702	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	123	PRO	CA-C-N	5.03	128.27	117.20
1	C	123	PRO	CA-C-N	5.03	128.26	117.20
1	A	684	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	C	240	TRP	CB-CG-CD1	-5.03	120.47	127.00
1	A	123	PRO	CA-C-N	5.03	128.26	117.20
1	B	684	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	240	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	B	468	ASN	N-CA-C	5.02	124.56	111.00
1	A	602	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	D	123	PRO	CA-C-N	5.01	128.23	117.20
1	D	602	VAL	CG1-CB-CG2	-5.00	102.89	110.90
1	B	240	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	C	602	VAL	CG1-CB-CG2	-5.00	102.90	110.90

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	415	TYR	Sidechain
1	A	51	ALA	Peptide
1	B	137	TYR	Sidechain
1	B	415	TYR	Sidechain
1	B	51	ALA	Peptide
1	C	137	TYR	Sidechain
1	C	415	TYR	Sidechain
1	C	51	ALA	Peptide
1	D	137	TYR	Sidechain
1	D	415	TYR	Sidechain
1	D	51	ALA	Peptide

5.2 Too-close contacts [\(i\)](#)

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	5746	0	5578	88	1
1	B	5746	0	5578	90	1
1	C	5746	0	5578	88	22
1	D	5746	0	5578	90	22
2	A	43	0	30	4	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
All	All	23156	0	22432	331	23

