



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:25 PM UTC

PDB ID : 1IPH / pdb_00001iph
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

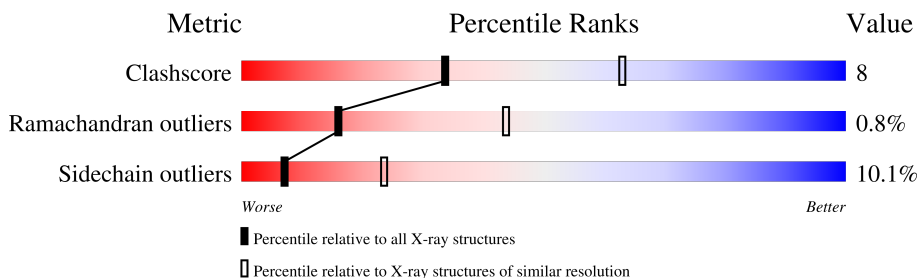
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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](#)

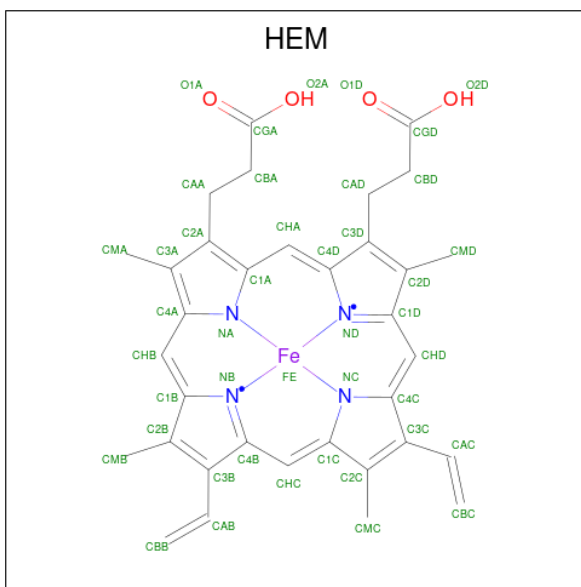
There are 2 unique types of molecules in this entry. The entry contains 23156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

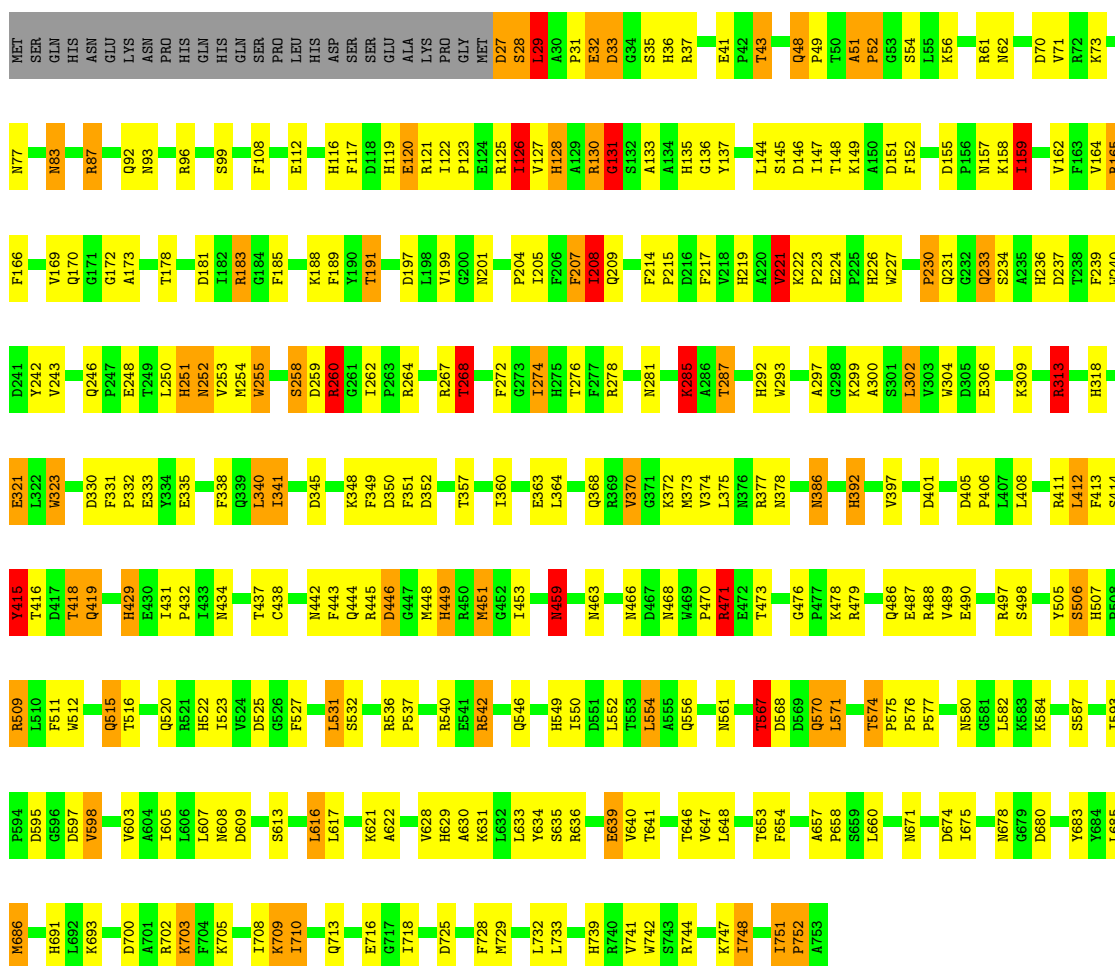
3 Residue-property plots

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.

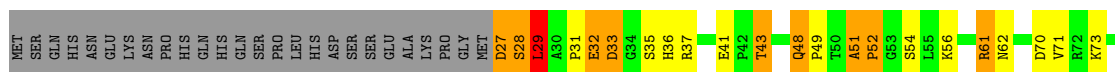
- Molecule 1: CATALASE HPII

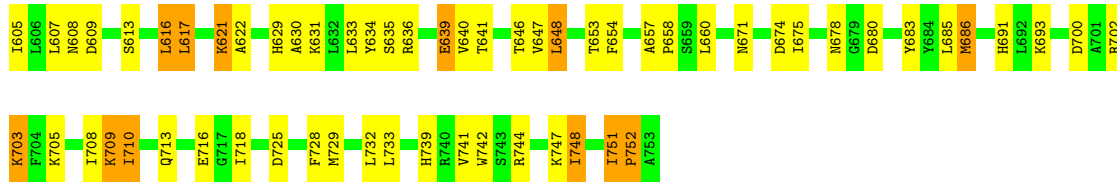
Chain A: 



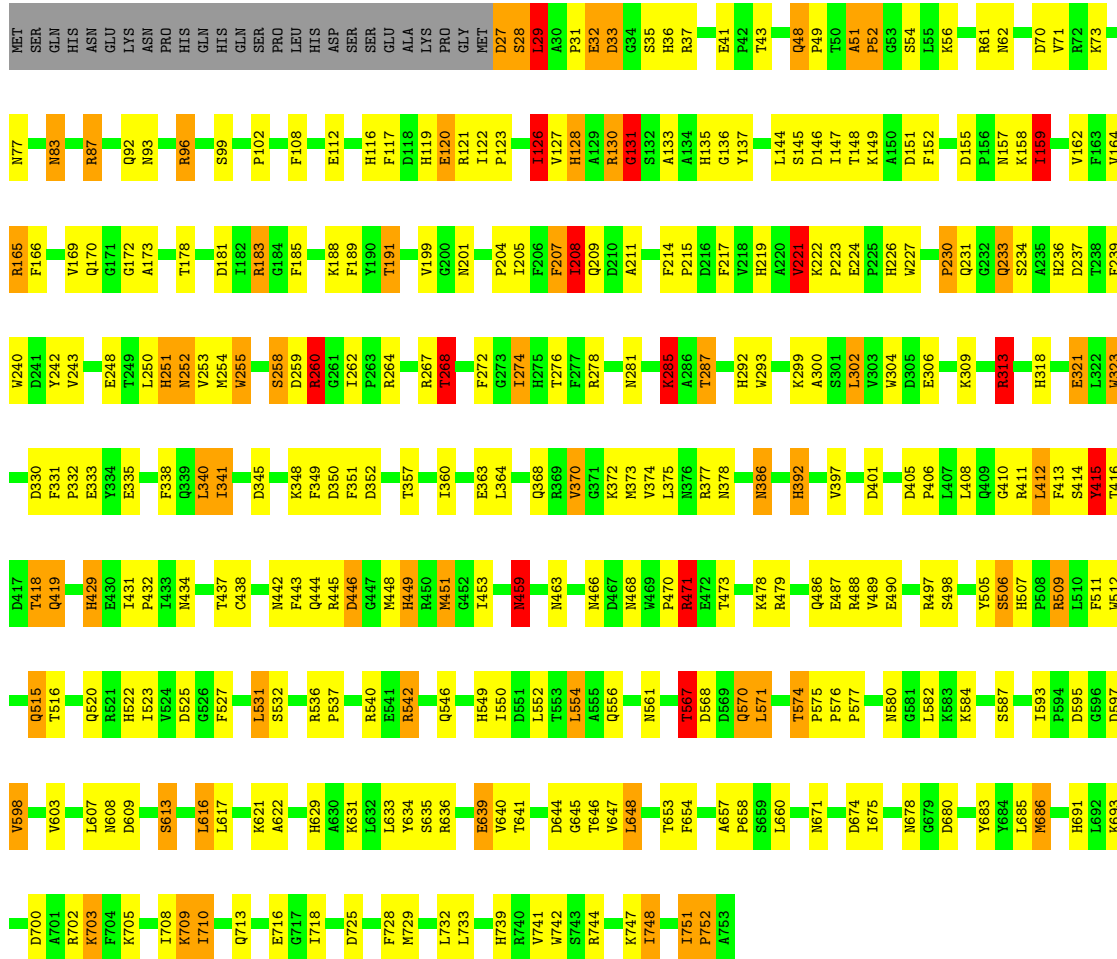
- Molecule 1: CATALASE HPII

Chain B: 





• 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	1.38	43/5902 (0.7%)	2.16	278/8024 (3.5%)
1	B	1.38	43/5902 (0.7%)	2.16	274/8024 (3.4%)
1	C	1.38	42/5902 (0.7%)	2.16	272/8024 (3.4%)
1	D	1.38	41/5902 (0.7%)	2.16	270/8024 (3.4%)
All	All	1.38	169/23608 (0.7%)	2.16	1094/32096 (3.4%)

