



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 03:46 AM EDT

PDB ID : 2QPD  
Title : An unexpected outcome of surface-engineering an integral membrane protein: Improved crystallization of cytochrome ba3 oxidase from *Thermus thermophilus*  
Authors : Liu, B.; Luna, V.M.; Chen, Y.; Stout, C.D.; Fee, J.A.  
Deposited on : 2007-07-23  
Resolution : 3.25 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

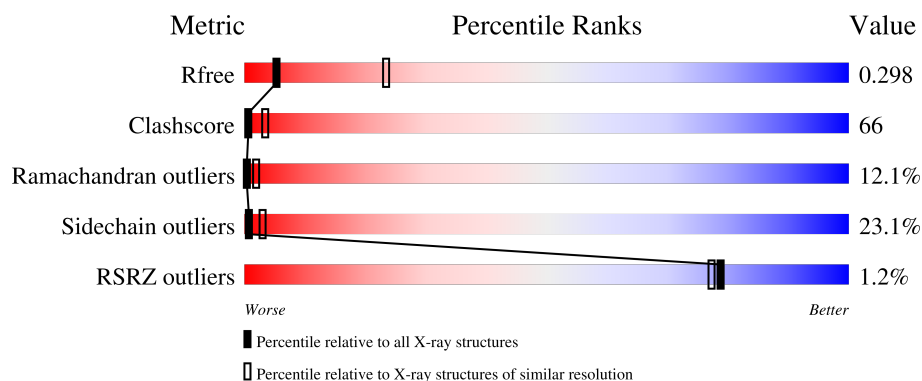
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	568	<div> <div></div> <div>20%51%23% . .</div> </div>
2	B	168	<div> <div></div> <div>23%52%20% . .</div> </div>
3	C	34	<div> <div>3%</div> <div>18%47%29% . .</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
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
1	A	557	Total	C	N	O	S	0	0	0
			4409	2985	709	699	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	216	234	4			

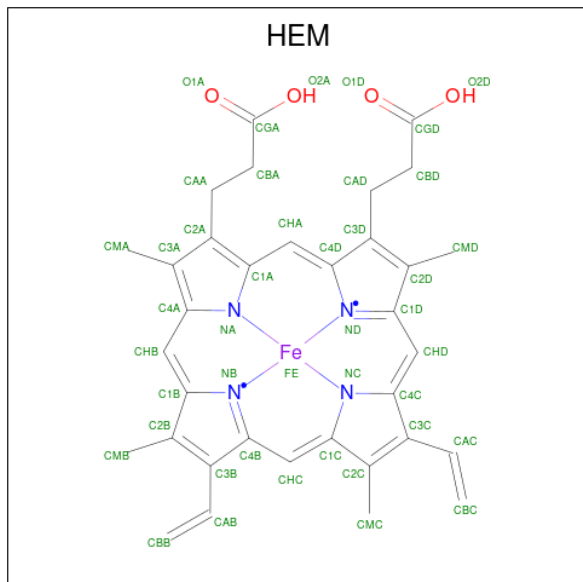
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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).

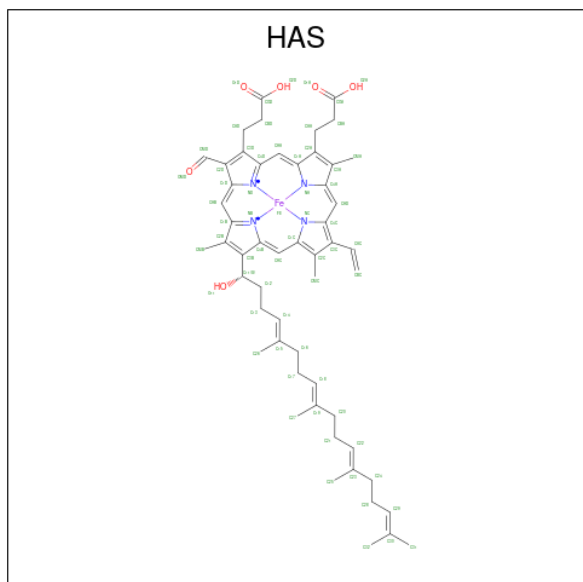
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



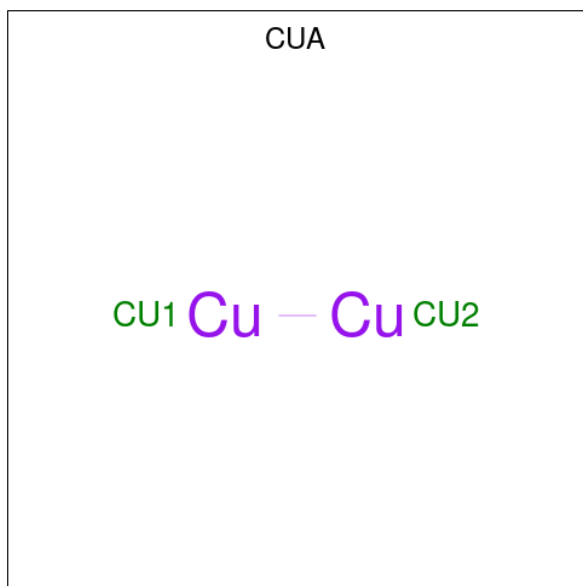
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



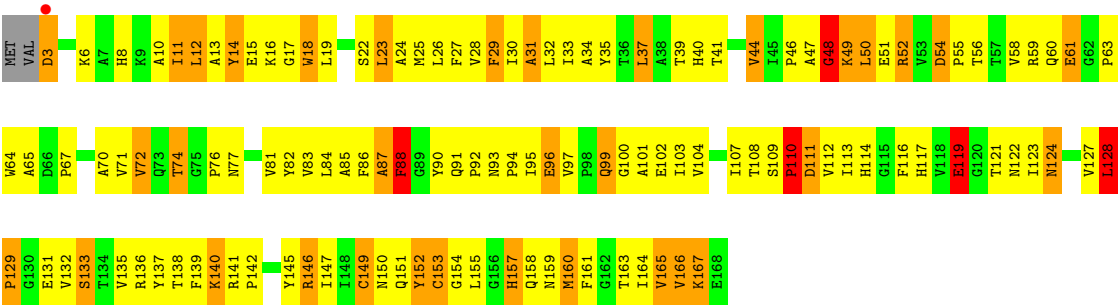
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

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

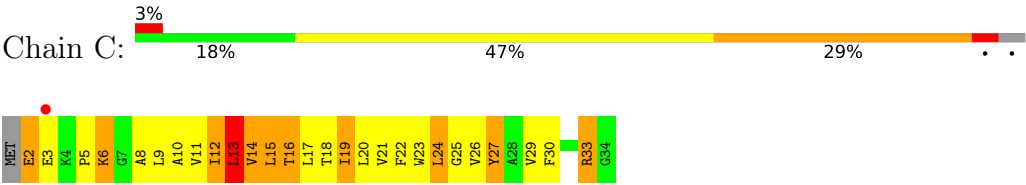


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			2	2		





● 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, $\alpha$ , $\beta$ , $\gamma$	115.19Å 115.19Å 149.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.25 19.98 – 3.01	Depositor EDS
% Data completeness (in resolution range)	77.2 (19.98-3.25) 77.2 (19.98-3.01)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.307 0.189 , 0.298	Depositor DCC
$R_{free}$ test set	780 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 81.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: CU1, HEM, HAS, CUA

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	1.07	1/4566 (0.0%)	1.19	23/6266 (0.4%)
2	B	1.09	2/1335 (0.1%)	1.22	6/1822 (0.3%)
3	C	1.21	0/265	1.24	2/359 (0.6%)
All	All	1.08	3/6166 (0.0%)	1.20	31/8447 (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	4
2	B	0	3
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	CYS	CB-SG	-6.39	1.71	1.82
2	B	29	PHE	CE1-CZ	6.35	1.49	1.37
1	A	248	TYR	CD1-CE1	6.19	1.48	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	50	LEU	CA-CB-CG	8.70	135.32	115.30
1	A	22	LEU	CA-CB-CG	-8.64	95.43	115.30
1	A	225	ARG	NE-CZ-NH2	8.40	124.50	120.30
2	B	128	LEU	CA-CB-CG	8.29	134.36	115.30
1	A	493	LEU	CA-CB-CG	7.95	133.58	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	33	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	401	LEU	CA-CB-CG	6.54	130.34	115.30
3	C	33	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	225	ARG	NE-CZ-NH1	-6.47	117.07	120.30
2	B	146	ARG	CB-CG-CD	-6.41	94.92	111.60
1	A	303	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	122	LEU	CA-CB-CG	6.34	129.88	115.30
1	A	220	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	19	LYS	CD-CE-NZ	6.14	125.81	111.70
1	A	220	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	327	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	37	LEU	CA-CB-CG	-6.05	101.39	115.30
1	A	437	VAL	CB-CA-C	-6.01	99.99	111.40
1	A	202	LEU	CA-CB-CG	5.91	128.90	115.30
2	B	23	LEU	CA-CB-CG	5.80	128.65	115.30
1	A	164	LEU	CA-CB-CG	-5.79	101.97	115.30
1	A	341	TRP	CA-CB-CG	-5.67	102.93	113.70
1	A	267	LEU	CA-CB-CG	-5.58	102.47	115.30
1	A	449	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	108	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	122	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	A	472	LEU	CB-CG-CD1	-5.27	102.04	111.00
2	B	88	PHE	CB-CA-C	5.06	120.52	110.40
2	B	146	ARG	CG-CD-NE	5.06	122.43	111.80
1	A	138	PRO	N-CA-C	5.03	125.17	112.10
1	A	561	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	ASN	Peptide
1	A	400	SER	Peptide
1	A	458	ASP	Peptide
1	A	503	GLU	Peptide
2	B	46	PRO	Peptide
2	B	48	GLY	Peptide
2	B	87	ALA	Peptide

## 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	4409	0	4516	648	0
2	B	1298	0	1280	162	0
3	C	259	0	279	40	0
4	A	1	0	0	0	0
5	A	43	0	30	9	0
6	A	65	0	61	33	0
7	B	2	0	0	0	0
All	All	6077	0	6166	813	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 66.

