



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:12 AM EST

PDB ID : 1QF7  
Title : STRUCTURE OF THE MUTANT HIS392GLN OF CATALASE HP11 FROM E. COLI  
Authors : Mate, M.J.; Loewen, P.C.; Fita, I.  
Deposited on : 1999-03-26  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

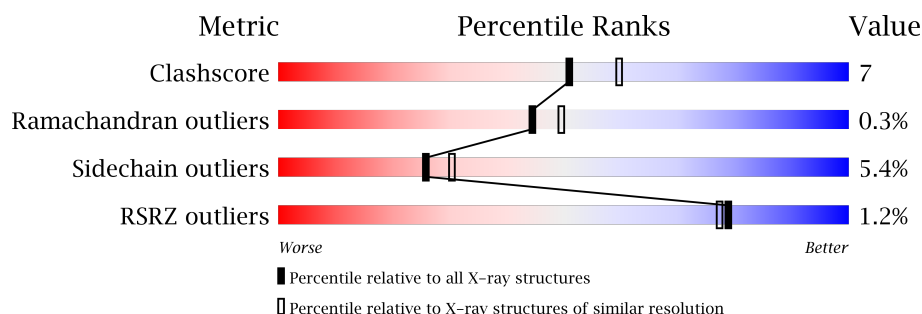
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 16%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>76%</span> <span>16%</span> <span>...</span> </div> </div>
1	B	753	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 75%, yellow 18%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>75%</span> <span>18%</span> <span>...</span> </div> </div>
1	C	753	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 75%, yellow 17%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>75%</span> <span>17%</span> <span>...</span> </div> </div>
1	D	753	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 17%, orange 5%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>76%</span> <span>17%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25843 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 PROTEIN (CATALASE HP11).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			
1	B	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			
1	C	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			
1	D	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLN	HIS	ENGINEERED MUTATION	UNP P21179
B	392	GLN	HIS	ENGINEERED MUTATION	UNP P21179
C	392	GLN	HIS	ENGINEERED MUTATION	UNP P21179
D	392	GLN	HIS	ENGINEERED MUTATION	UNP P21179

- 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
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

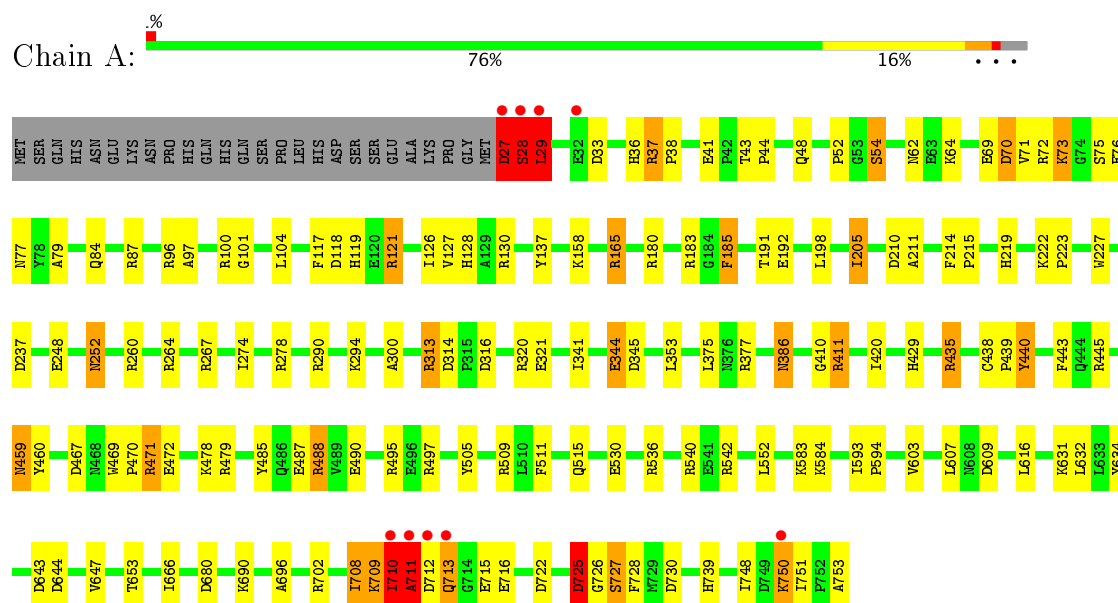
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	728	Total O 728 728	0	0
3	B	625	Total O 625 625	0	0
3	C	634	Total O 634 634	0	0
3	D	692	Total O 692 692	0	0

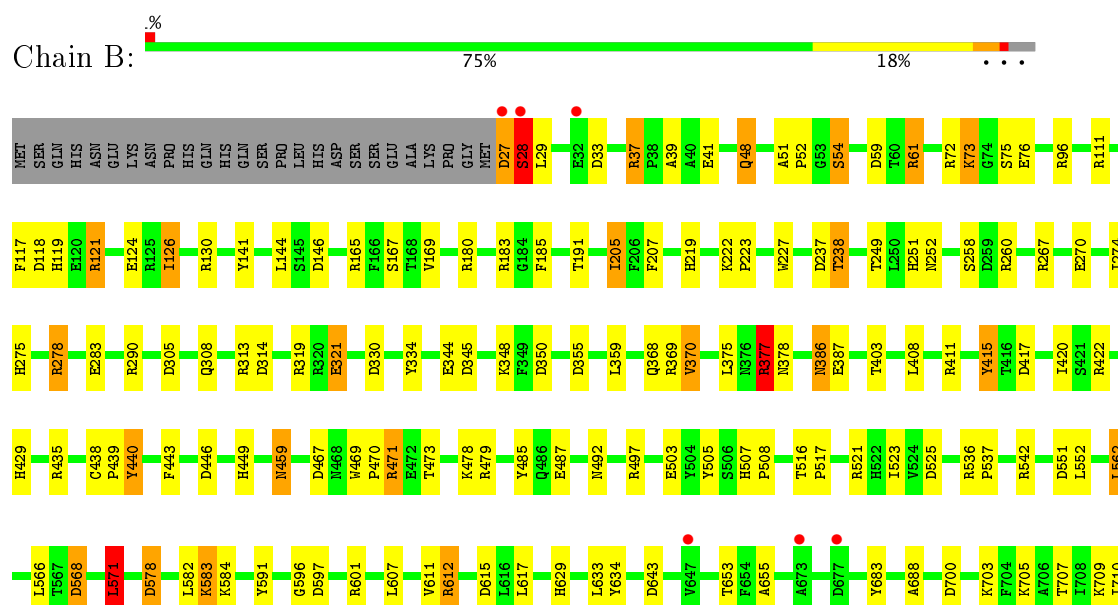
### 3 Residue-property plots

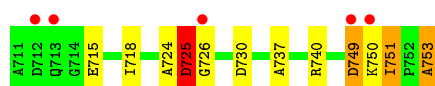
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: PROTEIN (CATALASE HP11)

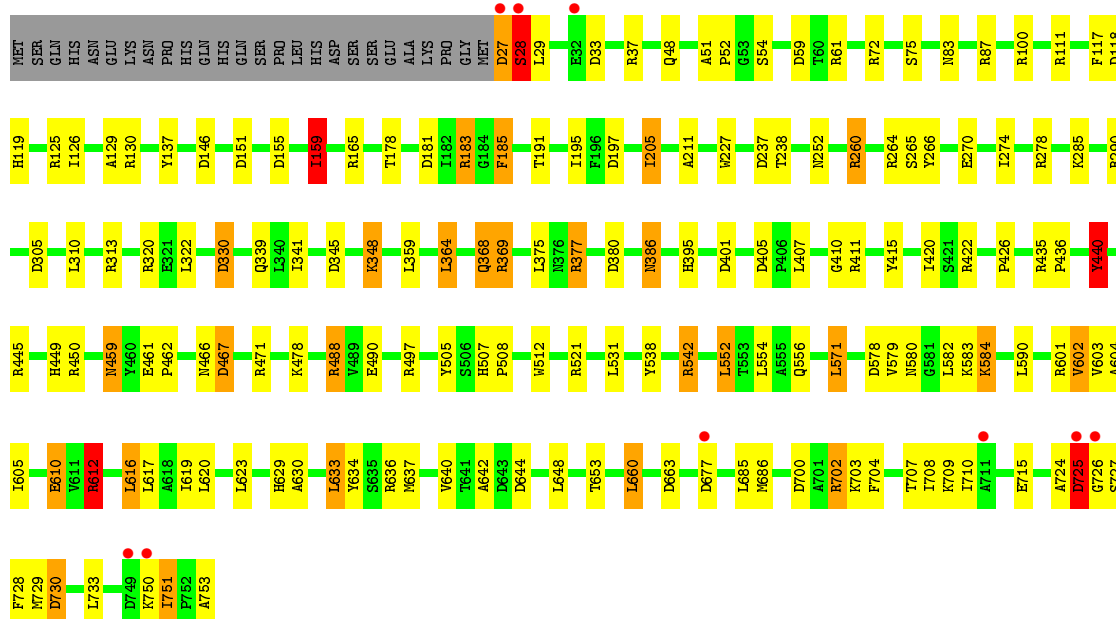
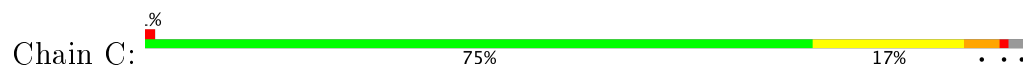