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 (331) 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:C:392:HIS:CD2	1:C:415:TYR:HB2	2.02	0.94
1:A:392:HIS:CD2	1:A:415:TYR:HB2	2.02	0.94
1:D:392:HIS:CD2	1:D:415:TYR:HB2	2.02	0.93
1:B:392:HIS:CD2	1:B:415:TYR:HB2	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ASN:ND2	1:C:285:LYS:HD3	1.94	0.82
1:B:281:ASN:ND2	1:B:285:LYS:HD3	1.95	0.82
1:A:281:ASN:ND2	1:A:285:LYS:HD3	1.95	0.81
1:D:281:ASN:ND2	1:D:285:LYS:HD3	1.94	0.80
1:A:509:ARG:HD2	1:A:576:PRO:HG2	1.64	0.80
1:D:509:ARG:HD2	1:D:576:PRO:HG2	1.64	0.78
1:C:509:ARG:HD2	1:C:576:PRO:HG2	1.64	0.78
1:B:509:ARG:HD2	1:B:576:PRO:HG2	1.64	0.77
1:C:710:ILE:HD13	1:C:718:ILE:HG13	1.68	0.76
1:D:710:ILE:HD13	1:D:718:ILE:HG13	1.68	0.76
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.68	0.75
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.68	0.75
1:C:392:HIS:HD2	1:C:415:TYR:CG	2.12	0.68
1:B:700:ASP:O	1:B:703:LYS:HG2	1.94	0.68
1:C:700:ASP:O	1:C:703:LYS:HG2	1.94	0.68
1:D:700:ASP:O	1:D:703:LYS:HG2	1.94	0.67
1:D:392:HIS:HD2	1:D:415:TYR:CG	2.12	0.67
1:B:392:HIS:HD2	1:B:415:TYR:CG	2.12	0.67
1:A:392:HIS:HD2	1:A:415:TYR:CG	2.12	0.67
1:A:700:ASP:O	1:A:703:LYS:HG2	1.94	0.66
1:B:392:HIS:CD2	1:B:415:TYR:CB	2.78	0.66
1:A:392:HIS:CD2	1:A:415:TYR:CB	2.78	0.66
1:D:392:HIS:CD2	1:D:415:TYR:CB	2.78	0.66
1:C:708:ILE:HG13	1:C:710:ILE:HD12	1.79	0.65
1:D:708:ILE:HG13	1:D:710:ILE:HD12	1.79	0.65
1:A:708:ILE:HG13	1:A:710:ILE:HD12	1.79	0.65
1:B:708:ILE:HG13	1:B:710:ILE:HD12	1.79	0.64
1:C:392:HIS:CD2	1:C:415:TYR:CB	2.78	0.64
1:B:392:HIS:HD2	1:B:415:TYR:HB2	1.61	0.64
1:A:338:PHE:HB3	1:A:340:LEU:HD13	1.82	0.62
1:C:338:PHE:HB3	1:C:340:LEU:HD13	1.82	0.62
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.82	0.62
1:B:338:PHE:HB3	1:B:340:LEU:HD13	1.82	0.62
1:C:264:ARG:HA	1:C:302:LEU:HD13	1.82	0.62
1:B:264:ARG:HA	1:B:302:LEU:HD13	1.82	0.61
1:D:392:HIS:HD2	1:D:415:TYR:CB	2.14	0.61
1:C:147:ILE:HA	1:C:285:LYS:HE3	1.82	0.61
1:C:568:ASP:HA	1:C:571:LEU:HD23	1.82	0.61
1:D:568:ASP:HA	1:D:571:LEU:HD23	1.82	0.61
1:A:392:HIS:HD2	1:A:415:TYR:CB	2.14	0.61
1:A:345:ASP:HA	1:A:348:LYS:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:HD2	1:A:415:TYR:HB2	1.61	0.60
1:A:147:ILE:HA	1:A:285:LYS:HE3	1.82	0.60
1:A:568:ASP:HA	1:A:571:LEU:HD23	1.82	0.60
1:B:147:ILE:HA	1:B:285:LYS:HE3	1.82	0.60
1:B:568:ASP:HA	1:B:571:LEU:HD23	1.82	0.60
1:D:345:ASP:HA	1:D:348:LYS:HD3	1.83	0.60
1:C:392:HIS:HD2	1:C:415:TYR:HB2	1.60	0.60
1:D:147:ILE:HA	1:D:285:LYS:HE3	1.82	0.60
1:D:264:ARG:HA	1:D:302:LEU:HD13	1.82	0.60
1:C:345:ASP:HA	1:C:348:LYS:HD3	1.83	0.59
1:A:264:ARG:HA	1:A:302:LEU:HD13	1.82	0.59
1:C:392:HIS:HD2	1:C:415:TYR:CB	2.14	0.59
1:B:131:GLY:HA2	1:B:166:PHE:O	2.03	0.59
1:A:516:THR:O	1:A:520:GLN:HG3	2.03	0.59
1:B:345:ASP:HA	1:B:348:LYS:HD3	1.83	0.59
1:D:516:THR:O	1:D:520:GLN:HG3	2.03	0.58
1:A:131:GLY:HA2	1:A:166:PHE:O	2.03	0.58
1:C:131:GLY:HA2	1:C:166:PHE:O	2.03	0.58
1:B:392:HIS:HD2	1:B:415:TYR:CB	2.14	0.58
1:C:516:THR:O	1:C:520:GLN:HG3	2.03	0.58
1:D:131:GLY:HA2	1:D:166:PHE:O	2.03	0.58
1:A:634:TYR:O	1:A:653:THR:HA	2.04	0.58
1:B:516:THR:O	1:B:520:GLN:HG3	2.03	0.57
1:B:634:TYR:O	1:B:653:THR:HA	2.04	0.57
1:C:634:TYR:O	1:C:653:THR:HA	2.04	0.57
1:D:264:ARG:HB3	1:D:268:THR:HG21	1.87	0.57
1:C:264:ARG:HB3	1:C:268:THR:HG21	1.87	0.56
1:A:264:ARG:HB3	1:A:268:THR:HG21	1.87	0.56
1:D:634:TYR:O	1:D:653:THR:HA	2.04	0.56
1:B:264:ARG:HB3	1:B:268:THR:HG21	1.87	0.56
1:B:515:GLN:HB2	1:B:520:GLN:HG2	1.88	0.55
1:D:392:HIS:HD2	1:D:415:TYR:HB2	1.60	0.55
1:C:333:GLU:HG2	1:C:374:VAL:HG22	1.89	0.55
1:C:515:GLN:HB2	1:C:520:GLN:HG2	1.89	0.55
1:A:333:GLU:HG2	1:A:374:VAL:HG22	1.89	0.55
1:B:333:GLU:HG2	1:B:374:VAL:HG22	1.89	0.55
1:A:449:HIS:CD2	1:A:451:MET:SD	3.00	0.55
1:A:515:GLN:HB2	1:A:520:GLN:HG2	1.89	0.55
1:C:449:HIS:CD2	1:C:451:MET:SD	3.00	0.55
1:A:537:PRO:HA	1:A:540:ARG:HG3	1.89	0.55
1:D:333:GLU:HG2	1:D:374:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:GLN:HB2	1:D:520:GLN:HG2	1.89	0.55
1:C:268:THR:HG23	1:C:300:ALA:H	1.72	0.54
1:D:537:PRO:HA	1:D:540:ARG:HG3	1.89	0.54
1:A:527:PHE:O	1:A:531:LEU:HB2	2.07	0.54
1:D:527:PHE:O	1:D:531:LEU:HB2	2.07	0.54
1:A:313:ARG:HG2	1:A:658:PRO:HG2	1.90	0.54
1:C:567:THR:HG22	1:C:570:GLN:H	1.73	0.54
1:D:313:ARG:HG2	1:D:658:PRO:HG2	1.90	0.54
1:B:221:VAL:HG13	1:B:239:PHE:CD1	2.43	0.54
1:D:449:HIS:CD2	1:D:451:MET:SD	3.00	0.54
1:C:221:VAL:HG13	1:C:239:PHE:CD1	2.43	0.54
1:B:567:THR:HG22	1:B:570:GLN:H	1.73	0.54
1:B:449:HIS:CD2	1:B:451:MET:SD	3.00	0.54
1:D:268:THR:HG23	1:D:300:ALA:H	1.72	0.54
1:A:221:VAL:HG13	1:A:239:PHE:CD1	2.43	0.53
1:A:268:THR:HG23	1:A:300:ALA:H	1.72	0.53
1:A:705:LYS:HE3	1:A:710:ILE:HG22	1.90	0.53
1:B:705:LYS:HE3	1:B:710:ILE:HG22	1.90	0.53
1:C:223:PRO:HG3	1:C:230:PRO:O	2.09	0.53
1:B:268:THR:HG23	1:B:300:ALA:H	1.72	0.53
1:D:705:LYS:HE3	1:D:710:ILE:HG22	1.91	0.53
1:A:258:SER:OG	1:A:260:ARG:HB2	2.09	0.53
1:A:567:THR:HG22	1:A:570:GLN:H	1.73	0.53
1:B:223:PRO:HG3	1:B:230:PRO:O	2.09	0.53
1:B:258:SER:OG	1:B:260:ARG:HB2	2.09	0.53
1:B:527:PHE:O	1:B:531:LEU:HB2	2.07	0.53
1:C:537:PRO:HA	1:C:540:ARG:HG3	1.89	0.53
1:A:223:PRO:HG3	1:A:230:PRO:O	2.09	0.53
1:D:258:SER:OG	1:D:260:ARG:HB2	2.09	0.53
1:C:258:SER:OG	1:C:260:ARG:HB2	2.09	0.53
1:D:267:ARG:HG2	1:D:332:PRO:HG3	1.91	0.53
1:B:267:ARG:HG2	1:B:332:PRO:HG3	1.91	0.53
1:B:537:PRO:HA	1:B:540:ARG:HG3	1.89	0.53
1:B:51:ALA:O	1:B:323:TRP:HZ2	1.92	0.53
1:C:527:PHE:O	1:C:531:LEU:HB2	2.07	0.53
1:D:567:THR:HG22	1:D:570:GLN:H	1.73	0.52
1:B:313:ARG:HG2	1:B:658:PRO:HG2	1.90	0.52
1:B:443:PHE:HD2	1:B:459:ASN:HA	1.75	0.52
1:C:267:ARG:HG2	1:C:332:PRO:HG3	1.91	0.52
1:C:313:ARG:HG2	1:C:658:PRO:HG2	1.90	0.52
1:C:705:LYS:HE3	1:C:710:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:PRO:HG3	1:D:230:PRO:O	2.09	0.52
1:B:231:GLN:O	1:B:233:GLN:HG3	2.09	0.52
1:B:639:GLU:HG3	1:B:647:VAL:HG13	1.92	0.52
1:C:639:GLU:HG3	1:C:647:VAL:HG13	1.92	0.52
1:C:51:ALA:O	1:C:323:TRP:HZ2	1.92	0.52
1:C:231:GLN:O	1:C:233:GLN:HG3	2.09	0.52
1:D:231:GLN:O	1:D:233:GLN:HG3	2.09	0.52
1:A:231:GLN:O	1:A:233:GLN:HG3	2.09	0.52
1:D:51:ALA:O	1:D:323:TRP:HZ2	1.92	0.52
1:D:221:VAL:HG13	1:D:239:PHE:CD1	2.43	0.52
1:A:51:ALA:O	1:A:323:TRP:HZ2	1.92	0.52
1:A:267:ARG:HG2	1:A:332:PRO:HG3	1.91	0.52
1:C:443:PHE:HD2	1:C:459:ASN:HA	1.75	0.52
1:D:443:PHE:HD2	1:D:459:ASN:HA	1.75	0.52
1:A:453:ILE:HD12	1:C:71:VAL:HG23	1.92	0.52
1:D:639:GLU:HG3	1:D:647:VAL:HG13	1.92	0.52
1:B:71:VAL:HG23	1:D:453:ILE:HD12	1.92	0.51
1:B:459:ASN:HD22	1:B:459:ASN:H	1.59	0.51
1:C:285:LYS:HE2	1:C:287:THR:OG1	2.11	0.51
1:A:639:GLU:HG3	1:A:647:VAL:HG13	1.92	0.51
1:B:453:ILE:HD12	1:D:71:VAL:HG23	1.92	0.51
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.44	0.51
1:C:459:ASN:H	1:C:459:ASN:HD22	1.59	0.51
1:D:285:LYS:HE2	1:D:287:THR:OG1	2.11	0.51
1:B:285:LYS:HE2	1:B:287:THR:OG1	2.11	0.51
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.44	0.51
1:A:71:VAL:HG23	1:C:453:ILE:HD12	1.92	0.51
1:A:443:PHE:HD2	1:A:459:ASN:HA	1.75	0.51
1:A:285:LYS:HE2	1:A:287:THR:OG1	2.11	0.50
1:A:459:ASN:HD22	1:A:459:ASN:H	1.59	0.50
1:C:418:THR:HG21	2:C:754:HEM:HBD1	1.93	0.50
1:B:418:THR:HG21	2:B:754:HEM:HBD1	1.93	0.50
1:B:490:GLU:HA	1:C:489:VAL:O	2.12	0.50
1:D:459:ASN:HD22	1:D:459:ASN:H	1.59	0.50
1:A:418:THR:HG21	2:A:754:HEM:HBD1	1.93	0.50
1:A:489:VAL:O	1:D:490:GLU:HA	2.12	0.50
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.44	0.50
1:A:471:ARG:NH2	1:C:27:ASP:N	2.60	0.50