All (813) 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	1.02	1.42
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.95	1.27
1:A:12:TYR:HA	1:A:16:PRO:HB3	1.21	1.20
1:A:102:ASN:OD1	1:A:105:LEU:HG	1.41	1.19
1:A:120:ALA:O	1:A:123:PRO:HD2	1.41	1.17
1:A:300:VAL:HG13	2:B:30:ILE:CD1	1.78	1.14
1:A:410:GLY:CA	1:A:502:ALA:HB2	1.77	1.13
1:A:385:PHE:CB	6:A:801:HAS:HMA2	1.81	1.10
1:A:388:GLN:HA	1:A:388:GLN:NE2	1.61	1.10
1:A:559:TRP:HB3	1:A:561:LEU:HD21	1.31	1.10
1:A:385:PHE:CG	6:A:801:HAS:HMA2	1.86	1.09
1:A:559:TRP:HB3	1:A:561:LEU:CD2	1.85	1.06
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.34	1.05
2:B:97:VAL:HG23	2:B:166:VAL:HG12	1.38	1.03
1:A:388:GLN:CA	1:A:388:GLN:HE21	1.68	1.02
1:A:300:VAL:HG13	2:B:30:ILE:HD13	1.36	1.02
1:A:526:ARG:HH21	1:A:529:PHE:HB2	1.21	1.02
1:A:518:ARG:HH21	1:A:518:ARG:HG3	1.26	0.98
1:A:101:PRO:HA	1:A:166:LEU:HD11	1.46	0.97
2:B:6:LYS:HE2	3:C:2:GLU:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:HIS:O	2:B:11:ILE:HG22	1.65	0.96
1:A:388:GLN:NE2	1:A:388:GLN:CA	2.25	0.94
2:B:149:CYS:HB3	2:B:160:MET:HG2	1.49	0.94
1:A:44:LEU:O	1:A:48:ASN:N	2.01	0.93
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.84	0.93
1:A:24:PHE:CD1	1:A:110:TRP:HD1	1.87	0.92
1:A:300:VAL:CG1	2:B:30:ILE:CD1	2.47	0.91
1:A:38:PHE:CZ	1:A:71:LEU:HD12	2.06	0.90
1:A:560:ARG:O	1:A:560:ARG:HG3	1.69	0.90
1:A:55:LEU:O	1:A:55:LEU:HG	1.70	0.89
1:A:78:ILE:HG22	1:A:79:VAL:N	1.84	0.89
1:A:271:LEU:CD1	1:A:308:PRO:HD3	2.03	0.88
1:A:135:PHE:O	1:A:137:PRO:HD3	1.72	0.88
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.61	0.88
2:B:97:VAL:HG23	2:B:166:VAL:CG1	2.04	0.87
1:A:34:VAL:O	1:A:37:LEU:HB2	1.74	0.87
1:A:271:LEU:HD13	1:A:308:PRO:HD3	1.57	0.87
1:A:313:ALA:HB2	6:A:801:HAS:H273	1.56	0.86
1:A:54:LEU:HD13	1:A:55:LEU:N	1.90	0.86
1:A:24:PHE:HD1	1:A:110:TRP:CD1	1.94	0.86
1:A:313:ALA:HB2	6:A:801:HAS:C27	2.05	0.86
1:A:412:PRO:HB3	1:A:501:LEU:HD13	1.58	0.86
1:A:423:ALA:O	1:A:427:LEU:HB2	1.76	0.86
1:A:486:TYR:O	1:A:490:SER:HB3	1.76	0.86
1:A:192:MET:HB2	1:A:273:LEU:HA	1.57	0.86
1:A:154:LEU:O	1:A:157:TRP:HB2	1.74	0.85
1:A:309:SER:O	6:A:801:HAS:C27	2.24	0.85
1:A:233:HIS:CE1	1:A:282:HIS:HE1	1.94	0.85
1:A:410:GLY:HA3	1:A:502:ALA:HB2	1.59	0.85
1:A:350:VAL:O	1:A:354:LEU:HD22	1.77	0.84
1:A:300:VAL:HG13	2:B:30:ILE:HD11	1.60	0.84
1:A:300:VAL:CG1	2:B:30:ILE:HD13	2.07	0.84
1:A:351:LEU:HA	1:A:354:LEU:HD23	1.57	0.84
1:A:233:HIS:CE1	1:A:282:HIS:CE1	2.65	0.83
2:B:149:CYS:CB	2:B:160:MET:HG2	2.07	0.83
1:A:24:PHE:HE1	1:A:110:TRP:HA	1.41	0.83
1:A:347:VAL:HG12	1:A:351:LEU:HD11	1.61	0.83
1:A:309:SER:O	6:A:801:HAS:H273	1.78	0.82
1:A:233:HIS:HB3	1:A:234:PRO:HD2	1.60	0.82
1:A:386:HIS:O	1:A:390:ALA:HB3	1.79	0.82
1:A:54:LEU:C	1:A:54:LEU:HD22	2.00	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASN:O	1:A:177:LYS:HB2	1.80	0.82
1:A:38:PHE:HZ	1:A:71:LEU:HD12	1.45	0.81
1:A:277:THR:H	1:A:278:PRO:HD3	1.43	0.81
1:A:559:TRP:CB	1:A:561:LEU:HD21	2.10	0.81
1:A:105:LEU:HB2	1:A:162:ILE:HD11	1.62	0.81
2:B:44:VAL:HG11	2:B:122:ASN:HB2	1.63	0.81
1:A:124:LEU:HD23	1:A:129:ALA:HB3	1.62	0.80
1:A:234:PRO:HD3	1:A:276:SER:O	1.81	0.80
1:A:498:LYS:N	1:A:499:PRO:HD3	1.97	0.80
1:A:24:PHE:CD1	1:A:110:TRP:CD1	2.68	0.79
1:A:63:GLN:HA	1:A:63:GLN:NE2	1.97	0.79
1:A:403:TRP:CZ3	1:A:404:LEU:HD13	2.17	0.79
3:C:8:ALA:O	3:C:11:VAL:HB	1.82	0.79
1:A:11:VAL:O	1:A:13:GLU:N	2.15	0.79
1:A:505:PRO:O	1:A:506:LEU:O	2.01	0.79
1:A:146:TYR:CE2	1:A:208:LEU:HD22	2.19	0.79
1:A:385:PHE:CD2	6:A:801:HAS:HMA2	2.17	0.79
1:A:410:GLY:HA2	1:A:502:ALA:CB	2.12	0.78
1:A:526:ARG:NH2	1:A:529:PHE:HB2	1.98	0.78
1:A:294:TRP:CZ2	1:A:544:PRO:HD2	2.19	0.78
1:A:184:TYR:CD2	1:A:266:ARG:HG2	2.17	0.78
1:A:385:PHE:CB	6:A:801:HAS:CMA	2.61	0.77
2:B:90:TYR:OH	2:B:149:CYS:HB2	1.84	0.77
1:A:340:PRO:O	1:A:342:ASP:N	2.18	0.77
1:A:374:VAL:HG21	3:C:30:PHE:HA	1.67	0.76
1:A:30:LEU:O	1:A:33:ILE:N	2.18	0.76
1:A:472:LEU:HD22	1:A:472:LEU:O	1.84	0.76
2:B:61:GLU:HA	2:B:65:ALA:HB2	1.65	0.76
1:A:406:PRO:HA	1:A:411:LYS:O	1.85	0.76
1:A:542:TYR:HB3	1:A:546:LEU:HD12	1.68	0.76
1:A:70:THR:HG23	1:A:132:LEU:HA	1.68	0.75
1:A:78:ILE:O	1:A:82:GLN:HB2	1.86	0.75
2:B:11:ILE:HG23	2:B:12:LEU:N	2.01	0.75
2:B:113:ILE:HG12	2:B:128:LEU:HD12	1.67	0.75
1:A:135:PHE:CZ	1:A:228:PHE:HE1	2.04	0.75