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 (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	392	HIS	CD2-NE2	-10.11	1.26	1.37
1	B	392	HIS	CD2-NE2	-10.11	1.26	1.37
1	D	392	HIS	CD2-NE2	-10.11	1.26	1.37
1	C	392	HIS	CD2-NE2	-10.05	1.26	1.37
1	C	159	ILE	CA-CB	9.44	1.67	1.54
1	D	159	ILE	CA-CB	9.44	1.67	1.54
1	A	159	ILE	CA-CB	9.43	1.67	1.54
1	B	159	ILE	CA-CB	9.40	1.67	1.54
1	D	126	ILE	CA-CB	8.88	1.66	1.54
1	A	126	ILE	CA-CB	8.87	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	126	ILE	CA-CB	8.83	1.66	1.54
1	B	126	ILE	CA-CB	8.83	1.66	1.54
1	B	318	HIS	CD2-NE2	-8.35	1.28	1.37
1	D	318	HIS	CD2-NE2	-8.34	1.28	1.37
1	C	318	HIS	CD2-NE2	-8.33	1.28	1.37
1	A	318	HIS	CD2-NE2	-8.32	1.28	1.37
1	B	523	ILE	CA-CB	8.07	1.63	1.54
1	A	523	ILE	CA-CB	8.04	1.63	1.54
1	D	523	ILE	CA-CB	8.02	1.63	1.54
1	C	523	ILE	CA-CB	8.01	1.63	1.54
1	C	219	HIS	CD2-NE2	-7.91	1.29	1.37
1	B	219	HIS	CD2-NE2	-7.90	1.29	1.37
1	A	219	HIS	CD2-NE2	-7.86	1.29	1.37
1	A	208	ILE	CA-CB	7.84	1.68	1.55
1	B	208	ILE	CA-CB	7.83	1.68	1.55
1	C	208	ILE	CA-CB	7.83	1.68	1.55
1	D	219	HIS	CD2-NE2	-7.83	1.29	1.37
1	D	208	ILE	CA-CB	7.82	1.68	1.55
1	C	243	VAL	CA-CB	7.72	1.62	1.54
1	A	243	VAL	CA-CB	7.72	1.62	1.54
1	D	243	VAL	CA-CB	7.70	1.62	1.54
1	B	243	VAL	CA-CB	7.69	1.62	1.54
1	C	236	HIS	CD2-NE2	-7.57	1.29	1.37
1	D	191	THR	CA-CB	7.54	1.65	1.53
1	A	191	THR	CA-CB	7.53	1.65	1.53
1	B	191	THR	CA-CB	7.52	1.65	1.53
1	D	236	HIS	CD2-NE2	-7.51	1.29	1.37
1	A	236	HIS	CD2-NE2	-7.50	1.29	1.37
1	B	236	HIS	CD2-NE2	-7.50	1.29	1.37
1	D	199	VAL	CA-CB	7.48	1.62	1.53
1	C	191	THR	CA-CB	7.48	1.65	1.53
1	C	199	VAL	CA-CB	7.40	1.62	1.53
1	B	199	VAL	CA-CB	7.39	1.62	1.53
1	A	199	VAL	CA-CB	7.38	1.62	1.53
1	A	449	HIS	CB-CG	7.28	1.60	1.50
1	B	449	HIS	CB-CG	7.27	1.60	1.50
1	D	449	HIS	CB-CG	7.27	1.60	1.50
1	C	449	HIS	CB-CG	7.20	1.60	1.50
1	D	36	HIS	CD2-NE2	-7.18	1.29	1.37
1	C	36	HIS	CD2-NE2	-7.13	1.30	1.37
1	A	36	HIS	CD2-NE2	-7.09	1.30	1.37
1	B	292	HIS	CD2-NE2	-7.06	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	HIS	CD2-NE2	-7.05	1.30	1.37
1	B	36	HIS	CD2-NE2	-7.04	1.30	1.37
1	D	292	HIS	CD2-NE2	-6.99	1.30	1.37
1	C	292	HIS	CD2-NE2	-6.97	1.30	1.37
1	B	691	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	691	HIS	CD2-NE2	-6.81	1.30	1.37
1	C	550	ILE	CA-CB	6.77	1.62	1.55
1	B	550	ILE	CA-CB	6.76	1.62	1.55
1	C	691	HIS	CD2-NE2	-6.75	1.30	1.37
1	D	550	ILE	CA-CB	6.75	1.62	1.55
1	A	276	THR	CA-CB	6.74	1.63	1.53
1	A	550	ILE	CA-CB	6.74	1.62	1.55
1	D	691	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	276	THR	CA-CB	6.71	1.63	1.53
1	D	276	THR	CA-CB	6.67	1.63	1.53
1	A	429	HIS	CD2-NE2	-6.65	1.30	1.37
1	C	276	THR	CA-CB	6.65	1.63	1.53
1	C	429	HIS	CD2-NE2	-6.63	1.30	1.37
1	B	429	HIS	CD2-NE2	-6.57	1.30	1.37
1	D	429	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	135	HIS	CD2-NE2	-6.54	1.30	1.37
1	C	135	HIS	CD2-NE2	-6.49	1.30	1.37
1	D	135	HIS	CD2-NE2	-6.48	1.30	1.37
1	A	135	HIS	CD2-NE2	-6.45	1.30	1.37
1	D	507	HIS	CD2-NE2	-6.45	1.30	1.37
1	D	116	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	507	HIS	CD2-NE2	-6.44	1.30	1.37
1	B	507	HIS	CD2-NE2	-6.43	1.30	1.37
1	C	116	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	116	HIS	CD2-NE2	-6.39	1.30	1.37
1	C	507	HIS	CD2-NE2	-6.38	1.30	1.37
1	B	116	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	251	HIS	CD2-NE2	-6.22	1.31	1.37
1	C	251	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	251	HIS	CD2-NE2	-6.20	1.31	1.37
1	D	251	HIS	CD2-NE2	-6.16	1.31	1.37
1	D	549	HIS	CD2-NE2	-6.15	1.31	1.37
1	B	549	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	549	HIS	CD2-NE2	-6.09	1.31	1.37
1	C	549	HIS	CD2-NE2	-6.09	1.31	1.37
1	D	164	VAL	CA-CB	6.02	1.63	1.54
1	B	226	HIS	CD2-NE2	-5.97	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	VAL	CA-CB	5.97	1.63	1.54
1	B	164	VAL	CA-CB	5.97	1.63	1.54
1	C	164	VAL	CA-CB	5.97	1.63	1.54
1	C	226	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	226	HIS	CD2-NE2	-5.92	1.31	1.37
1	D	226	HIS	CD2-NE2	-5.89	1.31	1.37
1	B	522	HIS	CD2-NE2	-5.89	1.31	1.37
1	D	522	HIS	CD2-NE2	-5.80	1.31	1.37
1	C	522	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	522	HIS	CD2-NE2	-5.73	1.31	1.37
1	A	292	HIS	CG-ND1	-5.68	1.31	1.38
1	A	675	ILE	CA-CB	5.67	1.62	1.54
1	B	675	ILE	CA-CB	5.66	1.61	1.54
1	C	675	ILE	CA-CB	5.65	1.61	1.54
1	C	292	HIS	CG-ND1	-5.63	1.32	1.38
1	D	675	ILE	CA-CB	5.60	1.61	1.54
1	D	292	HIS	CG-ND1	-5.60	1.32	1.38
1	B	119	HIS	CD2-NE2	-5.60	1.31	1.37
1	B	292	HIS	CG-ND1	-5.59	1.32	1.38
1	D	119	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	119	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	119	HIS	CD2-NE2	-5.54	1.31	1.37
1	A	112	GLU	CA-CB	-5.53	1.44	1.53
1	B	112	GLU	CA-CB	-5.52	1.44	1.53
1	D	112	GLU	CA-CB	-5.49	1.44	1.53
1	C	112	GLU	CA-CB	-5.48	1.44	1.53
1	B	507	HIS	CG-ND1	-5.42	1.32	1.38
1	C	507	HIS	CG-ND1	-5.40	1.32	1.38
1	D	507	HIS	CG-ND1	-5.39	1.32	1.38
1	A	507	HIS	CG-ND1	-5.39	1.32	1.38
1	B	629	HIS	CD2-NE2	-5.37	1.31	1.37
1	C	449	HIS	CG-CD2	5.35	1.41	1.35
1	D	629	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	449	HIS	CG-CD2	5.35	1.41	1.35
1	A	178	THR	CA-CB	5.34	1.59	1.52
1	D	178	THR	CA-CB	5.34	1.59	1.52
1	C	178	THR	CA-CB	5.33	1.59	1.52
1	A	629	HIS	CD2-NE2	-5.33	1.31	1.37
1	C	629	HIS	CD2-NE2	-5.33	1.31	1.37
1	D	449	HIS	CG-CD2	5.31	1.41	1.35
1	B	449	HIS	CG-CD2	5.31	1.41	1.35
1	B	178	THR	CA-CB	5.29	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	128	HIS	CD2-NE2	-5.26	1.32	1.37
1	B	128	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	397	VAL	CA-CB	5.22	1.59	1.55
1	A	640	VAL	CA-CB	5.21	1.61	1.54
1	A	128	HIS	CD2-NE2	-5.21	1.32	1.37
1	C	640	VAL	CA-CB	5.20	1.61	1.54
1	C	148	THR	CA-CB	5.20	1.62	1.53
1	D	640	VAL	CA-CB	5.19	1.61	1.54
1	C	397	VAL	CA-CB	5.17	1.59	1.55
1	D	397	VAL	CA-CB	5.17	1.59	1.55
1	A	148	THR	CA-CB	5.16	1.62	1.53
1	B	640	VAL	CA-CB	5.16	1.61	1.54
1	D	148	THR	CA-CB	5.15	1.62	1.53
1	B	148	THR	CA-CB	5.15	1.62	1.53
1	C	128	HIS	CD2-NE2	-5.15	1.32	1.37
1	B	397	VAL	CA-CB	5.12	1.59	1.55
1	D	377	ARG	CZ-NH1	5.11	1.40	1.32
1	A	119	HIS	CG-ND1	-5.09	1.32	1.38
1	D	511	PHE	CA-CB	5.08	1.61	1.53
1	A	511	PHE	CA-CB	5.08	1.61	1.53
1	C	449	HIS	CD2-NE2	-5.07	1.32	1.37
1	D	449	HIS	CD2-NE2	-5.07	1.32	1.37
1	B	377	ARG	CZ-NH1	5.06	1.39	1.32
1	B	449	HIS	CD2-NE2	-5.06	1.32	1.37
1	C	511	PHE	CA-CB	5.06	1.61	1.53
1	B	511	PHE	CA-CB	5.05	1.61	1.53
1	A	125	ARG	NE-CZ	5.04	1.38	1.33
1	B	125	ARG	NE-CZ	5.04	1.38	1.33
1	A	201	ASN	CA-CB	-5.04	1.46	1.53
1	A	377	ARG	CZ-NH1	5.03	1.39	1.32
1	C	377	ARG	CZ-NH1	5.01	1.39	1.32
1	C	125	ARG	NE-CZ	5.01	1.38	1.33
1	B	119	HIS	CG-ND1	-5.00	1.32	1.38

