



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 08:04 PM EDT

PDB ID : 3EH3  
Title : Structure of the reduced form of cytochrome ba3 oxidase from *Thermus thermophilus*  
Authors : Liu, B.; Chen, Y.; Doukov, T.; Soltis, S.M.; Stout, D.; Fee, J.A.  
Deposited on : 2008-09-11  
Resolution : 3.10 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

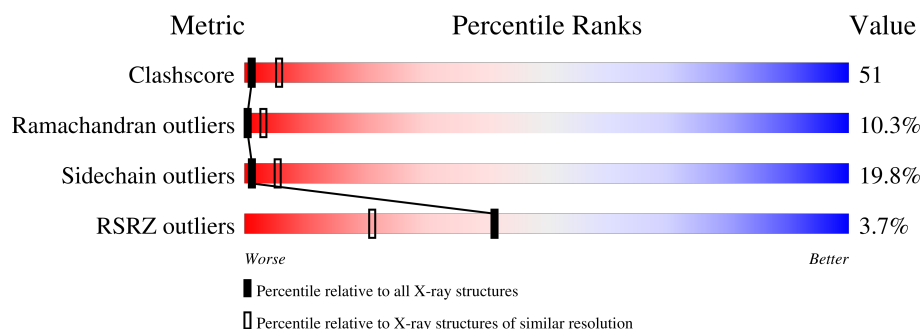
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	618	<div> <div>4%</div> <div> <div></div> <div>27%</div> <div>45%</div> <div>16%</div> <div>•</div> <div>10%</div> </div> </div>
2	B	166	<div> <div>2%</div> <div> <div></div> <div>35%</div> <div>42%</div> <div>21%</div> <div>•</div> </div> </div>
3	C	33	<div> <div>6%</div> <div> <div></div> <div>39%</div> <div>33%</div> <div>21%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEM	A	800	-	-	X	-
6	HAS	A	801	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6077 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4409	2985	709	699	16	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-55	SER	-	expression tag	UNP Q5SJ79
A	-54	GLU	-	expression tag	UNP Q5SJ79
A	-53	ILE	-	expression tag	UNP Q5SJ79
A	-52	SER	-	expression tag	UNP Q5SJ79
A	-51	ARG	-	expression tag	UNP Q5SJ79
A	-50	VAL	-	expression tag	UNP Q5SJ79
A	-49	TYR	-	expression tag	UNP Q5SJ79
A	-48	GLU	-	expression tag	UNP Q5SJ79
A	-47	ALA	-	expression tag	UNP Q5SJ79
A	-46	TYR	-	expression tag	UNP Q5SJ79
A	-45	PRO	-	expression tag	UNP Q5SJ79
A	-44	GLU	-	expression tag	UNP Q5SJ79
A	-43	LYS	-	expression tag	UNP Q5SJ79
A	-42	LYS	-	expression tag	UNP Q5SJ79
A	-41	ALA	-	expression tag	UNP Q5SJ79
A	-40	THR	-	expression tag	UNP Q5SJ79
A	-39	LEU	-	expression tag	UNP Q5SJ79
A	-38	TYR	-	expression tag	UNP Q5SJ79
A	-37	PHE	-	expression tag	UNP Q5SJ79
A	-36	LEU	-	expression tag	UNP Q5SJ79
A	-35	VAL	-	expression tag	UNP Q5SJ79
A	-34	LEU	-	expression tag	UNP Q5SJ79
A	-33	GLY	-	expression tag	UNP Q5SJ79
A	-32	PHE	-	expression tag	UNP Q5SJ79
A	-31	LEU	-	expression tag	UNP Q5SJ79
A	-30	ALA	-	expression tag	UNP Q5SJ79
A	-29	LEU	-	expression tag	UNP Q5SJ79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	ILE	-	expression tag	UNP Q5SJ79
A	-27	VAL	-	expression tag	UNP Q5SJ79
A	-26	GLY	-	expression tag	UNP Q5SJ79
A	-25	SER	-	expression tag	UNP Q5SJ79
A	-24	LEU	-	expression tag	UNP Q5SJ79
A	-23	PHE	-	expression tag	UNP Q5SJ79
A	-22	GLY	-	expression tag	UNP Q5SJ79
A	-21	PRO	-	expression tag	UNP Q5SJ79
A	-20	PHE	-	expression tag	UNP Q5SJ79
A	-19	GLN	-	expression tag	UNP Q5SJ79
A	-18	ALA	-	expression tag	UNP Q5SJ79
A	-17	LEU	-	expression tag	UNP Q5SJ79
A	-16	ASN	-	expression tag	UNP Q5SJ79
A	-15	TYR	-	expression tag	UNP Q5SJ79
A	-14	GLY	-	expression tag	UNP Q5SJ79
A	-13	ASN	-	expression tag	UNP Q5SJ79
A	-12	VAL	-	expression tag	UNP Q5SJ79
A	-11	ASP	-	expression tag	UNP Q5SJ79
A	-10	ALA	-	expression tag	UNP Q5SJ79
A	-9	TYR	-	expression tag	UNP Q5SJ79
A	-8	PRO	-	expression tag	UNP Q5SJ79
A	-7	LEU	-	expression tag	UNP Q5SJ79
A	-6	LEU	-	expression tag	UNP Q5SJ79
A	-5	MET	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79
A	258	ARG	LYS	engineered mutation	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	217	233	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	engineered mutation	UNP Q5SJ80

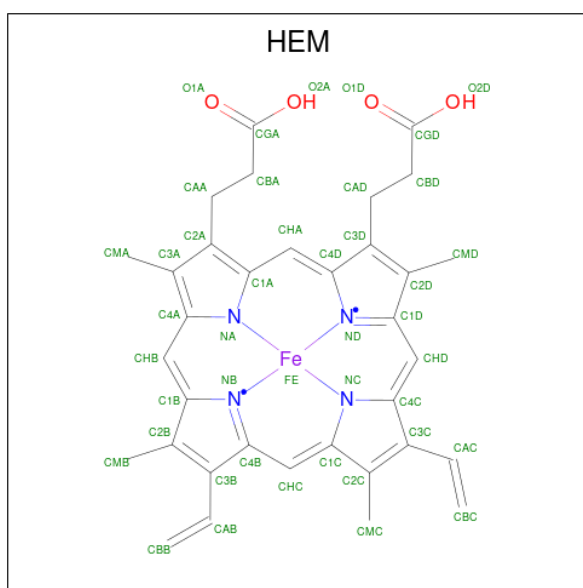
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

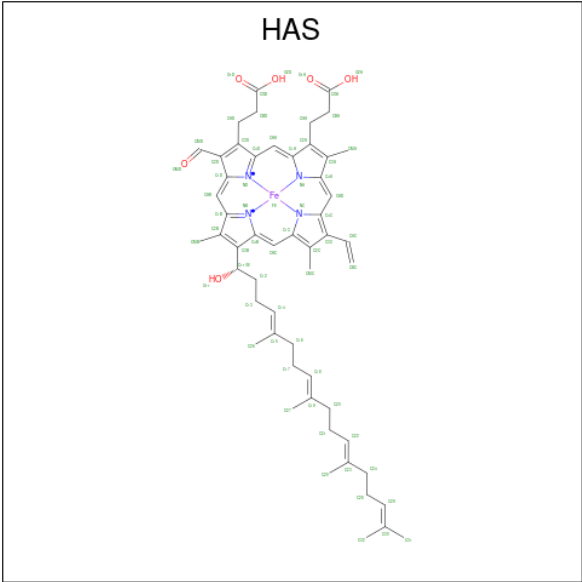
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



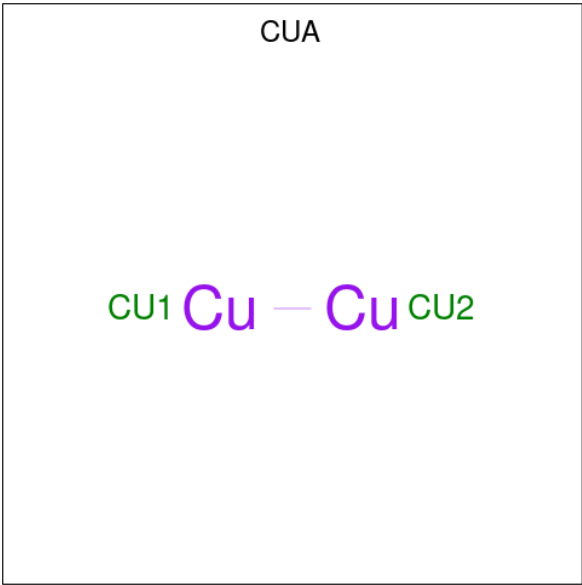
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula:  $C_{54}H_{64}FeN_4O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).