1:A:236:VAL:HA	1:A:239:TRP:CE3	2.21	0.75
2:B:34:ALA:HA	2:B:37:LEU:HD22	1.69	0.75
1:A:277:THR:N	1:A:278:PRO:CD	2.50	0.75
1:A:544:PRO:O	1:A:548:GLN:HG3	1.87	0.75
1:A:28:GLY:O	1:A:31:ALA:HB3	1.86	0.75
1:A:187:VAL:CG1	1:A:527:ILE:HD12	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:SER:HB3	2:B:129:PRO:HG3	1.69	0.75
1:A:389:VAL:HG22	5:A:800:HEM:CB	2.17	0.75
1:A:297:ILE:HG22	1:A:298:HIS:N	2.01	0.74
1:A:304:PHE:O	1:A:307:VAL:HG23	1.87	0.74
1:A:93:PRO:HB3	1:A:183:THR:HG23	1.70	0.74
1:A:112:MET:HB3	1:A:155:SER:HB2	1.69	0.73
1:A:236:VAL:CG2	1:A:237:TYR:H	2.02	0.73
2:B:11:ILE:CG2	2:B:12:LEU:H	2.00	0.73
3:C:11:VAL:HG12	3:C:12:ILE:N	2.02	0.73
1:A:317:ALA:HA	1:A:320:LEU:HD12	1.70	0.73
1:A:93:PRO:HG3	1:A:186:ALA:HB2	1.71	0.73
1:A:122:LEU:HA	1:A:125:LEU:CD1	2.18	0.73
1:A:412:PRO:HB3	1:A:501:LEU:CD1	2.19	0.73
2:B:154:GLY:O	2:B:157:HIS:HB2	1.89	0.73
1:A:244:TYR:OH	1:A:309:SER:HB3	1.89	0.73
1:A:270:LEU:HD22	1:A:524:MET:HG2	1.71	0.73
1:A:388:GLN:HE21	1:A:388:GLN:N	1.85	0.73
1:A:497:ARG:C	1:A:499:PRO:HD3	2.09	0.73
1:A:157:TRP:CZ2	1:A:194:PHE:HE2	2.07	0.73
1:A:91:TYR:CE2	1:A:408:LEU:HD21	2.22	0.73
1:A:389:VAL:HA	1:A:393:VAL:HG23	1.71	0.73
1:A:385:PHE:HB3	6:A:801:HAS:HMA2	1.71	0.72
1:A:52:TYR:N	1:A:53:PRO:CD	2.51	0.72
1:A:236:VAL:HG23	1:A:237:TYR:N	2.05	0.72
1:A:344:PRO:HG3	1:A:422:LEU:HD23	1.71	0.72
1:A:364:ILE:HG22	1:A:365:VAL:N	2.04	0.72
1:A:318:ALA:O	1:A:321:GLU:HB3	1.90	0.72
2:B:32:LEU:O	2:B:35:TYR:HB3	1.90	0.72
2:B:11:ILE:CG2	2:B:12:LEU:N	2.52	0.72
1:A:499:PRO:HB3	1:A:502:ALA:CB	2.20	0.71
3:C:26:VAL:O	3:C:29:VAL:N	2.22	0.71
1:A:356:PHE:CE2	6:A:801:HAS:H162	2.25	0.71
1:A:482:LEU:O	1:A:485:ILE:N	2.23	0.71
1:A:406:PRO:HD3	1:A:413:ILE:CD1	2.20	0.71
1:A:12:TYR:CA	1:A:16:PRO:HB3	2.13	0.70
1:A:544:PRO:HA	1:A:547:VAL:HG12	1.74	0.70
1:A:9:SER:OG	1:A:11:VAL:HG23	1.92	0.70
1:A:347:VAL:HG12	1:A:351:LEU:CD1	2.21	0.70
1:A:499:PRO:HB3	1:A:502:ALA:HB2	1.73	0.70
1:A:106:MET:N	1:A:162:ILE:HD11	2.07	0.70
1:A:389:VAL:HG22	5:A:800:HEM:HBC1	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ARG:O	2:B:65:ALA:HA	1.90	0.70
1:A:465:VAL:HA	1:A:468:VAL:HG23	1.73	0.70
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.21	0.69
1:A:23:TYR:HD1	1:A:107:TRP:HH2	1.39	0.69
1:A:181:LEU:HD13	1:A:262:ASP:OD1	1.93	0.69
1:A:411:LYS:HG2	1:A:497:ARG:HB3	1.74	0.69
1:A:497:ARG:HH21	1:A:499:PRO:HG2	1.58	0.68
1:A:24:PHE:HD1	1:A:110:TRP:HD1	1.27	0.68
1:A:385:PHE:CG	6:A:801:HAS:CMA	2.73	0.68
1:A:545:THR:O	1:A:549:LEU:HG	1.93	0.68
1:A:518:ARG:HH21	1:A:518:ARG:CG	2.03	0.68
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.23	0.68
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.29	0.68
1:A:370:THR:HA	1:A:373:TYR:CD1	2.29	0.68
1:A:122:LEU:HA	1:A:125:LEU:HD11	1.75	0.68
1:A:236:VAL:HG23	1:A:237:TYR:H	1.59	0.67
1:A:385:PHE:HB2	6:A:801:HAS:CMA	2.25	0.67
1:A:515:PRO:HD2	2:B:8:HIS:HD2	1.58	0.67
1:A:363:GLY:O	1:A:366:ASN:HB2	1.94	0.67
1:A:370:THR:HA	1:A:373:TYR:CE1	2.30	0.67
1:A:97:LEU:HD22	1:A:170:TRP:NE1	2.10	0.67
1:A:233:HIS:ND1	1:A:282:HIS:CE1	2.62	0.67
1:A:323:ALA:O	1:A:327:ARG:HG3	1.95	0.66
1:A:441:TRP:HB3	1:A:466:PRO:HB3	1.78	0.66
1:A:472:LEU:HD22	1:A:472:LEU:C	2.16	0.66
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.31	0.66
2:B:149:CYS:HB3	2:B:160:MET:CG	2.24	0.66
1:A:187:VAL:HG12	1:A:527:ILE:HD12	1.77	0.66
1:A:251:LEU:HA	1:A:254:GLN:HG3	1.77	0.66
1:A:386:HIS:HA	1:A:390:ALA:HB3	1.77	0.66
1:A:50:ASP:O	1:A:53:PRO:HD2	1.96	0.66
2:B:84:LEU:CD1	2:B:108:THR:HG23	2.26	0.66
1:A:251:LEU:HA	1:A:254:GLN:CG	2.26	0.66
1:A:386:HIS:HE1	5:A:800:HEM:C4D	2.14	0.66
1:A:147:LEU:O	1:A:151:VAL:HG23	1.95	0.65
1:A:388:GLN:HA	1:A:388:GLN:HE21	1.26	0.65
2:B:84:LEU:HD12	2:B:108:THR:O	1.97	0.65
1:A:236:VAL:CG2	1:A:237:TYR:N	2.59	0.65
1:A:404:LEU:O	1:A:408:LEU:HB2	1.97	0.65
1:A:526:ARG:HH21	1:A:529:PHE:CB	2.02	0.65
1:A:120:ALA:O	1:A:123:PRO:CD	2.33	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LEU:HA	3:C:12:ILE:CD1	2.27	0.65
1:A:297:ILE:O	1:A:300:VAL:N	2.30	0.65
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.32	0.65
1:A:385:PHE:HB2	6:A:801:HAS:HMA2	1.77	0.65
1:A:346:PHE:O	1:A:350:VAL:HG23	1.97	0.65
1:A:192:MET:HB2	1:A:273:LEU:CA	2.27	0.65
1:A:220:ASP:HB2	1:A:554:ASN:H	1.61	0.65