#### • Molecule 1: PROTEIN (CATALASE HP11)

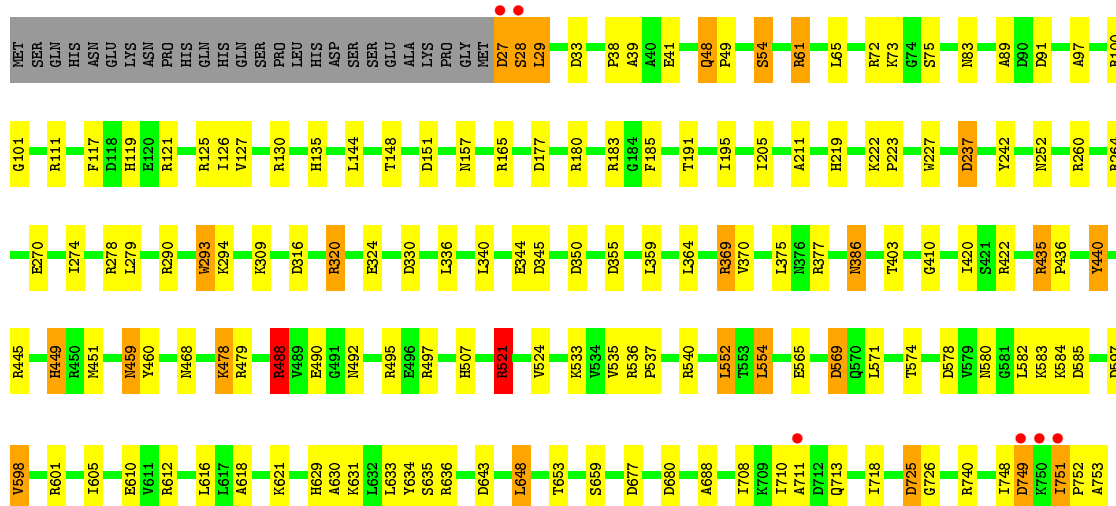
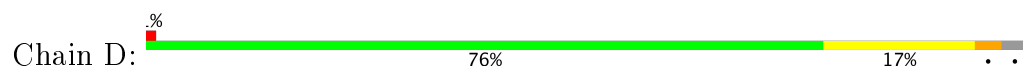




• Molecule 1: PROTEIN (CATALASE HP1I)



• Molecule 1: PROTEIN (CATALASE HP1I)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.40Å 132.92Å 121.67Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.04 – 2.19	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.20) 92.4 (20.04-2.19)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.144 , 0.210 0.143 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	12.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25843	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.77	1/5907 (0.0%)	1.70	117/8032 (1.5%)
1	B	0.74	1/5907 (0.0%)	1.64	109/8032 (1.4%)
1	C	0.75	1/5907 (0.0%)	1.65	84/8032 (1.0%)
1	D	0.73	0/5907	1.66	100/8032 (1.2%)
All	All	0.75	3/23628 (0.0%)	1.66	410/32128 (1.3%)

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	4
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	725	ASP	CA-CB	6.15	1.67	1.53
1	A	28	SER	CA-CB	5.47	1.61	1.52
1	B	753	ALA	C-O	5.05	1.32	1.23