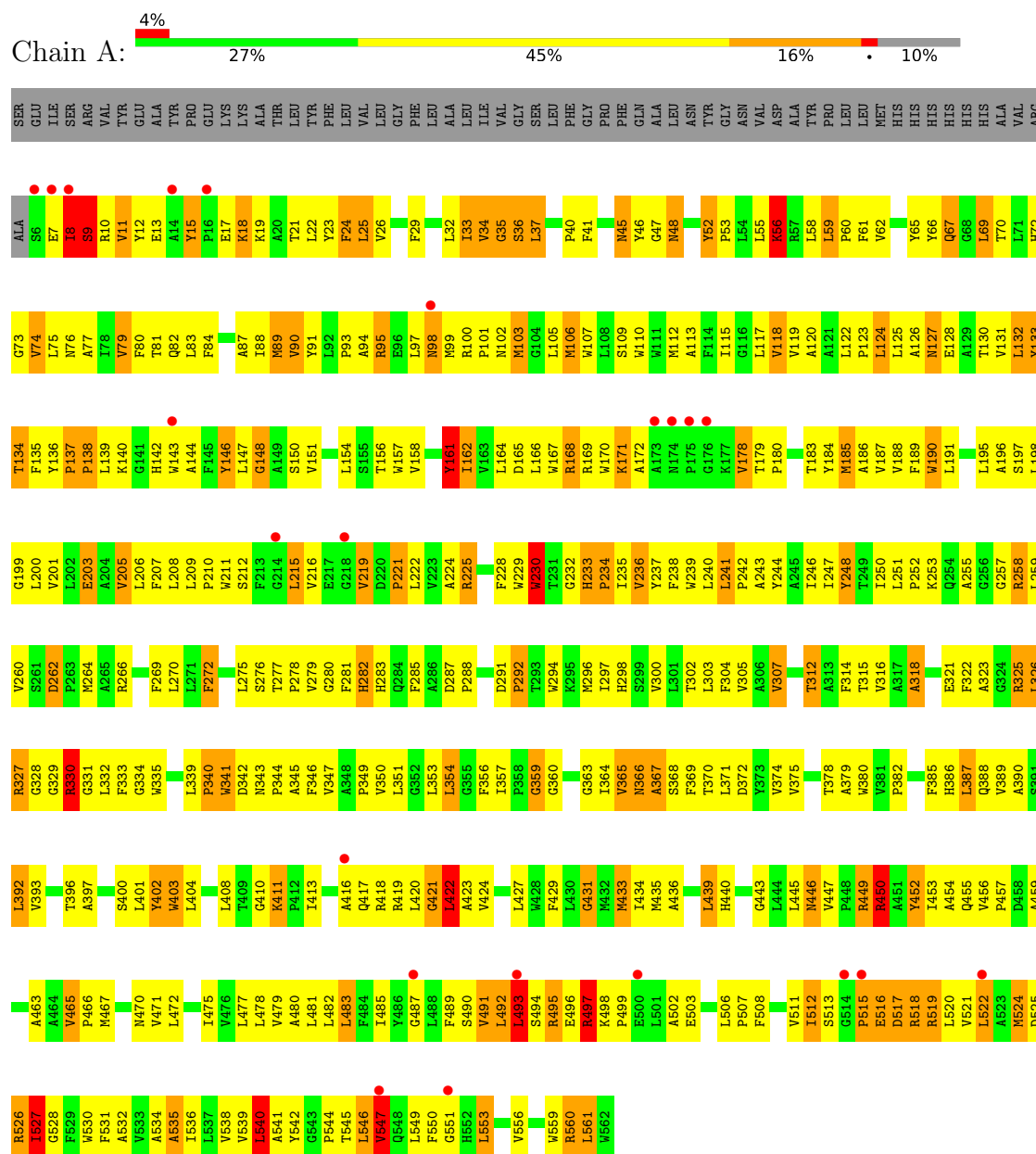


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
7	B	1	2	2	0	0

### 3 Residue-property plots

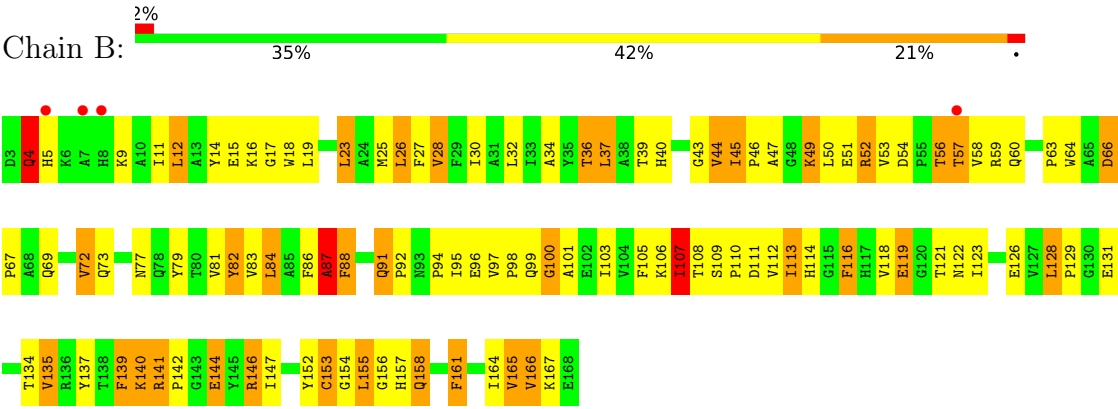
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Cytochrome c oxidase subunit 1

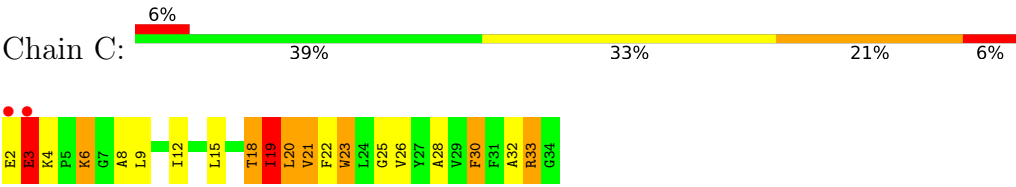


#### • Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 3: Cytochrome c oxidase polypeptide 2A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.75Å 119.75Å 150.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.10 19.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.99-3.10) 92.4 (19.99-2.95)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.300 0.209 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.0	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 129.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HAS, CUA, CU1

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	1.15	10/4566 (0.2%)	1.25	27/6266 (0.4%)
2	B	1.10	0/1335	1.20	8/1822 (0.4%)
3	C	1.20	0/265	1.31	2/359 (0.6%)
All	All	1.14	10/6166 (0.2%)	1.24	37/8447 (0.4%)