All (1094) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ASN	CA-CB-CG	12.68	125.28	112.60
1	C	201	ASN	CA-CB-CG	12.65	125.25	112.60
1	D	466	ASN	OD1-CG-ND2	-12.65	109.95	122.60
1	D	201	ASN	CA-CB-CG	12.65	125.25	112.60
1	B	201	ASN	CA-CB-CG	12.63	125.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	ASN	OD1-CG-ND2	-12.62	109.98	122.60
1	A	466	ASN	OD1-CG-ND2	-12.61	109.99	122.60
1	C	466	ASN	OD1-CG-ND2	-12.61	109.99	122.60
1	D	414	SER	N-CA-C	11.91	125.40	111.11
1	A	414	SER	N-CA-C	11.88	125.37	111.11
1	B	414	SER	N-CA-C	11.86	125.34	111.11
1	C	414	SER	N-CA-C	11.85	125.33	111.11
1	C	208	ILE	CA-CB-CG2	11.27	129.66	110.50
1	B	208	ILE	CA-CB-CG2	11.26	129.64	110.50
1	D	208	ILE	CA-CB-CG2	11.26	129.64	110.50
1	A	208	ILE	CA-CB-CG2	11.24	129.60	110.50
1	A	419	GLN	CA-CB-CG	-11.15	91.80	114.10
1	D	181	ASP	CA-CB-CG	11.14	123.74	112.60
1	D	419	GLN	CA-CB-CG	-11.14	91.83	114.10
1	B	419	GLN	CA-CB-CG	-11.12	91.85	114.10
1	C	419	GLN	CA-CB-CG	-11.12	91.86	114.10
1	B	181	ASP	CA-CB-CG	11.09	123.69	112.60
1	C	181	ASP	CA-CB-CG	11.09	123.69	112.60
1	A	181	ASP	CA-CB-CG	11.08	123.68	112.60
1	B	268	THR	N-CA-CB	-10.88	95.76	111.54
1	C	268	THR	N-CA-CB	-10.87	95.78	111.54
1	A	268	THR	N-CA-CB	-10.86	95.80	111.54
1	D	268	THR	N-CA-CB	-10.84	95.82	111.54
1	A	595	ASP	CA-CB-CG	10.81	123.41	112.60
1	B	350	ASP	CA-CB-CG	10.81	123.41	112.60
1	D	350	ASP	CA-CB-CG	10.78	123.38	112.60
1	C	595	ASP	CA-CB-CG	10.76	123.36	112.60
1	C	350	ASP	CA-CB-CG	10.76	123.36	112.60
1	B	595	ASP	CA-CB-CG	10.76	123.36	112.60
1	A	350	ASP	CA-CB-CG	10.75	123.35	112.60
1	D	595	ASP	CA-CB-CG	10.73	123.33	112.60
1	D	83	ASN	OD1-CG-ND2	-10.12	112.48	122.60
1	B	83	ASN	OD1-CG-ND2	-10.11	112.49	122.60
1	A	221	VAL	CB-CA-C	-10.11	98.27	112.22
1	C	83	ASN	OD1-CG-ND2	-10.11	112.49	122.60
1	A	83	ASN	OD1-CG-ND2	-10.09	112.51	122.60
1	C	221	VAL	CB-CA-C	-10.06	98.33	112.22
1	B	221	VAL	CB-CA-C	-10.06	98.33	112.22
1	D	221	VAL	CB-CA-C	-10.04	98.37	112.22
1	A	29	LEU	N-CA-C	-9.95	89.61	110.80
1	C	29	LEU	N-CA-C	-9.94	89.62	110.80
1	D	29	LEU	N-CA-C	-9.94	89.63	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	LEU	N-CA-C	-9.92	89.67	110.80
1	B	370	VAL	N-CA-CB	-9.86	98.75	112.35
1	C	370	VAL	N-CA-CB	-9.86	98.75	112.35
1	A	370	VAL	N-CA-CB	-9.84	98.77	112.35
1	D	370	VAL	N-CA-CB	-9.84	98.77	112.35
1	B	468	ASN	N-CA-C	9.75	124.56	112.47
1	D	201	ASN	CB-CG-ND2	-9.73	101.81	116.40
1	C	201	ASN	CB-CG-ND2	-9.71	101.83	116.40
1	B	201	ASN	CB-CG-ND2	-9.71	101.84	116.40
1	C	468	ASN	N-CA-C	9.70	124.50	112.47
1	A	201	ASN	CB-CG-ND2	-9.70	101.85	116.40
1	A	468	ASN	N-CA-C	9.67	124.47	112.47
1	D	468	ASN	N-CA-C	9.67	124.46	112.47
1	A	598	VAL	N-CA-C	-9.53	101.50	113.22
1	C	208	ILE	CA-CB-CG1	-9.52	94.22	110.40
1	D	598	VAL	N-CA-C	-9.51	101.52	113.22
1	A	208	ILE	CA-CB-CG1	-9.51	94.24	110.40
1	D	208	ILE	CA-CB-CG1	-9.50	94.24	110.40
1	B	208	ILE	CA-CB-CG1	-9.50	94.25	110.40
1	B	598	VAL	N-CA-C	-9.50	101.54	113.22
1	C	598	VAL	N-CA-C	-9.48	101.56	113.22
1	C	236	HIS	CA-CB-CG	9.45	123.25	113.80
1	A	236	HIS	CA-CB-CG	9.44	123.24	113.80
1	B	236	HIS	CA-CB-CG	9.40	123.20	113.80
1	D	236	HIS	CA-CB-CG	9.39	123.19	113.80
1	B	593	ILE	N-CA-C	-9.37	98.28	107.55
1	A	593	ILE	N-CA-C	-9.36	98.29	107.55
1	C	593	ILE	N-CA-C	-9.35	98.29	107.55
1	D	593	ILE	N-CA-C	-9.35	98.30	107.55
1	B	386	ASN	OD1-CG-ND2	-9.34	113.27	122.60
1	A	152	PHE	CA-CB-CG	9.33	123.13	113.80
1	C	152	PHE	CA-CB-CG	9.33	123.13	113.80
1	D	386	ASN	OD1-CG-ND2	-9.32	113.28	122.60
1	D	152	PHE	CA-CB-CG	9.32	123.12	113.80
1	B	152	PHE	CA-CB-CG	9.31	123.11	113.80
1	C	386	ASN	OD1-CG-ND2	-9.29	113.31	122.60
1	A	386	ASN	OD1-CG-ND2	-9.28	113.33	122.60
1	B	169	VAL	CA-C-O	-9.13	112.68	120.80
1	A	169	VAL	CA-C-O	-9.11	112.69	120.80
1	C	169	VAL	CA-C-O	-9.11	112.69	120.80
1	D	169	VAL	CA-C-O	-9.08	112.72	120.80
1	A	83	ASN	CB-CG-ND2	8.93	129.80	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASN	CB-CG-ND2	8.91	129.76	116.40
1	C	83	ASN	CB-CG-ND2	8.90	129.75	116.40
1	D	83	ASN	CB-CG-ND2	8.88	129.72	116.40
1	D	597	ASP	CA-CB-CG	8.75	121.35	112.60
1	A	597	ASP	CA-CB-CG	8.74	121.34	112.60
1	C	597	ASP	CA-CB-CG	8.69	121.29	112.60
1	B	597	ASP	CA-CB-CG	8.68	121.28	112.60
1	C	285	LYS	CG-CD-CE	8.64	131.17	111.30
1	B	285	LYS	CG-CD-CE	8.63	131.15	111.30
1	D	285	LYS	CG-CD-CE	8.63	131.14	111.30
1	A	285	LYS	CG-CD-CE	8.62	131.14	111.30
1	B	321	GLU	CA-CB-CG	8.57	131.24	114.10
1	A	321	GLU	CA-CB-CG	8.56	131.22	114.10
1	D	321	GLU	CA-CB-CG	8.56	131.22	114.10
1	C	321	GLU	CA-CB-CG	8.55	131.20	114.10
1	D	466	ASN	CB-CG-ND2	8.55	129.22	116.40
1	A	466	ASN	CB-CG-ND2	8.54	129.21	116.40
1	C	466	ASN	CB-CG-ND2	8.51	129.16	116.40
1	B	32	GLU	O-C-N	8.50	132.90	123.13
1	B	466	ASN	CB-CG-ND2	8.49	129.14	116.40
1	A	131	GLY	N-CA-C	8.48	133.28	113.18
1	C	131	GLY	N-CA-C	8.48	133.27	113.18
1	C	32	GLU	O-C-N	8.47	132.87	123.13
1	B	131	GLY	N-CA-C	8.47	133.25	113.18
1	D	131	GLY	N-CA-C	8.46	133.22	113.18
1	D	33	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	32	GLU	O-C-N	8.43	132.83	123.13
1	A	33	ASP	CA-CB-CG	8.42	121.02	112.60
1	D	32	GLU	O-C-N	8.41	132.80	123.13
1	B	33	ASP	CA-CB-CG	8.40	121.00	112.60
1	C	33	ASP	CA-CB-CG	8.38	120.98	112.60
1	C	27	ASP	CA-CB-CG	8.30	120.90	112.60
1	D	27	ASP	CA-CB-CG	8.28	120.88	112.60
1	A	27	ASP	CA-CB-CG	8.28	120.88	112.60
1	B	27	ASP	CA-CB-CG	8.25	120.85	112.60
1	D	183	ARG	NE-CZ-NH2	-8.19	111.83	119.20
1	A	126	ILE	CB-CG1-CD1	-8.18	96.62	113.80
1	C	183	ARG	NE-CZ-NH2	-8.18	111.84	119.20
1	C	126	ILE	CB-CG1-CD1	-8.17	96.64	113.80
1	D	126	ILE	CB-CG1-CD1	-8.17	96.64	113.80
1	B	126	ILE	CB-CG1-CD1	-8.17	96.65	113.80
1	A	183	ARG	NE-CZ-NH2	-8.11	111.90	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ARG	NE-CZ-NH2	-8.11	111.90	119.20
1	B	442	ASN	CA-C-O	-8.11	112.70	120.56
1	D	208	ILE	CB-CA-C	8.10	123.65	110.69
1	A	208	ILE	CB-CA-C	8.08	123.62	110.69
1	A	678	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	B	208	ILE	CB-CA-C	8.07	123.61	110.69
1	C	678	ASN	OD1-CG-ND2	-8.06	114.54	122.60
1	C	208	ILE	CB-CA-C	8.06	123.58	110.69
1	B	678	ASN	OD1-CG-ND2	-8.06	114.54	122.60
1	D	678	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	A	442	ASN	CA-C-O	-8.04	112.76	120.56
1	D	442	ASN	CA-C-O	-8.03	112.77	120.56
1	C	442	ASN	CA-C-O	-8.02	112.78	120.56
1	D	459	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	B	459	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	D	236	HIS	CB-CG-CD2	-8.00	120.81	131.20
1	B	236	HIS	CB-CG-CD2	-7.99	120.81	131.20
1	C	459	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	A	236	HIS	CB-CG-CD2	-7.96	120.86	131.20
1	C	236	HIS	CB-CG-CD2	-7.95	120.86	131.20
1	A	459	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	A	274	ILE	O-C-N	-7.93	112.66	122.57
1	B	570	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	D	570	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	C	570	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	C	274	ILE	O-C-N	-7.90	112.70	122.57
1	A	570	GLN	OE1-CD-NE2	-7.89	114.71	122.60
1	B	429	HIS	CB-CG-CD2	-7.88	120.96	131.20
1	D	274	ILE	O-C-N	-7.88	112.72	122.57
1	B	274	ILE	O-C-N	-7.87	112.73	122.57
1	A	429	HIS	CB-CG-CD2	-7.87	120.97	131.20
1	D	429	HIS	CB-CG-CD2	-7.86	120.99	131.20
1	A	331	PHE	CA-C-O	-7.85	112.40	120.02
1	D	145	SER	N-CA-C	7.85	121.95	112.38
1	C	429	HIS	CB-CG-CD2	-7.83	121.01	131.20
1	B	92	GLN	OE1-CD-NE2	-7.83	114.77	122.60
1	B	145	SER	N-CA-C	7.82	121.92	112.38
1	D	92	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	A	574	THR	CA-C-N	7.82	125.37	119.66
1	A	574	THR	C-N-CA	7.82	125.37	119.66
1	B	331	PHE	CA-C-O	-7.82	112.44	120.02
1	A	92	GLN	OE1-CD-NE2	-7.82	114.78	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	GLN	N-CA-C	7.81	120.92	111.40
1	A	145	SER	N-CA-C	7.80	121.90	112.38
1	C	92	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	D	170	GLN	N-CA-C	7.80	120.92	111.40
1	C	170	GLN	N-CA-C	7.80	120.91	111.40
1	C	331	PHE	CA-C-O	-7.79	112.46	120.02
1	D	331	PHE	CA-C-O	-7.79	112.46	120.02
1	C	145	SER	N-CA-C	7.78	121.88	112.38
1	B	386	ASN	CB-CG-ND2	7.78	128.07	116.40
1	A	170	GLN	N-CA-C	7.77	120.88	111.40
1	C	386	ASN	CB-CG-ND2	7.76	128.04	116.40
1	A	386	ASN	CB-CG-ND2	7.75	128.03	116.40
1	D	386	ASN	CB-CG-ND2	7.75	128.03	116.40
1	D	304	TRP	N-CA-C	7.73	120.38	111.11
1	B	574	THR	CA-C-N	7.72	125.30	119.66
1	B	574	THR	C-N-CA	7.72	125.30	119.66
1	D	70	ASP	CA-CB-CG	7.72	120.32	112.60
1	C	304	TRP	N-CA-C	7.72	120.37	111.11
1	B	70	ASP	CA-CB-CG	7.71	120.31	112.60
1	C	574	THR	CA-C-N	7.71	125.29	119.66
1	C	574	THR	C-N-CA	7.71	125.29	119.66
1	A	70	ASP	CA-CB-CG	7.71	120.31	112.60
1	D	574	THR	CA-C-N	7.71	125.29	119.66
1	D	574	THR	C-N-CA	7.71	125.29	119.66
1	B	546	GLN	OE1-CD-NE2	-7.70	114.91	122.60
1	A	304	TRP	N-CA-C	7.68	120.33	111.11
1	B	304	TRP	N-CA-C	7.68	120.33	111.11
1	C	70	ASP	CA-CB-CG	7.67	120.27	112.60
1	C	207	PHE	CA-CB-CG	7.67	121.47	113.80
1	C	546	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	B	62	ASN	CA-CB-CG	7.66	120.26	112.60
1	A	62	ASN	CA-CB-CG	7.64	120.25	112.60
1	D	62	ASN	CA-CB-CG	7.64	120.24	112.60
1	D	207	PHE	CA-CB-CG	7.64	121.44	113.80
1	A	207	PHE	CA-CB-CG	7.63	121.43	113.80
1	C	62	ASN	CA-CB-CG	7.63	120.23	112.60
1	A	546	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	C	183	ARG	NE-CZ-NH1	7.62	129.12	121.50
1	D	546	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	B	207	PHE	CA-CB-CG	7.61	121.41	113.80
1	D	183	ARG	NE-CZ-NH1	7.56	129.06	121.50
1	A	183	ARG	NE-CZ-NH1	7.55	129.05	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	ARG	NE-CZ-NH1	7.54	129.04	121.50
1	C	221	VAL	N-CA-CB	7.49	121.81	110.58
1	A	221	VAL	N-CA-CB	7.46	121.77	110.58
1	B	221	VAL	N-CA-CB	7.46	121.76	110.58
1	D	221	VAL	N-CA-CB	7.45	121.75	110.58
1	D	412	LEU	CA-C-O	-7.44	112.94	120.90
1	D	120	GLU	N-CA-C	7.43	120.33	111.33
1	D	587	SER	CA-CB-OG	7.43	125.96	111.10
1	B	120	GLU	N-CA-C	7.43	120.32	111.33
1	A	587	SER	CA-CB-OG	7.42	125.95	111.10
1	C	120	GLU	N-CA-C	7.42	120.31	111.33
1	A	412	LEU	CA-C-O	-7.42	112.96	120.90
1	B	587	SER	CA-CB-OG	7.42	125.94	111.10
1	A	120	GLU	N-CA-C	7.41	120.30	111.33
1	C	587	SER	CA-CB-OG	7.41	125.92	111.10
1	C	412	LEU	CA-C-O	-7.40	112.98	120.90
1	A	185	PHE	CA-CB-CG	7.35	121.15	113.80
1	D	185	PHE	CA-CB-CG	7.34	121.14	113.80
1	B	412	LEU	CA-C-O	-7.33	113.06	120.90
1	B	185	PHE	CA-CB-CG	7.31	121.11	113.80
1	C	185	PHE	CA-CB-CG	7.30	121.10	113.80
1	B	432	PRO	O-C-N	-7.28	113.87	122.24
1	B	473	THR	CA-C-N	7.27	124.97	119.66
1	B	473	THR	C-N-CA	7.27	124.97	119.66
1	C	252	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	C	432	PRO	O-C-N	-7.26	113.89	122.24
1	A	473	THR	CA-C-N	7.25	124.95	119.66
1	A	473	THR	C-N-CA	7.25	124.95	119.66
1	A	252	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	D	252	ASN	OD1-CG-ND2	-7.23	115.37	122.60
1	C	473	THR	CA-C-N	7.23	124.94	119.66
1	C	473	THR	C-N-CA	7.23	124.94	119.66
1	D	473	THR	CA-C-N	7.23	124.94	119.66
1	D	473	THR	C-N-CA	7.23	124.94	119.66
1	C	377	ARG	CA-CB-CG	-7.22	99.66	114.10
1	B	252	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	D	377	ARG	CA-CB-CG	-7.21	99.68	114.10
1	D	432	PRO	O-C-N	-7.21	113.95	122.24
1	B	208	ILE	N-CA-CB	-7.21	98.59	111.93
1	A	208	ILE	N-CA-CB	-7.21	98.60	111.93
1	B	377	ARG	CA-CB-CG	-7.21	99.69	114.10
1	C	208	ILE	N-CA-CB	-7.21	98.60	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	ILE	N-CA-CB	-7.21	98.60	111.93
1	A	377	ARG	CA-CB-CG	-7.20	99.71	114.10
1	A	432	PRO	O-C-N	-7.18	113.98	122.24
1	B	392	HIS	CA-C-N	7.16	126.86	119.56
1	B	392	HIS	C-N-CA	7.16	126.86	119.56
1	A	392	HIS	CA-C-N	7.12	126.82	119.56
1	A	392	HIS	C-N-CA	7.12	126.82	119.56
1	D	392	HIS	CA-C-N	7.09	126.79	119.56
1	D	392	HIS	C-N-CA	7.09	126.79	119.56
1	C	392	HIS	CA-C-N	7.08	126.78	119.56
1	C	392	HIS	C-N-CA	7.08	126.78	119.56
1	D	236	HIS	CB-CG-ND1	7.07	133.30	122.70
1	A	236	HIS	CB-CG-ND1	7.07	133.30	122.70
1	B	323	TRP	CG-CD2-CE3	7.06	140.96	133.90
1	B	236	HIS	CB-CG-ND1	7.05	133.28	122.70
1	C	236	HIS	CB-CG-ND1	7.04	133.25	122.70
1	A	434	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	323	TRP	CG-CD2-CE3	7.02	140.92	133.90
1	C	442	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	352	ASP	CA-CB-CG	7.01	119.61	112.60
1	B	434	ASN	CA-CB-CG	7.01	119.61	112.60
1	C	323	TRP	CG-CD2-CE3	7.00	140.90	133.90
1	D	434	ASN	CA-CB-CG	6.99	119.59	112.60
1	A	442	ASN	CA-CB-CG	6.99	119.59	112.60
1	B	442	ASN	CA-CB-CG	6.99	119.58	112.60
1	D	323	TRP	CG-CD2-CE3	6.99	140.88	133.90
1	D	442	ASN	CA-CB-CG	6.99	119.59	112.60
1	C	434	ASN	CA-CB-CG	6.97	119.57	112.60
1	B	352	ASP	CA-CB-CG	6.96	119.56	112.60
1	C	352	ASP	CA-CB-CG	6.95	119.55	112.60
1	D	525	ASP	CA-CB-CG	6.95	119.55	112.60
1	C	525	ASP	CA-CB-CG	6.95	119.55	112.60
1	D	352	ASP	CA-CB-CG	6.93	119.53	112.60
1	B	525	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	525	ASP	CA-CB-CG	6.91	119.51	112.60
1	C	377	ARG	NE-CZ-NH2	-6.88	113.00	119.20
1	B	419	GLN	N-CA-C	6.87	120.92	112.54
1	C	419	GLN	N-CA-C	6.87	120.92	112.54
1	B	331	PHE	CA-CB-CG	-6.86	106.94	113.80
1	C	446	ASP	N-CA-C	6.84	120.51	109.02
1	D	446	ASP	N-CA-C	6.84	120.50	109.02
1	C	331	PHE	CA-CB-CG	-6.83	106.97	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	ASP	N-CA-C	6.83	120.50	109.02
1	D	419	GLN	N-CA-C	6.83	120.88	112.54
1	A	419	GLN	N-CA-C	6.83	120.87	112.54
1	B	377	ARG	NE-CZ-NH2	-6.83	113.06	119.20
1	A	446	ASP	N-CA-C	6.82	120.48	109.02
1	D	331	PHE	CA-CB-CG	-6.82	106.98	113.80
1	A	119	HIS	CB-CG-CD2	-6.80	122.36	131.20
1	A	331	PHE	CA-CB-CG	-6.80	107.00	113.80
1	D	377	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	A	377	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	C	119	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	B	119	HIS	CB-CG-CD2	-6.79	122.37	131.20
1	A	233	GLN	CG-CD-NE2	6.79	126.58	116.40
1	B	233	GLN	CG-CD-NE2	6.79	126.58	116.40
1	D	233	GLN	CG-CD-NE2	6.78	126.57	116.40
1	D	119	HIS	CB-CG-CD2	-6.77	122.39	131.20
1	C	233	GLN	CG-CD-NE2	6.76	126.53	116.40
1	D	386	ASN	CA-CB-CG	6.72	119.32	112.60
1	C	386	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	437	THR	N-CA-C	-6.70	105.10	113.28
1	B	437	THR	N-CA-C	-6.69	105.12	113.28
1	C	437	THR	N-CA-C	-6.68	105.12	113.28
1	C	567	THR	CA-CB-OG1	-6.68	99.58	109.60
1	A	567	THR	CA-CB-OG1	-6.68	99.58	109.60
1	B	567	THR	CA-CB-OG1	-6.68	99.58	109.60
1	B	386	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	386	ASN	CA-CB-CG	6.67	119.27	112.60
1	D	437	THR	N-CA-C	-6.67	105.14	113.28
1	D	567	THR	CA-CB-OG1	-6.66	99.61	109.60
1	B	507	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	D	364	LEU	N-CA-C	-6.63	102.69	111.24
1	A	507	HIS	CB-CG-CD2	-6.63	122.59	131.20
1	A	364	LEU	N-CA-C	-6.62	102.70	111.24
1	C	364	LEU	N-CA-C	-6.61	102.71	111.24
1	B	364	LEU	N-CA-C	-6.59	102.74	111.24
1	C	507	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	D	507	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	C	183	ARG	CB-CG-CD	6.58	126.44	111.30
1	D	183	ARG	CB-CG-CD	6.58	126.42	111.30
1	B	183	ARG	CB-CG-CD	6.57	126.41	111.30
1	A	299	LYS	O-C-N	-6.56	115.85	123.27
1	A	183	ARG	CB-CG-CD	6.56	126.39	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	THR	CB-CA-C	6.56	121.41	111.18
1	C	268	THR	CB-CA-C	6.56	121.41	111.18
1	D	268	THR	CB-CA-C	6.55	121.41	111.18
1	B	299	LYS	O-C-N	-6.54	115.88	123.27
1	B	268	THR	CB-CA-C	6.53	121.36	111.18
1	A	556	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	C	299	LYS	O-C-N	-6.51	115.91	123.27
1	D	299	LYS	O-C-N	-6.51	115.91	123.27
1	B	556	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	C	471	ARG	NE-CZ-NH2	-6.48	113.36	119.20
1	C	556	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	D	471	ARG	NE-CZ-NH2	-6.48	113.37	119.20
1	D	556	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	A	739	HIS	CB-CG-CD2	-6.47	122.78	131.20
1	A	471	ARG	NE-CZ-NH2	-6.45	113.39	119.20
1	C	739	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	D	444	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	B	471	ARG	NE-CZ-NH2	-6.42	113.42	119.20
1	A	451	MET	CA-C-O	-6.42	112.17	120.00
1	B	444	GLN	OE1-CD-NE2	-6.42	116.18	122.60
1	B	466	ASN	N-CA-C	-6.41	102.83	111.87
1	B	739	HIS	CB-CG-CD2	-6.41	122.86	131.20
1	A	459	ASN	CB-CG-ND2	6.41	126.02	116.40
1	B	459	ASN	CB-CG-ND2	6.41	126.02	116.40
1	D	739	HIS	CB-CG-CD2	-6.41	122.86	131.20
1	B	451	MET	CA-C-O	-6.41	112.18	120.00
1	D	451	MET	CA-C-O	-6.41	112.18	120.00
1	C	451	MET	CA-C-O	-6.40	112.19	120.00