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.44	0.50
1:B:27:ASP:N	1:D:471:ARG:NH2	2.60	0.50
1:A:490:GLU:HA	1:D:489:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:VAL:HA	1:B:188:LYS:O	2.13	0.49
1:B:471:ARG:NH2	1:D:27:ASP:N	2.60	0.49
1:C:162:VAL:HA	1:C:188:LYS:O	2.13	0.49
1:A:27:ASP:N	1:C:471:ARG:NH2	2.60	0.49
1:A:162:VAL:HA	1:A:188:LYS:O	2.13	0.49
1:D:162:VAL:HA	1:D:188:LYS:O	2.13	0.49
1:D:418:THR:HG21	2:D:754:HEM:HBD1	1.93	0.49
1:B:489:VAL:O	1:C:490:GLU:HA	2.12	0.49
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.95	0.48
1:A:363:GLU:HB2	1:A:582:LEU:HD21	1.95	0.48
1:A:506:SER:HB3	1:A:577:PRO:O	2.14	0.48
1:D:506:SER:HB3	1:D:577:PRO:O	2.14	0.48
1:B:506:SER:HB3	1:B:577:PRO:O	2.14	0.48
1:D:214:PHE:HB3	1:D:215:PRO:HD3	1.96	0.48
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.96	0.48
1:B:214:PHE:HB3	1:B:215:PRO:HD3	1.96	0.48
1:A:128:HIS:O	1:A:165:ARG:NH2	2.47	0.47
1:B:128:HIS:O	1:B:165:ARG:NH2	2.47	0.47
1:C:214:PHE:HB3	1:C:215:PRO:HD3	1.96	0.47
1:C:506:SER:HB3	1:C:577:PRO:O	2.14	0.47
1:D:748:ILE:HA	1:D:751:ILE:HD13	1.96	0.47
1:C:255:TRP:HE3	1:C:260:ARG:HG2	1.80	0.47
1:B:363:GLU:HB2	1:B:582:LEU:HD21	1.95	0.47
1:C:128:HIS:O	1:C:165:ARG:NH2	2.47	0.47
1:D:128:HIS:O	1:D:165:ARG:NH2	2.47	0.47
1:A:641:THR:HA	1:A:646:THR:O	2.15	0.47
1:C:117:PHE:CE1	1:D:126:ILE:HD11	2.50	0.47
1:A:87:ARG:H	1:A:87:ARG:HG2	1.62	0.47
1:A:126:ILE:HD11	1:B:117:PHE:CE1	2.50	0.47
1:B:744:ARG:HA	1:B:747:LYS:HD2	1.97	0.47
1:C:363:GLU:HB2	1:C:582:LEU:HD21	1.95	0.47
1:C:748:ILE:HA	1:C:751:ILE:HD13	1.96	0.47
1:D:268:THR:HG23	1:D:300:ALA:N	2.30	0.47
1:D:641:THR:HA	1:D:646:THR:O	2.14	0.47
1:A:117:PHE:CE1	1:B:126:ILE:HD11	2.50	0.47
1:A:255:TRP:HE3	1:A:260:ARG:HG2	1.80	0.47
2:A:754:HEM:HMC1	2:A:754:HEM:HBC2	1.97	0.47
1:D:255:TRP:HE3	1:D:260:ARG:HG2	1.80	0.47
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.18	0.47
1:B:641:THR:HA	1:B:646:THR:O	2.14	0.47
1:D:744:ARG:HA	1:D:747:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:ILE:HA	1:B:751:ILE:HD13	1.96	0.46
2:C:754:HEM:HMC1	2:C:754:HEM:HBC2	1.97	0.46
1:A:268:THR:HG23	1:A:300:ALA:N	2.30	0.46
1:A:748:ILE:HA	1:A:751:ILE:HD13	1.96	0.46
1:C:126:ILE:HD11	1:D:117:PHE:CE1	2.50	0.46
1:D:710:ILE:CD1	1:D:718:ILE:HG13	2.43	0.46
1:B:255:TRP:HE3	1:B:260:ARG:HG2	1.80	0.46
1:C:641:THR:HA	1:C:646:THR:O	2.14	0.46
1:C:744:ARG:HA	1:C:747:LYS:HD2	1.97	0.46
2:D:754:HEM:HBC2	2:D:754:HEM:HMC1	1.97	0.46
1:A:278:ARG:HH22	1:A:487:GLU:CD	2.18	0.46
1:C:278:ARG:HH22	1:C:487:GLU:CD	2.18	0.46
1:A:710:ILE:CD1	1:A:718:ILE:HG13	2.43	0.46
1:C:710:ILE:CD1	1:C:718:ILE:HG13	2.43	0.46
1:C:268:THR:HG23	1:C:300:ALA:N	2.30	0.46
1:A:744:ARG:HA	1:A:747:LYS:HD2	1.97	0.45
1:B:268:THR:HG23	1:B:300:ALA:N	2.30	0.45
1:D:278:ARG:HH22	1:D:487:GLU:CD	2.18	0.45
2:B:754:HEM:HMC1	2:B:754:HEM:HBC2	1.97	0.45
1:C:126:ILE:HD12	1:D:121:ARG:NH2	2.32	0.45
1:A:126:ILE:HD12	1:B:121:ARG:NH2	2.31	0.45
1:D:87:ARG:H	1:D:87:ARG:HG2	1.62	0.45
1:A:121:ARG:NH2	1:B:126:ILE:HD12	2.32	0.45
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.43	0.45
1:C:121:ARG:NH2	1:D:126:ILE:HD12	2.31	0.44
1:A:234:SER:HB2	1:A:239:PHE:CD2	2.53	0.44
1:D:234:SER:HB2	1:D:239:PHE:CD2	2.53	0.44
1:B:234:SER:HB2	1:B:239:PHE:CD2	2.53	0.44
1:C:234:SER:HB2	1:C:239:PHE:CD2	2.53	0.44
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.54	0.43
1:A:449:HIS:HD2	1:A:451:MET:SD	2.41	0.43
1:B:708:ILE:H	1:B:708:ILE:HG12	1.73	0.43
1:A:255:TRP:CE3	1:A:260:ARG:HG2	2.54	0.43
2:A:754:HEM:HHD	2:A:754:HEM:HAC	1.83	0.43
1:B:43:THR:HG21	1:B:48:GLN:HG3	2.01	0.43
1:B:411:ARG:HG2	2:B:754:HEM:C2C	2.54	0.43
1:C:28:SER:O	1:C:29:LEU:HB2	2.19	0.43
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.54	0.43
1:B:449:HIS:HD2	1:B:451:MET:SD	2.41	0.43
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.53	0.43
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:TRP:CE3	1:C:260:ARG:HG2	2.54	0.42
1:B:130:ARG:HA	1:B:173:ALA:HA	2.02	0.42
1:C:43:THR:HG21	1:C:48:GLN:HG3	2.01	0.42
1:D:136:GLY:HA3	1:D:374:VAL:O	2.20	0.42
1:A:631:LYS:HB3	1:A:633:LEU:HD13	2.01	0.42
1:B:28:SER:O	1:B:29:LEU:HB2	2.19	0.42
1:B:255:TRP:CE3	1:B:260:ARG:HG2	2.54	0.42
1:D:449:HIS:HD2	1:D:451:MET:SD	2.41	0.42
1:C:411:ARG:HG2	2:C:754:HEM:C2C	2.54	0.42
1:D:255:TRP:CE3	1:D:260:ARG:HG2	2.54	0.42
1:C:130:ARG:HA	1:C:173:ALA:HA	2.01	0.42
1:D:43:THR:HG21	1:D:48:GLN:HG3	2.01	0.42
1:C:136:GLY:HA3	1:C:374:VAL:O	2.20	0.42
1:B:144:LEU:HD11	1:B:370:VAL:HG13	2.02	0.42
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.02	0.42
1:D:204:PRO:HB3	1:D:272:PHE:CD1	2.55	0.42
1:D:631:LYS:HB3	1:D:633:LEU:HD13	2.01	0.42
1:A:411:ARG:HG2	2:A:754:HEM:C2C	2.54	0.42
1:A:446:ASP:HB2	1:C:120:GLU:HG2	2.02	0.42
1:C:204:PRO:HB3	1:C:272:PHE:CD1	2.55	0.42
1:D:411:ARG:HG2	2:D:754:HEM:C2C	2.54	0.42
1:B:204:PRO:HB3	1:B:272:PHE:CD1	2.55	0.42
1:B:446:ASP:HB2	1:D:120:GLU:HG2	2.02	0.42
1:A:136:GLY:HA3	1:A:374:VAL:O	2.20	0.41
1:B:136:GLY:HA3	1:B:374:VAL:O	2.20	0.41
1:C:631:LYS:HB3	1:C:633:LEU:HD13	2.01	0.41
1:A:209:GLN:O	1:A:406:PRO:HG2	2.20	0.41
1:B:120:GLU:HG2	1:D:446:ASP:HB2	2.02	0.41
1:B:631:LYS:HB3	1:B:633:LEU:HD13	2.01	0.41
1:D:130:ARG:HA	1:D:173:ALA:HA	2.02	0.41
1:D:341:ILE:HD11	1:D:360:ILE:HD13	2.02	0.41
1:A:43:THR:HG21	1:A:48:GLN:HG3	2.01	0.41
1:A:605:ILE:HD12	1:A:630:ALA:HB1	2.02	0.41
1:B:209:GLN:O	1:B:406:PRO:HG2	2.20	0.41
1:A:204:PRO:HB3	1:A:272:PHE:CD1	2.55	0.41
1:A:130:ARG:HA	1:A:173:ALA:HA	2.02	0.41
1:A:341:ILE:HD11	1:A:360:ILE:HD13	2.02	0.41
1:A:120:GLU:HG2	1:C:446:ASP:HB2	2.02	0.41
1:C:333:GLU:HA	1:C:373:MET:O	2.21	0.41
1:C:341:ILE:HD11	1:C:360:ILE:HD13	2.02	0.41
1:D:28:SER:O	1:D:29:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:O	1:A:254:MET:HB2	2.21	0.41
1:C:582:LEU:HD12	1:C:582:LEU:HA	1.94	0.41
1:D:209:GLN:O	1:D:406:PRO:HG2	2.20	0.41
1:B:341:ILE:HD11	1:B:360:ILE:HD13	2.02	0.41
1:A:28:SER:O	1:A:29:LEU:HB2	2.19	0.41
1:B:207:PHE:C	1:B:208:ILE:HD12	2.41	0.41
1:B:429:HIS:CD2	1:D:83:ASN:HB3	2.56	0.41
1:C:117:PHE:CZ	1:D:126:ILE:HD11	2.56	0.41
1:C:449:HIS:HD2	1:C:451:MET:SD	2.41	0.41
1:D:207:PHE:C	1:D:208:ILE:HD12	2.41	0.41
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.51	0.41
1:A:117:PHE:CZ	1:B:126:ILE:HD11	2.56	0.41
1:A:144:LEU:HD11	1:A:370:VAL:HG13	2.02	0.41
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.51	0.41
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.57	0.41
1:C:209:GLN:O	1:C:406:PRO:HG2	2.20	0.41
1:C:605:ILE:HD12	1:C:630:ALA:HB1	2.03	0.41
1:C:639:GLU:HB2	1:C:648:LEU:O	2.21	0.41
1:D:251:HIS:O	1:D:254:MET:HB2	2.21	0.41
1:D:333:GLU:HA	1:D:373:MET:O	2.21	0.41
1:D:639:GLU:HB2	1:D:648:LEU:O	2.21	0.41
1:A:83:ASN:HB3	1:C:429:HIS:CD2	2.56	0.40
1:A:207:PHE:C	1:A:208:ILE:HD12	2.41	0.40
1:A:488:ARG:HH11	1:A:488:ARG:HD2	1.74	0.40
1:C:144:LEU:HD11	1:C:370:VAL:HG13	2.02	0.40
1:D:708:ILE:H	1:D:708:ILE:HG12	1.73	0.40
1:B:83:ASN:HB3	1:D:429:HIS:CD2	2.56	0.40
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.57	0.40
1:B:251:HIS:O	1:B:254:MET:HB2	2.21	0.40
1:B:751:ILE:HA	1:B:752:PRO:HD3	1.94	0.40
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.56	0.40
1:A:708:ILE:H	1:A:708:ILE:HG12	1.73	0.40
1:B:333:GLU:HA	1:B:373:MET:O	2.21	0.40
1:C:207:PHE:C	1:C:208:ILE:HD12	2.41	0.40
1:A:333:GLU:HA	1:A:373:MET:O	2.21	0.40
1:B:582:LEU:HD12	1:B:582:LEU:HA	1.94	0.40
1:B:605:ILE:HD12	1:B:630:ALA:HB1	2.02	0.40
1:C:87:ARG:H	1:C:87:ARG:HG2	1.62	0.40
1:D:96:ARG:HA	1:D:102:PRO:O	2.21	0.40
1:D:488:ARG:HH11	1:D:488:ARG:HD2	1.74	0.40