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	2
2	B	0	1
3	C	0	1
All	All	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	TYR	CE1-CZ	5.69	1.46	1.38
1	A	52	TYR	CD1-CE1	5.62	1.47	1.39
1	A	236	VAL	CB-CG2	5.52	1.64	1.52
1	A	230	TRP	CB-CG	5.43	1.60	1.50
1	A	56	LYS	CD-CE	5.42	1.64	1.51
1	A	205	VAL	CA-CB	5.40	1.66	1.54
1	A	190	TRP	CB-CG	-5.32	1.40	1.50
1	A	203	GLU	CG-CD	5.21	1.59	1.51
1	A	367	ALA	CA-CB	-5.16	1.41	1.52
1	A	335	TRP	CB-CG	-5.05	1.41	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	LEU	CA-CB-CG	9.98	138.26	115.30
1	A	387	LEU	CA-CB-CG	-9.97	92.37	115.30
3	C	20	LEU	CA-CB-CG	9.85	137.96	115.30
1	A	241	LEU	CB-CG-CD2	-9.82	94.31	111.00
1	A	449	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	492	LEU	CA-CB-CG	8.09	133.90	115.30
1	A	450	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	A	450	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	A	37	LEU	CA-CB-CG	6.93	131.25	115.30
1	A	449	ARG	CB-CG-CD	-6.62	94.38	111.60
2	B	146	ARG	CB-CG-CD	-6.59	94.46	111.60
1	A	374	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	522	LEU	CA-CB-CG	-6.24	100.96	115.30
1	A	307	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	A	540	LEU	CA-CB-CG	5.99	129.08	115.30
2	B	113	ILE	CB-CA-C	-5.79	100.01	111.60
2	B	84	LEU	CA-CB-CG	-5.70	102.19	115.30
3	C	20	LEU	CB-CG-CD2	5.66	120.63	111.00
1	A	520	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	307	VAL	CB-CA-C	5.62	122.08	111.40
2	B	19	LEU	CB-CG-CD2	5.57	120.46	111.00
2	B	12	LEU	CB-CG-CD1	5.53	120.40	111.00
1	A	117	LEU	CA-CB-CG	5.52	127.99	115.30
1	A	185	MET	CG-SD-CE	-5.44	91.49	100.20
1	A	493	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	282	HIS	N-CA-CB	5.28	120.11	110.60
1	A	215	LEU	CA-CB-CG	5.24	127.35	115.30
2	B	19	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	236	VAL	CG1-CB-CG2	5.22	119.25	110.90
1	A	435	MET	CA-CB-CG	-5.22	104.43	113.30
2	B	17	GLY	N-CA-C	-5.20	100.09	113.10
1	A	422	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	A	69	LEU	CB-CG-CD1	-5.15	102.25	111.00
1	A	74	VAL	CB-CA-C	-5.13	101.66	111.40
2	B	107	ILE	CG1-CB-CG2	5.09	122.60	111.40
1	A	449	ARG	CG-CD-NE	5.06	122.42	111.80
1	A	185	MET	CA-CB-CG	-5.00	104.79	113.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	8	ILE	Peptide
2	B	87	ALA	Peptide
3	C	33	ARG	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	4409	0	4516	507	0
2	B	1298	0	1282	140	0
3	C	259	0	279	30	0
4	A	1	0	0	0	0
5	A	43	0	30	25	0
6	A	65	0	61	21	0
7	B	2	0	0	0	0
All	All	6077	0	6168	623	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.84	1.31
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.77	1.17
1:A:101:PRO:HA	1:A:166:LEU:HD21	1.15	1.15
2:B:67:PRO:HB3	2:B:91:GLN:HG3	1.26	1.15
2:B:50:LEU:HD13	2:B:52:ARG:HE	1.17	1.08
1:A:497:ARG:HH21	1:A:499:PRO:HB3	1.15	1.06
1:A:178:VAL:HG22	1:A:522:LEU:HD11	1.39	1.05
1:A:22:LEU:O	1:A:26:VAL:HG23	1.59	1.03
1:A:11:VAL:HG22	1:A:503:GLU:OE2	1.58	1.03
1:A:115:ILE:O	1:A:119:VAL:HG23	1.61	1.01
1:A:225:ARG:HD3	1:A:287:ASP:OD1	1.60	1.01
2:B:52:ARG:HD2	2:B:131:GLU:OE1	1.62	0.99
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.79	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG12	1:A:512:ILE:HD12	1.46	0.97
1:A:235:ILE:O	1:A:238:PHE:HB3	1.66	0.95
1:A:518:ARG:O	1:A:522:LEU:HB2	1.66	0.95
1:A:97:LEU:CD2	1:A:180:PRO:HG2	1.97	0.95
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.52	0.95
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.44	0.94
1:A:454:ALA:O	1:A:457:PRO:HG3	1.64	0.94
1:A:99:MET:HE2	1:A:169:ARG:HE	1.31	0.93
1:A:18:LYS:NZ	1:A:18:LYS:HB3	1.85	0.91
5:A:800:HEM:HMB2	5:A:800:HEM:HBB2	1.54	0.90
2:B:122:ASN:HD21	3:C:33:ARG:HB2	1.32	0.90
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.03	0.89
1:A:560:ARG:O	1:A:560:ARG:HG3	1.73	0.89
1:A:97:LEU:HD21	1:A:180:PRO:HG2	1.53	0.89
1:A:456:VAL:HG23	1:A:456:VAL:O	1.70	0.89
1:A:330:ARG:HH21	1:A:330:ARG:HG3	1.38	0.87
1:A:8:ILE:HD12	1:A:9:SER:HB3	1.57	0.85
2:B:122:ASN:ND2	3:C:33:ARG:CB	2.40	0.85
1:A:158:VAL:HG12	1:A:162:ILE:HD11	1.59	0.85
1:A:413:ILE:HD11	1:A:491:VAL:HG11	1.59	0.85
1:A:497:ARG:NH2	1:A:499:PRO:HB3	1.92	0.84
1:A:477:LEU:HB3	5:A:800:HEM:HBB1	1.58	0.84
1:A:29:PHE:O	1:A:33:ILE:HG12	1.76	0.84
2:B:113:ILE:HD13	2:B:128:LEU:HD12	1.58	0.84
1:A:241:LEU:HD11	1:A:272:PHE:CD1	2.13	0.83
1:A:332:LEU:HG	1:A:332:LEU:O	1.80	0.82
1:A:281:PHE:CE2	1:A:542:TYR:HE1	1.97	0.82
1:A:230:TRP:HZ3	1:A:546:LEU:CD1	1.93	0.82
1:A:314:PHE:HD1	2:B:15:GLU:OE2	1.62	0.82
2:B:140:LYS:O	2:B:141:ARG:HB2	1.79	0.82
1:A:93:PRO:HG3	1:A:186:ALA:HB3	1.61	0.81
1:A:137:PRO:HG2	1:A:224:ALA:HB1	1.61	0.81
1:A:52:TYR:CE2	1:A:65:TYR:HA	2.16	0.81
1:A:138:PRO:HG2	2:B:112:VAL:HA	1.61	0.81
1:A:266:ARG:HB3	1:A:524:MET:CE	2.10	0.81
1:A:10:ARG:HA	1:A:13:GLU:HG2	1.64	0.80
1:A:389:VAL:HG22	5:A:800:HEM:CBC	2.11	0.80
2:B:122:ASN:ND2	3:C:33:ARG:HB2	1.97	0.80
1:A:489:PHE:O	1:A:493:LEU:HB2	1.82	0.79
1:A:126:ALA:O	1:A:127:ASN:HB2	1.82	0.79
1:A:35:GLY:O	1:A:37:LEU:N	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:CE2	1:A:125:LEU:HD23	2.18	0.79
1:A:134:THR:HG21	1:A:136:TYR:CZ	2.18	0.78
1:A:281:PHE:CE2	1:A:542:TYR:CE1	2.70	0.78
1:A:233:HIS:HB3	1:A:234:PRO:HD2	1.64	0.78
1:A:138:PRO:HD3	2:B:113:ILE:HG12	1.64	0.78
1:A:18:LYS:HB3	1:A:18:LYS:HZ2	1.46	0.78
1:A:325:ARG:HA	1:A:329:GLY:HA3	1.65	0.78
6:A:801:HAS:H161	3:C:15:LEU:HD11	1.65	0.78
1:A:59:LEU:HD22	1:A:61:PHE:CE1	2.18	0.77
1:A:477:LEU:HB3	5:A:800:HEM:CBB	2.14	0.77
1:A:389:VAL:HG22	5:A:800:HEM:HBC1	1.66	0.77
1:A:234:PRO:HD3	1:A:276:SER:O	1.85	0.77
1:A:482:LEU:HA	1:A:485:ILE:HD12	1.66	0.77
1:A:477:LEU:HD13	5:A:800:HEM:CBB	2.15	0.77
2:B:122:ASN:ND2	3:C:33:ARG:HB3	2.00	0.77
1:A:67:GLN:HG3	1:A:127:ASN:OD1	1.84	0.76
5:A:800:HEM:HBB2	5:A:800:HEM:CMB	2.14	0.76
1:A:135:PHE:HD1	1:A:135:PHE:O	1.69	0.76
1:A:11:VAL:HG21	1:A:497:ARG:HH22	1.50	0.76
1:A:402:TYR:CZ	1:A:421:GLY:HA2	2.21	0.76
1:A:136:TYR:CZ	1:A:225:ARG:NH1	2.54	0.76
1:A:372:ASP:OD2	6:A:801:HAS:O1D	2.03	0.76
1:A:146:TYR:CE2	1:A:208:LEU:HD22	2.21	0.76
1:A:168:ARG:HH11	1:A:171:LYS:HB3	1.49	0.76
2:B:14:TYR:OH	3:C:4:LYS:HG3	1.86	0.76
1:A:318:ALA:N	3:C:8:ALA:HB2	2.01	0.76
2:B:50:LEU:HD13	2:B:52:ARG:NE	1.98	0.75
1:A:101:PRO:HA	1:A:166:LEU:CD2	2.08	0.75
1:A:234:PRO:HG3	1:A:277:THR:HA	1.67	0.75
2:B:158:GLN:N	2:B:158:GLN:NE2	2.35	0.75
1:A:257:GLY:HA3	1:A:323:ALA:HB2	1.67	0.75
2:B:23:LEU:HD23	2:B:27:PHE:HE2	1.52	0.75
1:A:34:VAL:O	1:A:37:LEU:HB2	1.87	0.75
1:A:11:VAL:HG21	1:A:497:ARG:NH2	2.02	0.74
1:A:418:ARG:HH11	1:A:419:ARG:HD3	1.51	0.74
1:A:146:TYR:O	1:A:150:SER:HB3	1.87	0.74
1:A:266:ARG:HB3	1:A:524:MET:HE3	1.69	0.73
1:A:134:THR:HG21	1:A:136:TYR:CE1	2.22	0.73
1:A:135:PHE:HZ	1:A:200:LEU:HD11	1.53	0.73
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.23	0.73
1:A:135:PHE:O	1:A:135:PHE:CD1	2.41	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD23	1:A:79:VAL:HG21	1.70	0.73
2:B:67:PRO:HB3	2:B:91:GLN:CG	2.15	0.71
2:B:50:LEU:CD1	2:B:52:ARG:HE	2.01	0.71
1:A:349:PRO:HB3	1:A:396:THR:HG23	1.71	0.71
1:A:547:VAL:C	1:A:549:LEU:H	1.93	0.71
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.20	0.71
1:A:59:LEU:HD22	1:A:61:PHE:HE1	1.54	0.71
1:A:158:VAL:HG12	1:A:162:ILE:CD1	2.21	0.71
1:A:266:ARG:CB	1:A:524:MET:HE1	2.21	0.70
1:A:132:LEU:HD11	2:B:152:TYR:CB	2.21	0.70
2:B:83:VAL:HG11	2:B:116:PHE:HE1	1.57	0.70
1:A:314:PHE:CD1	2:B:15:GLU:OE2	2.44	0.70
1:A:260:VAL:HG12	1:A:512:ILE:CD1	2.21	0.70
2:B:94:PRO:HB2	2:B:165:VAL:HG23	1.72	0.70
1:A:561:LEU:HD23	1:A:561:LEU:N	2.07	0.69
1:A:139:LEU:HD23	2:B:112:VAL:HG11	1.74	0.69
2:B:97:VAL:O	2:B:166:VAL:HA	1.91	0.69
1:A:363:GLY:O	1:A:366:ASN:HB2	1.93	0.69
2:B:158:GLN:NE2	2:B:158:GLN:H	1.91	0.69
1:A:18:LYS:HZ1	1:A:408:LEU:HA	1.58	0.69
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.28	0.68
1:A:32:LEU:HB2	1:A:80:PHE:CD1	2.27	0.68
1:A:90:VAL:HG11	1:A:106:MET:HE3	1.74	0.68
1:A:515:PRO:HD2	1:A:516:GLU:HG2	1.74	0.68
1:A:101:PRO:O	1:A:103:MET:N	2.25	0.68
1:A:146:TYR:CD2	1:A:208:LEU:HB3	2.28	0.68
1:A:545:THR:O	1:A:549:LEU:HB2	1.94	0.68
1:A:146:TYR:HD2	1:A:208:LEU:HD13	1.58	0.68
1:A:266:ARG:HB2	1:A:524:MET:HE1	1.76	0.68
1:A:36:SER:O	1:A:481:LEU:HD22	1.94	0.68
1:A:197:SER:O	1:A:201:VAL:HG23	1.94	0.67
1:A:316:VAL:HG12	6:A:801:HAS:H251	1.76	0.67
1:A:56:LYS:HD3	1:A:62:VAL:O	1.94	0.67
1:A:506:LEU:O	1:A:508:PHE:N	2.23	0.67
1:A:93:PRO:HG3	1:A:186:ALA:CB	2.25	0.67
1:A:8:ILE:CD1	1:A:9:SER:HB3	2.24	0.67
1:A:456:VAL:O	1:A:456:VAL:CG2	2.42	0.67
1:A:37:LEU:O	1:A:40:PRO:HD2	1.95	0.66
1:A:178:VAL:HG22	1:A:522:LEU:CD1	2.21	0.66
1:A:90:VAL:HG11	1:A:106:MET:CE	2.25	0.66
2:B:79:TYR:CE2	2:B:98:PRO:HG2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:CD1	2:B:152:TYR:CB	2.74	0.66
1:A:233:HIS:CD2	1:A:237:TYR:CD2	2.85	0.65
1:A:465:VAL:HG22	1:A:466:PRO:HD3	1.77	0.65
1:A:69:LEU:HD11	5:A:800:HEM:CBD	2.27	0.65
1:A:300:VAL:HG22	2:B:30:ILE:HG12	1.79	0.65
1:A:230:TRP:CZ3	1:A:546:LEU:CD1	2.77	0.65
2:B:123:ILE:HD11	2:B:137:TYR:CG	2.32	0.65
1:A:84:PHE:CE1	1:A:397:ALA:HB1	2.32	0.65
1:A:230:TRP:O	1:A:234:PRO:HG2	1.96	0.65
1:A:70:THR:O	1:A:74:VAL:HG23	1.96	0.65
1:A:252:PRO:O	1:A:255:ALA:HB3	1.96	0.64
1:A:359:GLY:CA	1:A:388:GLN:NE2	2.61	0.64
2:B:40:HIS:O	2:B:43:GLY:N	2.23	0.64
1:A:132:LEU:HD11	2:B:152:TYR:HB2	1.78	0.64
1:A:455:GLN:C	1:A:457:PRO:HD3	2.18	0.64
1:A:84:PHE:CE1	1:A:397:ALA:CB	2.81	0.63
2:B:88:PHE:CG	2:B:156:GLY:HA3	2.33	0.63
1:A:203:GLU:OE2	1:A:228:PHE:HB2	1.98	0.63
1:A:359:GLY:C	1:A:388:GLN:HE22	2.01	0.63
1:A:17:GLU:HB3	1:A:103:MET:SD	2.38	0.63
1:A:195:LEU:HG	1:A:538:VAL:HG21	1.80	0.63
1:A:25:LEU:HD23	1:A:87:ALA:CB	2.28	0.63
1:A:146:TYR:HE2	1:A:208:LEU:HD22	1.64	0.63
1:A:243:ALA:HB1	1:A:396:THR:HG21	1.79	0.63
1:A:288:PRO:HD2	2:B:128:LEU:HD21	1.80	0.63
1:A:77:ALA:HB2	5:A:800:HEM:CMD	2.28	0.63
2:B:123:ILE:HD11	2:B:137:TYR:CD1	2.33	0.63
1:A:90:VAL:HG12	1:A:91:TYR:H	1.61	0.63
1:A:371:LEU:H	1:A:371:LEU:HD12	1.63	0.63
1:A:137:PRO:HG2	1:A:224:ALA:CB	2.29	0.62
2:B:14:TYR:CD2	3:C:9:LEU:HD21	2.35	0.62
2:B:63:PRO:HB2	2:B:82:TYR:CD2	2.34	0.62