1	C	459	ASN	CB-CG-ND2	6.40	126.00	116.40
1	D	252	ASN	CB-CG-ND2	6.40	126.00	116.40
1	A	252	ASN	CB-CG-ND2	6.40	126.00	116.40
1	B	116	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	C	116	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	C	444	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	D	135	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	A	135	HIS	CB-CG-CD2	-6.40	122.89	131.20
1	A	466	ASN	N-CA-C	-6.39	102.86	111.87
1	D	126	ILE	CA-C-O	-6.39	113.57	120.47
1	B	252	ASN	CB-CG-ND2	6.39	125.98	116.40
1	D	459	ASN	CB-CG-ND2	6.38	125.98	116.40
1	D	466	ASN	N-CA-C	-6.38	102.87	111.87
1	C	135	HIS	CB-CG-CD2	-6.38	122.91	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	252	ASN	CB-CG-ND2	6.38	125.97	116.40
1	B	135	HIS	CB-CG-CD2	-6.37	122.91	131.20
1	C	466	ASN	N-CA-C	-6.37	102.89	111.87
1	B	471	ARG	CB-CG-CD	6.37	125.94	111.30
1	A	116	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	D	116	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	C	126	ILE	CA-C-O	-6.36	113.61	120.47
1	C	471	ARG	CB-CG-CD	6.36	125.92	111.30
1	A	471	ARG	CB-CG-CD	6.35	125.91	111.30
1	A	444	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	D	471	ARG	CB-CG-CD	6.35	125.90	111.30
1	D	680	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	126	ILE	CA-C-O	-6.34	113.63	120.47
1	D	515	GLN	OE1-CD-NE2	-6.34	116.26	122.60
1	B	532	SER	CA-C-O	6.33	127.17	119.38
1	A	253	VAL	O-C-N	-6.33	115.73	121.87
1	B	126	ILE	CA-C-O	-6.32	113.64	120.47
1	D	532	SER	CA-C-O	6.32	127.16	119.38
1	A	515	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	B	253	VAL	O-C-N	-6.32	115.74	121.87
1	C	515	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	C	680	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	532	SER	CA-C-O	6.31	127.14	119.38
1	C	253	VAL	O-C-N	-6.31	115.75	121.87
1	C	532	SER	CA-C-O	6.31	127.14	119.38
1	A	680	ASP	CA-CB-CG	6.30	118.90	112.60
1	B	515	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	A	304	TRP	CA-C-O	-6.30	114.16	120.90
1	D	304	TRP	CA-C-O	-6.29	114.17	120.90
1	B	304	TRP	CA-C-O	-6.29	114.17	120.90
1	B	507	HIS	CB-CG-ND1	6.29	132.13	122.70
1	A	507	HIS	CB-CG-ND1	6.28	132.12	122.70
1	C	309	LYS	CB-CG-CD	-6.28	96.85	111.30
1	D	253	VAL	O-C-N	-6.28	115.78	121.87
1	A	309	LYS	CB-CG-CD	-6.28	96.86	111.30
1	D	309	LYS	CB-CG-CD	-6.28	96.87	111.30
1	B	680	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	309	LYS	CB-CG-CD	-6.27	96.88	111.30
1	C	693	LYS	CA-C-N	6.27	126.60	119.83
1	C	693	LYS	C-N-CA	6.27	126.60	119.83
1	A	446	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	507	HIS	CB-CG-ND1	6.25	132.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	TRP	CA-C-O	-6.25	114.21	120.90
1	D	250	LEU	N-CA-C	6.25	118.09	111.28
1	A	693	LYS	CA-C-N	6.25	126.58	119.83
1	A	693	LYS	C-N-CA	6.25	126.58	119.83
1	D	507	HIS	CB-CG-ND1	6.25	132.07	122.70
1	D	567	THR	N-CA-CB	-6.25	100.54	109.85
1	D	693	LYS	CA-C-N	6.25	126.58	119.83
1	D	693	LYS	C-N-CA	6.25	126.58	119.83
1	A	233	GLN	OE1-CD-NE2	-6.24	116.36	122.60
1	B	567	THR	N-CA-CB	-6.24	100.55	109.85
1	B	446	ASP	CA-CB-CG	6.24	118.84	112.60
1	B	250	LEU	N-CA-C	6.24	118.08	111.28
1	A	250	LEU	N-CA-C	6.23	118.07	111.28
1	A	463	ASN	CA-CB-CG	6.23	118.83	112.60
1	A	567	THR	N-CA-CB	-6.23	100.57	109.85
1	B	497	ARG	O-C-N	-6.23	116.12	123.22
1	C	446	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	250	LEU	N-CA-C	6.22	118.06	111.28
1	C	567	THR	N-CA-CB	-6.22	100.58	109.85
1	D	446	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	233	GLN	OE1-CD-NE2	-6.20	116.40	122.60
1	D	463	ASN	CA-CB-CG	6.20	118.80	112.60
1	D	233	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	C	497	ARG	O-C-N	-6.19	116.16	123.22
1	C	505	TYR	N-CA-C	6.19	122.42	114.56
1	D	728	PHE	CA-CB-CG	6.19	119.99	113.80
1	B	463	ASN	CA-CB-CG	6.19	118.79	112.60
1	C	728	PHE	CA-CB-CG	6.18	119.98	113.80
1	D	505	TYR	N-CA-C	6.18	122.42	114.56
1	C	463	ASN	CA-CB-CG	6.17	118.77	112.60
1	A	222	LYS	N-CA-C	6.17	118.96	110.01
1	B	693	LYS	CA-C-N	6.17	126.50	119.83
1	B	693	LYS	C-N-CA	6.17	126.50	119.83
1	C	233	GLN	OE1-CD-NE2	-6.17	116.43	122.60
1	D	29	LEU	CA-C-O	-6.17	111.69	120.51
1	D	222	LYS	N-CA-C	6.17	118.95	110.01
1	A	728	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	29	LEU	CA-C-O	-6.16	111.70	120.51
1	B	505	TYR	N-CA-C	6.16	122.39	114.56
1	C	716	GLU	CA-C-O	6.16	128.06	121.16
1	D	716	GLU	CA-C-O	6.15	128.05	121.16
1	B	716	GLU	CA-C-O	6.15	128.05	121.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	728	PHE	CA-CB-CG	6.15	119.95	113.80
1	B	29	LEU	CA-C-O	-6.15	111.72	120.51
1	C	29	LEU	CA-C-O	-6.14	111.72	120.51
1	A	716	GLU	CA-C-O	6.14	128.04	121.16
1	B	222	LYS	N-CA-C	6.14	118.92	110.01
1	C	222	LYS	N-CA-C	6.14	118.91	110.01
1	A	505	TYR	N-CA-C	6.13	122.35	114.56
1	B	165	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	B	165	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	A	165	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	226	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	165	ARG	NE-CZ-NH2	-6.08	113.73	119.20
1	A	449	HIS	CA-C-O	6.08	129.32	122.27
1	A	497	ARG	O-C-N	-6.06	116.13	123.16
1	C	165	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	A	629	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	B	449	HIS	CA-C-O	6.06	129.30	122.27
1	D	449	HIS	CA-C-O	6.05	129.29	122.27
1	C	629	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	D	497	ARG	O-C-N	-6.05	116.14	123.16
1	C	165	ARG	NE-CZ-NH2	-6.05	113.76	119.20
1	D	165	ARG	NE-CZ-NH1	6.04	127.54	121.50
1	D	629	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	654	PHE	CA-CB-CG	6.04	119.84	113.80
1	C	449	HIS	CA-C-O	6.04	129.28	122.27
1	C	226	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	C	237	ASP	N-CA-C	6.03	118.34	111.11
1	A	448	MET	N-CA-C	6.03	119.10	110.24
1	B	226	HIS	CB-CG-CD2	-6.03	123.37	131.20
1	B	448	MET	N-CA-C	6.02	119.09	110.24
1	B	629	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	D	165	ARG	NE-CZ-NH2	-6.02	113.78	119.20
1	B	259	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	636	ARG	N-CA-C	-6.01	99.93	109.07
1	A	636	ARG	N-CA-C	-6.01	99.93	109.07
1	C	636	ARG	N-CA-C	-6.01	99.93	109.07
1	D	259	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	549	HIS	CB-CG-CD2	-6.00	123.39	131.20
1	D	448	MET	N-CA-C	6.00	119.07	110.24
1	C	654	PHE	CA-CB-CG	6.00	119.80	113.80
1	D	226	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	B	468	ASN	N-CA-CB	-6.00	103.34	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	259	ASP	CA-CB-CG	6.00	118.60	112.60
1	D	468	ASN	N-CA-CB	-6.00	103.34	112.28
1	A	237	ASP	N-CA-C	5.99	118.30	111.11
1	B	636	ARG	N-CA-C	-5.99	99.96	109.07
1	C	468	ASN	N-CA-CB	-5.99	103.35	112.28
1	A	549	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	B	654	PHE	CA-CB-CG	5.99	119.79	113.80
1	D	149	LYS	CG-CD-CE	-5.99	97.53	111.30
1	D	32	GLU	CA-C-O	5.99	127.13	120.43
1	C	448	MET	N-CA-C	5.98	119.04	110.24
1	D	28	SER	N-CA-C	-5.98	98.06	110.80
1	D	654	PHE	CA-CB-CG	5.98	119.78	113.80
1	B	28	SER	N-CA-C	-5.98	98.06	110.80
1	D	237	ASP	N-CA-C	5.98	118.28	111.11
1	C	32	GLU	CA-C-O	5.97	127.12	120.43
1	C	149	LYS	CG-CD-CE	-5.97	97.56	111.30
1	C	567	THR	CA-CB-CG2	5.97	120.66	110.50
1	A	28	SER	N-CA-C	-5.97	98.08	110.80
1	A	567	THR	CA-CB-CG2	5.97	120.65	110.50
1	B	567	THR	CA-CB-CG2	5.97	120.65	110.50
1	C	549	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	C	28	SER	N-CA-C	-5.96	98.09	110.80
1	A	468	ASN	N-CA-CB	-5.96	103.39	112.28
1	A	149	LYS	CG-CD-CE	-5.96	97.59	111.30
1	D	567	THR	CA-CB-CG2	5.96	120.63	110.50
1	A	32	GLU	CA-C-O	5.96	127.10	120.43
1	B	149	LYS	CG-CD-CE	-5.96	97.60	111.30
1	D	549	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	B	237	ASP	N-CA-C	5.95	118.25	111.11
1	D	92	GLN	CB-CG-CD	5.94	122.70	112.60
1	C	92	GLN	CB-CG-CD	5.94	122.69	112.60
1	A	92	GLN	CB-CG-CD	5.93	122.68	112.60
1	B	92	GLN	CB-CG-CD	5.93	122.68	112.60
1	B	32	GLU	CA-C-O	5.93	127.07	120.43
1	C	170	GLN	CB-CG-CD	5.92	122.67	112.60
1	A	170	GLN	CB-CG-CD	5.92	122.66	112.60
1	D	674	ASP	O-C-N	-5.91	115.99	122.07
1	B	716	GLU	CB-CG-CD	5.90	122.64	112.60
1	A	674	ASP	O-C-N	-5.90	115.99	122.07
1	C	349	PHE	CA-C-N	-5.90	113.04	122.66
1	C	349	PHE	C-N-CA	-5.90	113.04	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	PHE	CA-C-N	-5.90	113.04	122.66
1	A	349	PHE	C-N-CA	-5.90	113.04	122.66
1	C	674	ASP	O-C-N	-5.90	115.99	122.07
1	D	255	TRP	CG-CD2-CE3	5.90	139.80	133.90
1	C	392	HIS	CB-CG-ND1	5.90	131.54	122.70
1	D	349	PHE	CA-C-N	-5.90	113.05	122.66
1	D	349	PHE	C-N-CA	-5.90	113.05	122.66
1	A	716	GLU	CB-CG-CD	5.89	122.62	112.60
1	B	392	HIS	CB-CG-ND1	5.89	131.53	122.70
1	D	392	HIS	CB-CG-ND1	5.89	131.53	122.70
1	C	512	TRP	CG-CD2-CE3	5.89	139.79	133.90
1	B	349	PHE	CA-C-N	-5.88	113.07	122.66
1	B	349	PHE	C-N-CA	-5.88	113.07	122.66
1	C	716	GLU	CB-CG-CD	5.88	122.60	112.60
1	B	170	GLN	CB-CG-CD	5.88	122.59	112.60
1	D	170	GLN	CB-CG-CD	5.88	122.59	112.60
1	B	512	TRP	CG-CD2-CE3	5.88	139.78	133.90
1	B	498	SER	CA-C-N	5.87	125.73	119.28
1	B	498	SER	C-N-CA	5.87	125.73	119.28
1	B	674	ASP	O-C-N	-5.87	116.03	122.07
1	D	716	GLU	CB-CG-CD	5.87	122.57	112.60
1	A	415	TYR	CA-CB-CG	5.86	124.45	113.90
1	A	498	SER	CA-C-N	5.86	125.73	119.28
1	A	498	SER	C-N-CA	5.86	125.73	119.28
1	A	255	TRP	CG-CD2-CE3	5.86	139.76	133.90
1	D	512	TRP	CG-CD2-CE3	5.86	139.76	133.90
1	A	392	HIS	CB-CG-ND1	5.86	131.49	122.70
1	C	285	LYS	CA-CB-CG	5.85	125.80	114.10
1	C	463	ASN	O-C-N	-5.85	116.25	123.33
1	A	463	ASN	O-C-N	-5.85	116.25	123.33
1	D	285	LYS	CA-CB-CG	5.84	125.78	114.10
1	A	512	TRP	CG-CD2-CE3	5.83	139.74	133.90
1	B	415	TYR	CA-CB-CG	5.83	124.40	113.90
1	C	255	TRP	CG-CD2-CE3	5.83	139.73	133.90
1	D	463	ASN	O-C-N	-5.83	116.27	123.33
1	A	285	LYS	CA-CB-CG	5.83	125.76	114.10
1	C	498	SER	CA-C-N	5.83	125.69	119.28
1	C	498	SER	C-N-CA	5.83	125.69	119.28
1	C	415	TYR	CA-CB-CG	5.83	124.39	113.90
1	B	255	TRP	CG-CD2-CE3	5.83	139.73	133.90
1	C	370	VAL	CB-CA-C	5.83	117.23	110.88
1	A	370	VAL	CB-CA-C	5.82	117.22	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	LYS	CA-CB-CG	5.82	125.74	114.10
1	D	445	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	A	96	ARG	NE-CZ-NH1	5.82	127.31	121.50
1	B	445	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	D	415	TYR	CA-CB-CG	5.81	124.36	113.90
1	C	96	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	B	463	ASN	O-C-N	-5.79	116.32	123.33
1	C	445	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	C	449	HIS	CA-CB-CG	5.79	119.58	113.80
1	B	370	VAL	CB-CA-C	5.78	117.18	110.88
1	B	449	HIS	CA-CB-CG	5.78	119.58	113.80
1	D	370	VAL	CB-CA-C	5.78	117.18	110.88
1	D	449	HIS	CA-CB-CG	5.77	119.57	113.80
1	B	96	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	D	96	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	D	498	SER	CA-C-N	5.76	125.61	119.28
1	D	498	SER	C-N-CA	5.76	125.61	119.28
1	A	445	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	A	449	HIS	CA-CB-CG	5.75	119.55	113.80
1	D	183	ARG	CA-CB-CG	5.75	125.60	114.10
1	B	183	ARG	CA-CB-CG	5.75	125.59	114.10
1	C	183	ARG	CA-CB-CG	5.75	125.59	114.10
1	A	183	ARG	CA-CB-CG	5.75	125.59	114.10
1	C	597	ASP	N-CA-C	-5.74	100.63	109.76
1	B	597	ASP	N-CA-C	-5.74	100.64	109.76
1	D	597	ASP	N-CA-C	-5.74	100.64	109.76
1	A	597	ASP	N-CA-C	-5.72	100.66	109.76
1	A	201	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	C	511	PHE	N-CA-C	-5.70	104.98	111.14
1	B	511	PHE	N-CA-C	-5.68	105.00	111.14
1	D	201	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	D	49	PRO	CB-CA-C	5.68	118.79	111.46
1	C	201	ASN	OD1-CG-ND2	5.68	128.28	122.60
1	D	133	ALA	N-CA-C	5.67	118.31	109.52
1	A	511	PHE	N-CA-C	-5.67	105.02	111.14
1	A	133	ALA	N-CA-C	5.66	118.30	109.52
1	A	438	CYS	CA-C-N	5.66	125.59	119.76
1	A	438	CYS	C-N-CA	5.66	125.59	119.76
1	C	49	PRO	CB-CA-C	5.66	118.77	111.46
1	D	511	PHE	N-CA-C	-5.66	105.03	111.14
1	A	49	PRO	CB-CA-C	5.66	118.76	111.46
1	C	133	ALA	N-CA-C	5.66	118.29	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	418	THR	N-CA-CB	-5.66	101.51	110.22
1	B	418	THR	N-CA-CB	-5.65	101.52	110.22
1	B	201	ASN	OD1-CG-ND2	5.65	128.25	122.60
1	B	49	PRO	CB-CA-C	5.65	118.74	111.46
1	C	378	ASN	CA-CB-CG	5.65	118.25	112.60
1	C	709	LYS	N-CA-C	5.64	118.90	111.28
1	A	258	SER	CA-CB-OG	5.64	122.38	111.10
1	B	258	SER	CA-CB-OG	5.64	122.37	111.10
1	A	418	THR	N-CA-CB	-5.63	101.54	110.22
1	D	258	SER	CA-CB-OG	5.63	122.36	111.10
1	C	438	CYS	CA-C-N	5.63	125.56	119.76
1	C	438	CYS	C-N-CA	5.63	125.56	119.76
1	A	709	LYS	N-CA-C	5.63	118.88	111.28
1	B	133	ALA	N-CA-C	5.63	118.24	109.52
1	C	258	SER	CA-CB-OG	5.63	122.35	111.10
1	D	378	ASN	CA-CB-CG	5.62	118.22	112.60
1	A	378	ASN	CA-CB-CG	5.62	118.22	112.60
1	C	123	PRO	CA-C-O	-5.62	115.01	121.36
1	B	709	LYS	N-CA-C	5.62	118.87	111.28
1	C	207	PHE	O-C-N	-5.62	114.77	122.46
1	A	207	PHE	O-C-N	-5.61	114.77	122.46
1	D	709	LYS	N-CA-C	5.61	118.86	111.28
1	D	438	CYS	CA-C-N	5.61	125.54	119.76
1	D	438	CYS	C-N-CA	5.61	125.54	119.76
1	A	123	PRO	CA-C-O	-5.61	115.02	121.36
1	B	438	CYS	CA-C-N	5.60	125.53	119.76
1	B	438	CYS	C-N-CA	5.60	125.53	119.76
1	B	123	PRO	CA-C-O	-5.60	115.03	121.36
1	C	418	THR	N-CA-CB	-5.60	101.60	110.22
1	C	370	VAL	N-CA-C	5.59	119.97	113.42
1	D	123	PRO	CA-C-O	-5.59	115.04	121.36
1	A	370	VAL	N-CA-C	5.59	119.96	113.42
1	B	378	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	370	VAL	N-CA-C	5.59	119.96	113.42
1	B	207	PHE	O-C-N	-5.58	114.81	122.46
1	C	128	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	C	96	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	370	VAL	N-CA-C	5.58	119.95	113.42
1	D	242	TYR	N-CA-C	-5.58	105.28	111.36
1	B	242	TYR	N-CA-C	-5.58	105.28	111.36
1	D	207	PHE	O-C-N	-5.58	114.82	122.46
1	C	287	THR	CA-C-O	-5.57	114.34	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	PHE	CA-CB-CG	5.57	119.37	113.80
1	D	287	THR	CA-C-O	-5.57	114.35	120.36
1	A	96	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	B	287	THR	CA-C-O	-5.57	114.35	120.36
1	A	287	THR	CA-C-O	-5.56	114.36	120.36
1	A	351	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	242	TYR	N-CA-C	-5.56	105.30	111.36
1	A	108	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	242	TYR	N-CA-C	-5.56	105.30	111.36
1	A	556	GLN	CG-CD-NE2	5.55	124.72	116.40
1	B	128	HIS	CB-CG-CD2	-5.55	123.99	131.20
1	C	351	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	561	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	D	431	ILE	N-CA-C	-5.54	102.92	108.96
1	B	431	ILE	N-CA-C	-5.54	102.92	108.96
1	D	128	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	B	108	PHE	CA-CB-CG	5.54	119.34	113.80
1	C	77	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	C	636	ARG	CA-CB-CG	5.53	125.17	114.10
1	D	77	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	D	122	ILE	O-C-N	-5.53	114.80	121.10
1	B	96	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	C	431	ILE	N-CA-C	-5.52	102.95	108.96
1	B	556	GLN	CG-CD-NE2	5.51	124.67	116.40
1	B	636	ARG	CA-CB-CG	5.51	125.13	114.10
1	A	122	ILE	O-C-N	-5.51	114.81	121.10
1	A	431	ILE	N-CA-C	-5.51	102.95	108.96
1	C	556	GLN	CG-CD-NE2	5.51	124.67	116.40
1	A	128	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	D	413	PHE	CA-C-O	5.51	126.60	120.82
1	A	636	ARG	CA-CB-CG	5.50	125.11	114.10
1	B	77	ASN	OD1-CG-ND2	-5.50	117.09	122.60
1	A	219	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	D	219	HIS	CB-CG-CD2	-5.50	124.05	131.20
1	D	351	PHE	CA-CB-CG	5.50	119.30	113.80
1	C	122	ILE	O-C-N	-5.50	114.83	121.10
1	D	561	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	616	LEU	N-CA-C	5.50	117.28	111.28
1	D	556	GLN	CG-CD-NE2	5.50	124.65	116.40
1	D	636	ARG	CA-CB-CG	5.50	125.10	114.10
1	A	77	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	B	219	HIS	CB-CG-CD2	-5.50	124.05	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	B	122	ILE	O-C-N	-5.50	114.83	121.10
1	D	108	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	702	ARG	CB-CG-CD	-5.49	98.66	111.30
1	B	616	LEU	N-CA-C	5.49	117.27	111.28
1	C	702	ARG	CB-CG-CD	-5.49	98.67	111.30
1	C	155	ASP	CA-CB-CG	5.49	118.09	112.60
1	C	219	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	C	616	LEU	N-CA-C	5.49	117.26	111.28
1	B	155	ASP	CA-CB-CG	5.49	118.08	112.60
1	D	702	ARG	CB-CG-CD	-5.49	98.68	111.30
1	B	413	PHE	CA-C-O	5.48	126.58	120.82
1	D	131	GLY	O-C-N	-5.48	115.57	122.70
1	C	108	PHE	CA-CB-CG	5.48	119.28	113.80