All (23) symmetry-related close contacts are listed below. The label for Atom-2 includes the

symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:621:LYS:CD	1:D:644:ASP:OD1[2_544]	0.48	1.72
1:C:621:LYS:CB	1:D:644:ASP:OD2[2_544]	0.57	1.63
1:C:621:LYS:CG	1:D:644:ASP:CG[2_544]	0.64	1.56
1:C:621:LYS:NZ	1:D:613:SER:OG[2_544]	0.79	1.41
1:C:617:LEU:CD2	1:D:646:THR:CA[2_544]	0.92	1.28
1:C:621:LYS:CE	1:D:613:SER:OG[2_544]	1.22	0.98
1:C:621:LYS:CG	1:D:644:ASP:OD1[2_544]	1.28	0.92
1:C:621:LYS:CD	1:D:644:ASP:CG[2_544]	1.29	0.91
1:C:621:LYS:CG	1:D:644:ASP:OD2[2_544]	1.43	0.77
1:C:617:LEU:CG	1:D:645:GLY:O[2_544]	1.45	0.75
1:C:621:LYS:CB	1:D:644:ASP:CG[2_544]	1.48	0.72
1:C:617:LEU:CD2	1:D:646:THR:N[2_544]	1.58	0.62
1:C:617:LEU:CB	1:D:645:GLY:O[2_544]	1.61	0.59
1:C:621:LYS:CG	1:D:644:ASP:CB[2_544]	1.71	0.49
1:C:621:LYS:NZ	1:D:613:SER:CB[2_544]	1.94	0.26
1:C:617:LEU:CD2	1:D:645:GLY:O[2_544]	1.97	0.23
1:C:617:LEU:CD2	1:D:646:THR:C[2_544]	1.97	0.23
1:C:617:LEU:CD2	1:D:645:GLY:C[2_544]	2.02	0.18
1:C:621:LYS:CE	1:D:644:ASP:OD1[2_544]	2.03	0.17
1:C:621:LYS:CE	1:D:644:ASP:CG[2_544]	2.04	0.16
1:C:621:LYS:CA	1:D:644:ASP:OD2[2_544]	2.04	0.16
1:A:476:GLY:CA	1:B:61:ARG:NH2[2_545]	2.05	0.15
1:C:621:LYS:CD	1:D:644:ASP:OD2[2_544]	2.18	0.02