2:B:92:PRO:HG2	2:B:95:ILE:HG13	1.79	0.62
1:A:260:VAL:CG2	2:B:11:ILE:HG21	2.30	0.62
1:A:90:VAL:HG12	1:A:91:TYR:N	2.15	0.61
1:A:368:SER:OG	3:C:23:TRP:NE1	2.33	0.61
1:A:266:ARG:CB	1:A:524:MET:CE	2.76	0.61
1:A:359:GLY:C	1:A:388:GLN:NE2	2.54	0.61
1:A:90:VAL:CG1	1:A:91:TYR:N	2.62	0.61
2:B:27:PHE:HA	2:B:30:ILE:HD12	1.81	0.61
2:B:155:LEU:N	2:B:155:LEU:HD23	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LYS:NZ	1:A:408:LEU:HA	2.15	0.61
1:A:35:GLY:C	1:A:37:LEU:H	2.03	0.61
1:A:101:PRO:CA	1:A:166:LEU:HD21	2.10	0.61
1:A:46:TYR:OH	1:A:449:ARG:HA	2.00	0.61
1:A:12:TYR:HA	1:A:15:TYR:O	2.00	0.61
1:A:497:ARG:O	1:A:499:PRO:HD3	2.00	0.61
1:A:115:ILE:HA	1:A:118:VAL:HG23	1.82	0.61
1:A:433:MET:O	1:A:436:ALA:HB3	2.01	0.61
1:A:195:LEU:HD21	1:A:535:ALA:N	2.15	0.61
1:A:132:LEU:HD11	2:B:152:TYR:CG	2.35	0.60
1:A:69:LEU:HD11	5:A:800:HEM:HBD1	1.83	0.60
1:A:240:LEU:HD22	6:A:801:HAS:CMC	2.30	0.60
1:A:260:VAL:CG1	1:A:512:ILE:HD12	2.25	0.60
1:A:146:TYR:O	1:A:150:SER:CB	2.49	0.60
1:A:427:LEU:O	1:A:431:GLY:N	2.35	0.60
2:B:103:ILE:HD13	2:B:139:PHE:HD1	1.66	0.60
1:A:260:VAL:HA	1:A:512:ILE:HB	1.84	0.60
1:A:497:ARG:HE	1:A:499:PRO:HG3	1.67	0.60
1:A:235:ILE:HG12	1:A:239:TRP:NE1	2.17	0.59
1:A:277:THR:N	1:A:278:PRO:HD2	2.17	0.59
1:A:366:ASN:ND2	6:A:801:HAS:HBD1	2.17	0.59
1:A:294:TRP:CZ3	1:A:297:ILE:HG21	2.37	0.59
1:A:450:ARG:NE	5:A:800:HEM:O2D	2.33	0.59
1:A:281:PHE:HE2	1:A:542:TYR:HE1	1.46	0.59
1:A:154:LEU:O	1:A:157:TRP:HB2	2.01	0.59
1:A:89:MET:HG2	1:A:242:PRO:HG3	1.84	0.59
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.85	0.59
2:B:45:ILE:O	2:B:46:PRO:C	2.39	0.59
1:A:138:PRO:HD2	1:A:139:LEU:H	1.67	0.59
1:A:459:ALA:O	2:B:146:ARG:NH1	2.30	0.59
1:A:281:PHE:CD1	1:A:298:HIS:CE1	2.91	0.59
1:A:411:LYS:HD3	1:A:496:GLU:O	2.03	0.59
1:A:73:GLY:HA3	1:A:133:TYR:HB3	1.85	0.59
1:A:99:MET:CE	1:A:169:ARG:HE	2.11	0.59
1:A:132:LEU:HD13	1:A:450:ARG:CZ	2.33	0.58
1:A:138:PRO:CG	2:B:112:VAL:HA	2.32	0.58
1:A:411:LYS:HE2	1:A:495:ARG:NH2	2.18	0.58
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.86	0.58
1:A:356:PHE:CE1	1:A:388:GLN:OE1	2.57	0.58
1:A:387:LEU:HD11	1:A:436:ALA:HB1	1.85	0.58
2:B:82:TYR:N	2:B:82:TYR:CD1	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:HB2	5:A:800:HEM:HMD2	1.86	0.58
1:A:302:THR:HG21	1:A:367:ALA:HB1	1.85	0.58
2:B:119:GLU:OE2	2:B:146:ARG:NH2	2.36	0.58
1:A:178:VAL:CG2	1:A:522:LEU:HD11	2.24	0.58
1:A:52:TYR:N	1:A:53:PRO:HD2	2.19	0.57
1:A:545:THR:C	1:A:547:VAL:H	2.07	0.57
1:A:230:TRP:CZ3	1:A:546:LEU:HD11	2.39	0.57
2:B:113:ILE:CD1	2:B:128:LEU:HD12	2.29	0.57
1:A:236:VAL:HG23	1:A:237:TYR:N	2.19	0.57
2:B:64:TRP:NE1	2:B:82:TYR:HB3	2.20	0.57
2:B:88:PHE:CD2	2:B:156:GLY:HA3	2.39	0.57
2:B:144:GLU:HA	2:B:164:ILE:O	2.04	0.57
1:A:302:THR:O	1:A:305:VAL:HG12	2.05	0.57
1:A:330:ARG:HH21	1:A:330:ARG:CG	2.14	0.57
1:A:241:LEU:HD11	1:A:272:PHE:CE1	2.40	0.57
1:A:386:HIS:HA	1:A:390:ALA:HB3	1.87	0.57
3:C:19:ILE:O	3:C:19:ILE:HG22	2.04	0.57
1:A:143:TRP:HA	1:A:212:SER:OG	2.05	0.56
1:A:264:MET:SD	2:B:15:GLU:HG2	2.45	0.56
1:A:411:LYS:HD2	1:A:494:SER:O	2.04	0.56
1:A:420:LEU:HD11	1:A:483:LEU:HD23	1.88	0.56
1:A:545:THR:O	1:A:547:VAL:N	2.32	0.56
1:A:211:TRP:CD2	1:A:219:VAL:CG2	2.89	0.56
1:A:471:VAL:O	1:A:475:ILE:HG13	2.06	0.56
1:A:277:THR:HG22	1:A:538:VAL:HG22	1.86	0.56
2:B:49:LYS:HD3	2:B:49:LYS:C	2.26	0.56
1:A:244:TYR:CZ	1:A:312:THR:HG21	2.41	0.56
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.41	0.56
1:A:347:VAL:HG12	1:A:351:LEU:HD12	1.88	0.56
1:A:76:ASN:O	1:A:81:THR:HG23	2.06	0.55
1:A:340:PRO:O	1:A:342:ASP:N	2.39	0.55
2:B:86:PHE:O	2:B:88:PHE:N	2.38	0.55
1:A:97:LEU:HD21	1:A:180:PRO:CG	2.33	0.55
2:B:54:ASP:OD1	2:B:57:THR:HG23	2.05	0.55
2:B:66:ASP:OD2	2:B:69:GLN:CG	2.53	0.55
1:A:135:PHE:CE1	1:A:208:LEU:HD11	2.41	0.55
1:A:339:LEU:O	1:A:341:TRP:N	2.38	0.55
2:B:58:VAL:HG22	2:B:64:TRP:HB2	1.87	0.55
1:A:32:LEU:HD13	1:A:80:PHE:CE1	2.42	0.55
1:A:138:PRO:HG3	2:B:129:PRO:HG3	1.89	0.55
5:A:800:HEM:HMB2	5:A:800:HEM:CBB	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:VAL:C	1:A:549:LEU:N	2.60	0.55
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.89	0.55
1:A:477:LEU:HD13	5:A:800:HEM:HBB2	1.88	0.54
1:A:56:LYS:O	1:A:60:PRO:HA	2.08	0.54
2:B:58:VAL:CG2	2:B:64:TRP:HE3	2.20	0.54
1:A:243:ALA:O	1:A:247:ILE:HG13	2.06	0.54
1:A:191:LEU:HB3	1:A:531:PHE:CD2	2.42	0.54
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.88	0.54
1:A:25:LEU:HD23	1:A:87:ALA:HB3	1.90	0.54
1:A:46:TYR:HA	1:A:453:ILE:HD11	1.89	0.54
1:A:161:TYR:HD1	1:A:162:ILE:N	2.06	0.54
1:A:402:TYR:OH	1:A:421:GLY:HA2	2.08	0.54
2:B:58:VAL:CG2	2:B:64:TRP:CE3	2.90	0.54
1:A:105:LEU:O	1:A:158:VAL:HG11	2.07	0.54
2:B:88:PHE:CD1	2:B:156:GLY:HA3	2.42	0.54
1:A:69:LEU:CD1	5:A:800:HEM:HBD1	2.38	0.54
1:A:233:HIS:O	1:A:234:PRO:C	2.46	0.54
1:A:243:ALA:HB1	1:A:396:THR:CG2	2.38	0.54
1:A:387:LEU:HD12	1:A:440:HIS:HE1	1.73	0.54
2:B:103:ILE:HD13	2:B:139:PHE:CD1	2.43	0.54
1:A:132:LEU:CD1	2:B:152:TYR:CG	2.91	0.53
1:A:240:LEU:HD22	6:A:801:HAS:HMC2	1.88	0.53
1:A:314:PHE:CD2	3:C:12:ILE:HD13	2.43	0.53
3:C:15:LEU:O	3:C:19:ILE:CG1	2.56	0.53
1:A:402:TYR:CE1	1:A:421:GLY:HA3	2.44	0.53
2:B:47:ALA:HB3	2:B:134:THR:HB	1.91	0.53
1:A:178:VAL:HG12	1:A:179:THR:N	2.23	0.53
1:A:359:GLY:CA	1:A:388:GLN:HE22	2.21	0.53
2:B:99:GLN:O	2:B:101:ALA:N	2.41	0.53
1:A:420:LEU:HD21	1:A:487:GLY:HA3	1.89	0.53
1:A:88:ILE:HG13	1:A:246:ILE:HD11	1.90	0.53
1:A:288:PRO:HD2	2:B:128:LEU:CD2	2.39	0.53
2:B:66:ASP:OD2	2:B:69:GLN:HG3	2.09	0.53
1:A:93:PRO:CG	1:A:186:ALA:CB	2.87	0.53
1:A:207:PHE:CZ	1:A:550:PHE:HE2	2.27	0.53
1:A:77:ALA:HB1	1:A:239:TRP:CH2	2.44	0.52
1:A:234:PRO:CD	1:A:276:SER:O	2.57	0.52
1:A:525:ASP:C	1:A:527:ILE:H	2.12	0.52
1:A:385:PHE:CE2	6:A:801:HAS:HAA1	2.43	0.52
1:A:69:LEU:HD11	5:A:800:HEM:HBD2	1.91	0.52
1:A:233:HIS:O	1:A:235:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ASN:ND2	1:A:65:TYR:CE1	2.77	0.52
1:A:277:THR:CG2	1:A:538:VAL:HG22	2.40	0.52
1:A:347:VAL:HG12	1:A:351:LEU:CD1	2.39	0.52
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.44	0.52
1:A:21:THR:OG1	1:A:91:TYR:HB2	2.09	0.52
1:A:24:PHE:HZ	1:A:109:SER:HB3	1.75	0.52
1:A:59:LEU:HB3	1:A:61:PHE:CD1	2.45	0.52
1:A:77:ALA:HB1	1:A:239:TRP:CZ2	2.45	0.52
1:A:235:ILE:O	1:A:238:PHE:CB	2.51	0.52
1:A:322:PHE:HZ	2:B:4:GLN:OE1	1.92	0.52
1:A:449:ARG:HD2	1:A:450:ARG:HD2	1.91	0.52
1:A:375:VAL:O	1:A:378:THR:HG23	2.10	0.52
2:B:44:VAL:O	2:B:135:VAL:HG12	2.09	0.52
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.45	0.52
1:A:45:ASN:O	1:A:48:ASN:N	2.40	0.52
1:A:72:HIS:HE1	5:A:800:HEM:C4B	2.28	0.52
1:A:66:TYR:CD2	2:B:152:TYR:CE1	2.97	0.51
1:A:294:TRP:HZ2	1:A:544:PRO:HG2	1.73	0.51
1:A:418:ARG:NH1	1:A:419:ARG:HD3	2.24	0.51
1:A:481:LEU:O	1:A:485:ILE:HG13	2.10	0.51
1:A:12:TYR:CE2	1:A:19:LYS:HB2	2.45	0.51
1:A:247:ILE:HG21	1:A:353:LEU:HD11	1.91	0.51
1:A:445:LEU:O	1:A:446:ASN:HB2	2.11	0.51
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.25	0.51
1:A:75:LEU:HA	1:A:79:VAL:CG2	2.40	0.51
1:A:126:ALA:O	1:A:127:ASN:CB	2.56	0.51
1:A:84:PHE:CZ	1:A:397:ALA:HB2	2.45	0.51
1:A:450:ARG:HH11	5:A:800:HEM:CGD	2.24	0.51
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.75	0.51
1:A:343:ASN:O	1:A:344:PRO:C	2.46	0.51
1:A:128:GLU:O	1:A:142:HIS:N	2.44	0.51
1:A:365:VAL:HG11	3:C:26:VAL:HG11	1.93	0.51
2:B:37:LEU:CD1	2:B:45:ILE:HD11	2.40	0.51
1:A:82:GLN:NE2	1:A:156:THR:HG23	2.26	0.50
1:A:93:PRO:CG	1:A:186:ALA:HB3	2.36	0.50
1:A:248:TYR:HE2	1:A:315:THR:HG21	1.76	0.50
1:A:561:LEU:HD23	1:A:561:LEU:H	1.75	0.50
1:A:140:LYS:HG3	1:A:211:TRP:CH2	2.46	0.50
1:A:225:ARG:HH22	2:B:126:GLU:CD	2.13	0.50
1:A:560:ARG:H	1:A:561:LEU:HD23	1.77	0.50
2:B:53:VAL:HG23	2:B:54:ASP:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:TRP:O	1:A:532:ALA:N	2.44	0.50
1:A:561:LEU:CD1	2:B:87:ALA:CB	2.89	0.50
2:B:72:VAL:CG2	2:B:72:VAL:O	2.59	0.50
1:A:55:LEU:O	1:A:56:LYS:C	2.49	0.50
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.40	0.50
2:B:72:VAL:O	2:B:72:VAL:HG22	2.12	0.50
1:A:316:VAL:HG12	6:A:801:HAS:C25	2.42	0.50
1:A:402:TYR:CZ	1:A:421:GLY:CA	2.92	0.50
1:A:477:LEU:CB	5:A:800:HEM:CBB	2.86	0.50
1:A:477:LEU:HD12	5:A:800:HEM:HMB3	1.92	0.50
1:A:367:ALA:HB2	6:A:801:HAS:OMD	2.11	0.50
1:A:47:GLY:HA2	1:A:467:MET:O	2.11	0.50
2:B:94:PRO:HB2	2:B:165:VAL:CG2	2.39	0.50
1:A:132:LEU:HD13	1:A:450:ARG:NH2	2.26	0.49
1:A:343:ASN:OD1	1:A:343:ASN:C	2.50	0.49
1:A:262:ASP:OD2	1:A:266:ARG:NE	2.45	0.49
1:A:211:TRP:CD2	1:A:219:VAL:HG22	2.48	0.49
1:A:228:PHE:C	1:A:228:PHE:CD2	2.86	0.49
1:A:236:VAL:HG12	1:A:239:TRP:CE3	2.48	0.49
1:A:346:PHE:O	1:A:349:PRO:HD2	2.12	0.49
1:A:357:ILE:HG23	3:C:15:LEU:HA	1.94	0.49
1:A:12:TYR:CZ	1:A:19:LYS:HB2	2.48	0.49
1:A:360:GLY:HA3	6:A:801:HAS:C14	2.42	0.49
1:A:402:TYR:CE1	1:A:421:GLY:CA	2.95	0.49
2:B:23:LEU:O	2:B:27:PHE:HD2	1.95	0.49
1:A:84:PHE:CZ	1:A:397:ALA:CB	2.96	0.49
1:A:427:LEU:HB2	1:A:480:ALA:HB2	1.93	0.49
1:A:561:LEU:N	1:A:561:LEU:CD2	2.75	0.49
1:A:8:ILE:CD1	1:A:9:SER:H	2.26	0.49
1:A:281:PHE:CE1	1:A:298:HIS:CE1	3.01	0.49
1:A:321:GLU:O	1:A:322:PHE:C	2.51	0.49
1:A:517:ASP:O	1:A:519:ARG:N	2.46	0.49
1:A:518:ARG:HA	1:A:521:VAL:HB	1.94	0.49
1:A:77:ALA:HB2	5:A:800:HEM:HMD3	1.94	0.49
1:A:184:TYR:CD2	1:A:266:ARG:HG2	2.48	0.49
1:A:258:ARG:O	1:A:259:LEU:C	2.48	0.49
1:A:21:THR:HG22	1:A:408:LEU:CD1	2.43	0.48
2:B:54:ASP:O	2:B:58:VAL:HB	2.14	0.48
1:A:365:VAL:O	1:A:367:ALA:N	2.47	0.48
1:A:70:THR:OG1	1:A:132:LEU:HA	2.12	0.48
1:A:191:LEU:HD13	1:A:531:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:O	1:A:139:LEU:C	2.51	0.48
1:A:342:ASP:HB2	1:A:418:ARG:NH2	2.29	0.48
1:A:497:ARG:O	1:A:499:PRO:CD	2.62	0.48
1:A:189:PHE:HE1	1:A:242:PRO:HD3	1.79	0.48
1:A:303:LEU:HB3	2:B:26:LEU:HG	1.95	0.48
1:A:539:VAL:O	1:A:540:LEU:C	2.51	0.48
1:A:389:VAL:HB	6:A:801:HAS:CB	2.43	0.48
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.96	0.48
2:B:32:LEU:O	2:B:36:THR:HG23	2.13	0.48
2:B:34:ALA:HA	2:B:37:LEU:HB2	1.94	0.48
1:A:89:MET:HE3	1:A:186:ALA:HA	1.96	0.48
1:A:146:TYR:CD2	1:A:208:LEU:HD13	2.45	0.48
1:A:230:TRP:HZ3	1:A:546:LEU:HD12	1.77	0.48
1:A:136:TYR:CE1	1:A:225:ARG:NH1	2.76	0.48