1	C	561	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	B	702	ARG	CB-CG-CD	-5.47	98.71	111.30
1	D	616	LEU	N-CA-C	5.47	117.25	111.28
1	B	536	ARG	CA-C-N	5.47	125.30	119.28
1	B	536	ARG	C-N-CA	5.47	125.30	119.28
1	C	536	ARG	CA-C-N	5.47	125.30	119.28
1	C	536	ARG	C-N-CA	5.47	125.30	119.28
1	C	128	HIS	O-C-N	-5.47	115.09	122.41
1	C	131	GLY	O-C-N	-5.46	115.60	122.70
1	A	155	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	561	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	D	442	ASN	O-C-N	-5.45	116.61	122.88
1	C	413	PHE	CA-C-O	5.45	126.54	120.82
1	D	536	ARG	CA-C-N	5.44	125.26	119.28
1	D	536	ARG	C-N-CA	5.44	125.26	119.28
1	A	131	GLY	O-C-N	-5.44	115.63	122.70
1	B	603	VAL	CG1-CB-CG2	-5.44	98.84	110.80
1	B	116	HIS	CB-CG-ND1	5.43	130.85	122.70
1	B	131	GLY	O-C-N	-5.43	115.64	122.70
1	D	32	GLU	CA-C-N	5.43	131.91	121.54
1	D	32	GLU	C-N-CA	5.43	131.91	121.54
1	D	155	ASP	CA-CB-CG	5.43	118.03	112.60
1	D	603	VAL	CG1-CB-CG2	-5.43	98.86	110.80
1	A	536	ARG	CA-C-N	5.42	125.25	119.28
1	A	536	ARG	C-N-CA	5.42	125.25	119.28
1	A	116	HIS	CB-CG-ND1	5.42	130.83	122.70
1	B	128	HIS	O-C-N	-5.42	115.14	122.41
1	B	240	TRP	CG-CD2-CE3	5.42	139.32	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	ASN	O-C-N	-5.42	116.64	122.88
1	A	128	HIS	O-C-N	-5.42	115.15	122.41
1	C	603	VAL	CG1-CB-CG2	-5.42	98.88	110.80
1	C	703	LYS	CB-CA-C	-5.42	101.47	110.68
1	A	603	VAL	CG1-CB-CG2	-5.42	98.88	110.80
1	B	703	LYS	CB-CA-C	-5.42	101.47	110.68
1	C	304	TRP	CE2-CD2-CG	-5.42	100.70	107.20
1	D	128	HIS	O-C-N	-5.42	115.15	122.41
1	A	416	THR	CA-CB-OG1	-5.42	101.48	109.60
1	C	116	HIS	CB-CG-ND1	5.42	130.82	122.70
1	D	703	LYS	CB-CA-C	-5.42	101.47	110.68
1	A	413	PHE	CA-C-O	5.41	126.50	120.82
1	A	703	LYS	CB-CA-C	-5.41	101.48	110.68
1	B	304	TRP	CD2-CE2-CZ2	-5.41	116.99	122.40
1	D	31	PRO	CA-C-N	-5.41	114.99	122.30
1	D	31	PRO	C-N-CA	-5.41	114.99	122.30
1	D	240	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	A	32	GLU	CA-C-N	5.41	131.87	121.54
1	A	32	GLU	C-N-CA	5.41	131.87	121.54
1	B	304	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	D	116	HIS	CB-CG-ND1	5.41	130.81	122.70
1	D	686	MET	N-CA-C	5.41	118.09	111.82
1	A	686	MET	N-CA-C	5.40	118.08	111.82
1	A	221	VAL	CA-CB-CG1	-5.39	101.23	110.40
1	B	31	PRO	CA-C-N	-5.39	115.02	122.30
1	B	31	PRO	C-N-CA	-5.39	115.02	122.30
1	B	32	GLU	CA-C-N	5.39	131.84	121.54
1	B	32	GLU	C-N-CA	5.39	131.84	121.54
1	B	702	ARG	CG-CD-NE	5.39	123.87	112.00
1	B	372	LYS	CB-CG-CD	-5.39	98.90	111.30
1	C	32	GLU	CA-C-N	5.39	131.84	121.54
1	C	32	GLU	C-N-CA	5.39	131.84	121.54
1	B	416	THR	CA-CB-OG1	-5.39	101.52	109.60
1	C	686	MET	N-CA-C	5.39	118.07	111.82
1	C	702	ARG	CG-CD-NE	5.39	123.86	112.00
1	D	304	TRP	CD2-CE2-CZ2	-5.39	117.01	122.40
1	D	304	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	A	31	PRO	CA-C-N	-5.38	115.03	122.30
1	A	31	PRO	C-N-CA	-5.38	115.03	122.30
1	B	323	TRP	CE2-CD2-CG	-5.38	100.74	107.20
1	D	416	THR	CA-CB-OG1	-5.38	101.53	109.60
1	D	702	ARG	CG-CD-NE	5.38	123.84	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	ILE	CB-CA-C	-5.38	104.69	111.04
1	A	702	ARG	CG-CD-NE	5.38	123.84	112.00
1	C	304	TRP	CD2-CE2-CZ2	-5.38	117.02	122.40
1	A	304	TRP	CE2-CD2-CG	-5.38	100.75	107.20
1	C	119	HIS	CB-CG-ND1	5.38	130.76	122.70
1	D	401	ASP	CA-CB-CG	5.38	117.97	112.60
1	B	686	MET	N-CA-C	5.37	118.05	111.82
1	D	221	VAL	CA-CB-CG1	-5.37	101.27	110.40
1	D	372	LYS	CB-CG-CD	-5.37	98.94	111.30
1	B	36	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	B	251	HIS	CA-C-O	-5.37	115.18	120.82
1	C	372	LYS	CB-CG-CD	-5.37	98.96	111.30
1	A	372	LYS	CB-CG-CD	-5.37	98.96	111.30
1	A	442	ASN	O-C-N	-5.37	116.71	122.88
1	A	330	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	221	VAL	CA-CB-CG1	-5.36	101.28	110.40
1	C	221	VAL	CA-CB-CG1	-5.36	101.28	110.40
1	C	36	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	304	TRP	CD2-CE2-CZ2	-5.36	117.04	122.40
1	A	323	TRP	CE2-CD2-CG	-5.36	100.77	107.20
1	C	31	PRO	CA-C-N	-5.36	115.06	122.30
1	C	31	PRO	C-N-CA	-5.36	115.06	122.30
1	C	416	THR	CA-CB-OG1	-5.36	101.56	109.60
1	D	36	HIS	CB-CG-CD2	-5.36	124.23	131.20
1	A	119	HIS	CB-CG-ND1	5.36	130.73	122.70
1	C	593	ILE	CB-CA-C	-5.35	104.72	111.04
1	A	27	ASP	N-CA-C	-5.35	96.01	111.00
1	B	119	HIS	CB-CG-ND1	5.35	130.73	122.70
1	A	240	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	A	251	HIS	CA-C-O	-5.35	115.20	120.82
1	A	401	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	119	HIS	CB-CG-ND1	5.35	130.72	122.70
1	B	27	ASP	N-CA-C	-5.35	96.03	111.00
1	C	401	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	27	ASP	N-CA-C	-5.35	96.03	111.00
1	D	251	HIS	CA-C-O	-5.35	115.21	120.82
1	C	27	ASP	N-CA-C	-5.34	96.04	111.00
1	D	593	ILE	CB-CA-C	-5.34	104.73	111.04
1	A	515	GLN	CG-CD-NE2	5.34	124.41	116.40
1	B	515	GLN	CG-CD-NE2	5.34	124.41	116.40
1	C	240	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	C	251	HIS	CA-C-O	-5.34	115.22	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	515	GLN	CG-CD-NE2	5.34	124.41	116.40
1	B	401	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	725	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	341	ILE	CA-C-N	5.33	125.24	119.85
1	C	341	ILE	C-N-CA	5.33	125.24	119.85
1	D	323	TRP	CE2-CD2-CG	-5.33	100.80	107.20
1	B	330	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	593	ILE	CB-CA-C	-5.33	104.75	111.04
1	C	323	TRP	CE2-CD2-CG	-5.33	100.81	107.20
1	D	93	ASN	O-C-N	5.33	129.45	123.27
1	B	608	ASN	N-CA-C	-5.33	101.39	108.74
1	B	341	ILE	CA-C-N	5.33	125.23	119.85
1	B	341	ILE	C-N-CA	5.33	125.23	119.85
1	A	36	HIS	CB-CG-CD2	-5.32	124.28	131.20
1	A	512	TRP	CB-CG-CD1	-5.32	118.92	126.90
1	B	306	GLU	CA-C-N	5.32	127.41	120.28
1	B	306	GLU	C-N-CA	5.32	127.41	120.28
1	C	306	GLU	CA-C-N	5.32	127.41	120.28
1	C	306	GLU	C-N-CA	5.32	127.41	120.28
1	D	512	TRP	CB-CG-CD1	-5.32	118.92	126.90
1	C	608	ASN	N-CA-C	-5.32	101.40	108.74
1	C	725	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	515	GLN	CG-CD-NE2	5.32	124.38	116.40
1	C	609	ASP	N-CA-C	5.32	119.61	113.18
1	D	608	ASN	N-CA-C	-5.32	101.40	108.74
1	B	357	THR	CA-CB-CG2	5.32	119.54	110.50
1	A	341	ILE	CA-C-N	5.31	125.22	119.85
1	A	341	ILE	C-N-CA	5.31	125.22	119.85
1	A	608	ASN	N-CA-C	-5.31	101.41	108.74
1	B	442	ASN	O-C-N	-5.31	116.77	122.88
1	B	512	TRP	CB-CG-CD1	-5.31	118.93	126.90
1	D	330	ASP	CA-CB-CG	5.31	117.91	112.60
1	D	725	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	35	SER	N-CA-C	5.31	122.11	110.80
1	B	405	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	330	ASP	CA-CB-CG	5.31	117.91	112.60
1	C	52	PRO	CA-C-N	5.31	125.99	119.99
1	C	52	PRO	C-N-CA	5.31	125.99	119.99
1	D	357	THR	CA-CB-CG2	5.31	119.52	110.50
1	B	575	PRO	N-CA-C	5.30	115.56	110.47
1	C	35	SER	N-CA-C	5.30	122.10	110.80
1	C	224	GLU	CB-CG-CD	5.30	121.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	306	GLU	CA-C-N	5.30	127.39	120.28
1	D	306	GLU	C-N-CA	5.30	127.39	120.28
1	A	609	ASP	N-CA-C	5.30	119.59	113.18
1	C	357	THR	CA-CB-CG2	5.30	119.51	110.50
1	D	341	ILE	CA-C-N	5.30	125.20	119.85
1	D	341	ILE	C-N-CA	5.30	125.20	119.85
1	A	725	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	93	ASN	O-C-N	5.30	129.42	123.27
1	A	35	SER	N-CA-C	5.29	122.07	110.80
1	A	449	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	D	405	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	575	PRO	N-CA-C	5.29	115.55	110.47
1	A	224	GLU	CB-CG-CD	5.29	121.59	112.60
1	D	52	PRO	CA-C-N	5.29	125.97	119.99
1	D	52	PRO	C-N-CA	5.29	125.97	119.99
1	B	609	ASP	N-CA-C	5.29	119.57	113.18
1	A	357	THR	CA-CB-CG2	5.28	119.48	110.50
1	B	93	ASN	O-C-N	5.28	129.40	123.27
1	A	52	PRO	CA-C-N	5.28	125.96	119.99
1	A	52	PRO	C-N-CA	5.28	125.96	119.99
1	C	575	PRO	N-CA-C	5.28	115.54	110.47
1	D	35	SER	N-CA-C	5.28	122.05	110.80
1	D	224	GLU	CB-CG-CD	5.28	121.58	112.60
1	D	449	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	A	306	GLU	CA-C-N	5.27	127.35	120.28
1	A	306	GLU	C-N-CA	5.27	127.35	120.28
1	C	405	ASP	CA-CB-CG	5.27	117.87	112.60
1	D	609	ASP	N-CA-C	5.27	119.56	113.18
1	B	224	GLU	CB-CG-CD	5.27	121.56	112.60
1	C	512	TRP	CB-CG-CD1	-5.27	119.00	126.90
1	A	93	ASN	O-C-N	5.27	129.38	123.27
1	C	449	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	405	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	52	PRO	CA-C-N	5.26	125.93	119.99
1	B	52	PRO	C-N-CA	5.26	125.93	119.99
1	B	449	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	D	486	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	A	151	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	392	HIS	CG-CD2-NE2	5.24	112.44	107.20
1	C	151	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	486	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	D	255	TRP	CE2-CD2-CG	-5.23	100.92	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	392	HIS	CG-CD2-NE2	5.23	112.43	107.20
1	B	392	HIS	ND1-CG-CD2	-5.23	100.87	106.10
1	C	748	ILE	N-CA-C	5.23	119.40	112.76
1	B	486	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	B	392	HIS	CG-CD2-NE2	5.22	112.42	107.20
1	D	542	ARG	O-C-N	-5.22	116.58	122.12
1	A	217	PHE	CA-CB-CG	-5.22	108.58	113.80
1	A	255	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	C	262	ILE	O-C-N	-5.22	115.15	121.10
1	D	748	ILE	N-CA-C	5.22	119.38	112.76
1	A	575	PRO	N-CA-C	5.21	115.48	110.47
1	B	748	ILE	N-CA-C	5.21	119.37	112.76
1	D	392	HIS	ND1-CG-CD2	-5.21	100.89	106.10
1	B	512	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	C	255	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	C	486	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	B	554	LEU	N-CA-C	-5.20	104.68	111.02
1	B	151	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	201	ASN	CB-CA-C	-5.20	100.72	111.22
1	C	217	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	217	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	255	TRP	CE2-CD2-CG	-5.20	100.97	107.20
1	C	37	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	D	37	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	D	151	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	99	SER	N-CA-C	5.19	119.10	112.87
1	D	99	SER	N-CA-C	5.19	119.10	112.87
1	A	201	ASN	CB-CA-C	-5.19	100.74	111.22
1	B	201	ASN	CB-CA-C	-5.19	100.74	111.22
1	D	201	ASN	CB-CA-C	-5.19	100.74	111.22
1	A	748	ILE	N-CA-C	5.18	119.34	112.76
1	A	512	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	D	262	ILE	O-C-N	-5.18	115.19	121.10
1	A	392	HIS	ND1-CG-CD2	-5.18	100.92	106.10
1	A	99	SER	N-CA-C	5.18	119.08	112.87
1	C	512	TRP	CE2-CD2-CG	-5.18	100.99	107.20
1	C	392	HIS	CG-CD2-NE2	5.17	112.38	107.20
1	B	262	ILE	O-C-N	-5.17	115.20	121.10
1	B	657	ALA	CA-C-N	5.17	126.30	119.84
1	B	657	ALA	C-N-CA	5.17	126.30	119.84
1	C	99	SER	N-CA-C	5.17	119.07	112.87
1	C	542	ARG	O-C-N	-5.17	116.64	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	554	LEU	N-CA-C	-5.16	104.72	111.02
1	B	37	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	C	657	ALA	CA-C-N	5.16	126.29	119.84
1	C	657	ALA	C-N-CA	5.16	126.29	119.84
1	D	512	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	D	657	ALA	CA-C-N	5.16	126.29	119.84
1	D	657	ALA	C-N-CA	5.16	126.29	119.84
1	A	293	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	D	217	PHE	CA-CB-CG	-5.16	108.64	113.80
1	B	293	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	A	262	ILE	O-C-N	-5.15	115.23	121.10
1	A	37	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	B	570	GLN	CG-CD-NE2	5.15	124.12	116.40
1	C	158	LYS	N-CA-CB	-5.15	101.93	110.47
1	D	570	GLN	CG-CD-NE2	5.15	124.12	116.40
1	A	710	ILE	N-CA-C	5.14	116.38	108.71
1	C	570	GLN	CG-CD-NE2	5.14	124.11	116.40
1	C	710	ILE	N-CA-C	5.14	116.38	108.71
1	D	554	LEU	N-CA-C	-5.14	104.74	111.02
1	B	542	ARG	O-C-N	-5.14	116.67	122.12
1	D	158	LYS	N-CA-CB	-5.14	101.94	110.47
1	A	189	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	479	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	D	313	ARG	N-CA-C	5.14	116.88	111.28
1	A	554	LEU	N-CA-C	-5.14	104.75	111.02
1	A	542	ARG	O-C-N	-5.14	116.68	122.12
1	A	657	ALA	CA-C-N	5.14	126.26	119.84
1	A	657	ALA	C-N-CA	5.14	126.26	119.84
1	B	159	ILE	CB-CG1-CD1	-5.14	103.01	113.80
1	C	159	ILE	CB-CG1-CD1	-5.14	103.02	113.80
1	C	189	PHE	CA-CB-CG	5.14	118.94	113.80
1	C	392	HIS	ND1-CG-CD2	-5.14	100.96	106.10
1	D	471	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	B	158	LYS	N-CA-CB	-5.13	101.95	110.47
1	B	471	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	C	293	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	C	172	GLY	O-C-N	-5.12	117.31	122.59
1	D	172	GLY	O-C-N	-5.12	117.31	122.59
1	D	189	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	580	ASN	CB-CG-ND2	5.12	124.09	116.40
1	D	710	ILE	N-CA-C	5.12	116.34	108.71
1	C	742	TRP	CB-CG-CD1	-5.12	119.22	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ILE	CB-CG1-CD1	-5.12	103.05	113.80
1	A	172	GLY	O-C-N	-5.12	117.32	122.59
1	C	260	ARG	CA-CB-CG	5.12	124.34	114.10
1	A	54	SER	CB-CA-C	-5.12	102.30	110.79
1	A	158	LYS	N-CA-CB	-5.12	101.97	110.47
1	A	471	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	B	189	PHE	CA-CB-CG	5.12	118.92	113.80
1	C	471	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	742	TRP	CB-CG-CD1	-5.12	119.23	126.90
1	B	54	SER	CB-CA-C	-5.12	102.30	110.79
1	B	710	ILE	N-CA-C	5.12	116.33	108.71
1	B	227	TRP	CG-CD1-NE1	-5.11	103.55	110.20
1	B	260	ARG	CA-CB-CG	5.11	124.33	114.10
1	D	159	ILE	CB-CG1-CD1	-5.11	103.06	113.80
1	C	580	ASN	CB-CG-ND2	5.11	124.07	116.40
1	C	54	SER	CB-CA-C	-5.11	102.31	110.79
1	D	54	SER	CB-CA-C	-5.11	102.31	110.79
1	C	313	ARG	N-CA-C	5.11	116.85	111.28
1	A	157	ASN	N-CA-C	5.11	119.38	113.20
1	C	479	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	D	293	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	A	570	GLN	CG-CD-NE2	5.10	124.05	116.40
1	B	580	ASN	CB-CG-ND2	5.10	124.05	116.40
1	B	742	TRP	CB-CG-CD1	-5.10	119.25	126.90
1	D	742	TRP	CB-CG-CD1	-5.10	119.25	126.90
1	B	157	ASN	N-CA-C	5.10	119.37	113.20
1	D	157	ASN	N-CA-C	5.10	119.37	113.20
1	A	580	ASN	CB-CG-ND2	5.10	124.04	116.40
1	D	479	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	C	157	ASN	N-CA-C	5.09	119.36	113.20
1	A	260	ARG	CA-CB-CG	5.09	124.28	114.10
1	A	293	TRP	CG-CD1-NE1	-5.09	103.59	110.20
1	D	335	GLU	CA-CB-CG	-5.09	103.92	114.10
1	B	293	TRP	CG-CD1-NE1	-5.08	103.59	110.20
1	B	313	ARG	N-CA-C	5.08	116.82	111.28
1	D	260	ARG	CA-CB-CG	5.08	124.27	114.10
1	A	227	TRP	CG-CD1-NE1	-5.08	103.59	110.20
1	C	293	TRP	CG-CD1-NE1	-5.08	103.59	110.20
1	D	671	ASN	OD1-CG-ND2	-5.08	117.52	122.60
1	D	227	TRP	CG-CD1-NE1	-5.08	103.60	110.20
1	A	313	ARG	N-CA-C	5.08	116.81	111.28
1	B	335	GLU	CA-CB-CG	-5.07	103.95	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	293	TRP	CG-CD1-NE1	-5.07	103.61	110.20
1	A	335	GLU	CA-CB-CG	-5.07	103.97	114.10
1	B	479	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	C	330	ASP	N-CA-C	-5.07	102.02	109.62
1	B	172	GLY	O-C-N	-5.06	117.38	122.59
1	C	335	GLU	CA-CB-CG	-5.06	103.98	114.10
1	D	728	PHE	N-CA-C	-5.06	105.04	111.11
1	B	330	ASP	N-CA-C	-5.06	102.03	109.62
1	B	671	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	C	227	TRP	CG-CD1-NE1	-5.05	103.63	110.20
1	C	671	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	671	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	D	41	GLU	CA-C-O	-5.05	115.46	120.26
1	A	728	PHE	N-CA-C	-5.05	105.05	111.11
1	A	741	VAL	O-C-N	-5.04	116.27	122.57
1	B	728	PHE	N-CA-C	-5.04	105.06	111.11
1	C	728	PHE	N-CA-C	-5.04	105.06	111.11
1	C	41	GLU	CA-C-O	-5.04	115.48	120.26
1	B	246	GLN	CA-C-N	5.03	126.13	119.84
1	B	246	GLN	C-N-CA	5.03	126.13	119.84
1	A	330	ASP	N-CA-C	-5.03	102.08	109.62
1	D	330	ASP	N-CA-C	-5.03	102.08	109.62
1	B	741	VAL	O-C-N	-5.02	116.29	122.57
1	A	43	THR	CA-C-N	5.02	125.55	120.38
1	A	43	THR	C-N-CA	5.02	125.55	120.38
1	B	41	GLU	CA-C-O	-5.02	115.49	120.26
1	D	741	VAL	O-C-N	-5.02	116.30	122.57
1	A	41	GLU	CA-C-O	-5.02	115.49	120.26
1	C	43	THR	CA-C-N	5.01	125.54	120.38
1	C	43	THR	C-N-CA	5.01	125.54	120.38
1	A	197	ASP	CA-C-O	-5.01	115.00	120.36
1	A	246	GLN	CA-C-N	5.01	126.10	119.84
1	A	246	GLN	C-N-CA	5.01	126.10	119.84
1	A	297	ALA	N-CA-C	-5.01	106.59	113.30
1	A	691	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	C	741	VAL	O-C-N	-5.00	116.31	122.57
1	A	628	VAL	O-C-N	-5.00	117.63	122.93
1	B	43	THR	CA-C-N	5.00	125.53	120.38
1	B	43	THR	C-N-CA	5.00	125.53	120.38