1:A:112:MET:CB	1:A:155:SER:HB2	2.26	0.64
1:A:225:ARG:HA	1:A:228:PHE:HB3	1.80	0.64
1:A:464:ALA:HB3	1:A:465:VAL:HG12	1.78	0.64
1:A:523:ALA:O	1:A:526:ARG:HB2	1.98	0.64
2:B:117:HIS:HD2	2:B:124:ASN:HB2	1.63	0.64
2:B:153:CYS:SG	2:B:157:HIS:HA	2.37	0.64
1:A:38:PHE:O	1:A:39:GLY:C	2.35	0.64
1:A:105:LEU:HD23	1:A:105:LEU:N	2.11	0.64
1:A:453:ILE:HD13	1:A:454:ALA:N	2.13	0.64
1:A:505:PRO:O	1:A:506:LEU:C	2.35	0.64
1:A:560:ARG:O	1:A:560:ARG:CG	2.42	0.64
2:B:82:TYR:CD1	2:B:82:TYR:N	2.65	0.64
1:A:192:MET:CB	1:A:273:LEU:HA	2.26	0.64
1:A:271:LEU:HD12	1:A:308:PRO:HD3	1.79	0.64
3:C:13:LEU:O	3:C:16:THR:HB	1.97	0.64
1:A:88:ILE:O	1:A:90:VAL:N	2.30	0.64
1:A:170:TRP:CE3	1:A:171:LYS:HA	2.33	0.64
1:A:410:GLY:CA	1:A:502:ALA:CB	2.68	0.64
1:A:24:PHE:HE1	1:A:110:TRP:CA	2.09	0.63
1:A:466:PRO:O	1:A:469:PHE:HB2	1.98	0.63
2:B:152:TYR:HA	2:B:157:HIS:CD2	2.32	0.63
1:A:199:GLY:HA3	1:A:230:TRP:CG	2.34	0.63
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.13	0.63
1:A:75:LEU:O	1:A:79:VAL:HB	1.98	0.63
1:A:30:LEU:O	1:A:31:ALA:C	2.37	0.63
1:A:403:TRP:HZ3	1:A:404:LEU:HD13	1.62	0.63
1:A:332:LEU:HA	3:C:6:LYS:HE3	1.81	0.62
1:A:402:TYR:CE1	1:A:413:ILE:HG21	2.34	0.62
1:A:550:PHE:HA	1:A:553:LEU:CD2	2.28	0.62
1:A:105:LEU:HB2	1:A:162:ILE:CD1	2.28	0.62
1:A:251:LEU:HD12	1:A:254:GLN:HG3	1.80	0.62
1:A:343:ASN:O	1:A:347:VAL:HG23	2.00	0.62
1:A:199:GLY:HA3	1:A:230:TRP:HB3	1.82	0.62
3:C:9:LEU:HA	3:C:12:ILE:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HA	1:A:152:PHE:HA	1.81	0.62
1:A:262:ASP:N	1:A:263:PRO:HD2	2.14	0.62
2:B:131:GLU:HG3	2:B:132:VAL:N	2.14	0.62
1:A:28:GLY:N	1:A:83:LEU:HD13	2.15	0.62
1:A:442:ALA:O	1:A:445:LEU:HB2	2.00	0.62
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.34	0.62
1:A:233:HIS:O	1:A:236:VAL:HG22	1.99	0.62
1:A:407:ASN:ND2	1:A:506:LEU:HD23	2.15	0.62
1:A:56:LYS:O	1:A:59:LEU:O	2.18	0.62
2:B:90:TYR:CZ	2:B:147:ILE:HG22	2.34	0.62
1:A:133:TYR:OH	6:A:801:HAS:O1A	2.17	0.61
1:A:357:ILE:HG22	1:A:358:PRO:N	2.14	0.61
3:C:26:VAL:O	3:C:27:TYR:C	2.39	0.61
1:A:390:ALA:HA	5:A:800:HEM:HBC2	1.81	0.61
1:A:220:ASP:HB2	1:A:554:ASN:C	2.21	0.61
1:A:347:VAL:CG1	1:A:351:LEU:HD11	2.29	0.61
1:A:94:ALA:O	1:A:97:LEU:N	2.30	0.60
1:A:122:LEU:O	1:A:123:PRO:C	2.37	0.60
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.65	0.60
2:B:147:ILE:O	2:B:161:PHE:HA	2.01	0.60
1:A:54:LEU:HD22	1:A:54:LEU:O	2.00	0.60
1:A:405:LEU:O	1:A:406:PRO:C	2.37	0.60
1:A:544:PRO:O	1:A:548:GLN:CG	2.49	0.60
2:B:102:GLU:HA	2:B:138:THR:HG23	1.84	0.60
1:A:196:ALA:O	1:A:198:LEU:N	2.34	0.60
1:A:364:ILE:O	1:A:365:VAL:C	2.38	0.60
1:A:59:LEU:HB3	1:A:61:PHE:CE1	2.36	0.60
1:A:38:PHE:HA	1:A:41:PHE:HD1	1.66	0.60
1:A:154:LEU:O	1:A:157:TRP:N	2.35	0.60
1:A:187:VAL:HG11	1:A:527:ILE:HD12	1.83	0.60
1:A:189:PHE:O	1:A:191:LEU:N	2.35	0.59
1:A:277:THR:N	1:A:278:PRO:HD3	2.11	0.59
1:A:432:MET:O	1:A:436:ALA:N	2.27	0.59
1:A:108:LEU:O	1:A:112:MET:HG3	2.01	0.59
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.90	0.59
1:A:355:GLY:O	1:A:358:PRO:HG2	2.02	0.59
2:B:30:ILE:HA	2:B:33:ILE:HD12	1.82	0.59
1:A:511:VAL:HG12	1:A:512:ILE:C	2.23	0.59
1:A:550:PHE:HA	1:A:553:LEU:HD21	1.83	0.59
1:A:244:TYR:O	1:A:248:TYR:HB2	2.02	0.59
1:A:335:TRP:O	1:A:339:LEU:HD22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:PRO:HA	2:B:166:VAL:O	2.02	0.59
1:A:334:GLY:O	1:A:336:ILE:N	2.35	0.58
1:A:546:LEU:O	1:A:550:PHE:HD1	1.86	0.58
2:B:110:PRO:O	2:B:111:ASP:HB3	2.02	0.58
1:A:20:ALA:HB3	1:A:106:MET:CE	2.32	0.58
1:A:134:THR:O	1:A:135:PHE:CD1	2.56	0.58
1:A:536:ILE:HG22	1:A:537:LEU:HD23	1.85	0.58
1:A:184:TYR:CE2	1:A:266:ARG:HG2	2.38	0.58
2:B:70:ALA:O	2:B:81:VAL:HA	2.04	0.58
2:B:90:TYR:CE1	2:B:147:ILE:HG22	2.39	0.58
1:A:74:VAL:O	1:A:78:ILE:HB	2.04	0.58
1:A:52:TYR:O	1:A:56:LYS:N	2.36	0.58
1:A:554:ASN:HD22	2:B:52:ARG:HG3	1.68	0.58
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.16	0.58
2:B:157:HIS:O	2:B:160:MET:HB3	2.04	0.58
1:A:135:PHE:CZ	1:A:228:PHE:CE1	2.90	0.58
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.39	0.57
1:A:451:ALA:O	1:A:453:ILE:N	2.34	0.57
1:A:140:LYS:HE3	1:A:211:TRP:CE2	2.38	0.57
2:B:63:PRO:HG2	2:B:82:TYR:CE2	2.39	0.57
2:B:101:ALA:O	2:B:103:ILE:HD12	2.04	0.57
1:A:235:ILE:O	1:A:235:ILE:HG12	2.03	0.57