1:A:389:VAL:HG13	1:A:390:ALA:N	2.29	0.48
1:A:559:TRP:HB3	1:A:561:LEU:CD2	2.44	0.48
1:A:281:PHE:H	1:A:298:HIS:CD2	2.32	0.48
1:A:420:LEU:O	1:A:421:GLY:C	2.52	0.48
2:B:23:LEU:HD23	2:B:27:PHE:CE2	2.39	0.48
1:A:59:LEU:HB3	1:A:61:PHE:CE1	2.49	0.47
1:A:322:PHE:HZ	2:B:4:GLN:CD	2.17	0.47
1:A:330:ARG:HG3	1:A:330:ARG:NH2	2.17	0.47
1:A:161:TYR:O	1:A:164:LEU:N	2.47	0.47
1:A:167:TRP:O	1:A:167:TRP:CG	2.66	0.47
1:A:387:LEU:HD11	1:A:436:ALA:CB	2.43	0.47
1:A:449:ARG:O	1:A:450:ARG:HB2	2.13	0.47
2:B:83:VAL:O	2:B:84:LEU:HD12	2.14	0.47
1:A:561:LEU:CD1	2:B:87:ALA:HB2	2.44	0.47
3:C:15:LEU:O	3:C:19:ILE:HG13	2.14	0.47
3:C:18:THR:O	3:C:22:PHE:HB2	2.14	0.47
1:A:248:TYR:HH	1:A:312:THR:HG1	1.62	0.47
1:A:302:THR:CG2	1:A:367:ALA:HB1	2.44	0.47
1:A:325:ARG:NH1	1:A:331:GLY:O	2.47	0.47
1:A:344:PRO:N	1:A:422:LEU:HD23	2.28	0.47
1:A:72:HIS:CE1	5:A:800:HEM:C4B	3.02	0.47
1:A:137:PRO:O	1:A:221:PRO:HB3	2.14	0.47
1:A:167:TRP:O	1:A:167:TRP:CD1	2.68	0.47
1:A:233:HIS:CB	1:A:234:PRO:CD	2.81	0.47
1:A:233:HIS:ND1	1:A:282:HIS:CE1	2.81	0.47
1:A:413:ILE:CD1	1:A:491:VAL:HG11	2.38	0.47
2:B:114:HIS:CE1	2:B:153:CYS:CB	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PHE:CZ	2:B:4:GLN:OE1	2.68	0.47
2:B:153:CYS:SG	2:B:157:HIS:HB2	2.54	0.47
1:A:257:GLY:CA	1:A:323:ALA:HB2	2.40	0.47
1:A:318:ALA:H	3:C:8:ALA:HB2	1.78	0.47
1:A:325:ARG:O	1:A:326:LEU:C	2.54	0.47
2:B:113:ILE:HG23	2:B:128:LEU:CD1	2.45	0.47
1:A:33:ILE:HG23	1:A:485:ILE:HG12	1.97	0.47
1:A:323:ALA:O	1:A:327:ARG:HG3	2.15	0.47
2:B:94:PRO:CB	2:B:165:VAL:CG2	2.93	0.47
1:A:222:LEU:HG	1:A:549:LEU:HD11	1.96	0.46
1:A:340:PRO:C	1:A:342:ASP:H	2.18	0.46
1:A:559:TRP:HB3	1:A:561:LEU:HD21	1.97	0.46
2:B:152:TYR:CZ	2:B:154:GLY:HA2	2.51	0.46
1:A:123:PRO:HG3	1:A:144:ALA:CB	2.30	0.46
1:A:364:ILE:HG22	3:C:23:TRP:CD1	2.51	0.46
2:B:52:ARG:N	2:B:52:ARG:CD	2.77	0.46
1:A:17:GLU:CB	1:A:103:MET:SD	3.04	0.46
1:A:45:ASN:HD21	1:A:452:TYR:HA	1.80	0.46
1:A:139:LEU:HD23	2:B:112:VAL:CG1	2.42	0.46
1:A:70:THR:HG21	1:A:130:THR:HA	1.97	0.46
1:A:236:VAL:CG2	1:A:237:TYR:N	2.79	0.46
1:A:378:THR:O	1:A:382:PRO:HD2	2.15	0.46
2:B:158:GLN:N	2:B:158:GLN:HE21	2.09	0.46
3:C:25:GLY:O	3:C:28:ALA:HB3	2.16	0.46
1:A:19:LYS:C	1:A:21:THR:N	2.68	0.46
1:A:75:LEU:O	1:A:79:VAL:HB	2.15	0.46
1:A:344:PRO:CA	1:A:422:LEU:HD23	2.46	0.46
1:A:456:VAL:N	1:A:457:PRO:HD3	2.31	0.46
1:A:463:ALA:HB3	1:A:467:MET:HE3	1.98	0.46
1:A:561:LEU:HD13	2:B:87:ALA:CB	2.45	0.46
1:A:61:PHE:CZ	1:A:62:VAL:HG23	2.51	0.46
1:A:477:LEU:CD1	5:A:800:HEM:HBB2	2.46	0.46
1:A:328:GLY:O	1:A:330:ARG:NH2	2.49	0.46
2:B:114:HIS:HE1	2:B:153:CYS:CB	2.27	0.46
1:A:207:PHE:HZ	1:A:550:PHE:HE2	1.64	0.45
2:B:95:ILE:HG22	2:B:97:VAL:HG13	1.97	0.45
1:A:9:SER:OG	1:A:11:VAL:HB	2.15	0.45
1:A:294:TRP:NE1	1:A:544:PRO:HB2	2.31	0.45
1:A:518:ARG:HG2	1:A:522:LEU:HD13	1.99	0.45
1:A:525:ASP:C	1:A:527:ILE:N	2.69	0.45
1:A:132:LEU:HD12	2:B:152:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:THR:O	2:B:60:GLN:NE2	2.46	0.45
1:A:95:ARG:NH1	1:A:98:ASN:OD1	2.43	0.45
1:A:132:LEU:CD1	2:B:152:TYR:HB3	2.47	0.45
1:A:8:ILE:HD12	1:A:9:SER:N	2.31	0.45
1:A:365:VAL:O	1:A:366:ASN:C	2.54	0.45
2:B:82:TYR:N	2:B:82:TYR:HD1	2.13	0.45
1:A:19:LYS:C	1:A:21:THR:H	2.20	0.45
1:A:238:PHE:O	1:A:240:LEU:N	2.50	0.45
1:A:445:LEU:HA	1:A:445:LEU:HD23	1.38	0.45
2:B:28:VAL:HG12	2:B:32:LEU:HD12	1.97	0.45
1:A:70:THR:HG22	1:A:124:LEU:HD21	1.98	0.45
1:A:525:ASP:O	1:A:527:ILE:N	2.41	0.45
1:A:208:LEU:O	1:A:212:SER:CB	2.64	0.45
1:A:303:LEU:O	2:B:26:LEU:HD21	2.17	0.45
2:B:118:VAL:HB	2:B:123:ILE:HB	1.99	0.45
1:A:247:ILE:HG23	1:A:251:LEU:HD23	1.99	0.45
1:A:350:VAL:HG11	6:A:801:HAS:H312	1.99	0.45
1:A:515:PRO:HD2	1:A:516:GLU:H	1.82	0.45
1:A:251:LEU:O	1:A:252:PRO:C	2.55	0.45
1:A:294:TRP:CZ3	1:A:541:ALA:HA	2.51	0.45
1:A:351:LEU:HB3	1:A:429:PHE:CG	2.52	0.45
1:A:41:PHE:CD1	1:A:55:LEU:HD13	2.52	0.44
1:A:512:ILE:HG22	1:A:512:ILE:O	2.17	0.44
2:B:44:VAL:O	2:B:135:VAL:CG1	2.65	0.44
3:C:20:LEU:O	3:C:21:VAL:C	2.56	0.44
1:A:262:ASP:HB2	1:A:511:VAL:CG1	2.46	0.44
1:A:270:LEU:HD11	1:A:530:TRP:CG	2.52	0.44
1:A:366:ASN:HB3	6:A:801:HAS:C2D	2.47	0.44
2:B:14:TYR:CE2	3:C:9:LEU:HD11	2.52	0.44
1:A:167:TRP:CZ3	1:A:527:ILE:HG21	2.52	0.44
1:A:423:ALA:O	1:A:424:VAL:C	2.56	0.44
2:B:107:ILE:O	2:B:108:THR:HB	2.17	0.44
1:A:400:SER:O	1:A:404:LEU:HB3	2.17	0.44
2:B:158:GLN:O	2:B:161:PHE:HE1	1.99	0.44
1:A:15:TYR:HB2	1:A:18:LYS:HG3	1.99	0.44
1:A:21:THR:HG22	1:A:408:LEU:HD13	2.00	0.44
2:B:39:THR:HB	2:B:40:HIS:ND1	2.33	0.44
1:A:325:ARG:HA	1:A:329:GLY:CA	2.42	0.44
1:A:344:PRO:O	1:A:345:ALA:C	2.55	0.44
1:A:356:PHE:CD1	1:A:392:LEU:HD22	2.53	0.44
1:A:239:TRP:HZ3	6:A:801:HAS:HMA1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:LEU:HD12	2:B:84:LEU:HA	1.71	0.44
1:A:183:THR:O	1:A:187:VAL:N	2.50	0.43
1:A:304:PHE:O	1:A:307:VAL:N	2.39	0.43
1:A:61:PHE:HE2	1:A:125:LEU:HD23	1.74	0.43
1:A:106:MET:HG3	1:A:162:ILE:HG21	2.00	0.43
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.53	0.43
1:A:359:GLY:HA3	1:A:388:GLN:HE22	1.80	0.43
1:A:447:VAL:CG1	1:A:453:ILE:HD13	2.49	0.43
1:A:489:PHE:HD2	1:A:493:LEU:HD22	1.84	0.43
1:A:526:ARG:O	1:A:527:ILE:C	2.56	0.43
2:B:18:TRP:CD2	3:C:12:ILE:HD12	2.53	0.43
1:A:206:LEU:O	1:A:207:PHE:CG	2.72	0.43
1:A:379:ALA:HB3	1:A:443:GLY:N	2.32	0.43
2:B:94:PRO:CB	2:B:165:VAL:HG23	2.45	0.43
1:A:82:GLN:HG3	1:A:238:PHE:CE1	2.53	0.43
1:A:120:ALA:O	1:A:124:LEU:HB2	2.18	0.43
1:A:382:PRO:O	1:A:386:HIS:ND1	2.49	0.43
1:A:99:MET:HE1	1:A:169:ARG:HB3	2.00	0.43
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.33	0.43
1:A:132:LEU:HD12	2:B:152:TYR:HB3	2.01	0.43
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.54	0.43
1:A:229:TRP:CZ3	1:A:283:HIS:CE1	3.06	0.43
1:A:342:ASP:C	1:A:422:LEU:HD21	2.39	0.43
1:A:208:LEU:O	1:A:212:SER:HB3	2.19	0.43
1:A:186:ALA:O	1:A:190:TRP:CD1	2.72	0.42
1:A:255:ALA:O	1:A:327:ARG:HD3	2.18	0.42
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.19	0.42
1:A:497:ARG:O	1:A:497:ARG:HG3	2.19	0.42
1:A:524:MET:HE2	1:A:524:MET:HB2	1.90	0.42
2:B:106:LYS:HG2	2:B:134:THR:HG23	2.01	0.42
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.79	0.42
1:A:168:ARG:NH1	1:A:172:ALA:HB2	2.34	0.42
1:A:270:LEU:HD22	1:A:524:MET:HG2	2.01	0.42
1:A:294:TRP:HA	1:A:294:TRP:CE3	2.53	0.42
1:A:330:ARG:CG	1:A:330:ARG:NH2	2.77	0.42
1:A:209:LEU:HB2	1:A:210:PRO:HD2	2.02	0.42
1:A:561:LEU:HD13	2:B:87:ALA:HB1	2.02	0.42
2:B:83:VAL:HG11	2:B:116:PHE:CE1	2.45	0.42
1:A:52:TYR:O	1:A:56:LYS:N	2.40	0.42
1:A:238:PHE:O	1:A:242:PRO:HD3	2.19	0.42
1:A:318:ALA:H	3:C:8:ALA:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:THR:HB	3:C:30:PHE:CE1	2.53	0.42
1:A:545:THR:C	1:A:547:VAL:N	2.72	0.42
2:B:107:ILE:HD13	2:B:116:PHE:CE1	2.54	0.42
3:C:3:GLU:HB3	3:C:4:LYS:H	1.57	0.42
1:A:99:MET:SD	1:A:170:TRP:HB2	2.60	0.42
1:A:60:PRO:C	1:A:62:VAL:N	2.73	0.42
1:A:185:MET:HG2	1:A:269:PHE:CD1	2.54	0.42
2:B:52:ARG:HD2	2:B:52:ARG:N	2.35	0.42
1:A:371:LEU:HD12	1:A:371:LEU:N	2.30	0.42
1:A:418:ARG:HH11	1:A:419:ARG:CD	2.27	0.42
1:A:184:TYR:O	1:A:188:VAL:HG22	2.20	0.42
1:A:233:HIS:HB3	1:A:234:PRO:HD3	1.97	0.42
1:A:248:TYR:OH	1:A:312:THR:HA	2.20	0.42
1:A:302:THR:HG21	1:A:367:ALA:CB	2.48	0.42
1:A:385:PHE:HB3	6:A:801:HAS:C4A	2.49	0.42
2:B:119:GLU:OE2	2:B:146:ARG:HD3	2.20	0.42
1:A:260:VAL:HG23	2:B:11:ILE:HG21	2.00	0.42
1:A:540:LEU:O	1:A:544:PRO:HD2	2.19	0.42
3:C:15:LEU:O	3:C:19:ILE:HG12	2.20	0.42
1:A:133:TYR:OH	6:A:801:HAS:HBA2	2.20	0.42
1:A:360:GLY:N	1:A:388:GLN:HE22	2.18	0.42
2:B:63:PRO:HG2	2:B:64:TRP:CE3	2.55	0.42
2:B:109:SER:HA	2:B:110:PRO:HD2	1.70	0.42
3:C:22:PHE:O	3:C:23:TRP:C	2.57	0.42
1:A:65:TYR:HB2	1:A:452:TYR:CD1	2.54	0.41
1:A:190:TRP:CE3	1:A:190:TRP:HA	2.54	0.41
1:A:364:ILE:HD13	3:C:19:ILE:CG2	2.50	0.41
2:B:121:THR:O	3:C:33:ARG:HD3	2.20	0.41
1:A:66:TYR:CD2	2:B:152:TYR:HE1	2.38	0.41
1:A:230:TRP:CE3	1:A:546:LEU:HD11	2.55	0.41
1:A:318:ALA:CA	3:C:8:ALA:HB2	2.50	0.41
2:B:95:ILE:CG2	2:B:97:VAL:HG13	2.51	0.41
2:B:161:PHE:CD1	2:B:161:PHE:N	2.88	0.41
1:A:80:PHE:CD2	1:A:80:PHE:C	2.93	0.41
1:A:130:THR:HG22	1:A:130:THR:O	2.20	0.41
1:A:229:TRP:HA	1:A:232:GLY:HA3	2.02	0.41
1:A:445:LEU:O	1:A:446:ASN:CB	2.68	0.41
1:A:477:LEU:CD1	5:A:800:HEM:CBB	2.93	0.41
2:B:28:VAL:O	2:B:32:LEU:HD12	2.20	0.41
1:A:354:LEU:HA	1:A:354:LEU:HD12	1.54	0.41
1:A:439:LEU:HD12	1:A:439:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:GLN:HG2	2:B:100:GLY:N	2.35	0.41
1:A:161:TYR:O	1:A:165:ASP:N	2.32	0.41
1:A:236:VAL:HG23	1:A:237:TYR:CD2	2.55	0.41
1:A:385:PHE:CG	6:A:801:HAS:HMA2	2.55	0.41
1:A:527:ILE:HG22	1:A:528:GLY:N	2.35	0.41
1:A:549:LEU:C	1:A:551:GLY:H	2.24	0.41
2:B:15:GLU:O	2:B:18:TRP:HB3	2.21	0.41
1:A:411:LYS:H	1:A:411:LYS:HG2	1.62	0.41
2:B:81:VAL:HG11	2:B:95:ILE:HG12	2.03	0.41
1:A:147:LEU:O	1:A:151:VAL:N	2.53	0.41
1:A:322:PHE:CE1	1:A:512:ILE:HD11	2.56	0.41
1:A:378:THR:O	1:A:379:ALA:C	2.59	0.41
1:A:418:ARG:NH1	1:A:419:ARG:CD	2.84	0.41
2:B:58:VAL:HG22	2:B:64:TRP:HE3	1.85	0.41
1:A:132:LEU:HD12	2:B:152:TYR:CB	2.51	0.41
1:A:221:PRO:HD2	1:A:222:LEU:H	1.86	0.41
1:A:232:GLY:O	1:A:235:ILE:HG22	2.21	0.41
2:B:37:LEU:HD11	2:B:45:ILE:HD11	2.02	0.41
2:B:44:VAL:H	2:B:44:VAL:HG22	1.56	0.41
1:A:60:PRO:C	1:A:62:VAL:H	2.24	0.41
1:A:248:TYR:O	1:A:259:LEU:HD13	2.21	0.41
1:A:275:LEU:HD13	1:A:304:PHE:HB3	2.02	0.41
1:A:530:TRP:C	1:A:532:ALA:N	2.74	0.41
1:A:33:ILE:HG12	1:A:33:ILE:H	1.74	0.40
2:B:114:HIS:CE1	2:B:153:CYS:HB3	2.56	0.40
1:A:385:PHE:CD2	6:A:801:HAS:HAA1	2.55	0.40
1:A:417:GLN:O	1:A:421:GLY:N	2.38	0.40
1:A:467:MET:O	1:A:471:VAL:HG23	2.21	0.40
1:A:89:MET:HG3	1:A:189:PHE:CZ	2.57	0.40
1:A:178:VAL:CG2	1:A:522:LEU:CD1	2.92	0.40
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.08	0.40
1:A:367:ALA:CA	6:A:801:HAS:OMD	2.69	0.40
2:B:63:PRO:CB	2:B:82:TYR:CD2	3.04	0.40
1:A:288:PRO:CD	2:B:128:LEU:CD2	2.99	0.40
1:A:375:VAL:HB	1:A:380:TRP:CG	2.57	0.40
2:B:105:PHE:HB2	2:B:135:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	555/618 (90%)	385 (69%)	108 (20%)	62 (11%)	0	2
2	B	164/166 (99%)	131 (80%)	23 (14%)	10 (6%)	1	9
3	C	31/33 (94%)	24 (77%)	2 (6%)	5 (16%)	0	0
All	All	750/817 (92%)	540 (72%)	133 (18%)	77 (10%)	0	3