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain
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	94	1
1	B	5746	0	5578	95	1
1	C	5746	0	5578	95	22
1	D	5746	0	5578	96	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	351	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 8.

All (351) 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:B:683:TYR:HA	1:B:686:MET:HE3	1.81	0.62
1:A:338:PHE:HB3	1:A:340:LEU:HD13	1.82	0.62
1:A:683:TYR:HA	1:A:686:MET:HE3	1.81	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:683:TYR:HA	1:C:686:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:ASP:HA	1:D:571:LEU:HD23	1.82	0.61
1:D:683:TYR:HA	1:D:686:MET:HE3	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:278:ARG:HH22	1:C:487:GLU:CD	2.18	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:278:ARG:HH22	1:B:487:GLU:CD	2.18	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:278:ARG:HH22	1:A:487:GLU:CD	2.18	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:278:ARG:HH22	1:D:487:GLU:CD	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:622:ALA:HB3	1:C:729:MET:HE2	1.96	0.48
1:A:506:SER:HB3	1:A:577:PRO:O	2.14	0.48
1:B:622:ALA:HB3	1:B:729:MET:HE2	1.96	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:D:622:ALA:HB3	1:D:729:MET:HE2	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:622:ALA:HB3	1:A:729:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:752:PRO:HB2	1:D:686:MET:HE1	1.98	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:A:752:PRO:HB2	1:B:686:MET:HE1	1.98	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:207:PHE:C	1:D:208:ILE:HD12	2.41	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:207:PHE:C	1:A:208:ILE:HD12	2.41	0.45
1:A:126:ILE:HD12	1:B:121:ARG:NH2	2.31	0.45
1:B:207:PHE:C	1:B:208:ILE:HD12	2.41	0.45
1:C:207:PHE:C	1:C:208:ILE:HD12	2.41	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:A:686:MET:HE1	1:B:752:PRO:HB2	1.98	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:254:MET:HE3	1:A:254:MET:HB3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:MET:HE1	1:D:752:PRO:HB2	1.98	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
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:C:254:MET:HE3	1:C:254:MET:HB3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:254:MET:HE3	1:D:254:MET:HB3	1.86	0.41
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:159:ILE:C	1:C:159:ILE:HD12	2.47	0.40
1:C:451:MET:HE3	1:C:451:MET:HB3	1.93	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:159:ILE:C	1:B:159:ILE:HD12	2.47	0.40
1:B:333:GLU:HA	1:B:373:MET:O	2.21	0.40
1:D:159:ILE:C	1:D:159:ILE:HD12	2.47	0.40
1:A:159:ILE:C	1:A:159:ILE:HD12	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	16	44
1	B	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	16	44
1	C	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	16	44
1	D	725/753 (96%)	685 (94%)	34 (5%)	6 (1%)	16	44
All	All	2900/3012 (96%)	2740 (94%)	136 (5%)	24 (1%)	16	44