2:B:71:VAL:O	2:B:72:VAL:HG12	2.03	0.57
2:B:149:CYS:SG	2:B:160:MET:HG2	2.44	0.57
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.40	0.57
1:A:472:LEU:C	1:A:472:LEU:CD2	2.73	0.57
1:A:24:PHE:CE1	1:A:110:TRP:HA	2.31	0.57
1:A:515:PRO:HD2	2:B:8:HIS:CD2	2.39	0.57
1:A:35:GLY:CA	1:A:75:LEU:HD12	2.34	0.57
1:A:267:LEU:O	1:A:268:ALA:C	2.41	0.56
1:A:381:VAL:HB	1:A:382:PRO:CD	2.35	0.56
1:A:45:ASN:ND2	1:A:65:TYR:CZ	2.73	0.56
1:A:52:TYR:H	1:A:53:PRO:CD	2.18	0.56
1:A:260:VAL:HA	1:A:512:ILE:HD13	1.87	0.56
1:A:351:LEU:HA	1:A:354:LEU:CD2	2.33	0.56
1:A:381:VAL:O	1:A:384:HIS:HB3	2.05	0.56
2:B:83:VAL:HG12	2:B:84:LEU:N	2.19	0.56
1:A:91:TYR:OH	1:A:407:ASN:OD1	2.22	0.56
1:A:453:ILE:HD13	1:A:453:ILE:C	2.26	0.56
1:A:405:LEU:O	1:A:408:LEU:N	2.38	0.56
1:A:24:PHE:CD2	1:A:86:GLN:HB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.41	0.56
1:A:44:LEU:HD12	1:A:51:ALA:HB2	1.88	0.56
1:A:395:LEU:HD21	1:A:428:TRP:CD1	2.40	0.56
2:B:90:TYR:OH	2:B:149:CYS:CB	2.52	0.56
1:A:23:TYR:CD1	1:A:107:TRP:HH2	2.23	0.55
1:A:157:TRP:CZ2	1:A:194:PHE:CE2	2.91	0.55
1:A:344:PRO:HG3	1:A:422:LEU:CD2	2.36	0.55
2:B:56:THR:O	2:B:60:GLN:NE2	2.39	0.55
1:A:226:THR:HG23	1:A:281:PHE:HE2	1.70	0.55
1:A:467:MET:HA	1:A:470:ASN:HD22	1.71	0.55
1:A:442:ALA:O	1:A:447:VAL:HG23	2.06	0.55
1:A:365:VAL:O	1:A:367:ALA:N	2.39	0.55
1:A:481:LEU:HD12	1:A:481:LEU:O	2.05	0.55
1:A:44:LEU:C	1:A:47:GLY:H	2.10	0.55
1:A:515:PRO:CD	2:B:8:HIS:HD2	2.18	0.55
1:A:277:THR:H	1:A:278:PRO:CD	2.07	0.55
1:A:297:ILE:C	1:A:299:SER:N	2.59	0.55
1:A:135:PHE:CE1	1:A:228:PHE:CE1	2.95	0.55
1:A:106:MET:O	1:A:109:SER:HB3	2.07	0.55
2:B:88:PHE:HE2	2:B:153:CYS:SG	2.30	0.55
1:A:64:SER:O	1:A:65:TYR:C	2.44	0.55
1:A:184:TYR:CE2	1:A:266:ARG:HB3	2.42	0.55
1:A:81:THR:OG1	1:A:239:TRP:CD1	2.54	0.55
2:B:11:ILE:O	2:B:12:LEU:C	2.46	0.55
2:B:82:TYR:H	2:B:82:TYR:HD1	1.51	0.54
3:C:10:ALA:O	3:C:14:VAL:HG23	2.07	0.54
1:A:192:MET:HB2	1:A:273:LEU:CB	2.36	0.54
1:A:191:LEU:HB3	1:A:531:PHE:CD2	2.42	0.54
1:A:282:HIS:NE2	1:A:283:HIS:CD2	2.76	0.54
1:A:386:HIS:HA	1:A:390:ALA:CB	2.37	0.54
1:A:497:ARG:HH21	1:A:499:PRO:CG	2.20	0.54
2:B:27:PHE:O	2:B:31:ALA:N	2.29	0.54
3:C:10:ALA:O	3:C:13:LEU:HB3	2.07	0.54
1:A:52:TYR:N	1:A:53:PRO:HD2	2.21	0.54
1:A:89:MET:O	1:A:93:PRO:HG2	2.06	0.54
1:A:406:PRO:HD3	1:A:413:ILE:HD12	1.88	0.54
2:B:116:PHE:O	2:B:116:PHE:CD2	2.61	0.54
1:A:465:VAL:O	1:A:468:VAL:HG23	2.08	0.54
1:A:135:PHE:O	1:A:137:PRO:CD	2.52	0.54
1:A:234:PRO:HG3	1:A:277:THR:HA	1.90	0.54
1:A:532:ALA:O	1:A:536:ILE:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:VAL:HG13	1:A:548:GLN:H	1.71	0.54
1:A:89:MET:HB3	1:A:190:TRP:NE1	2.23	0.54
1:A:122:LEU:HA	1:A:125:LEU:HD12	1.89	0.54
1:A:267:LEU:HD12	1:A:270:LEU:HB3	1.89	0.54
1:A:398:MET:O	1:A:401:LEU:HB2	2.08	0.54
1:A:285:PHE:CE1	1:A:369:PHE:HA	2.43	0.54
1:A:41:PHE:HE2	1:A:54:LEU:HD11	1.72	0.54
1:A:124:LEU:CD2	1:A:129:ALA:HB3	2.34	0.54
1:A:153:VAL:O	1:A:154:LEU:C	2.44	0.54
1:A:346:PHE:O	1:A:349:PRO:HD2	2.08	0.54
1:A:371:LEU:HD23	3:C:26:VAL:HG12	1.89	0.54
1:A:511:VAL:HG12	1:A:512:ILE:O	2.06	0.54
6:A:801:HAS:HHA	6:A:801:HAS:CBA	2.38	0.54
2:B:58:VAL:HG13	2:B:59:ARG:N	2.23	0.54
1:A:498:LYS:N	1:A:499:PRO:CD	2.71	0.54
2:B:158:GLN:HG2	2:B:158:GLN:O	2.07	0.54
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.89	0.53
2:B:88:PHE:CE2	2:B:153:CYS:SG	3.01	0.53
1:A:559:TRP:CB	1:A:561:LEU:CD2	2.74	0.53
2:B:3:ASP:N	2:B:6:LYS:HB3	2.22	0.53
2:B:40:HIS:CD2	2:B:41:THR:CG2	2.91	0.53
2:B:157:HIS:ND1	2:B:157:HIS:C	2.59	0.53
1:A:21:THR:O	1:A:25:LEU:HB2	2.08	0.53
1:A:50:ASP:O	1:A:53:PRO:CD	2.56	0.53
1:A:170:TRP:HE3	1:A:171:LYS:HA	1.74	0.53
1:A:222:LEU:HD12	1:A:222:LEU:O	2.08	0.53
1:A:410:GLY:HA3	1:A:499:PRO:HB3	1.90	0.53
1:A:206:LEU:HB2	1:A:207:PHE:CD2	2.44	0.53
1:A:41:PHE:CE1	1:A:55:LEU:HD13	2.44	0.53
1:A:313:ALA:HB2	6:A:801:HAS:C19	2.39	0.53
1:A:324:GLY:O	1:A:329:GLY:N	2.40	0.53
1:A:506:LEU:O	1:A:508:PHE:N	2.42	0.53
2:B:11:ILE:HG22	2:B:12:LEU:H	1.72	0.53
1:A:97:LEU:O	1:A:99:MET:HG3	2.08	0.53
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.43	0.53
2:B:28:VAL:O	2:B:31:ALA:HB3	2.09	0.53
1:A:220:ASP:CB	1:A:554:ASN:H	2.22	0.53
1:A:236:VAL:HA	1:A:239:TRP:CD2	2.43	0.53
2:B:24:ALA:O	2:B:28:VAL:HG23	2.09	0.53
1:A:184:TYR:CG	1:A:184:TYR:O	2.61	0.52