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	36	SER
1	A	102	ASN
1	A	127	ASN
1	A	161	TYR
1	A	162	ILE
1	A	178	VAL
1	A	205	VAL
1	A	330	ARG
1	A	366	ASN
1	A	369	PHE
1	A	446	ASN
1	A	498	LYS
1	A	512	ILE
1	A	517	ASP
1	A	518	ARG
1	A	534	ALA
1	A	546	LEU
2	B	88	PHE
2	B	141	ARG
1	A	79	VAL
1	A	89	MET
1	A	98	ASN
1	A	103	MET

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Mol	Chain	Res	Type
1	A	113	ALA
1	A	132	LEU
1	A	148	GLY
1	A	198	LEU
1	A	340	PRO
1	A	365	VAL
1	A	393	VAL
1	A	402	TYR
1	A	421	GLY
1	A	497	ARG
1	A	507	PRO
1	A	527	ILE
2	B	87	ALA
2	B	100	GLY
2	B	111	ASP
3	C	21	VAL
3	C	32	ALA
1	A	8	ILE
1	A	9	SER
1	A	94	ALA
1	A	138	PRO
1	A	199	GLY
1	A	233	HIS
1	A	292	PRO
1	A	341	TRP
1	A	392	LEU
1	A	515	PRO
2	B	4	GLN
1	A	112	MET
1	A	196	ALA
1	A	234	PRO
1	A	326	LEU
1	A	403	TRP
1	A	416	ALA
1	A	526	ARG
1	A	553	LEU
3	C	3	GLU
1	A	35	GLY
1	A	535	ALA
2	B	28	VAL
2	B	51	GLU
2	B	73	GLN