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

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Mol	Chain	Res	Type
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%)	550 (90%)	62 (10%)	7 23
1	B	612/636 (96%)	550 (90%)	62 (10%)	7 23
1	C	612/636 (96%)	550 (90%)	62 (10%)	7 23
1	D	612/636 (96%)	550 (90%)	62 (10%)	7 23
All	All	2448/2544 (96%)	2200 (90%)	248 (10%)	7 23

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	GLU
1	A	48	GLN
1	A	56	LYS
1	A	61	ARG
1	A	73	LYS
1	A	87	ARG

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Mol	Chain	Res	Type
1	A	126	ILE
1	A	127	VAL
1	A	146	ASP
1	A	159	ILE
1	A	183	ARG
1	A	191	THR
1	A	205	ILE
1	A	208	ILE
1	A	221	VAL
1	A	230	PRO
1	A	248	GLU
1	A	252	ASN
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	368	GLN
1	A	375	LEU
1	A	386	ASN
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	542	ARG
1	A	552	LEU
1	A	554	LEU
1	A	567	THR
1	A	571	LEU
1	A	574	THR
1	A	584	LYS
1	A	598	VAL
1	A	607	LEU
1	A	613	SER

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Mol	Chain	Res	Type
1	A	616	LEU
1	A	617	LEU
1	A	621	LYS
1	A	635	SER
1	A	639	GLU
1	A	648	LEU
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	A	751	ILE
1	B	29	LEU
1	B	32	GLU
1	B	48	GLN
1	B	56	LYS
1	B	61	ARG
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	183	ARG
1	B	191	THR
1	B	205	ILE
1	B	208	ILE
1	B	221	VAL
1	B	230	PRO
1	B	248	GLU
1	B	252	ASN
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	368	GLN
1	B	375	LEU
1	B	386	ASN

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Mol	Chain	Res	Type
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	542	ARG
1	B	552	LEU
1	B	554	LEU
1	B	567	THR
1	B	571	LEU
1	B	574	THR
1	B	584	LYS
1	B	598	VAL
1	B	607	LEU
1	B	613	SER
1	B	616	LEU
1	B	617	LEU
1	B	621	LYS
1	B	635	SER
1	B	639	GLU
1	B	648	LEU
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	B	751	ILE
1	C	29	LEU
1	C	32	GLU
1	C	48	GLN
1	C	56	LYS
1	C	61	ARG
1	C	73	LYS
1	C	87	ARG
1	C	126	ILE
1	C	127	VAL

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Mol	Chain	Res	Type
1	C	146	ASP
1	C	159	ILE
1	C	183	ARG
1	C	191	THR
1	C	205	ILE
1	C	208	ILE
1	C	221	VAL
1	C	230	PRO
1	C	248	GLU
1	C	252	ASN
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	368	GLN
1	C	375	LEU
1	C	386	ASN
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	542	ARG
1	C	552	LEU
1	C	554	LEU
1	C	567	THR
1	C	571	LEU
1	C	574	THR
1	C	584	LYS
1	C	598	VAL
1	C	607	LEU
1	C	613	SER
1	C	616	LEU
1	C	617	LEU

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Mol	Chain	Res	Type
1	C	621	LYS
1	C	635	SER
1	C	639	GLU
1	C	648	LEU
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	C	751	ILE
1	D	29	LEU
1	D	32	GLU
1	D	48	GLN
1	D	56	LYS
1	D	61	ARG
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	183	ARG
1	D	191	THR
1	D	205	ILE
1	D	208	ILE
1	D	221	VAL
1	D	230	PRO
1	D	248	GLU
1	D	252	ASN
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	368	GLN
1	D	375	LEU
1	D	386	ASN
1	D	408	LEU
1	D	412	LEU

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Mol	Chain	Res	Type
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	542	ARG
1	D	552	LEU
1	D	554	LEU
1	D	567	THR
1	D	571	LEU
1	D	574	THR
1	D	584	LYS
1	D	598	VAL
1	D	607	LEU
1	D	613	SER
1	D	616	LEU
1	D	617	LEU
1	D	621	LYS
1	D	635	SER
1	D	639	GLU
1	D	648	LEU
1	D	660	LEU
1	D	685	LEU
1	D	709	LYS
1	D	713	GLN
1	D	732	LEU
1	D	733	LEU
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	252	ASN
1	A	386	ASN
1	A	392	HIS
1	A	429	HIS
1	A	449	HIS
1	A	459	ASN

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Mol	Chain	Res	Type
1	A	507	HIS
1	A	572	ASN
1	A	629	HIS
1	B	77	ASN
1	B	84	GLN
1	B	252	ASN
1	B	386	ASN
1	B	392	HIS
1	B	429	HIS
1	B	449	HIS
1	B	459	ASN
1	B	572	ASN
1	B	629	HIS
1	C	84	GLN
1	C	231	GLN
1	C	252	ASN
1	C	386	ASN
1	C	392	HIS
1	C	429	HIS
1	C	449	HIS
1	C	459	ASN
1	C	507	HIS
1	C	572	ASN
1	C	629	HIS
1	D	84	GLN
1	D	231	GLN
1	D	252	ASN
1	D	386	ASN
1	D	392	HIS
1	D	429	HIS
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	572	ASN
1	D	580	ASN
1	D	629	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	754	1	50,50,50	1.36	8 (16%)	67,82,82	1.41	6 (8%)
2	HEM	A	754	1	50,50,50	1.36	8 (16%)	67,82,82	1.41	6 (8%)
2	HEM	D	754	1	50,50,50	1.37	8 (16%)	67,82,82	1.40	6 (8%)
2	HEM	C	754	1	50,50,50	1.36	8 (16%)	67,82,82	1.41	5 (7%)

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	B	754	1	-	1/14/54/54	-
2	HEM	A	754	1	-	1/14/54/54	-
2	HEM	D	754	1	-	1/14/54/54	-
2	HEM	C	754	1	-	1/14/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	754	HEM	CBB-CAB	2.97	1.44	1.30
2	C	754	HEM	CBB-CAB	2.96	1.44	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	754	HEM	CBB-CAB	2.96	1.44	1.30
2	A	754	HEM	CBB-CAB	2.95	1.44	1.30
2	A	754	HEM	CBC-CAC	2.88	1.44	1.30
2	D	754	HEM	CBC-CAC	2.88	1.44	1.30
2	B	754	HEM	CBC-CAC	2.87	1.44	1.30
2	C	754	HEM	CBC-CAC	2.86	1.44	1.30
2	D	754	HEM	CAB-C3B	-2.86	1.39	1.47
2	C	754	HEM	CAB-C3B	-2.85	1.39	1.47
2	B	754	HEM	CAB-C3B	-2.83	1.39	1.47
2	A	754	HEM	CAB-C3B	-2.82	1.39	1.47
2	C	754	HEM	O2D-CGD	-2.74	1.21	1.30
2	D	754	HEM	CAC-C3C	-2.72	1.40	1.47
2	B	754	HEM	CAC-C3C	-2.72	1.40	1.47
2	A	754	HEM	O2D-CGD	-2.71	1.21	1.30
2	A	754	HEM	CAC-C3C	-2.71	1.40	1.47
2	C	754	HEM	CAC-C3C	-2.70	1.40	1.47
2	D	754	HEM	O2D-CGD	-2.70	1.21	1.30
2	B	754	HEM	O2D-CGD	-2.69	1.21	1.30
2	C	754	HEM	C3C-C4C	-2.67	1.41	1.46
2	B	754	HEM	C3C-C4C	-2.66	1.41	1.46
2	A	754	HEM	C3C-C4C	-2.65	1.41	1.46
2	D	754	HEM	C3C-C4C	-2.62	1.41	1.46
2	D	754	HEM	CMC-C2C	2.23	1.55	1.50
2	B	754	HEM	CMC-C2C	2.19	1.55	1.50
2	C	754	HEM	CMC-C2C	2.17	1.55	1.50
2	A	754	HEM	CMC-C2C	2.16	1.55	1.50
2	D	754	HEM	O2A-CGA	-2.15	1.23	1.30
2	A	754	HEM	O2A-CGA	-2.13	1.23	1.30
2	C	754	HEM	O2A-CGA	-2.12	1.23	1.30
2	B	754	HEM	O2A-CGA	-2.11	1.23	1.30

All (23) 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	112.53
2	B	754	HEM	CBD-CAD-C3D	-7.17	92.71	112.53
2	A	754	HEM	CBD-CAD-C3D	-7.16	92.73	112.53
2	C	754	HEM	CBD-CAD-C3D	-7.16	92.74	112.53
2	C	754	HEM	C3B-C2B-C1B	-2.68	104.39	106.41
2	B	754	HEM	C3B-C2B-C1B	-2.66	104.41	106.41
2	A	754	HEM	C3B-C2B-C1B	-2.65	104.42	106.41
2	D	754	HEM	C3B-C2B-C1B	-2.61	104.45	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754	HEM	CHC-C1C-NC	-2.28	121.97	124.45
2	D	754	HEM	CHC-C1C-NC	-2.23	122.02	124.45
2	C	754	HEM	CHC-C1C-NC	-2.23	122.03	124.45
2	A	754	HEM	CHC-C1C-NC	-2.22	122.04	124.45
2	D	754	HEM	CAC-C3C-C4C	-2.15	119.69	124.82
2	A	754	HEM	CAC-C3C-C4C	-2.14	119.70	124.82
2	B	754	HEM	CAC-C3C-C4C	-2.14	119.72	124.82
2	C	754	HEM	CAC-C3C-C4C	-2.13	119.72	124.82
2	B	754	HEM	C2B-C1B-NB	2.05	112.19	109.84
2	C	754	HEM	C2B-C1B-NB	2.03	112.17	109.84
2	A	754	HEM	C1D-C2D-C3D	-2.02	104.86	106.98
2	D	754	HEM	C2B-C1B-NB	2.01	112.15	109.84
2	A	754	HEM	C4D-C3D-C2D	2.01	109.81	106.89
2	B	754	HEM	C1D-C2D-C3D	-2.00	104.88	106.98
2	D	754	HEM	C1D-C2D-C3D	-2.00	104.88	106.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	754	HEM	C2C-C3C-CAC-CBC
2	B	754	HEM	C2C-C3C-CAC-CBC
2	C	754	HEM	C2C-C3C-CAC-CBC
2	D	754	HEM	C2C-C3C-CAC-CBC