1:A:63:GLN:NE2	1:A:63:GLN:CA	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HB2	1:A:80:PHE:CD1	2.44	0.52
1:A:352:GLY:HA2	1:A:395:LEU:HD12	1.91	0.52
1:A:199:GLY:CA	1:A:230:TRP:CG	2.92	0.52
1:A:375:VAL:O	1:A:377:ASN:N	2.42	0.52
1:A:111:TRP:O	1:A:115:ILE:HD13	2.09	0.52
1:A:329:GLY:HA3	1:A:335:TRP:HA	1.91	0.52
1:A:20:ALA:HB3	1:A:106:MET:HE2	1.91	0.52
1:A:41:PHE:O	1:A:43:ALA:N	2.43	0.52
1:A:314:PHE:HD2	3:C:12:ILE:HD12	1.75	0.52
1:A:374:VAL:CG2	3:C:30:PHE:HA	2.38	0.52
1:A:375:VAL:O	1:A:376:HIS:C	2.47	0.52
1:A:262:ASP:HB3	1:A:263:PRO:CD	2.40	0.52
1:A:410:GLY:HA3	1:A:499:PRO:HG3	1.92	0.52
2:B:64:TRP:CH2	2:B:132:VAL:HG21	2.45	0.52
2:B:74:THR:O	2:B:74:THR:OG1	2.26	0.52
2:B:109:SER:HB3	2:B:129:PRO:CG	2.38	0.52
1:A:74:VAL:O	1:A:79:VAL:HG23	2.09	0.51
1:A:294:TRP:CH2	1:A:544:PRO:HD2	2.45	0.51
1:A:302:THR:O	1:A:305:VAL:N	2.42	0.51
1:A:520:LEU:HG	1:A:521:VAL:N	2.25	0.51
2:B:24:ALA:O	2:B:25:MET:C	2.49	0.51
1:A:27:LEU:HD23	1:A:83:LEU:HD22	1.91	0.51
2:B:54:ASP:OD1	2:B:54:ASP:C	2.49	0.51
1:A:218:GLY:O	1:A:555:PRO:HB3	2.09	0.51
1:A:356:PHE:HE2	6:A:801:HAS:H162	1.74	0.51
1:A:151:VAL:O	1:A:152:PHE:C	2.48	0.51
1:A:161:TYR:O	1:A:165:ASP:N	2.33	0.51
1:A:406:PRO:CD	1:A:413:ILE:CD1	2.88	0.51
2:B:84:LEU:HG	2:B:110:PRO:HD3	1.93	0.51
2:B:90:TYR:HH	2:B:149:CYS:HB2	1.75	0.51
1:A:459:ALA:O	2:B:146:ARG:NH1	2.37	0.51
1:A:52:TYR:H	1:A:53:PRO:HD3	1.76	0.51
2:B:35:TYR:C	2:B:35:TYR:CD1	2.76	0.51
1:A:21:THR:HG21	1:A:91:TYR:CB	2.40	0.51
1:A:223:VAL:HG12	1:A:549:LEU:HD12	1.93	0.51
1:A:412:PRO:CB	1:A:501:LEU:HD13	2.35	0.51
1:A:428:TRP:CD1	1:A:428:TRP:C	2.84	0.51
2:B:55:PRO:HB3	2:B:109:SER:O	2.11	0.51
1:A:340:PRO:C	1:A:342:ASP:H	2.15	0.51
1:A:402:TYR:HE1	1:A:413:ILE:HG21	1.75	0.51
1:A:18:LYS:NZ	1:A:504:ALA:HB2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:O	1:A:117:LEU:N	2.34	0.50
2:B:72:VAL:CG2	2:B:72:VAL:O	2.59	0.50
1:A:134:THR:HG22	1:A:228:PHE:CE2	2.46	0.50
1:A:129:ALA:O	1:A:131:VAL:HG22	2.11	0.50
1:A:388:GLN:HB3	6:A:801:HAS:HMC3	1.92	0.50
1:A:465:VAL:O	1:A:466:PRO:C	2.50	0.50
1:A:18:LYS:HZ1	1:A:504:ALA:CB	2.24	0.50
1:A:18:LYS:HZ1	1:A:504:ALA:HB3	1.77	0.50
1:A:70:THR:HG23	1:A:132:LEU:CA	2.38	0.50
1:A:211:TRP:HZ2	1:A:558:GLY:HA3	1.76	0.50
2:B:158:GLN:OE1	2:B:158:GLN:N	2.41	0.50
1:A:162:ILE:O	1:A:166:LEU:HD12	2.11	0.50
1:A:417:GLN:HA	1:A:420:LEU:HB3	1.92	0.50
2:B:11:ILE:HG23	2:B:12:LEU:H	1.68	0.50
2:B:111:ASP:OD2	2:B:112:VAL:N	2.38	0.50
3:C:5:PRO:O	3:C:9:LEU:HD12	2.12	0.50
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.94	0.50
2:B:116:PHE:O	2:B:116:PHE:HD2	1.94	0.50
1:A:463:ALA:O	1:A:465:VAL:N	2.45	0.49
1:A:512:ILE:N	1:A:512:ILE:CD1	2.75	0.49
2:B:116:PHE:CE1	2:B:147:ILE:HD13	2.46	0.49
2:B:157:HIS:C	2:B:159:ASN:H	2.15	0.49
1:A:220:ASP:HB2	1:A:554:ASN:N	2.27	0.49
2:B:14:TYR:HE1	3:C:5:PRO:HD2	1.77	0.49
1:A:516:GLU:O	1:A:518:ARG:N	2.41	0.49
1:A:192:MET:HB2	1:A:273:LEU:CD1	2.42	0.49
1:A:91:TYR:O	1:A:95:ARG:HG2	2.12	0.49
1:A:357:ILE:HG22	1:A:358:PRO:CD	2.43	0.49
1:A:154:LEU:O	1:A:157:TRP:CB	2.55	0.49
1:A:201:VAL:O	1:A:205:VAL:HG23	2.12	0.49
1:A:233:HIS:CD2	1:A:233:HIS:C	2.86	0.49
1:A:253:LYS:O	1:A:253:LYS:HG3	2.11	0.49
1:A:386:HIS:CE1	5:A:800:HEM:C4D	2.98	0.49
1:A:472:LEU:O	1:A:472:LEU:CD2	2.55	0.49
1:A:23:TYR:O	1:A:24:PHE:C	2.51	0.49
1:A:386:HIS:CA	1:A:390:ALA:HB3	2.41	0.49
1:A:89:MET:HB3	1:A:190:TRP:CE2	2.48	0.49
1:A:23:TYR:C	1:A:25:LEU:N	2.63	0.49
1:A:233:HIS:CB	1:A:234:PRO:CD	2.89	0.49
2:B:90:TYR:CZ	2:B:147:ILE:CG2	2.96	0.48
3:C:9:LEU:O	3:C:10:ALA:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CE1	1:A:228:PHE:CD1	3.02	0.48
1:A:171:LYS:NZ	1:A:177:LYS:O	2.25	0.48
1:A:353:LEU:O	1:A:356:PHE:HB3	2.13	0.48
2:B:32:LEU:O	2:B:33:ILE:C	2.52	0.48
2:B:86:PHE:CD1	2:B:86:PHE:C	2.86	0.48
1:A:27:LEU:O	1:A:28:GLY:C	2.50	0.48
1:A:181:LEU:O	1:A:185:MET:N	2.46	0.48
1:A:192:MET:CG	1:A:273:LEU:HA	2.44	0.48
1:A:233:HIS:CD2	1:A:237:TYR:CD2	3.01	0.48
1:A:412:PRO:HG3	1:A:501:LEU:HD11	1.95	0.48
2:B:151:GLN:O	2:B:153:CYS:N	2.46	0.48
1:A:238:PHE:O	1:A:242:PRO:HD2	2.13	0.48
1:A:385:PHE:CD2	6:A:801:HAS:HAA2	2.48	0.48
1:A:407:ASN:HD21	1:A:506:LEU:HD23	1.77	0.48
1:A:12:TYR:CG	1:A:19:LYS:HG3	2.49	0.48
1:A:18:LYS:HZ3	1:A:504:ALA:HB2	1.77	0.48
1:A:501:LEU:H	1:A:501:LEU:HG	1.40	0.48