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Mol	Chain	Res	Type
2	B	139	PHE
1	A	45	ASN
1	A	318	ALA
1	A	479	VAL
1	A	547	VAL
3	C	6	LYS
3	C	19	ILE
1	A	431	GLY
1	A	221	PRO
1	A	359	GLY
1	A	34	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/503 (90%)	376 (83%)	77 (17%)	2	9
2	B	136/136 (100%)	98 (72%)	38 (28%)	0	1
3	C	26/26 (100%)	19 (73%)	7 (27%)	0	1
All	All	615/665 (92%)	493 (80%)	122 (20%)	1	5

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	ILE
1	A	9	SER
1	A	15	TYR
1	A	18	LYS
1	A	24	PHE
1	A	25	LEU
1	A	33	ILE
1	A	48	ASN
1	A	56	LYS
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	67	GLN
1	A	90	VAL
1	A	95	ARG
1	A	100	ARG
1	A	106	MET
1	A	107	TRP
1	A	118	VAL
1	A	122	LEU
1	A	124	LEU
1	A	131	VAL
1	A	133	TYR
1	A	134	THR
1	A	146	TYR
1	A	161	TYR
1	A	168	ARG
1	A	171	LYS
1	A	215	LEU
1	A	216	VAL
1	A	219	VAL
1	A	225	ARG
1	A	230	TRP
1	A	248	TYR
1	A	253	LYS
1	A	258	ARG
1	A	262	ASP
1	A	272	PHE
1	A	279	VAL
1	A	291	ASP
1	A	292	PRO
1	A	296	MET
1	A	312	THR
1	A	325	ARG
1	A	327	ARG
1	A	330	ARG
1	A	354	LEU
1	A	401	LEU
1	A	411	LYS
1	A	422	LEU
1	A	433	MET
1	A	434	ILE
1	A	439	LEU
1	A	450	ARG

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Mol	Chain	Res	Type
1	A	452	TYR
1	A	465	VAL
1	A	470	ASN
1	A	472	LEU
1	A	478	LEU
1	A	483	LEU
1	A	490	SER
1	A	491	VAL
1	A	492	LEU
1	A	493	LEU
1	A	495	ARG
1	A	497	ARG
1	A	513	SER
1	A	516	GLU
1	A	519	ARG
1	A	524	MET
1	A	527	ILE
1	A	536	ILE
1	A	540	LEU
1	A	547	VAL
1	A	553	LEU
1	A	556	VAL
1	A	560	ARG
1	A	561	LEU
2	B	4	GLN
2	B	5	HIS
2	B	9	LYS
2	B	12	LEU
2	B	16	LYS
2	B	23	LEU
2	B	25	MET
2	B	26	LEU
2	B	36	THR
2	B	37	LEU
2	B	44	VAL
2	B	45	ILE
2	B	49	LYS
2	B	52	ARG
2	B	56	THR
2	B	57	THR
2	B	59	ARG
2	B	66	ASP

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Mol	Chain	Res	Type
2	B	72	VAL
2	B	77	ASN
2	B	82	TYR
2	B	91	GLN
2	B	96	GLU
2	B	107	ILE
2	B	116	PHE
2	B	119	GLU
2	B	128	LEU
2	B	135	VAL
2	B	140	LYS
2	B	144	GLU
2	B	147	ILE
2	B	153	CYS
2	B	155	LEU
2	B	158	GLN
2	B	161	PHE
2	B	165	VAL
2	B	166	VAL
2	B	167	LYS
3	C	2	GLU
3	C	3	GLU
3	C	6	LYS
3	C	18	THR
3	C	19	ILE
3	C	23	TRP
3	C	30	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	254	GLN
1	A	298	HIS
1	A	388	GLN
1	A	440	HIS
1	A	446	ASN
2	B	73	GLN
2	B	77	ASN
2	B	91	GLN
2	B	114	HIS
2	B	122	ASN

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Mol	Chain	Res	Type
2	B	158	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
6	HAS	A	801	1	56,72,72	4.22	22 (39%)	50,109,109	4.04	29 (58%)
5	HEM	A	800	1	27,50,50	2.90	13 (48%)	17,82,82	3.07	8 (47%)
7	CUA	B	802	2	0,1,1	-	-	-		

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
6	HAS	A	801	1	-	6/35/122/122	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	800	1	-	2/6/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C1B-NB	-13.25	1.31	1.49
6	A	801	HAS	C1D-ND	-11.36	1.34	1.49
6	A	801	HAS	C3D-C2D	10.80	1.47	1.34
6	A	801	HAS	C4D-ND	-10.11	1.35	1.49
6	A	801	HAS	C4B-NB	-8.74	1.37	1.49
6	A	801	HAS	C4A-C3A	8.69	1.50	1.38
6	A	801	HAS	C1A-C2A	7.46	1.48	1.38
6	A	801	HAS	C3C-CAC	-7.46	1.32	1.47
5	A	800	HEM	C3D-C2D	7.17	1.58	1.37
6	A	801	HAS	C1D-C2D	-6.18	1.41	1.51
5	A	800	HEM	C3C-C2C	-5.21	1.33	1.40
5	A	800	HEM	C4B-NB	5.02	1.46	1.36
6	A	801	HAS	CHD-C4A	-4.71	1.46	1.51
5	A	800	HEM	C3B-CAB	4.66	1.57	1.47
5	A	800	HEM	C3C-CAC	4.40	1.56	1.47
6	A	801	HAS	C2B-C3B	4.20	1.37	1.34
6	A	801	HAS	CHC-C4B	-3.92	1.46	1.53
6	A	801	HAS	CMD-C2D	3.83	1.51	1.44
5	A	800	HEM	C3B-C2B	-3.73	1.35	1.40
6	A	801	HAS	C3C-C2C	3.70	1.45	1.40
6	A	801	HAS	CHD-C4C	-3.51	1.47	1.51
5	A	800	HEM	C4D-C3D	3.38	1.50	1.42
5	A	800	HEM	CMB-C2B	3.32	1.59	1.51
5	A	800	HEM	CMD-C2D	3.08	1.58	1.51
6	A	801	HAS	C1C-C2C	2.84	1.42	1.38
6	A	801	HAS	CAA-C2A	-2.63	1.48	1.52
6	A	801	HAS	CHA-C4D	-2.57	1.48	1.53
6	A	801	HAS	C2A-C3A	2.54	1.45	1.37
5	A	800	HEM	CAD-C3D	2.48	1.56	1.52
5	A	800	HEM	C1B-C2B	2.32	1.47	1.42
6	A	801	HAS	FE-NC	2.25	2.11	1.95
6	A	801	HAS	FE-NA	2.15	2.11	1.95
5	A	800	HEM	CMC-C2C	2.02	1.56	1.51
6	A	801	HAS	C11-C3B	-2.01	1.48	1.51
5	A	800	HEM	C1C-C2C	2.00	1.47	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C12-C11-C3B	-10.34	100.75	114.11
6	A	801	HAS	CHB-C1B-NB	10.05	123.43	110.94
6	A	801	HAS	CHB-C1D-ND	8.01	120.90	110.94
5	A	800	HEM	CAA-CBA-CGA	-7.47	100.13	112.67
6	A	801	HAS	C4C-CHD-C4A	7.18	130.39	112.87
6	A	801	HAS	CHA-C4D-ND	6.96	123.88	110.75
6	A	801	HAS	CAD-CBD-CGD	-6.82	101.23	112.67
6	A	801	HAS	CAA-CBA-CGA	-6.79	101.27	112.67
6	A	801	HAS	CHC-C4B-NB	6.20	122.44	110.75
6	A	801	HAS	C27-C19-C20	6.03	125.41	115.27
5	A	800	HEM	C4C-C3C-C2C	5.73	110.90	106.90
6	A	801	HAS	CHC-C1C-C2C	-5.37	120.16	129.45
6	A	801	HAS	C4A-C3A-C2A	-5.09	100.39	105.81
6	A	801	HAS	C1D-CHB-C1B	4.86	130.18	116.15
6	A	801	HAS	C24-C28-C29	-4.37	97.52	111.88
5	A	800	HEM	C1D-C2D-C3D	-4.23	104.05	107.00
6	A	801	HAS	CHD-C4A-C3A	-4.20	122.51	129.53
6	A	801	HAS	C32-C30-C31	3.87	123.16	114.60
6	A	801	HAS	C21-C22-C23	-3.76	118.61	127.66
5	A	800	HEM	CAD-CBD-CGD	-3.75	106.39	112.67
6	A	801	HAS	CAA-C2A-C1A	3.49	129.75	127.30
6	A	801	HAS	C31-C30-C29	-3.45	112.66	122.65
6	A	801	HAS	OMD-CMD-C2D	3.41	128.71	124.39
6	A	801	HAS	C27-C19-C18	-3.25	115.35	123.68
6	A	801	HAS	C4C-C3C-C2C	3.20	109.31	104.41
6	A	801	HAS	CHD-C4C-C3C	-2.97	125.71	129.61
5	A	800	HEM	CMA-C3A-C4A	-2.95	123.93	128.46
6	A	801	HAS	CBD-CAD-C3D	-2.93	109.16	114.35
5	A	800	HEM	CBD-CAD-C3D	2.69	117.43	112.48
6	A	801	HAS	CHB-C1B-C2B	2.63	122.90	114.70
6	A	801	HAS	C12-C13-C14	2.53	118.92	112.23
6	A	801	HAS	C13-C14-C15	-2.24	122.26	127.66
5	A	800	HEM	CBA-CAA-C2A	-2.24	108.36	112.49
6	A	801	HAS	O11-C11-C3B	2.23	116.00	110.36
6	A	801	HAS	C24-C23-C22	2.22	125.61	121.12
5	A	800	HEM	CMD-C2D-C3D	2.15	129.00	124.94
6	A	801	HAS	C26-C15-C14	-2.01	118.52	123.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
5	A	800	HEM	C4D-C3D-CAD-CBD
6	A	801	HAS	C2D-C3D-CAD-CBD
6	A	801	HAS	C4D-C3D-CAD-CBD
6	A	801	HAS	C11-C12-C13-C14
6	A	801	HAS	C25-C23-C24-C28
6	A	801	HAS	C22-C23-C24-C28
6	A	801	HAS	C23-C24-C28-C29