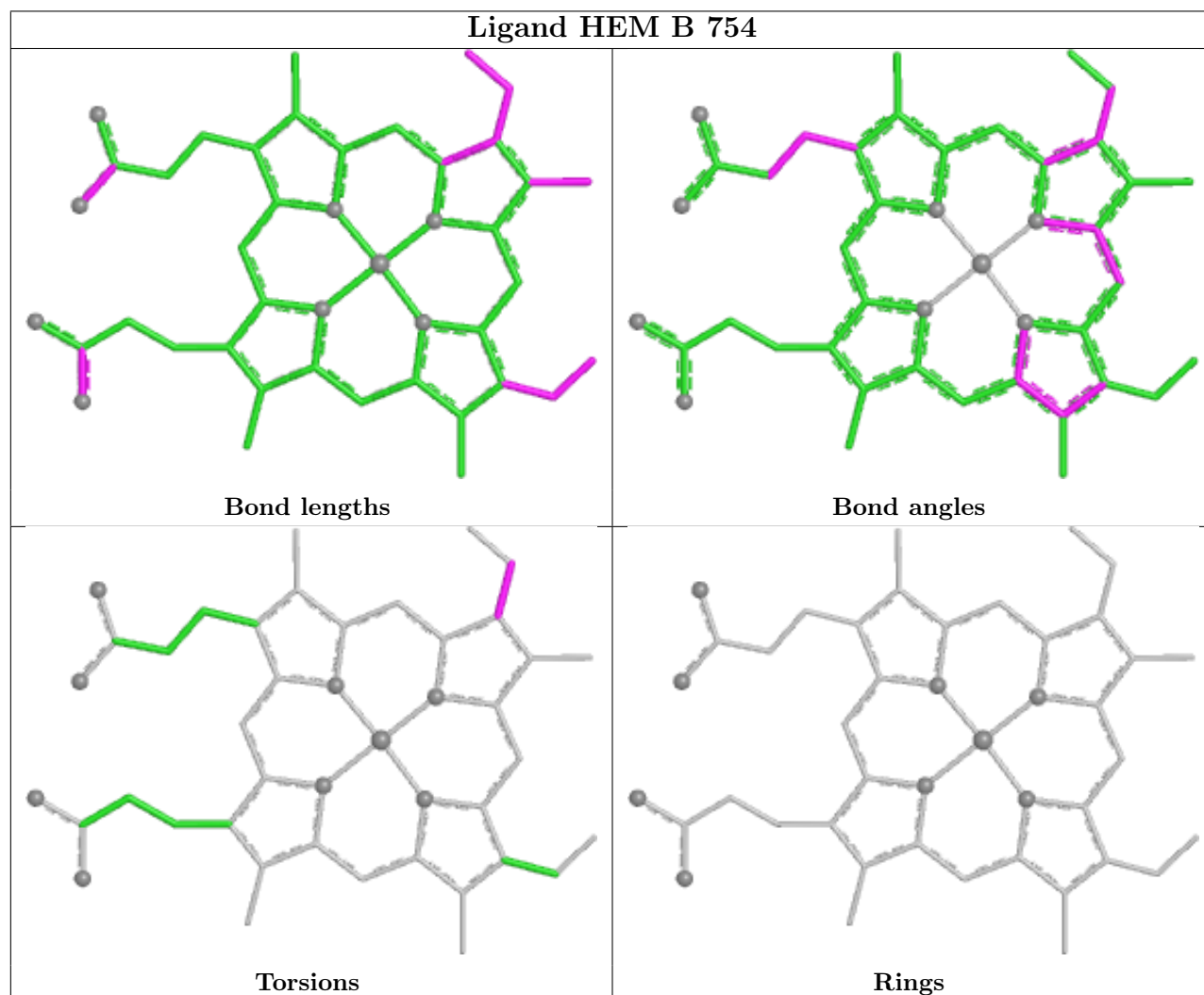
There are no ring outliers.

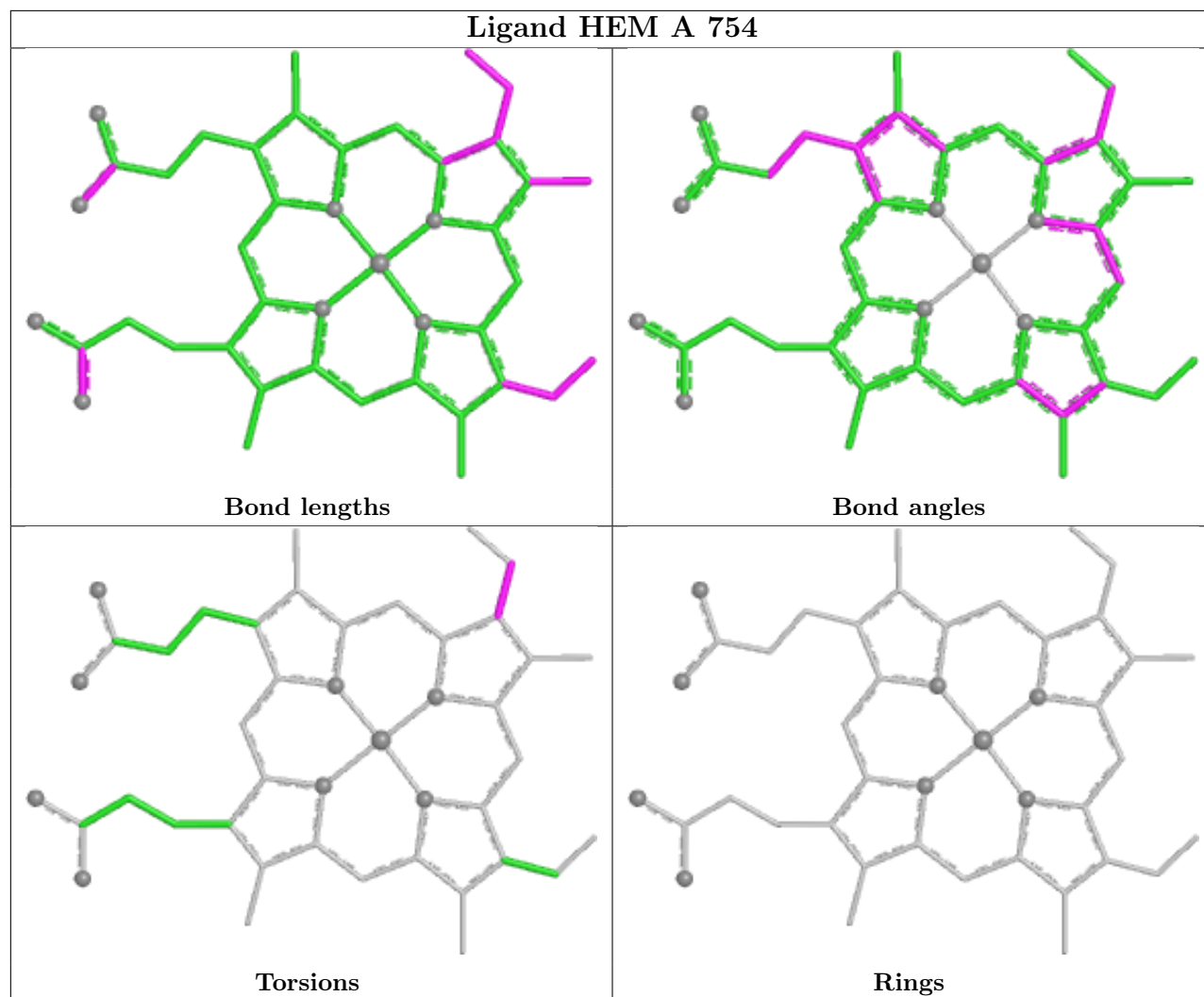
4 monomers are involved in 13 short contacts:

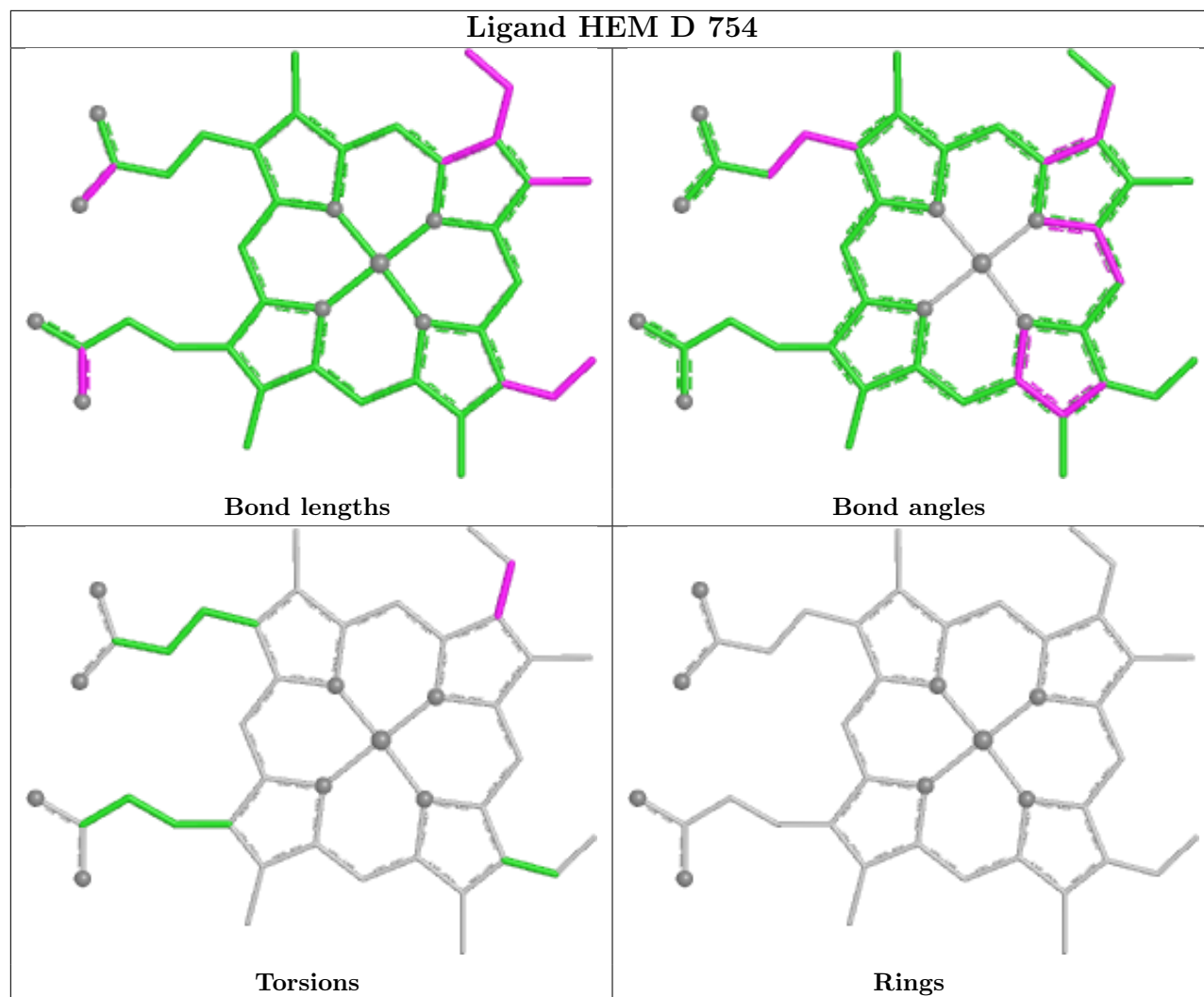
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	754	HEM	3	0
2	A	754	HEM	4	0
2	D	754	HEM	3	0
2	C	754	HEM	3	0

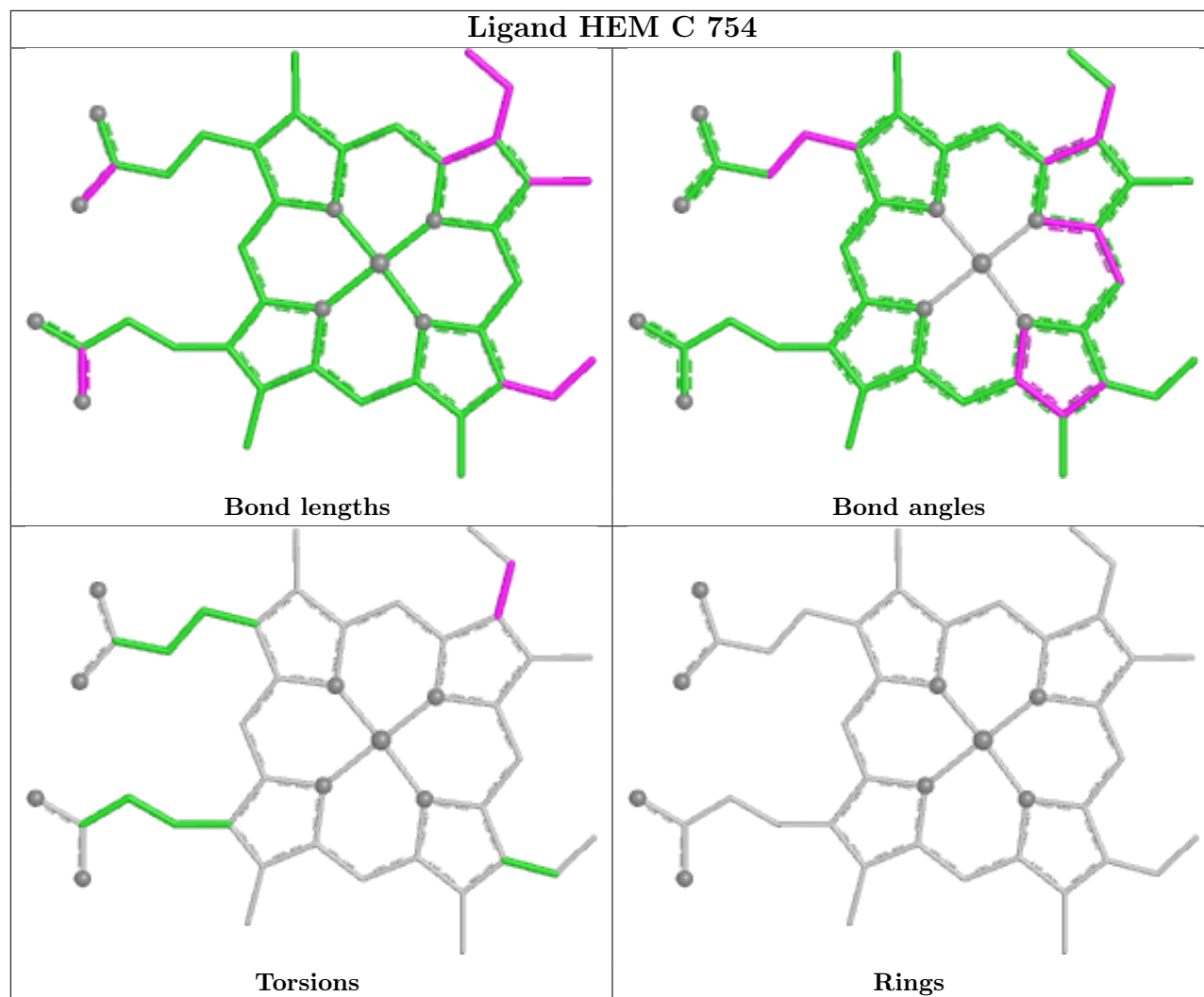
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.