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	19 49
1	B	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	19 49
1	C	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	19 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	19	49
All	All	2900/3012 (96%)	2740 (94%)	136 (5%)	24 (1%)	19	49

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	B	33	ASP
1	C	33	ASP
1	D	33	ASP
1	A	130	ARG
1	A	131	GLY
1	B	130	ARG
1	B	131	GLY
1	C	130	ARG
1	C	131	GLY
1	D	130	ARG
1	D	131	GLY
1	B	274	ILE
1	C	274	ILE
1	A	274	ILE
1	D	274	ILE
1	A	752	PRO
1	B	752	PRO
1	C	752	PRO
1	D	752	PRO
1	A	52	PRO
1	B	52	PRO
1	C	52	PRO
1	D	52	PRO

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%)	549 (90%)	63 (10%)	7	21
1	B	612/636 (96%)	549 (90%)	63 (10%)	7	21
1	C	612/636 (96%)	549 (90%)	63 (10%)	7	21
1	D	612/636 (96%)	549 (90%)	63 (10%)	7	21
All	All	2448/2544 (96%)	2196 (90%)	252 (10%)	7	21

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	37	ARG
1	A	56	LYS
1	A	73	LYS
1	A	87	ARG
1	A	126	ILE
1	A	127	VAL
1	A	146	ASP
1	A	159	ILE
1	A	165	ARG
1	A	183	ARG
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	208	ILE
1	A	221	VAL
1	A	227	TRP
1	A	230	PRO
1	A	237	ASP
1	A	252	ASN
1	A	259	ASP
1	A	260	ARG
1	A	268	THR
1	A	285	LYS
1	A	302	LEU
1	A	313	ARG
1	A	321	GLU
1	A	340	LEU
1	A	348	LYS
1	A	368	GLN
1	A	375	LEU
1	A	377	ARG
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	408	LEU
1	A	412	LEU
1	A	415	TYR
1	A	419	GLN
1	A	459	ASN
1	A	471	ARG
1	A	478	LYS
1	A	506	SER
1	A	509	ARG
1	A	531	LEU
1	A	552	LEU
1	A	554	LEU
1	A	567	THR
1	A	574	THR
1	A	589	SER
1	A	598	VAL
1	A	607	LEU
1	A	613	SER
1	A	616	LEU
1	A	617	LEU
1	A	635	SER
1	A	639	GLU
1	A	648	LEU
1	A	659	SER
1	A	660	LEU
1	A	685	LEU
1	A	709	LYS
1	A	713	GLN
1	A	732	LEU
1	A	733	LEU
1	B	32	GLU
1	B	37	ARG
1	B	56	LYS
1	B	73	LYS
1	B	87	ARG
1	B	126	ILE
1	B	127	VAL
1	B	146	ASP
1	B	159	ILE
1	B	165	ARG
1	B	183	ARG
1	B	185	PHE

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Mol	Chain	Res	Type
1	B	191	THR
1	B	205	ILE
1	B	208	ILE
1	B	221	VAL
1	B	227	TRP
1	B	230	PRO
1	B	237	ASP
1	B	252	ASN
1	B	259	ASP
1	B	260	ARG
1	B	268	THR
1	B	285	LYS
1	B	302	LEU
1	B	313	ARG
1	B	321	GLU
1	B	340	LEU
1	B	348	LYS
1	B	368	GLN
1	B	375	LEU
1	B	377	ARG
1	B	386	ASN
1	B	408	LEU
1	B	412	LEU
1	B	415	TYR
1	B	419	GLN
1	B	459	ASN
1	B	471	ARG
1	B	478	LYS
1	B	506	SER
1	B	509	ARG
1	B	531	LEU
1	B	552	LEU
1	B	554	LEU
1	B	567	THR
1	B	574	THR
1	B	589	SER
1	B	598	VAL
1	B	607	LEU
1	B	613	SER
1	B	616	LEU
1	B	617	LEU
1	B	635	SER

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Mol	Chain	Res	Type
1	B	639	GLU
1	B	648	LEU
1	B	659	SER
1	B	660	LEU
1	B	685	LEU
1	B	709	LYS
1	B	713	GLN
1	B	732	LEU
1	B	733	LEU
1	C	32	GLU
1	C	37	ARG
1	C	56	LYS
1	C	73	LYS
1	C	87	ARG
1	C	126	ILE
1	C	127	VAL
1	C	146	ASP
1	C	159	ILE
1	C	165	ARG
1	C	183	ARG
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	208	ILE
1	C	221	VAL
1	C	227	TRP
1	C	230	PRO
1	C	237	ASP
1	C	252	ASN
1	C	259	ASP
1	C	260	ARG
1	C	268	THR
1	C	285	LYS
1	C	302	LEU
1	C	313	ARG
1	C	321	GLU
1	C	340	LEU
1	C	348	LYS
1	C	368	GLN
1	C	375	LEU
1	C	377	ARG
1	C	386	ASN

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Mol	Chain	Res	Type
1	C	408	LEU
1	C	412	LEU
1	C	415	TYR
1	C	419	GLN
1	C	459	ASN
1	C	471	ARG
1	C	478	LYS
1	C	506	SER
1	C	509	ARG
1	C	531	LEU
1	C	552	LEU
1	C	554	LEU
1	C	567	THR
1	C	574	THR
1	C	589	SER
1	C	598	VAL
1	C	607	LEU
1	C	613	SER
1	C	616	LEU
1	C	617	LEU
1	C	635	SER
1	C	639	GLU
1	C	648	LEU
1	C	659	SER
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	713	GLN
1	C	732	LEU
1	C	733	LEU
1	D	32	GLU
1	D	37	ARG
1	D	56	LYS
1	D	73	LYS
1	D	87	ARG
1	D	126	ILE
1	D	127	VAL
1	D	146	ASP
1	D	159	ILE
1	D	165	ARG
1	D	183	ARG
1	D	185	PHE

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Mol	Chain	Res	Type
1	D	191	THR
1	D	205	ILE
1	D	208	ILE
1	D	221	VAL
1	D	227	TRP
1	D	230	PRO
1	D	237	ASP
1	D	252	ASN
1	D	259	ASP
1	D	260	ARG
1	D	268	THR
1	D	285	LYS
1	D	302	LEU
1	D	313	ARG
1	D	321	GLU
1	D	340	LEU
1	D	348	LYS
1	D	368	GLN
1	D	375	LEU
1	D	377	ARG
1	D	386	ASN
1	D	408	LEU
1	D	412	LEU
1	D	415	TYR
1	D	419	GLN
1	D	459	ASN
1	D	471	ARG
1	D	478	LYS
1	D	506	SER
1	D	509	ARG
1	D	531	LEU
1	D	552	LEU
1	D	554	LEU
1	D	567	THR
1	D	574	THR
1	D	589	SER
1	D	598	VAL
1	D	607	LEU
1	D	613	SER
1	D	616	LEU
1	D	617	LEU
1	D	635	SER