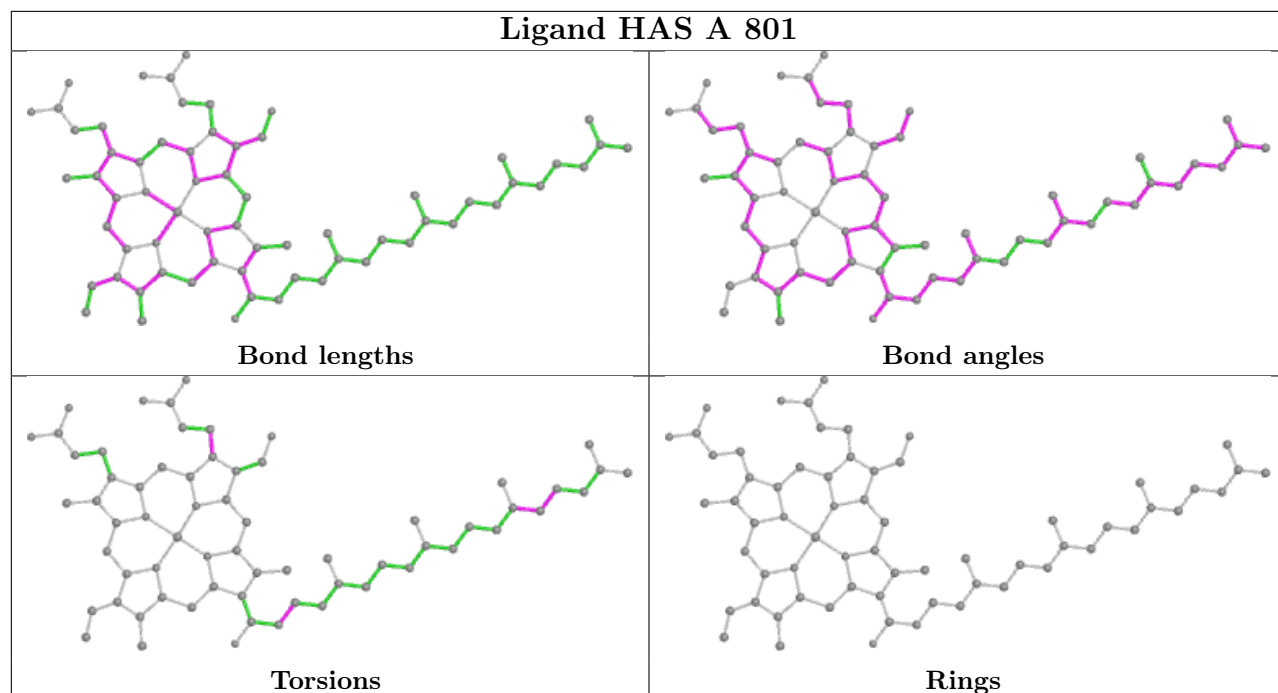
There are no ring outliers.

2 monomers are involved in 46 short contacts:

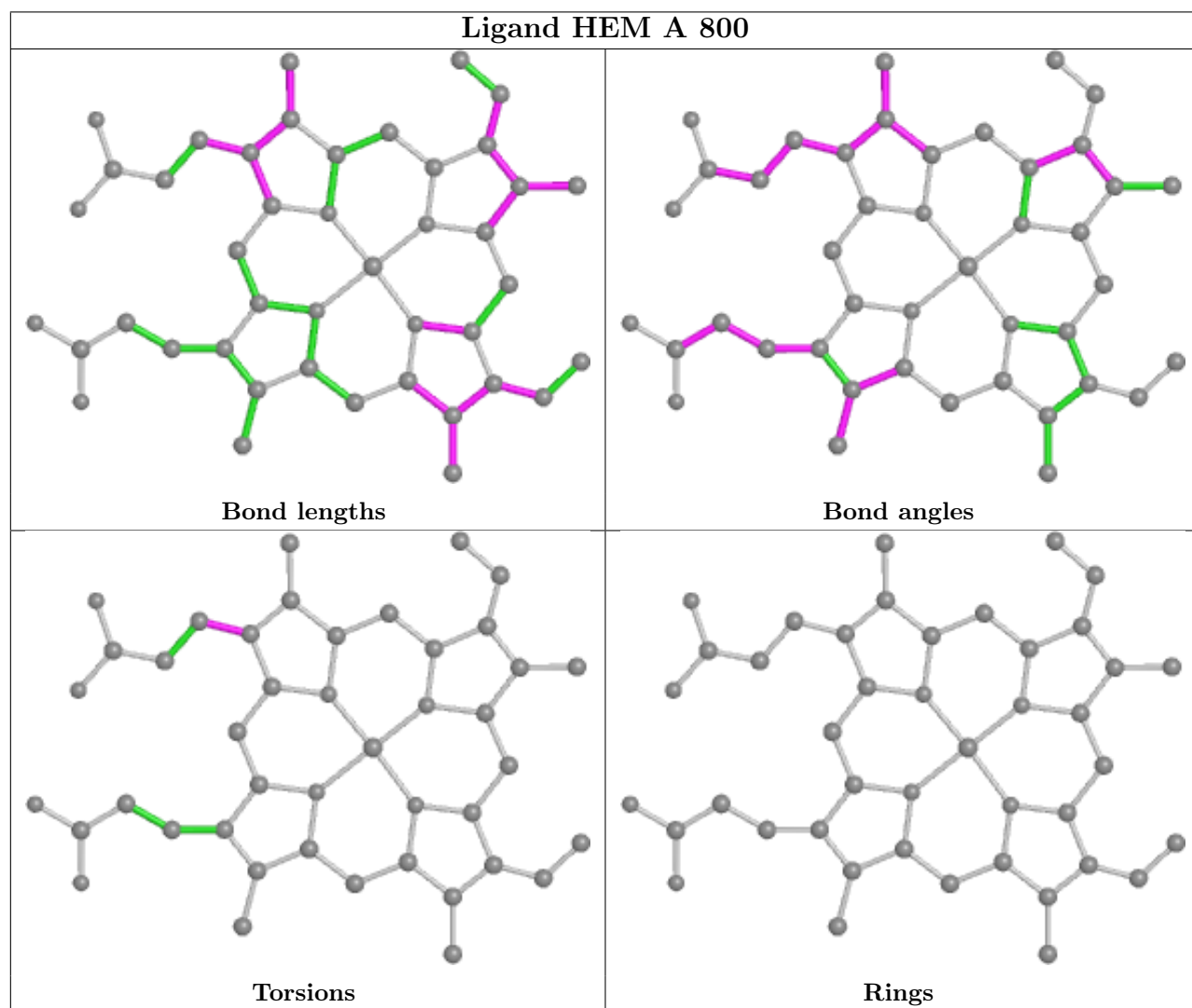
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	801	HAS	21	0
5	A	800	HEM	25	0

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.

## Ligand HAS A 801



## Ligand HEM A 800



## 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	557/618 (90%)	-0.02	22 (3%) 39 20	66, 98, 130, 159	0
2	B	166/166 (100%)	0.04	4 (2%) 59 37	75, 98, 134, 192	0
3	C	33/33 (100%)	-0.26	2 (6%) 21 9	73, 88, 128, 146	0
All	All	756/817 (92%)	-0.02	28 (3%) 41 21	66, 98, 133, 192	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	SER	15.0
1	A	7	GLU	12.0
1	A	493	LEU	6.0
2	B	5	HIS	4.6
1	A	14	ALA	4.6
1	A	175	PRO	3.6
1	A	174	ASN	3.2
3	C	2	GLU	3.1
1	A	551	GLY	2.9
1	A	522	LEU	2.8
1	A	487	GLY	2.7
2	B	7	ALA	2.6
1	A	218	GLY	2.6
1	A	16	PRO	2.6
2	B	8	HIS	2.5
1	A	143	TRP	2.5
1	A	514	GLY	2.4
1	A	173	ALA	2.4
1	A	8	ILE	2.4
1	A	98	ASN	2.3
1	A	515	PRO	2.3
1	A	500	GLU	2.3
1	A	214	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	3	GLU	2.1
1	A	547	VAL	2.1
1	A	176	GLY	2.1
1	A	416	ALA	2.1
2	B	57	THR	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

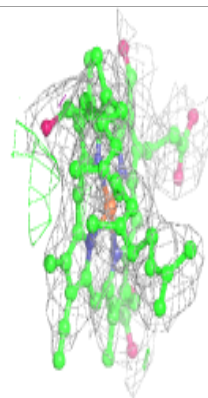
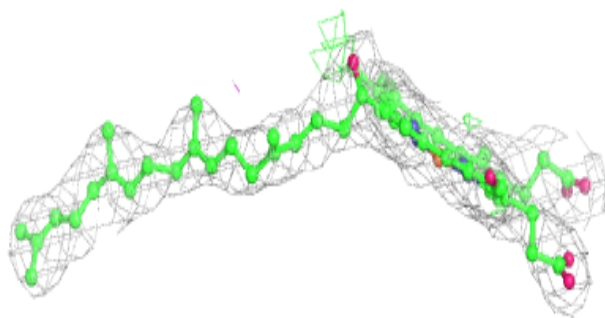
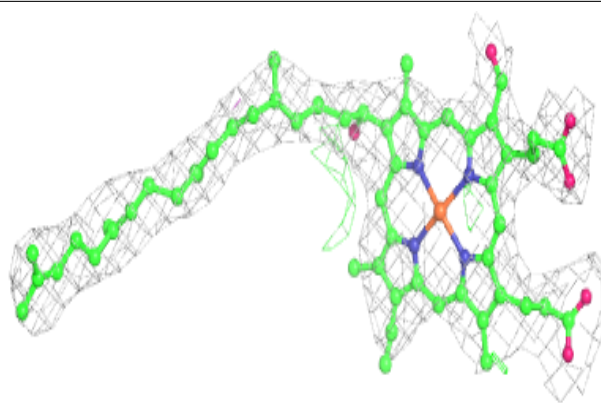
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	HAS	A	801	65/65	0.96	0.19	65,82,93,95	0
5	HEM	A	800	43/43	0.97	0.18	66,79,100,118	0
4	CU1	A	803	1/1	0.98	0.15	97,97,97,97	0
7	CUA	B	802	2/2	0.99	0.09	103,103,103,118	0

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

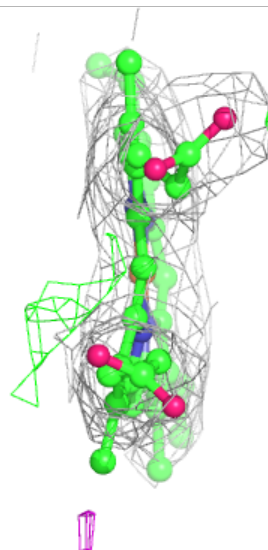
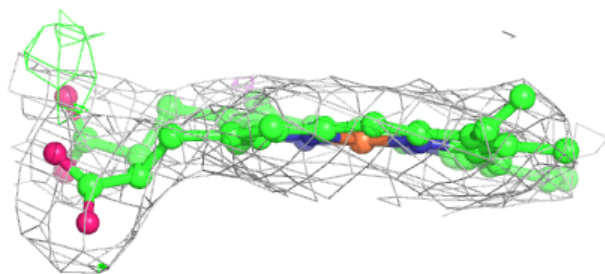
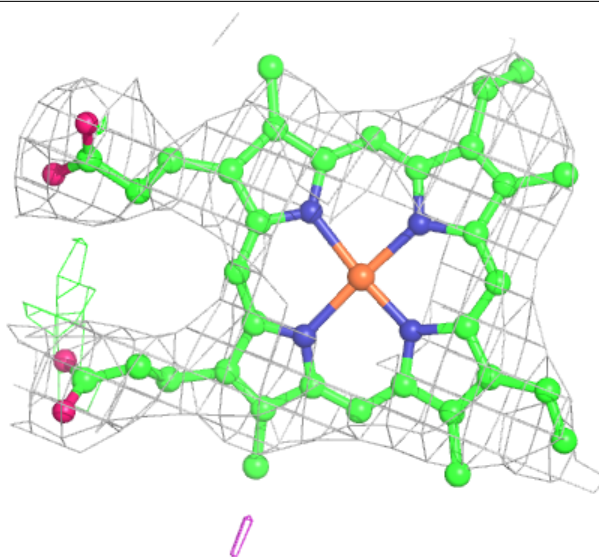
**Electron density around HAS A 801:**

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



**Electron density around HEM A 800:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.