2:B:40:HIS:CD2	2:B:41:THR:HG22	2.49	0.48
1:A:44:LEU:O	1:A:47:GLY:N	2.47	0.48
1:A:300:VAL:CG1	2:B:30:ILE:HD11	2.29	0.48
2:B:51:GLU:O	2:B:51:GLU:HG2	2.12	0.48
2:B:58:VAL:CG1	2:B:59:ARG:N	2.76	0.48
1:A:555:PRO:O	1:A:556:VAL:HG13	2.14	0.48
1:A:54:LEU:HD13	1:A:55:LEU:H	1.75	0.48
1:A:119:VAL:HG12	1:A:148:GLY:CA	2.44	0.48
1:A:164:LEU:HD23	1:A:167:TRP:HB3	1.94	0.48
1:A:405:LEU:HA	1:A:405:LEU:HD12	1.39	0.48
2:B:35:TYR:CD1	2:B:35:TYR:O	2.67	0.48
2:B:99:GLN:HG3	2:B:99:GLN:O	2.13	0.48
2:B:40:HIS:CD2	2:B:41:THR:HG23	2.48	0.48
2:B:72:VAL:O	2:B:72:VAL:HG23	2.14	0.48
1:A:86:GLN:HG3	1:A:156:THR:HG22	1.95	0.48
1:A:348:ALA:O	1:A:349:PRO:C	2.50	0.48
1:A:426:TRP:O	1:A:430:LEU:HD13	2.14	0.48
1:A:78:ILE:HG22	1:A:79:VAL:H	1.72	0.47
1:A:526:ARG:NH2	1:A:529:PHE:CB	2.71	0.47
1:A:197:SER:O	1:A:201:VAL:HB	2.15	0.47
1:A:229:TRP:CZ3	1:A:283:HIS:ND1	2.82	0.47
1:A:477:LEU:HD13	5:A:800:HEM:HMB3	1.94	0.47
1:A:552:HIS:ND1	1:A:552:HIS:N	2.62	0.47
1:A:162:ILE:O	1:A:165:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:O	1:A:190:TRP:C	2.52	0.47
1:A:499:PRO:HB3	1:A:502:ALA:HB3	1.95	0.47
1:A:512:ILE:N	1:A:512:ILE:HD12	2.30	0.47
2:B:138:THR:O	2:B:140:LYS:NZ	2.37	0.47
1:A:437:VAL:O	1:A:441:TRP:HB2	2.14	0.47
1:A:27:LEU:HD23	1:A:83:LEU:CD2	2.44	0.47
1:A:41:PHE:C	1:A:43:ALA:N	2.66	0.47
1:A:156:THR:O	1:A:160:ILE:HG13	2.14	0.47
1:A:518:ARG:HG3	1:A:518:ARG:NH2	2.05	0.47
1:A:23:TYR:HD1	1:A:107:TRP:CH2	2.25	0.47
1:A:246:ILE:O	1:A:250:ILE:HB	2.15	0.47
1:A:288:PRO:HD2	2:B:128:LEU:HD22	1.95	0.47
1:A:356:PHE:CD1	1:A:392:LEU:HD23	2.50	0.47
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.93	0.47
1:A:378:THR:OG1	1:A:380:TRP:HB2	2.14	0.47
1:A:386:HIS:CE1	5:A:800:HEM:C1A	3.02	0.47
2:B:10:ALA:O	2:B:11:ILE:C	2.53	0.47
2:B:32:LEU:HB3	3:C:27:TYR:CZ	2.50	0.47
2:B:137:TYR:CD1	2:B:138:THR:N	2.82	0.47
3:C:16:THR:O	3:C:20:LEU:HG	2.15	0.47
1:A:300:VAL:HG11	2:B:30:ILE:CD1	2.43	0.47
1:A:316:VAL:O	1:A:317:ALA:C	2.52	0.47
1:A:542:TYR:N	1:A:542:TYR:CD2	2.83	0.47
1:A:264:MET:HA	1:A:264:MET:CE	2.45	0.47
2:B:13:ALA:HA	2:B:16:LYS:NZ	2.30	0.47
1:A:152:PHE:O	1:A:155:SER:HB3	2.14	0.47
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.96	0.47
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.69	0.47
1:A:381:VAL:HG12	1:A:385:PHE:CE2	2.50	0.47
1:A:411:LYS:CG	1:A:497:ARG:HB3	2.44	0.47
1:A:497:ARG:HE	1:A:499:PRO:HG2	1.80	0.47
1:A:548:GLN:HB3	1:A:549:LEU:H	1.50	0.47
2:B:55:PRO:CB	2:B:110:PRO:HA	2.45	0.47
1:A:21:THR:HG21	1:A:91:TYR:HB3	1.97	0.46
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.96	0.46
1:A:182:VAL:O	1:A:182:VAL:HG12	2.14	0.46
1:A:429:PHE:O	1:A:433:MET:HG2	2.15	0.46
1:A:439:LEU:O	1:A:440:HIS:C	2.52	0.46
3:C:17:LEU:HD23	3:C:17:LEU:HA	1.66	0.46
1:A:81:THR:CB	1:A:239:TRP:CD1	2.98	0.46
1:A:185:MET:CE	1:A:265:ALA:HB1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLY:HA3	1:A:335:TRP:HB2	1.98	0.46
1:A:406:PRO:O	1:A:410:GLY:N	2.46	0.46
1:A:487:GLY:O	1:A:488:LEU:C	2.52	0.46
1:A:29:PHE:O	1:A:32:LEU:HB3	2.16	0.46
1:A:59:LEU:HB3	1:A:61:PHE:CD1	2.50	0.46
2:B:32:LEU:HB2	3:C:23:TRP:HH2	1.80	0.46
2:B:145:TYR:CE1	2:B:166:VAL:CG2	2.98	0.46
1:A:82:GLN:CD	1:A:152:PHE:HE2	2.19	0.46
1:A:199:GLY:HA3	1:A:230:TRP:CB	2.44	0.46
1:A:258:ARG:HB3	1:A:510:GLU:O	2.15	0.46
1:A:325:ARG:NH1	1:A:331:GLY:O	2.48	0.46
1:A:425:VAL:HG12	1:A:426:TRP:N	2.31	0.46
1:A:427:LEU:O	1:A:480:ALA:HB2	2.15	0.46
1:A:518:ARG:CG	1:A:518:ARG:NH2	2.70	0.46
2:B:32:LEU:HB2	3:C:23:TRP:CH2	2.51	0.46
2:B:18:TRP:CZ2	3:C:12:ILE:HB	2.50	0.46
2:B:85:ALA:HB3	2:B:127:VAL:HG11	1.98	0.46
1:A:47:GLY:HA2	1:A:470:ASN:HB2	1.96	0.46
1:A:135:PHE:CE1	1:A:228:PHE:HE1	2.34	0.46
1:A:164:LEU:O	1:A:168:ARG:HB2	2.16	0.46
1:A:229:TRP:CZ3	1:A:283:HIS:CG	3.04	0.46
1:A:346:PHE:CZ	1:A:350:VAL:HG21	2.51	0.46
3:C:13:LEU:HD12	3:C:17:LEU:HG	1.97	0.46
1:A:179:THR:HG22	1:A:183:THR:HB	1.97	0.46
2:B:54:ASP:OD1	2:B:54:ASP:O	2.33	0.46
2:B:81:VAL:O	2:B:81:VAL:HG12	2.15	0.46
1:A:134:THR:HG22	1:A:228:PHE:CZ	2.51	0.46
1:A:300:VAL:HA	1:A:303:LEU:HD12	1.98	0.46
1:A:456:VAL:HG23	1:A:456:VAL:O	2.16	0.46
1:A:23:TYR:C	1:A:110:TRP:HE1	2.19	0.46
1:A:143:TRP:CE3	1:A:213:PHE:HE2	2.33	0.46
1:A:35:GLY:N	1:A:75:LEU:HD12	2.30	0.45
1:A:259:LEU:O	1:A:512:ILE:HD13	2.15	0.45