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Mol	Chain	Res	Type
1	D	639	GLU
1	D	648	LEU
1	D	659	SER
1	D	660	LEU
1	D	685	LEU
1	D	709	LYS
1	D	713	GLN
1	D	732	LEU
1	D	733	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	386	ASN
1	A	392	HIS
1	A	429	HIS
1	A	449	HIS
1	A	459	ASN
1	B	368	GLN
1	B	386	ASN
1	B	392	HIS
1	B	429	HIS
1	B	449	HIS
1	B	459	ASN
1	C	368	GLN
1	C	386	ASN
1	C	392	HIS
1	C	429	HIS
1	C	449	HIS
1	C	459	ASN
1	D	368	GLN
1	D	386	ASN
1	D	392	HIS
1	D	429	HIS
1	D	449	HIS
1	D	459	ASN

5.3.3 RNA

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 monosaccharides 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	A	754	1	41,50,50	1.56	11 (26%)	45,82,82	1.67	6 (13%)
2	HEM	D	754	1	41,50,50	1.57	11 (26%)	45,82,82	1.66	5 (11%)
2	HEM	B	754	1	41,50,50	1.55	11 (26%)	45,82,82	1.67	5 (11%)
2	HEM	C	754	1	41,50,50	1.56	11 (26%)	45,82,82	1.67	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	754	1	-	1/12/54/54	-
2	HEM	D	754	1	-	1/12/54/54	-
2	HEM	B	754	1	-	1/12/54/54	-
2	HEM	C	754	1	-	1/12/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	754	HEM	C3C-CAC	-3.75	1.40	1.47
2	B	754	HEM	C3C-CAC	-3.75	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	754	HEM	C3C-CAC	-3.73	1.40	1.47
2	C	754	HEM	C3C-CAC	-3.72	1.40	1.47
2	D	754	HEM	C1A-NA	3.15	1.42	1.36
2	A	754	HEM	C1A-NA	3.13	1.42	1.36
2	C	754	HEM	C1A-NA	3.13	1.42	1.36
2	B	754	HEM	C1A-NA	3.10	1.42	1.36
2	D	754	HEM	CBB-CAB	2.90	1.44	1.30
2	C	754	HEM	CBB-CAB	2.89	1.44	1.30
2	B	754	HEM	CBB-CAB	2.89	1.44	1.30
2	A	754	HEM	CBB-CAB	2.88	1.44	1.30
2	D	754	HEM	CAB-C3B	-2.82	1.39	1.47
2	C	754	HEM	CAB-C3B	-2.81	1.39	1.47
2	B	754	HEM	CAB-C3B	-2.79	1.39	1.47
2	A	754	HEM	CAB-C3B	-2.78	1.39	1.47
2	C	754	HEM	O2D-CGD	-2.67	1.21	1.30
2	A	754	HEM	O2D-CGD	-2.64	1.21	1.30
2	D	754	HEM	O2D-CGD	-2.63	1.21	1.30
2	B	754	HEM	O2D-CGD	-2.62	1.21	1.30
2	D	754	HEM	C3C-C2C	-2.39	1.37	1.40
2	B	754	HEM	C3C-C2C	-2.35	1.37	1.40
2	C	754	HEM	C3C-C2C	-2.33	1.37	1.40
2	A	754	HEM	C3C-C2C	-2.33	1.37	1.40
2	D	754	HEM	CHA-C4D	2.27	1.40	1.35
2	C	754	HEM	CHA-C4D	2.27	1.40	1.35
2	A	754	HEM	CBC-CAC	2.26	1.44	1.29
2	D	754	HEM	CBC-CAC	2.26	1.44	1.29
2	B	754	HEM	CBC-CAC	2.25	1.44	1.29
2	B	754	HEM	CHA-C4D	2.25	1.40	1.35
2	C	754	HEM	CBC-CAC	2.25	1.44	1.29
2	A	754	HEM	CHA-C4D	2.24	1.40	1.35
2	A	754	HEM	C2C-C1C	2.18	1.47	1.42
2	B	754	HEM	CHB-C1B	2.17	1.40	1.35
2	C	754	HEM	C2C-C1C	2.17	1.47	1.42
2	D	754	HEM	CHB-C1B	2.17	1.40	1.35
2	A	754	HEM	CHB-C1B	2.16	1.40	1.35
2	C	754	HEM	CHB-C1B	2.15	1.40	1.35
2	B	754	HEM	C2C-C1C	2.14	1.47	1.42
2	D	754	HEM	C2C-C1C	2.14	1.47	1.42
2	D	754	HEM	O2A-CGA	-2.09	1.23	1.30
2	A	754	HEM	O2A-CGA	-2.07	1.23	1.30
2	C	754	HEM	O2A-CGA	-2.06	1.23	1.30
2	B	754	HEM	O2A-CGA	-2.05	1.23	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	754	HEM	CBD-CAD-C3D	-7.17	92.71	112.63
2	B	754	HEM	CBD-CAD-C3D	-7.17	92.71	112.63
2	A	754	HEM	CBD-CAD-C3D	-7.16	92.73	112.63
2	C	754	HEM	CBD-CAD-C3D	-7.16	92.74	112.63
2	B	754	HEM	C4B-CHC-C1C	2.98	126.49	122.56
2	C	754	HEM	C4B-CHC-C1C	2.96	126.47	122.56
2	D	754	HEM	C4B-CHC-C1C	2.96	126.47	122.56
2	A	754	HEM	C4B-CHC-C1C	2.96	126.47	122.56
2	C	754	HEM	C3B-C2B-C1B	-2.82	104.39	106.49
2	B	754	HEM	C3B-C2B-C1B	-2.80	104.41	106.49
2	A	754	HEM	C3B-C2B-C1B	-2.78	104.42	106.49
2	D	754	HEM	C3B-C2B-C1B	-2.75	104.45	106.49
2	A	754	HEM	CBA-CAA-C2A	2.43	116.77	112.62
2	D	754	HEM	CBA-CAA-C2A	2.43	116.77	112.62
2	B	754	HEM	CBA-CAA-C2A	2.42	116.75	112.62
2	C	754	HEM	CBA-CAA-C2A	2.41	116.73	112.62
2	C	754	HEM	C4B-C3B-C2B	2.36	108.99	107.11
2	A	754	HEM	C4B-C3B-C2B	2.36	108.99	107.11
2	B	754	HEM	C4B-C3B-C2B	2.35	108.98	107.11
2	D	754	HEM	C4B-C3B-C2B	2.32	108.95	107.11
2	A	754	HEM	C4D-C3D-C2D	2.00	109.81	106.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	754	HEM	CAA-CBA-CGA-O1A
2	B	754	HEM	CAA-CBA-CGA-O1A
2	D	754	HEM	CAA-CBA-CGA-O1A
2	C	754	HEM	CAA-CBA-CGA-O1A