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	542	ARG	CD-NE-CZ	37.39	175.94	123.60
1	D	488	ARG	CD-NE-CZ	24.67	158.14	123.60
1	D	61	ARG	CD-NE-CZ	23.79	156.90	123.60
1	A	27	ASP	CA-CB-CG	20.44	158.37	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	ARG	NE-CZ-NH1	-19.28	110.66	120.30
1	C	725	ASP	N-CA-C	19.13	162.65	111.00
1	B	377	ARG	NE-CZ-NH2	18.76	129.68	120.30
1	A	710	ILE	CB-CA-C	18.62	148.84	111.60
1	D	488	ARG	NE-CZ-NH1	18.15	129.38	120.30
1	A	471	ARG	NE-CZ-NH2	18.08	129.34	120.30
1	A	29	LEU	CA-C-O	16.71	155.19	120.10
1	D	278	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	A	542	ARG	NE-CZ-NH2	-15.17	112.71	120.30
1	A	260	ARG	NE-CZ-NH2	-14.82	112.89	120.30
1	C	445	ARG	NE-CZ-NH1	14.72	127.66	120.30
1	A	130	ARG	NE-CZ-NH1	14.69	127.64	120.30
1	D	536	ARG	NE-CZ-NH1	-14.29	113.16	120.30
1	A	29	LEU	CA-C-N	-13.58	87.32	117.20
1	D	61	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	B	28	SER	N-CA-CB	13.41	130.62	110.50
1	D	601	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	A	27	ASP	O-C-N	-13.26	101.49	122.70
1	A	70	ASP	CB-CG-OD2	13.13	130.12	118.30
1	C	411	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	C	521	ARG	NE-CZ-NH2	-12.80	113.90	120.30
1	A	712	ASP	CB-CA-C	12.63	135.66	110.40
1	B	313	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	D	125	ARG	NE-CZ-NH2	-12.23	114.19	120.30
1	D	130	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	B	707	THR	N-CA-CB	11.91	132.94	110.30
1	A	37	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	C	601	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	C	471	ARG	NE-CZ-NH2	11.63	126.12	120.30
1	B	61	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	C	725	ASP	CB-CG-OD1	11.41	128.57	118.30
1	D	29	LEU	CB-CA-C	11.32	131.71	110.20
1	C	27	ASP	CA-CB-CG	-11.27	88.60	113.40
1	C	59	ASP	CB-CG-OD1	11.21	128.39	118.30
1	B	612	ARG	CD-NE-CZ	11.18	139.25	123.60
1	A	713	GLN	N-CA-CB	-10.79	91.18	110.60
1	D	449	HIS	CA-CB-CG	10.76	131.89	113.60
1	A	278	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	D	643	ASP	CB-CG-OD1	10.59	127.83	118.30
1	B	521	ARG	CD-NE-CZ	10.59	138.42	123.60
1	C	467	ASP	CB-CG-OD1	10.55	127.80	118.30
1	D	33	ASP	CB-CG-OD2	-10.54	108.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	LEU	CB-CA-C	10.31	129.79	110.20
1	B	121	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	644	ASP	CB-CG-OD1	10.21	127.49	118.30
1	A	28	SER	CA-C-N	-10.14	94.89	117.20
1	A	121	ARG	CD-NE-CZ	10.06	137.69	123.60
1	A	27	ASP	CB-CG-OD1	10.00	127.30	118.30
1	C	725	ASP	CB-CA-C	-10.00	90.40	110.40
1	D	369	ARG	CD-NE-CZ	9.94	137.52	123.60
1	A	260	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	C	725	ASP	N-CA-CB	-9.89	92.80	110.60
1	D	345	ASP	CB-CG-OD1	9.85	127.16	118.30
1	B	29	LEU	CB-CA-C	9.78	128.78	110.20
1	B	521	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	B	130	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	B	96	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	A	712	ASP	N-CA-CB	-9.65	93.23	110.60
1	A	180	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	D	725	ASP	CB-CG-OD1	9.63	126.97	118.30
1	D	278	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	D	521	ARG	NE-CZ-NH2	9.53	125.07	120.30
1	D	180	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	B	72	ARG	NE-CZ-NH2	-9.49	115.55	120.30
1	A	28	SER	C-N-CA	-9.48	97.99	121.70
1	C	72	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	313	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	601	ARG	CD-NE-CZ	9.29	136.60	123.60
1	D	440	TYR	CB-CG-CD2	9.26	126.55	121.00
1	D	177	ASP	CB-CG-OD1	9.25	126.63	118.30
1	A	28	SER	CB-CA-C	-9.24	92.55	110.10
1	C	445	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	121	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	D	479	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	D	242	TYR	CB-CG-CD1	9.08	126.45	121.00
1	D	320	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	A	479	ARG	CD-NE-CZ	9.05	136.28	123.60
1	D	125	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	710	ILE	O-C-N	-8.92	108.43	122.70
1	B	59	ASP	CB-CG-OD2	8.86	126.27	118.30
1	D	680	ASP	CB-CG-OD1	8.85	126.26	118.30
1	C	636	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	C	33	ASP	CB-CG-OD1	8.64	126.08	118.30
1	D	180	ARG	NE-CZ-NH2	-8.59	116.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	ASP	CB-CG-OD1	8.56	126.01	118.30
1	D	242	TYR	CB-CG-CD2	-8.54	115.88	121.00
1	D	290	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	C	27	ASP	N-CA-C	8.48	133.90	111.00
1	A	536	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	91	ASP	CB-CG-OD1	8.41	125.87	118.30
1	D	740	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	712	ASP	O-C-N	-8.40	109.26	122.70
1	B	612	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	D	264	ARG	CD-NE-CZ	8.37	135.31	123.60
1	D	61	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	D	290	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	467	ASP	CB-CG-OD1	8.34	125.80	118.30
1	A	540	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	A	28	SER	N-CA-CB	8.30	122.95	110.50
1	D	28	SER	C-N-CA	-8.29	100.97	121.70
1	D	636	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	C	27	ASP	CB-CG-OD2	8.27	125.75	118.30
1	D	260	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	712	ASP	CB-CG-OD1	8.23	125.71	118.30
1	D	440	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	A	471	ARG	NE-CZ-NH1	-8.17	116.21	120.30
1	D	598	VAL	N-CA-CB	-8.17	93.52	111.50
1	A	33	ASP	CB-CG-OD1	8.16	125.64	118.30
1	D	497	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	488	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	B	440	TYR	CB-CG-CD2	8.10	125.86	121.00
1	A	183	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	710	ILE	CA-C-O	8.04	136.98	120.10
1	C	305	ASP	CB-CG-OD1	8.03	125.52	118.30
1	C	663	ASP	CB-CG-OD2	8.02	125.52	118.30
1	C	111	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	321	GLU	CA-CB-CG	7.97	130.94	113.40
1	B	28	SER	CA-C-N	-7.97	99.67	117.20
1	D	355	ASP	CB-CG-OD1	7.96	125.47	118.30
1	B	180	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	96	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	D	753	ALA	CA-C-O	-7.89	103.52	120.10
1	B	440	TYR	CB-CG-CD1	-7.89	116.27	121.00
1	C	130	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	C	290	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	64	LYS	CD-CE-NZ	7.76	129.55	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	D	740	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	37	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	130	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	C	278	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	495	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	C	542	ARG	CA-CB-CG	7.65	130.22	113.40
1	C	27	ASP	CB-CG-OD1	-7.63	111.44	118.30
1	B	141	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	A	96	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	B	260	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	479	ARG	CD-NE-CZ	7.57	134.20	123.60
1	B	417	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	C	405	ASP	CB-CG-OD2	7.55	125.09	118.30
1	D	260	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	D	121	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	28	SER	O-C-N	7.52	134.73	122.70
1	B	355	ASP	CB-CG-OD1	7.51	125.06	118.30
1	B	601	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	B	73	LYS	CA-CB-CG	7.46	129.81	113.40
1	A	445	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	B	37	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	B	542	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	C	100	ARG	N-CA-CB	7.40	123.92	110.60
1	B	551	ASP	CB-CG-OD1	-7.36	111.67	118.30
1	C	28	SER	C-N-CA	-7.34	103.35	121.70
1	A	130	ARG	NH1-CZ-NH2	-7.33	111.34	119.40
1	A	542	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	29	LEU	N-CA-C	7.33	130.78	111.00
1	C	440	TYR	CB-CG-CD1	-7.29	116.62	121.00
1	B	314	ASP	CB-CG-OD1	7.27	124.85	118.30
1	C	663	ASP	CB-CG-OD1	-7.26	111.77	118.30
1	A	712	ASP	CA-C-O	7.23	135.28	120.10
1	C	440	TYR	CB-CG-CD2	7.18	125.31	121.00
1	D	488	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	169	VAL	CG1-CB-CG2	-7.16	99.44	110.90
1	B	27	ASP	CA-C-O	7.11	135.03	120.10
1	C	725	ASP	CA-CB-CG	7.10	129.03	113.40
1	B	597	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	710	ILE	CA-CB-CG1	7.09	124.47	111.00
1	D	597	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	485	TYR	CB-CG-CD1	-7.07	116.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	753	ALA	CA-C-O	-7.07	105.25	120.10
1	A	730	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	96	ARG	NH1-CZ-NH2	7.05	127.15	119.40
1	D	725	ASP	N-CA-C	7.04	130.02	111.00
1	D	111	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	D	260	ARG	NH1-CZ-NH2	7.04	127.14	119.40
1	B	542	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	D	264	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	753	ALA	CA-C-O	-7.01	105.37	120.10
1	A	183	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	350	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	B	643	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	28	SER	O-C-N	6.94	133.81	122.70
1	B	37	ARG	CD-NE-CZ	6.94	133.31	123.60
1	B	76	GLU	OE1-CD-OE2	6.92	131.61	123.30
1	A	344	GLU	CA-CB-CG	6.91	128.60	113.40
1	C	181	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	29	LEU	C-N-CA	6.89	138.93	121.70
1	C	369	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	B	111	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	137	TYR	CB-CG-CD2	6.87	125.12	121.00
1	D	100	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	72	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	27	ASP	N-CA-C	6.84	129.46	111.00
1	B	505	TYR	CB-CG-CD1	-6.84	116.90	121.00
1	C	320	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	D	183	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	146	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	339	GLN	N-CA-CB	6.82	122.88	110.60
1	B	267	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	28	SER	CA-CB-OG	6.80	129.56	111.20
1	B	27	ASP	CA-CB-CG	-6.78	98.48	113.40
1	B	617	LEU	CB-CA-C	-6.77	97.33	110.20
1	B	28	SER	O-C-N	6.76	133.51	122.70
1	A	711	ALA	O-C-N	-6.74	111.92	122.70
1	A	488	ARG	NH1-CZ-NH2	6.68	126.75	119.40
1	A	320	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	D	344	GLU	CB-CA-C	-6.66	97.07	110.40
1	C	320	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	725	ASP	N-CA-C	6.64	128.94	111.00