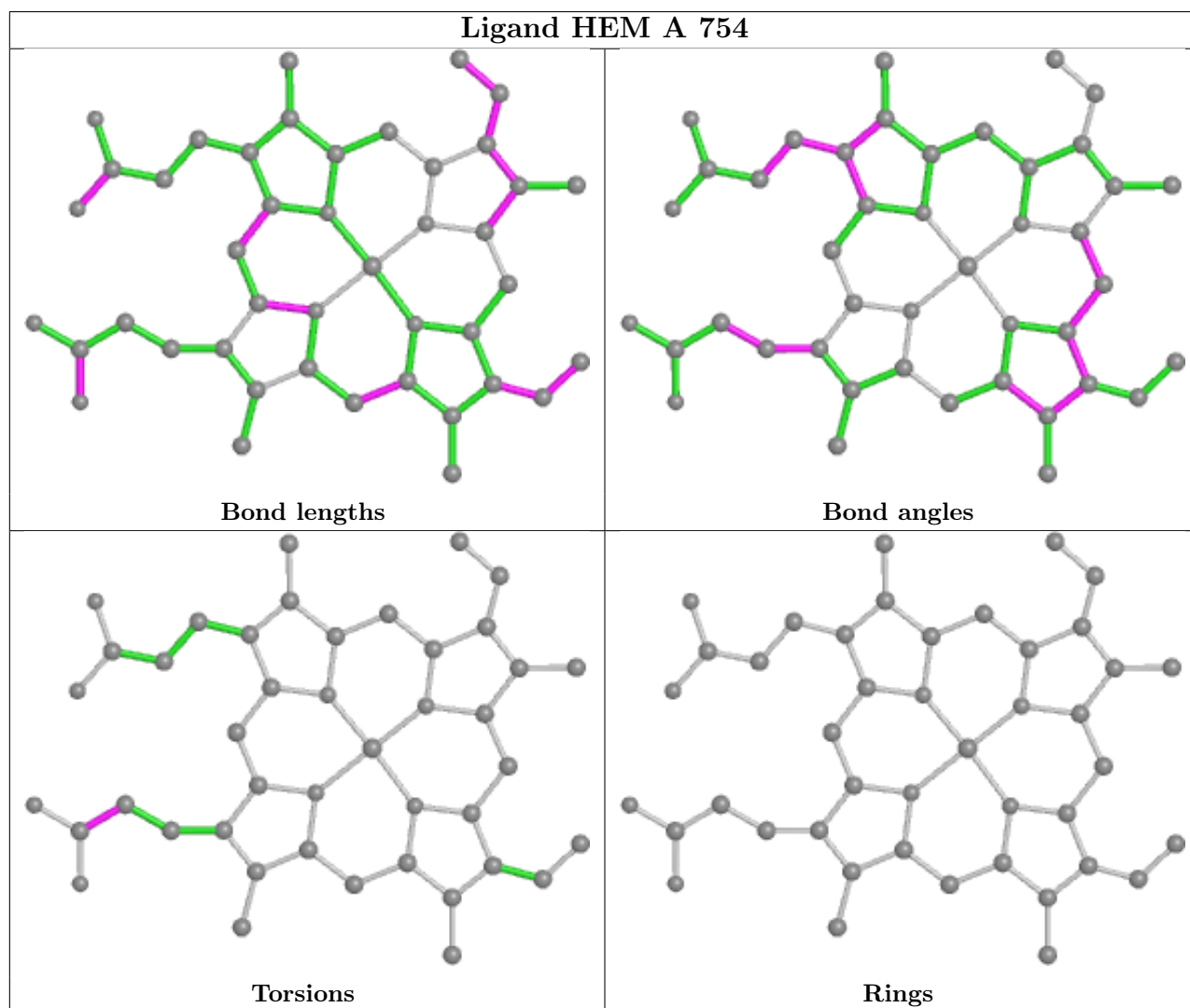
There are no ring outliers.

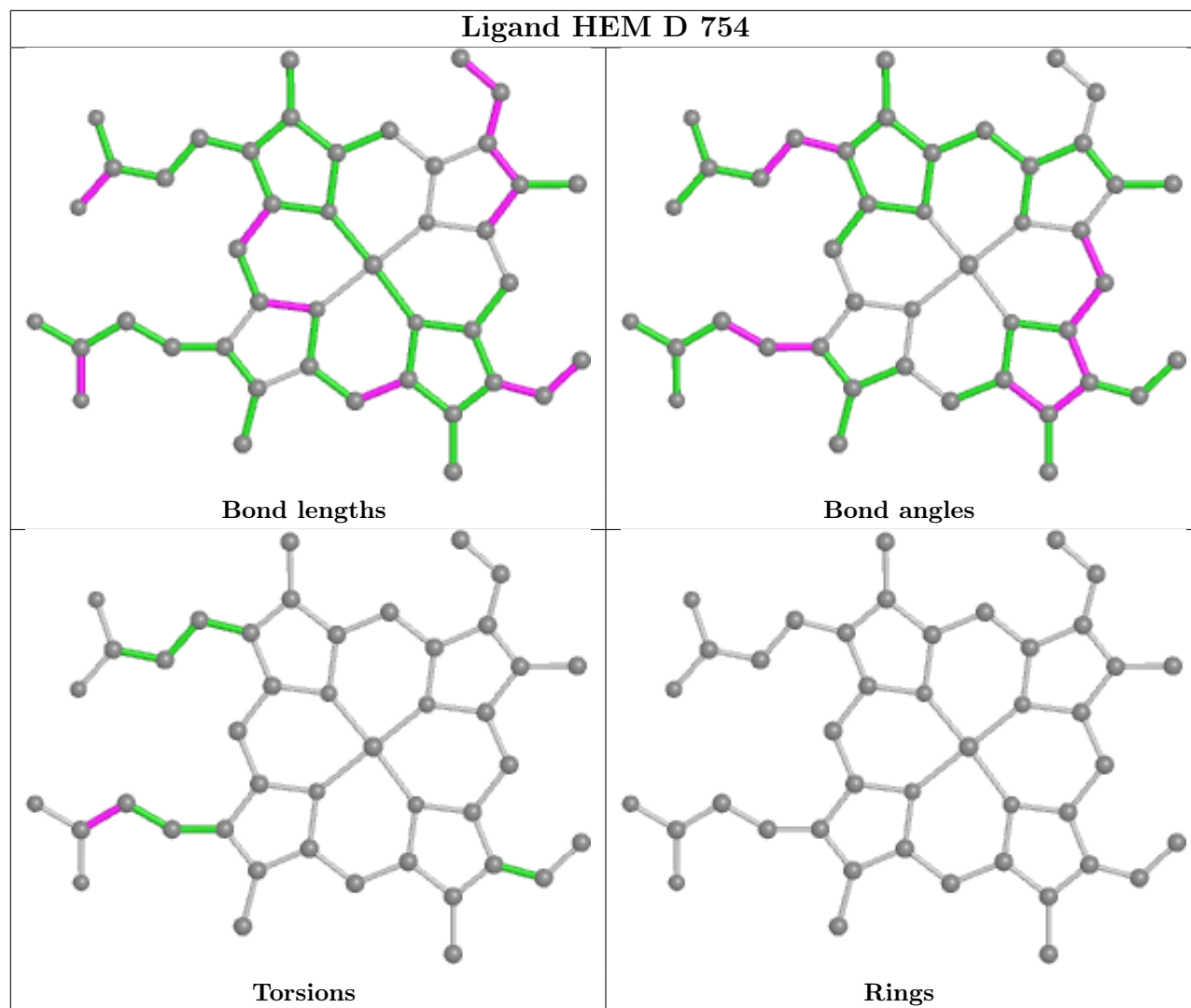
4 monomers are involved in 13 short contacts:

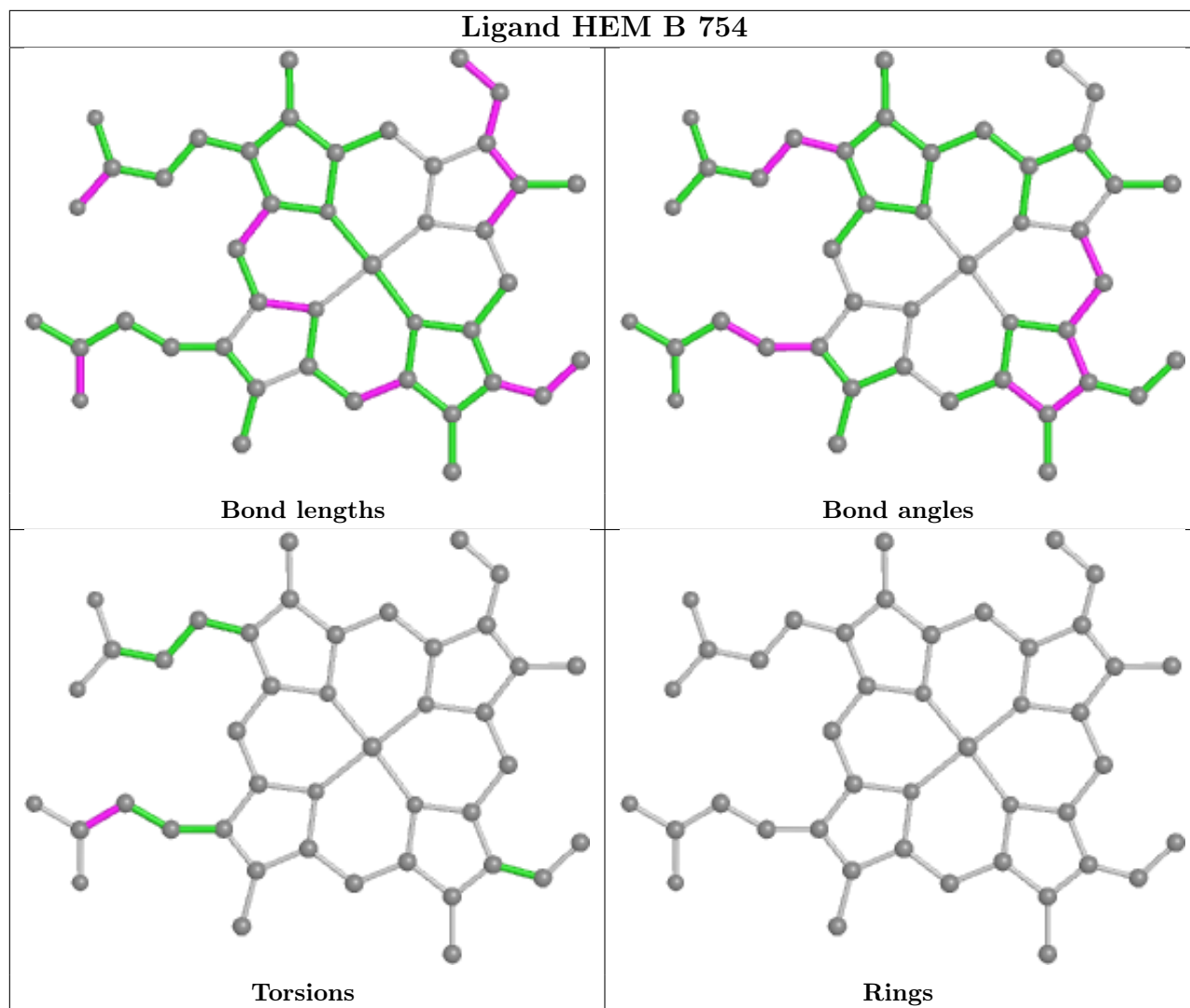
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	754	HEM	4	0
2	D	754	HEM	3	0
2	B	754	HEM	3	0
2	C	754	HEM	3	0

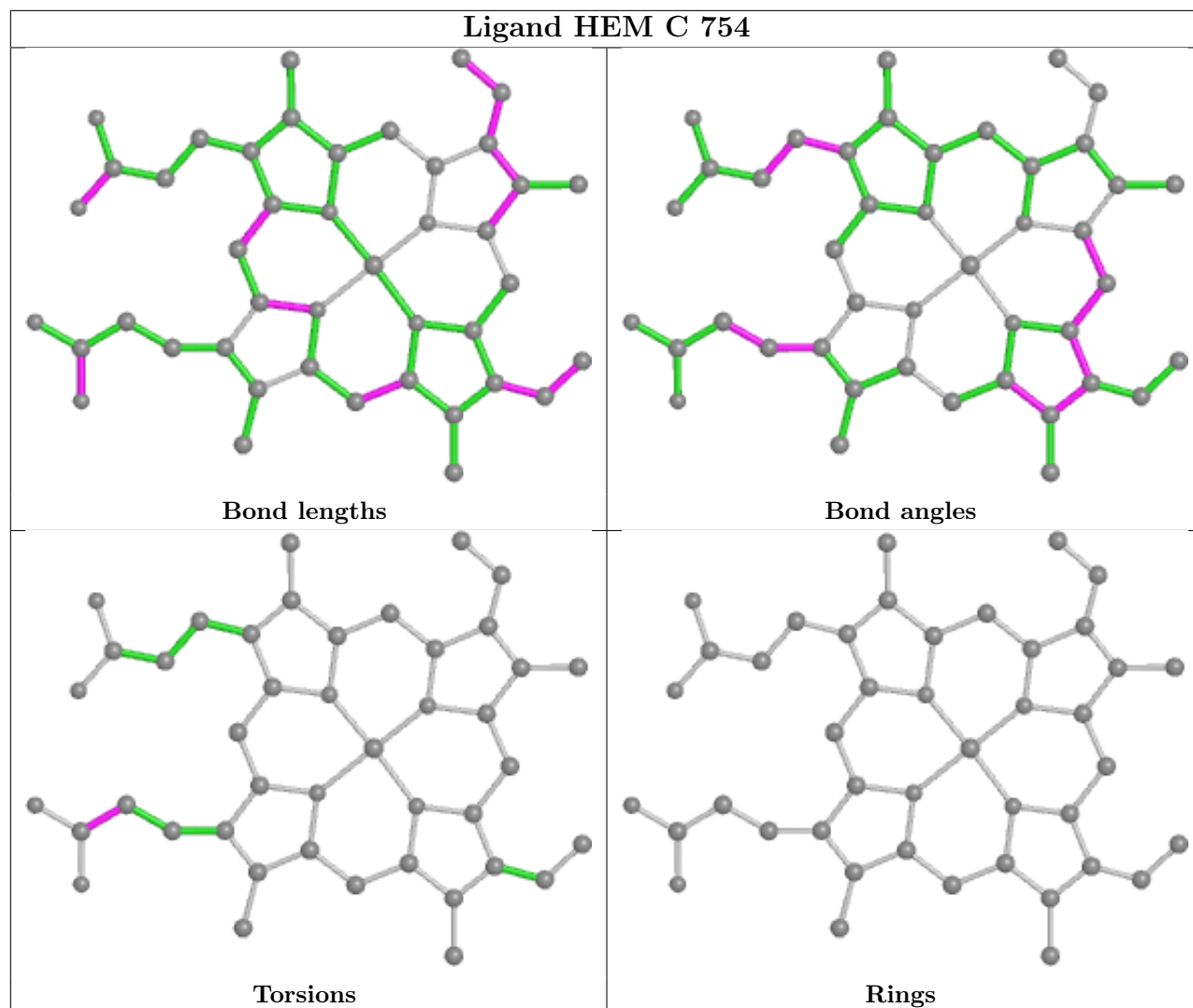
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.