1	B	521	ARG	NH1-CZ-NH2	-6.61	112.13	119.40
1	D	445	ARG	CD-NE-CZ	6.61	132.85	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	702	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	700	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	488	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	C	640	VAL	N-CA-CB	6.57	125.95	111.50
1	A	29	LEU	CA-CB-CG	6.56	130.39	115.30
1	C	54	SER	CB-CA-C	6.56	122.56	110.10
1	C	146	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	290	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	680	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	615	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	497	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	479	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	377	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	727	SER	N-CA-CB	-6.44	100.84	110.50
1	A	411	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	319	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	536	ARG	NH1-CZ-NH2	6.43	126.47	119.40
1	D	479	ARG	NE-CZ-NH1	-6.43	117.09	120.30
1	B	41	GLU	OE1-CD-OE2	-6.42	115.59	123.30
1	A	100	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	B	467	ASP	CB-CG-OD1	6.35	124.01	118.30
1	B	683	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	B	411	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	28	SER	O-C-N	6.33	132.83	122.70
1	A	320	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	509	ARG	NE-CZ-NH2	6.31	123.46	120.30
1	D	554	LEU	CA-CB-CG	6.31	129.81	115.30
1	B	33	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	100	ARG	CD-NE-CZ	6.28	132.38	123.60
1	A	487	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	B	37	ARG	CA-CB-CG	6.25	127.14	113.40
1	D	435	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	612	ARG	CD-NE-CZ	6.21	132.29	123.60
1	B	305	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	568	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	403	THR	N-CA-CB	6.20	122.07	110.30
1	D	61	ARG	CB-CG-CD	6.19	127.69	111.60
1	A	702	ARG	CD-NE-CZ	6.17	132.24	123.60
1	A	70	ASP	OD1-CG-OD2	-6.13	111.65	123.30
1	B	334	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	D	677	ASP	CB-CG-OD1	6.12	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	237	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	350	ASP	CB-CA-C	-6.11	98.19	110.40
1	A	709	LYS	C-N-CA	-6.08	106.49	121.70
1	A	711	ALA	CA-C-O	6.08	132.88	120.10
1	D	540	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	41	GLU	CA-CB-CG	6.08	126.78	113.40
1	B	141	TYR	CB-CG-CD1	6.06	124.63	121.00
1	B	683	TYR	CB-CG-CD2	6.03	124.61	121.00
1	A	314	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	677	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	B	167	SER	N-CA-CB	-5.96	101.56	110.50
1	A	643	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	497	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	D	569	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	C	401	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	319	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	264	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	87	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	D	100	ARG	CG-CD-NE	5.92	124.23	111.80
1	D	369	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	278	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	D	711	ALA	CA-C-O	5.88	132.46	120.10
1	D	151	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	435	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	345	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	495	ARG	CD-NE-CZ	5.86	131.81	123.60
1	A	479	ARG	CG-CD-NE	5.83	124.03	111.80
1	A	710	ILE	N-CA-CB	-5.81	97.44	110.80
1	A	100	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	644	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	B	290	ARG	N-CA-CB	5.79	121.02	110.60
1	A	79	ALA	N-CA-CB	-5.78	102.01	110.10
1	A	609	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	753	ALA	CA-C-O	-5.77	107.98	120.10
1	B	59	ASP	CA-CB-CG	-5.77	100.71	113.40
1	B	54	SER	CB-CA-C	5.77	121.06	110.10
1	C	730	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	C	422	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	725	ASP	N-CA-C	5.75	126.51	111.00
1	B	525	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	28	SER	C-N-CA	-5.73	107.37	121.70
1	C	636	ARG	NE-CZ-NH1	5.73	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	185	PHE	CB-CG-CD1	5.70	124.79	120.80
1	D	324	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	D	497	ARG	CD-NE-CZ	5.66	131.53	123.60
1	B	551	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	740	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	69	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	D	725	ASP	CA-CB-CG	5.63	125.79	113.40
1	A	530	GLU	OE1-CD-OE2	-5.62	116.55	123.30
1	C	677	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	591	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	C	602	VAL	CB-CA-C	-5.61	100.75	111.40
1	B	290	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	568	ASP	N-CA-CB	-5.60	100.52	110.60
1	B	688	ALA	CB-CA-C	-5.58	101.72	110.10
1	C	642	ALA	CB-CA-C	-5.58	101.72	110.10
1	D	422	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	73	LYS	CD-CE-NZ	-5.56	98.92	111.70
1	C	330	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	27	ASP	CA-C-N	-5.55	105.00	117.20
1	C	579	VAL	CG1-CB-CG2	5.54	119.76	110.90
1	A	727	SER	CB-CA-C	5.53	120.61	110.10
1	A	264	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	377	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	183	ARG	CG-CD-NE	5.52	123.39	111.80
1	B	377	ARG	CA-CB-CG	-5.51	101.28	113.40
1	B	124	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	C	48	GLN	CA-CB-CG	5.51	125.52	113.40
1	C	644	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	100	ARG	CG-CD-NE	5.49	123.34	111.80
1	D	612	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	730	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	749	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	D	725	ASP	CA-C-N	5.46	127.12	116.20
1	D	618	ALA	N-CA-CB	5.45	117.73	110.10
1	A	505	TYR	CB-CG-CD2	5.45	124.27	121.00
1	C	377	ARG	CD-NE-CZ	-5.44	115.98	123.60
1	B	355	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	27	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	403	THR	N-CA-CB	5.40	120.56	110.30
1	A	248	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	B	422	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	538	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	D	369	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	197	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	749	ASP	N-CA-CB	-5.35	100.97	110.60
1	D	111	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	D	578	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	54	SER	CA-CB-OG	-5.34	96.78	111.20
1	C	87	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	210	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	183	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	72	ARG	CD-NE-CZ	5.33	131.07	123.60
1	B	238	THR	CA-CB-CG2	-5.33	104.93	112.40
1	B	471	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	B	37	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	B	446	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	29	LEU	N-CA-CB	-5.29	99.81	110.40
1	A	165	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	387	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	D	350	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	C	111	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	505	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	D	316	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	62	ASN	CB-CA-C	5.27	120.94	110.40
1	A	278	ARG	CD-NE-CZ	5.27	130.98	123.60
1	C	265	SER	N-CA-CB	-5.27	102.60	110.50
1	B	715	GLU	CA-CB-CG	5.26	124.97	113.40
1	C	197	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	C	380	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	636	ARG	NH1-CZ-NH2	-5.24	113.63	119.40
1	C	407	LEU	CB-CG-CD2	-5.24	102.10	111.00
1	C	364	LEU	O-C-N	-5.21	114.36	122.70
1	A	722	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	54	SER	O-C-N	-5.21	114.37	122.70
1	B	497	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	267	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	C	368	GLN	CB-CG-CD	5.20	125.13	111.60
1	B	503	GLU	OE1-CD-OE2	-5.20	117.06	123.30
1	B	707	THR	CB-CA-C	-5.20	97.56	111.60
1	C	260	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	660	LEU	N-CA-CB	-5.19	100.02	110.40
1	C	264	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	647	VAL	CG1-CB-CG2	-5.17	102.62	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	LYS	CA-CB-CG	5.16	124.76	113.40
1	B	278	ARG	CD-NE-CZ	5.16	130.83	123.60
1	C	159	ILE	CB-CG1-CD1	-5.16	99.46	113.90
1	C	538	TYR	CB-CG-CD1	5.16	124.09	121.00
1	C	159	ILE	CB-CA-C	5.15	121.90	111.60
1	A	497	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	316	ASP	CB-CG-OD2	5.14	122.92	118.30
1	D	270	GLU	OE1-CD-OE2	-5.14	117.14	123.30
1	B	485	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	D	293	TRP	N-CA-CB	5.13	119.83	110.60
1	A	440	TYR	CB-CG-CD1	-5.12	117.92	121.00
1	D	54	SER	CB-CA-C	5.11	119.80	110.10
1	B	578	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	569	ASP	N-CA-CB	5.09	119.77	110.60
1	D	648	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	571	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	29	LEU	N-CA-CB	-5.07	100.26	110.40
1	D	478	LYS	CA-CB-CG	5.07	124.55	113.40
1	C	151	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	270	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	A	185	PHE	CB-CG-CD1	5.05	124.33	120.80
1	D	725	ASP	CA-C-O	-5.05	109.50	120.10
1	C	612	ARG	CG-CD-NE	5.05	122.40	111.80
1	A	716	GLU	CA-CB-CG	5.04	124.48	113.40
1	A	472	GLU	OE1-CD-OE2	5.02	129.32	123.30
1	B	724	ALA	C-N-CA	5.02	134.25	121.70
1	D	585	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	488	ARG	NH1-CZ-NH2	-5.01	113.89	119.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ASP	Mainchain,Peptide
1	A	28	SER	Mainchain
1	A	711	ALA	Mainchain
1	D	157	ASN	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5748	0	5586	81	0
1	B	5748	0	5586	84	0
1	C	5748	0	5586	86	0
1	D	5748	0	5586	85	1
2	A	43	0	30	4	0
2	B	43	0	30	6	0
2	C	43	0	30	4	0
2	D	43	0	30	7	0
3	A	728	0	0	7	2
3	B	625	0	0	14	0
3	C	634	0	0	13	1
3	D	692	0	0	10	2
All	All	25843	0	22464	298	3

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 (298) 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:725:ASP:HB2	1:C:728:PHE:HB3	1.30	1.08
1:B:583:LYS:HE2	1:B:583:LYS:H	1.25	0.98
1:C:724:ALA:O	1:C:725:ASP:HB3	1.65	0.96
1:B:415:TYR:HB2	3:B:1378:HOH:O	1.64	0.95
1:D:369:ARG:HB2	3:D:1392:HOH:O	1.76	0.86
1:A:126[B]:ILE:HD12	1:A:127:VAL:HG22	1.58	0.84
1:A:726:GLY:HA3	3:A:1398:HOH:O	1.77	0.84
1:D:126[B]:ILE:HD11	2:D:754:HEM:CMD	2.08	0.84
1:B:368:GLN:HB2	3:B:1245:HOH:O	1.78	0.83
1:B:583:LYS:CE	1:B:583:LYS:H	1.91	0.82
1:B:126[A]:ILE:HD11	1:C:118:ASP:O	1.80	0.82
1:D:710:ILE:HD13	1:D:718:ILE:HG13	1.62	0.82
1:D:126[B]:ILE:HD11	2:D:754:HEM:HMD1	1.66	0.77
1:C:126[B]:ILE:HD11	2:C:754:HEM:CMD	2.14	0.77
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ARG:NH1	3:B:1296:HOH:O	2.13	0.74
1:C:126[B]:ILE:HD11	2:C:754:HEM:HMD1	1.69	0.74
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.70	0.73
1:A:27:ASP:CB	1:A:28:SER:HA	2.19	0.72
1:D:28:SER:H	1:D:29:LEU:HD23	1.55	0.71
1:C:386:ASN:HD22	1:C:386:ASN:C	1.94	0.70
1:D:39:ALA:H	1:D:48:GLN:NE2	1.89	0.70
1:B:126[B]:ILE:HD11	2:B:754:HEM:CMD	2.21	0.70
1:A:28:SER:O	1:A:29:LEU:CB	2.39	0.70
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.73	0.70
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.74	0.69
1:D:726:GLY:O	3:D:1205:HOH:O	2.11	0.69
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.27	0.69
1:A:708:ILE:O	1:A:710:ILE:HB	1.93	0.69
1:B:369:ARG:HG2	3:B:1115:HOH:O	1.91	0.69
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.75	0.68
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.74	0.68
1:A:27:ASP:N	3:A:1362:HOH:O	2.26	0.67
1:C:488:ARG:HH21	1:D:492:ASN:ND2	1.93	0.67
1:D:126[B]:ILE:HD11	2:D:754:HEM:HMD2	1.76	0.67
1:A:70:ASP:OD1	1:A:71:VAL:HG13	1.95	0.67
1:B:583:LYS:N	1:B:583:LYS:HE2	2.05	0.66
3:B:904:HOH:O	1:C:126[A]:ILE:HD11	1.96	0.66
1:A:386:ASN:HD22	1:A:386:ASN:C	1.98	0.66
1:B:117:PHE:CE2	1:C:126[B]:ILE:HD12	2.31	0.65
1:C:704:PHE:O	1:C:707:THR:HG22	1.96	0.65
1:D:165:ARG:HE	1:D:386:ASN:HD21	1.46	0.64
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.61	0.63
3:B:924:HOH:O	1:D:73:LYS:HE2	1.97	0.63
1:A:751:ILE:O	1:A:751:ILE:HD12	1.98	0.63
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.14	0.63
1:B:330:ASP:OD2	1:B:629:HIS:HE1	1.82	0.62
1:A:73:LYS:NZ	1:C:440:TYR:OH	2.30	0.62
1:A:126[B]:ILE:HD13	1:D:117:PHE:CE2	2.34	0.62
1:B:37:ARG:HD2	3:B:1319:HOH:O	1.98	0.62
1:A:488:ARG:NE	1:A:490:GLU:OE2	2.26	0.62
1:D:330:ASP:OD2	1:D:629:HIS:HE1	1.84	0.61
1:D:28:SER:H	1:D:29:LEU:CD2	2.12	0.61
1:B:386:ASN:C	1:B:386:ASN:HD22	2.03	0.61
1:A:126[B]:ILE:CD1	1:A:127:VAL:HG22	2.29	0.61
1:C:266:TYR:HB2	3:C:1191:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:HIS:HB2	1:D:449:HIS:CE1	2.35	0.61
1:D:27:ASP:HB2	1:D:29:LEU:HD21	1.83	0.61
1:B:126[B]:ILE:HD11	2:B:754:HEM:HMD1	1.82	0.60
3:A:1472:HOH:O	1:D:126[A]:ILE:HD11	2.01	0.60
1:C:552:LEU:HD13	1:C:556:GLN:NE2	2.16	0.60
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.85	0.59
1:C:345:ASP:HA	1:C:348:LYS:HD3	1.85	0.59
1:B:165:ARG:HE	1:B:386:ASN:HD21	1.48	0.59
1:A:341:ILE:HD12	1:A:353:LEU:HD21	1.85	0.59
1:B:126[B]:ILE:HD11	2:B:754:HEM:HMD2	1.84	0.58
1:D:274:ILE:HD12	2:D:754:HEM:HMB1	1.84	0.58
1:D:386:ASN:C	1:D:386:ASN:HD22	2.06	0.58
1:A:435:ARG:NH1	3:A:1137:HOH:O	2.25	0.58
1:D:631:LYS:HE2	3:D:1261:HOH:O	2.04	0.57
1:B:126[B]:ILE:HD13	1:C:118:ASP:HA	1.86	0.57
1:C:126[B]:ILE:HD11	2:C:754:HEM:HMD2	1.86	0.57
1:D:631:LYS:HG3	1:D:633:LEU:HD13	1.85	0.57
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.39	0.57
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.86	0.57
1:C:435:ARG:HD3	3:C:1120:HOH:O	2.05	0.57
1:D:751:ILE:HD13	1:D:752:PRO:HD2	1.85	0.57
1:D:126[B]:ILE:CD1	2:D:754:HEM:HMD1	2.34	0.56
1:B:751:ILE:HD12	1:B:753:ALA:HB2	1.86	0.56
1:B:562:LEU:HA	1:C:637:MET:HB2	1.87	0.56
1:A:37:ARG:NH2	1:C:466:ASN:HA	2.20	0.56
1:B:725:ASP:OD1	1:B:726:GLY:N	2.39	0.56
1:C:330:ASP:OD2	1:C:629:HIS:HE1	1.89	0.56
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.21	0.56
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.37	0.55
1:B:118:ASP:HA	1:C:126[B]:ILE:HD13	1.87	0.55
1:C:178:THR:HG21	1:C:310:LEU:HD23	1.88	0.55
1:B:345:ASP:HA	1:B:348:LYS:HD2	1.89	0.55
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.21	0.55
1:C:709:LYS:N	1:C:709:LYS:HD2	2.22	0.55
1:C:604:ALA:HB1	1:C:633:LEU:HD22	1.89	0.55
1:A:118:ASP:HA	1:D:126[B]:ILE:HD13	1.89	0.55
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.37	0.55
1:A:710:ILE:HG12	1:A:715:GLU:OE1	2.07	0.54
1:B:39:ALA:N	1:B:48:GLN:OE1	2.34	0.54
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.39	0.54
1:A:583:LYS:O	1:A:584:LYS:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASP:CG	3:C:873:HOH:O	2.46	0.54
1:B:126[A]:ILE:HD13	3:C:1387:HOH:O	2.08	0.54
1:B:749:ASP:OD2	1:B:750:LYS:HE2	2.08	0.54
1:A:165:ARG:HE	1:A:386:ASN:HD21	1.56	0.53
1:B:377:ARG:NH2	3:B:1296:HOH:O	2.40	0.53
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.91	0.53
1:C:629:HIS:HD2	3:C:1054:HOH:O	1.91	0.53
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.90	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.57	0.53
1:A:28:SER:O	1:A:29:LEU:CG	2.57	0.52
1:B:377:ARG:NH1	1:B:378:ASN:O	2.42	0.52
1:B:27:ASP:CG	1:D:468:ASN:HD22	2.13	0.52
1:A:126[B]:ILE:HD11	2:A:754:HEM:CMD	2.40	0.52
1:D:574:THR:HG22	3:D:1363:HOH:O	2.09	0.52
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.40	0.52
1:A:76:GLU:O	1:A:77:ASN:HB2	2.08	0.52
1:A:28:SER:C	1:A:29:LEU:CG	2.79	0.52
1:B:126[B]:ILE:HD12	1:C:117:PHE:CE2	2.45	0.52
1:C:183:ARG:HG2	3:C:1381:HOH:O	2.08	0.52
1:C:488:ARG:HH21	1:D:492:ASN:HD21	1.54	0.52
1:C:700:ASP:O	1:C:703:LYS:HG3	2.10	0.52
1:B:207:PHE:O	1:B:249:THR:HA	2.10	0.51
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.90	0.51
1:B:344:GLU:H	1:B:344:GLU:CD	2.14	0.51
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.46	0.51
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.14	0.51
1:B:578:ASP:HB3	1:B:582:LEU:O	2.10	0.51
1:A:36:HIS:CD2	1:A:36:HIS:H	2.29	0.50
1:B:377:ARG:CZ	3:B:1296:HOH:O	2.58	0.50
1:D:751:ILE:HD13	1:D:752:PRO:CD	2.41	0.50
1:B:634:TYR:O	1:B:653:THR:HA	2.11	0.50
1:D:435:ARG:HD3	3:D:1135:HOH:O	2.11	0.50
3:A:919:HOH:O	1:C:52:PRO:HG3	2.12	0.50
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.93	0.50
1:B:629:HIS:HD2	3:B:1059:HOH:O	1.94	0.49
3:C:1104:HOH:O	1:D:488:ARG:HD2	2.11	0.49
1:D:629:HIS:HD2	3:D:1068:HOH:O	1.95	0.49
1:C:322:LEU:HB2	3:C:1191:HOH:O	2.11	0.49
1:C:725:ASP:O	1:C:725:ASP:OD1	2.29	0.49
1:C:725:ASP:O	1:C:725:ASP:CG	2.48	0.49
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HG2	1:D:126[A]:ILE:HD13	1.95	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.27	0.49
1:B:583:LYS:CD	1:B:583:LYS:H	2.26	0.48
1:D:710:ILE:CD1	1:D:718:ILE:HG13	2.38	0.48
1:C:619:ILE:O	1:C:623:LEU:HG	2.14	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.12	0.48
1:C:205:ILE:H	1:C:205:ILE:HD13	1.78	0.48
1:B:274:ILE:HD12	2:B:754:HEM:HMB1	1.95	0.47
1:C:602:VAL:HG12	1:C:603:VAL:N	2.30	0.47
1:A:750:LYS:HB3	1:A:750:LYS:HZ2	1.80	0.47
2:B:754:HEM:CMB	2:B:754:HEM:HBB2	2.45	0.47
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.96	0.47
1:D:748:ILE:O	1:D:751:ILE:HG22	2.14	0.47
1:B:27:ASP:N	1:B:27:ASP:OD1	2.47	0.47
1:C:238:THR:HB	1:D:460:TYR:CE1	2.49	0.47
1:B:507:HIS:N	1:B:508:PRO:HD2	2.29	0.47
1:A:84:GLN:HG3	1:C:395:HIS:CD2	2.50	0.47
1:C:616:LEU:HD22	1:C:620:LEU:HG	1.96	0.47
1:A:27:ASP:OD1	1:A:28:SER:HB3	2.15	0.47
1:B:165:ARG:HE	1:B:386:ASN:ND2	2.12	0.47
1:C:274:ILE:HD12	2:C:754:HEM:HMB1	1.96	0.47
1:D:533:LYS:NZ	3:D:1366:HOH:O	2.48	0.47
1:A:117:PHE:CE2	1:D:126[B]:ILE:HD12	2.50	0.46
1:D:459:ASN:H	1:D:459:ASN:HD22	1.62	0.46
1:A:127:VAL:O	1:A:128:HIS:HB2	2.15	0.46
1:C:386:ASN:C	1:C:386:ASN:ND2	2.66	0.46
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.51	0.46
1:D:583:LYS:HB2	1:D:583:LYS:HZ3	1.80	0.46
1:D:659:SER:HB2	1:D:688:ALA:HB2	1.97	0.46
1:A:411:ARG:HG2	2:A:754:HEM:C2C	2.51	0.46
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.97	0.46
1:A:28:SER:C	1:A:29:LEU:HG	2.36	0.46
1:B:583:LYS:O	1:B:584:LYS:HB3	2.16	0.46
1:C:449:HIS:HB2	3:C:1285:HOH:O	2.14	0.46
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.98	0.46
1:A:725:ASP:CG	1:A:726:GLY:H	2.16	0.46
1:D:359:LEU:H	1:D:507:HIS:HD2	1.64	0.46
1:B:308:GLN:OE1	1:C:313:ARG:NH1	2.48	0.46
1:B:368:GLN:NE2	3:B:1141:HOH:O	2.45	0.46
1:D:708:ILE:HG13	1:D:710:ILE:HD12	1.97	0.46
1:B:607:LEU:HD22	1:B:611:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:TRP:CZ3	1:D:336:LEU:HB2	2.52	0.45
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.86	0.45
1:A:52:PRO:HG3	3:C:961:HOH:O	2.17	0.45
1:C:578:ASP:HB2	1:C:582:LEU:O	2.17	0.45
1:A:126[A]:ILE:HD11	3:D:1446:HOH:O	2.17	0.45
1:A:488:ARG:HA	1:B:492:ASN:HD22	1.81	0.45
1:B:469:TRP:CE3	1:B:471:ARG:HG3	2.52	0.45
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.99	0.45
1:A:435:ARG:HD3	3:A:1137:HOH:O	2.16	0.45
1:B:258:SER:HA	1:B:523:ILE:HG12	1.99	0.45
1:C:727:SER:HA	1:C:730:ASP:OD2	2.16	0.45
1:A:725:ASP:CG	1:A:726:GLY:N	2.65	0.44
1:C:507:HIS:N	1:C:508:PRO:HD2	2.32	0.44
1:B:275:HIS:CD2	1:B:408:LEU:HB2	2.52	0.44
1:A:488:ARG:HA	1:B:492:ASN:ND2	2.33	0.44
1:C:165:ARG:HE	1:C:386:ASN:HD21	1.65	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.34	0.44
1:C:507:HIS:N	1:C:508:PRO:CD	2.80	0.44
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.48	0.44
1:D:631:LYS:HG3	1:D:633:LEU:CD1	2.46	0.44
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.53	0.44
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.48	0.44
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.53	0.43
1:C:725:ASP:OD2	1:C:729:MET:N	2.23	0.43
1:A:29:LEU:HA	1:C:467:ASP:OD1	2.18	0.43
1:D:708:ILE:CD1	1:D:710:ILE:HD12	2.49	0.43
1:D:725:ASP:O	3:D:1207:HOH:O	2.21	0.43
1:B:27:ASP:CG	1:D:468:ASN:ND2	2.72	0.43
1:C:461:GLU:HB2	1:C:462:PRO:HA	1.99	0.43
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.72	0.43
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.53	0.43
1:B:435:ARG:HD3	3:B:1136:HOH:O	2.18	0.43
1:C:610:GLU:O	1:C:610:GLU:HG3	2.18	0.43
1:D:97:ALA:O	1:D:101:GLY:HA3	2.19	0.43
1:A:748:ILE:O	1:A:751:ILE:HG13	2.18	0.43
1:C:725:ASP:OD2	1:C:726:GLY:O	2.37	0.43
1:D:222:LYS:HB3	1:D:223:PRO:HD2	2.00	0.43
1:A:104:LEU:HB3	3:C:775:HOH:O	2.19	0.43
1:C:552:LEU:HD22	1:C:552:LEU:O	2.18	0.43
1:D:583:LYS:O	1:D:584:LYS:HB3	2.18	0.43
2:A:754:HEM:CMC	2:A:754:HEM:HBC2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.49	0.43
1:D:320:ARG:HD3	3:D:916:HOH:O	2.18	0.43
1:A:313:ARG:NH2	1:D:309:LYS:HD2	2.34	0.43
1:B:121:ARG:HG2	1:C:126[A]:ILE:HD13	2.01	0.43
1:C:702:ARG:HE	1:C:702:ARG:HB2	1.66	0.43
1:A:73:LYS:HZ3	1:C:450:ARG:NH2	2.17	0.43
1:A:603:VAL:HG11	1:A:666:ILE:HD12	2.01	0.42
1:A:725:ASP:OD1	1:A:726:GLY:N	2.52	0.42
1:A:205:ILE:H	1:A:205:ILE:HD13	1.83	0.42
1:C:260:ARG:HD3	1:C:590:LEU:HD21	2.01	0.42
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.91	0.42
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.54	0.42
1:B:655:ALA:HB3	3:B:1324:HOH:O	2.20	0.42
1:A:511:PHE:O	1:A:515:GLN:HG2	2.18	0.42
1:B:377:ARG:HH11	1:B:377:ARG:HD2	1.37	0.42
1:B:536:ARG:HA	1:B:537:PRO:HD3	1.85	0.42
1:C:512:TRP:CZ3	1:C:554:LEU:HD13	2.54	0.42
1:C:602:VAL:HG21	3:C:1312:HOH:O	2.20	0.42
3:B:1136:HOH:O	1:D:451:MET:HE1	2.20	0.42
1:A:36:HIS:HE1	3:A:1329:HOH:O	2.01	0.42
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.00	0.42
1:C:341:ILE:HD12	1:C:341:ILE:N	2.35	0.42
1:C:724:ALA:O	1:C:725:ASP:CB	2.49	0.42
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.01	0.42
1:A:709:LYS:O	1:A:710:ILE:HB	2.15	0.42
1:B:222:LYS:HB3	1:B:223:PRO:HD2	2.01	0.42
1:B:705:LYS:HE3	1:B:710:ILE:HG22	2.02	0.42
1:B:51:ALA:HB1	1:B:52:PRO:HD2	2.01	0.42
1:C:126[A]:ILE:HG12	3:C:899:HOH:O	2.20	0.42
1:A:43:THR:HB	1:A:44:PRO:HD2	2.02	0.41
1:B:126[B]:ILE:CD1	2:B:754:HEM:HMD1	2.50	0.41
1:D:535:VAL:O	1:D:537:PRO:HD3	2.19	0.41
1:B:386:ASN:C	1:B:386:ASN:ND2	2.73	0.41
1:B:596:GLY:HA3	1:B:737:ALA:O	2.20	0.41
1:C:125:ARG:HB2	1:C:129:ALA:HA	2.01	0.41
1:D:195:ILE:HD11	1:D:436:PRO:HA	2.01	0.41
1:D:72:ARG:HD2	1:D:72:ARG:HH11	1.64	0.41
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.41
2:D:754:HEM:HBB2	2:D:754:HEM:CMB	2.50	0.41
1:B:27:ASP:CB	1:D:468:ASN:HD22	2.33	0.41
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:NH1	1:C:270:GLU:OE1	2.45	0.41
1:D:48:GLN:HB3	1:D:49:PRO:HD2	2.01	0.41
1:A:460:TYR:CE1	1:B:238:THR:HB	2.55	0.41
1:D:27:ASP:HB2	1:D:29:LEU:CD2	2.49	0.41
1:A:158:LYS:HE2	1:A:192:GLU:OE1	2.19	0.41
1:A:459:ASN:C	1:A:459:ASN:HD22	2.24	0.41
1:D:165:ARG:HE	1:D:386:ASN:ND2	2.14	0.41
2:D:754:HEM:HBB2	2:D:754:HEM:HMB1	2.03	0.41
1:A:126[B]:ILE:HD13	1:D:117:PHE:CZ	2.55	0.41
1:A:300:ALA:HB1	1:A:739:HIS:CE1	2.56	0.41
1:C:634:TYR:O	1:C:653:THR:HA	2.20	0.41
1:D:521:ARG:HH21	1:D:524:VAL:HG11	1.84	0.41
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.55	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41
1:B:473:THR:O	1:D:89:ALA:HA	2.21	0.41
1:B:725:ASP:HB2	1:B:726:GLY:H	1.55	0.41
1:D:126[B]:ILE:HD13	1:D:126[B]:ILE:HG21	1.85	0.41
1:A:97:ALA:O	1:A:101:GLY:HA3	2.20	0.41
1:C:359:LEU:H	1:C:507:HIS:CD2	2.39	0.41
1:C:605:ILE:HD12	1:C:630:ALA:HB1	2.03	0.41
1:D:148:THR:HB	1:D:279:LEU:HB3	2.01	0.41
1:D:634:TYR:O	1:D:653:THR:HA	2.21	0.41
1:D:634:TYR:CG	1:D:635:SER:N	2.89	0.41
1:D:748:ILE:HG13	1:D:749:ASP:N	2.36	0.41
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.57	0.40
1:D:364:LEU:HD11	1:D:580:ASN:HB2	2.03	0.40
1:B:275:HIS:CG	1:B:408:LEU:HB2	2.56	0.40
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.50	0.40
1:C:490:GLU:OE2	1:D:488:ARG:NH2	2.54	0.40
1:A:126[B]:ILE:HD12	1:A:127:VAL:N	2.36	0.40
1:A:274:ILE:HD12	2:A:754:HEM:HMB1	2.04	0.40
1:B:205:ILE:H	1:B:205:ILE:HD13	1.86	0.40
1:B:144:LEU:HD21	1:B:370:VAL:HG22	2.03	0.40
1:B:516:THR:HB	1:B:517:PRO:CD	2.52	0.40
1:A:709:LYS:O	1:A:710:ILE:CB	2.60	0.40
1:B:429:HIS:CG	1:D:83:ASN:HB3	2.56	0.40
1:C:612:ARG:HB2	1:C:612:ARG:NH1	2.37	0.40

All (3) 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)
3:A:1360:HOH:O	3:D:1418:HOH:O[1_455]	2.06	0.14
1:D:28:SER:CA	3:C:1326:HOH:O[2_555]	2.07	0.13
3:A:1133:HOH:O	3:D:1418:HOH:O[1_455]	2.12	0.08

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/753 (96%)	703 (97%)	19 (3%)	4 (1%)	28	29
1	B	726/753 (96%)	701 (97%)	22 (3%)	3 (0%)	38	41
1	C	726/753 (96%)	705 (97%)	19 (3%)	2 (0%)	44	49
1	D	726/753 (96%)	700 (96%)	25 (3%)	1 (0%)	55	63
All	All	2904/3012 (96%)	2809 (97%)	85 (3%)	10 (0%)	44	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	725	ASP
1	A	711	ALA
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	B	75	SER
1	C	28	SER
1	D	75	SER
1	A	29	LEU
1	B	28	SER

### 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	613/636 (96%)	587 (96%)	26 (4%)	34	43
1	B	613/636 (96%)	580 (95%)	33 (5%)	26	30
1	C	613/636 (96%)	572 (93%)	41 (7%)	19	21
1	D	613/636 (96%)	579 (94%)	34 (6%)	25	29
All	All	2452/2544 (96%)	2318 (94%)	134 (6%)	26	29

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	48	GLN
1	A	54	SER
1	A	185	PHE
1	A	191	THR
1	A	198	LEU
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	294	LYS
1	A	321	GLU
1	A	344	GLU
1	A	375	LEU
1	A	386	ASN
1	A	440	TYR
1	A	459	ASN
1	A	478	LYS
1	A	552	LEU
1	A	616	LEU
1	A	708	ILE
1	A	710	ILE
1	A	713	GLN
1	A	727	SER
1	A	750	LYS
1	B	28	SER
1	B	48	GLN

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Mol	Chain	Res	Type
1	B	54	SER
1	B	61	ARG
1	B	73	LYS
1	B	126[A]	ILE
1	B	126[B]	ILE
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	283	GLU
1	B	321	GLU
1	B	370	VAL
1	B	375	LEU
1	B	377	ARG
1	B	386	ASN
1	B	415	TYR
1	B	440	TYR
1	B	459	ASN
1	B	478	LYS
1	B	562	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	633	LEU
1	B	703	LYS
1	B	709	LYS
1	B	751	ILE
1	C	28	SER
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	285	LYS

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Mol	Chain	Res	Type
1	C	348	LYS
1	C	368	GLN
1	C	369	ARG
1	C	375	LEU
1	C	377	ARG
1	C	386	ASN
1	C	415	TYR
1	C	426	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	531	LEU
1	C	542	ARG
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	715	GLU
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	27	ASP
1	D	41	GLU
1	D	48	GLN
1	D	54	SER
1	D	61	ARG
1	D	127	VAL
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN

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Mol	Chain	Res	Type
1	D	294	LYS
1	D	340	LEU
1	D	375	LEU
1	D	386	ASN
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS
1	D	488	ARG
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	565	GLU
1	D	569	ASP
1	D	582	LEU
1	D	598	VAL
1	D	610	GLU
1	D	616	LEU
1	D	621	LYS
1	D	648	LEU
1	D	713	GLN
1	D	749	ASP
1	D	751	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	386	ASN
1	A	459	ASN
1	A	515	GLN
1	B	157	ASN
1	B	252	ASN
1	B	368	GLN
1	B	386	ASN
1	B	459	ASN
1	B	492	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	386	ASN
1	C	459	ASN

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Mol	Chain	Res	Type
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	386	ASN
1	D	449	HIS
1	D	459	ASN
1	D	492	ASN
1	D	507	HIS
1	D	546	GLN
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 carbohydrates 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	28,50,50	1.98	7 (25%)	17,82,82	1.67	5 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	754	1,3	28,50,50	2.14	9 (32%)	17,82,82	1.87	5 (29%)
2	HEM	C	754	1	28,50,50	2.13	9 (32%)	17,82,82	1.65	4 (23%)
2	HEM	D	754	1	28,50,50	2.10	6 (21%)	17,82,82	1.65	5 (29%)

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	-	0/6/54/54	0/0/8/8
2	HEM	B	754	1,3	-	0/6/54/54	0/0/8/8
2	HEM	C	754	1	-	0/6/54/54	0/0/8/8
2	HEM	D	754	1	-	0/6/54/54	0/0/8/8

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	754	HEM	C3B-C2B	-6.32	1.32	1.40
2	D	754	HEM	C3B-C2B	-5.31	1.33	1.40
2	B	754	HEM	C3B-C2B	-5.15	1.33	1.40
2	B	754	HEM	C3C-C2C	-5.10	1.33	1.40
2	A	754	HEM	C3B-C2B	-4.87	1.33	1.40
2	D	754	HEM	C3C-C2C	-4.34	1.34	1.40
2	A	754	HEM	C3C-C2C	-4.02	1.35	1.40
2	C	754	HEM	C3C-C2C	-3.73	1.35	1.40
2	B	754	HEM	C3D-C2D	-2.07	1.31	1.37
2	C	754	HEM	CMA-C3A	2.13	1.56	1.51
2	B	754	HEM	CMC-C2C	2.15	1.56	1.51
2	B	754	HEM	C1B-NB	2.18	1.39	1.36
2	C	754	HEM	C1C-NC	2.29	1.39	1.36
2	B	754	HEM	CAA-C2A	2.35	1.56	1.52
2	C	754	HEM	C1B-NB	2.36	1.39	1.36
2	D	754	HEM	CMB-C2B	2.36	1.56	1.51
2	A	754	HEM	CMB-C2B	2.42	1.56	1.51
2	B	754	HEM	CAD-C3D	2.45	1.57	1.52
2	D	754	HEM	C1C-NC	2.46	1.39	1.36
2	A	754	HEM	CMD-C2D	2.48	1.56	1.51
2	C	754	HEM	CAD-C3D	2.69	1.57	1.52
2	C	754	HEM	CMB-C2B	2.80	1.57	1.51
2	A	754	HEM	C1C-NC	2.84	1.40	1.36
2	A	754	HEM	C3B-CAB	3.26	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	754	HEM	C3B-CAB	3.32	1.54	1.47
2	A	754	HEM	C3C-CAC	3.44	1.54	1.47
2	C	754	HEM	C3C-CAC	3.45	1.54	1.47
2	B	754	HEM	C3C-CAC	3.80	1.55	1.47
2	D	754	HEM	C3C-CAC	3.81	1.55	1.47
2	B	754	HEM	C3B-CAB	3.89	1.55	1.47
2	D	754	HEM	C3B-CAB	4.27	1.56	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754	HEM	CMD-C2D-C1D	-4.31	121.84	128.46
2	C	754	HEM	CMD-C2D-C1D	-3.43	123.19	128.46
2	A	754	HEM	CMD-C2D-C1D	-3.41	123.23	128.46
2	D	754	HEM	CMD-C2D-C1D	-3.33	123.35	128.46
2	B	754	HEM	CMA-C3A-C4A	-2.59	124.48	128.46
2	A	754	HEM	CMA-C3A-C4A	-2.59	124.49	128.46
2	C	754	HEM	CMA-C3A-C4A	-2.46	124.68	128.46
2	B	754	HEM	CMB-C2B-C3B	2.04	128.68	124.89
2	A	754	HEM	CAD-CBD-CGD	2.05	116.16	112.66
2	A	754	HEM	CMB-C2B-C3B	2.05	128.70	124.89
2	D	754	HEM	CMB-C2B-C3B	2.18	128.93	124.89
2	A	754	HEM	CMD-C2D-C3D	2.23	129.15	124.94
2	B	754	HEM	CMC-C2C-C3C	2.27	129.10	124.89
2	D	754	HEM	CMD-C2D-C3D	2.30	129.28	124.94
2	C	754	HEM	CMD-C2D-C3D	2.31	129.30	124.94
2	C	754	HEM	CMB-C2B-C3B	2.37	129.30	124.89
2	D	754	HEM	CBA-CAA-C2A	2.48	117.23	112.48
2	D	754	HEM	CAD-CBD-CGD	3.09	117.94	112.66
2	B	754	HEM	CMD-C2D-C3D	3.24	131.04	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	754	HEM	4	0
2	B	754	HEM	6	0
2	C	754	HEM	4	0
2	D	754	HEM	7	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	727/753 (96%)	-0.70	9 (1%) 79 77	8, 16, 34, 64	0
1	B	727/753 (96%)	-0.63	11 (1%) 74 72	9, 17, 35, 63	0
1	C	727/753 (96%)	-0.66	9 (1%) 79 77	9, 17, 35, 63	0
1	D	727/753 (96%)	-0.75	6 (0%) 86 85	10, 16, 34, 62	0
All	All	2908/3012 (96%)	-0.68	35 (1%) 79 77	8, 16, 35, 64	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	ASP	8.7
1	A	28	SER	8.4
1	C	27	ASP	7.0
1	A	27	ASP	7.0
1	A	712	ASP	5.7
1	D	27	ASP	4.9
1	C	28	SER	4.7
1	D	28	SER	4.7
1	A	713	GLN	4.4
1	B	28	SER	4.3
1	C	726	GLY	4.1
1	B	750	LYS	4.1
1	D	750	LYS	3.6
1	A	711	ALA	3.6
1	B	677	ASP	3.5
1	C	725	ASP	3.3
1	A	710	ILE	3.2
1	C	711	ALA	3.2
1	A	750	LYS	3.0
1	A	32	GLU	2.9
1	B	713	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	749	ASP	2.8
1	B	726	GLY	2.8
1	B	712	ASP	2.7
1	C	749	ASP	2.7
1	C	677	ASP	2.5
1	C	750	LYS	2.5
1	D	749	ASP	2.4
1	B	647	VAL	2.3
1	B	32	GLU	2.3
1	C	32	GLU	2.2
1	D	751	ILE	2.1
1	A	29	LEU	2.1
1	B	673	ALA	2.0
1	D	711	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	B	754	43/43	0.98	0.09	0.11	10,15,19,27	0
2	HEM	D	754	43/43	0.97	0.09	-0.11	11,14,19,28	0
2	HEM	A	754	43/43	0.98	0.08	-0.15	11,14,19,28	0
2	HEM	C	754	43/43	0.98	0.09	-0.20	10,15,19,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.