2:B:24:ALA:O	2:B:27:PHE:N	2.49	0.45
2:B:83:VAL:HG13	2:B:91:GLN:O	2.16	0.45
1:A:137:PRO:HG3	1:A:208:LEU:HD21	1.97	0.45
1:A:184:TYR:CE2	1:A:266:ARG:CB	2.99	0.45
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.52	0.45
1:A:170:TRP:HE3	1:A:171:LYS:CA	2.28	0.45
1:A:182:VAL:O	1:A:182:VAL:CG1	2.64	0.45
1:A:251:LEU:HA	1:A:254:GLN:HG2	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:HIS:CD2	1:A:283:HIS:N	2.84	0.45
1:A:410:GLY:HA2	1:A:502:ALA:CA	2.45	0.45
2:B:44:VAL:HB	2:B:122:ASN:O	2.15	0.45
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.60	0.45
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.68	0.45
1:A:361:ALA:O	1:A:365:VAL:HG23	2.17	0.45
2:B:16:LYS:O	2:B:17:GLY:C	2.54	0.45
2:B:121:THR:HA	3:C:33:ARG:HB3	1.98	0.45
1:A:119:VAL:HG12	1:A:148:GLY:HA2	1.99	0.45
1:A:266:ARG:CD	1:A:521:VAL:HG13	2.47	0.45
1:A:405:LEU:HB3	1:A:406:PRO:CD	2.46	0.45
1:A:409:THR:C	1:A:411:LYS:H	2.20	0.45
3:C:33:ARG:HH21	3:C:33:ARG:HD2	1.59	0.45
1:A:69:LEU:HD11	5:A:800:HEM:CBA	2.46	0.45
1:A:308:PRO:O	1:A:312:THR:N	2.50	0.45
2:B:96:GLU:HA	2:B:165:VAL:HG23	1.97	0.45
1:A:207:PHE:CD1	1:A:219:VAL:HG13	2.52	0.45
1:A:382:PRO:O	1:A:386:HIS:HB2	2.17	0.45
1:A:385:PHE:HB2	6:A:801:HAS:HMA1	1.98	0.45
1:A:428:TRP:CD1	1:A:429:PHE:N	2.85	0.45
2:B:27:PHE:HA	2:B:30:ILE:HG13	1.99	0.45
1:A:210:PRO:HB2	1:A:216:VAL:HG22	1.99	0.45
1:A:418:ARG:HB3	1:A:418:ARG:CZ	2.46	0.45
1:A:477:LEU:HA	1:A:480:ALA:HB3	1.99	0.45
2:B:110:PRO:O	2:B:111:ASP:CB	2.65	0.45
1:A:91:TYR:CE2	1:A:408:LEU:CD2	2.97	0.45
1:A:96:GLU:OE1	1:A:180:PRO:HB2	2.17	0.45
1:A:97:LEU:O	1:A:98:ASN:C	2.56	0.45
1:A:192:MET:SD	1:A:192:MET:C	2.96	0.45
1:A:235:ILE:HA	1:A:238:PHE:HB3	1.99	0.45
1:A:310:LEU:HD22	2:B:18:TRP:CZ2	2.52	0.45
1:A:351:LEU:HD21	1:A:426:TRP:CH2	2.51	0.45
1:A:225:ARG:HA	1:A:228:PHE:CB	2.45	0.44
1:A:228:PHE:CD2	1:A:228:PHE:C	2.90	0.44
2:B:97:VAL:CG2	2:B:166:VAL:CG1	2.87	0.44
1:A:18:LYS:NZ	1:A:504:ALA:CB	2.79	0.44
1:A:84:PHE:CE1	1:A:397:ALA:HA	2.52	0.44
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.54	0.44
3:C:15:LEU:O	3:C:19:ILE:HG13	2.16	0.44
1:A:266:ARG:HD2	1:A:521:VAL:HG13	2.00	0.44
1:A:308:PRO:O	1:A:311:MET:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:CE1	1:A:312:THR:HG23	2.52	0.44
1:A:413:ILE:HG13	1:A:491:VAL:HG21	2.00	0.44
2:B:103:ILE:HD13	2:B:139:PHE:HD1	1.82	0.44
1:A:15:TYR:HA	1:A:100:ARG:HH11	1.82	0.44
1:A:238:PHE:O	1:A:242:PRO:CD	2.66	0.44
1:A:404:LEU:HD12	1:A:404:LEU:HA	1.70	0.44
1:A:302:THR:O	1:A:303:LEU:C	2.54	0.44
1:A:543:GLY:HA3	1:A:544:PRO:HD3	1.84	0.44
2:B:99:GLN:HE21	2:B:100:GLY:N	2.16	0.44
1:A:414:SER:OG	1:A:416:ALA:HB3	2.17	0.44
1:A:514:GLY:CA	2:B:8:HIS:CD2	3.01	0.44
2:B:67:PRO:HB3	2:B:91:GLN:HG2	2.00	0.44
1:A:121:ALA:O	1:A:125:LEU:HD11	2.18	0.44
1:A:164:LEU:HD21	1:A:167:TRP:HE3	1.83	0.44
1:A:207:PHE:HD1	1:A:219:VAL:HG13	1.82	0.44
1:A:12:TYR:CD1	1:A:19:LYS:HG3	2.53	0.43
1:A:117:LEU:O	1:A:120:ALA:HB3	2.17	0.43
1:A:288:PRO:CD	2:B:128:LEU:HD22	2.48	0.43
1:A:292:PRO:HD3	2:B:48:GLY:HA3	2.00	0.43
1:A:318:ALA:O	1:A:321:GLU:N	2.50	0.43
1:A:127:ASN:CG	1:A:127:ASN:O	2.57	0.43
1:A:220:ASP:HA	1:A:221:PRO:HD2	1.69	0.43
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.99	0.43
1:A:354:LEU:HD22	1:A:354:LEU:H	1.83	0.43
1:A:377:ASN:HB3	2:B:150:ASN:HB2	2.00	0.43
1:A:379:ALA:O	1:A:380:TRP:C	2.55	0.43
1:A:386:HIS:C	1:A:390:ALA:HB3	2.38	0.43
2:B:64:TRP:CD1	2:B:83:VAL:O	2.71	0.43
3:C:11:VAL:C	3:C:13:LEU:N	2.70	0.43
1:A:282:HIS:CG	6:A:801:HAS:OMD	2.72	0.43
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.61	0.43
1:A:309:SER:O	6:A:801:HAS:H272	2.17	0.43
2:B:119:GLU:OE2	2:B:146:ARG:HD3	2.18	0.43
1:A:26:VAL:O	1:A:29:PHE:HB2	2.18	0.43
1:A:95:ARG:HH11	1:A:504:ALA:CB	2.30	0.43
1:A:230:TRP:HA	1:A:542:TYR:CZ	2.53	0.43
2:B:149:CYS:O	2:B:157:HIS:HE1	2.01	0.43
1:A:79:VAL:HA	1:A:152:PHE:HZ	1.81	0.43
1:A:109:SER:O	1:A:112:MET:HB2	2.19	0.43
1:A:241:LEU:HD11	1:A:272:PHE:CE1	2.54	0.43
1:A:248:TYR:OH	1:A:312:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:HD13	1:A:408:LEU:HB3	2.01	0.43
1:A:259:LEU:CD1	1:A:261:SER:H	2.31	0.43
1:A:231:THR:O	1:A:234:PRO:HG2	2.19	0.43
1:A:353:LEU:HB3	6:A:801:HAS:C24	2.48	0.43
1:A:406:PRO:CD	1:A:413:ILE:HD13	2.49	0.43
1:A:26:VAL:O	1:A:30:LEU:HG	2.18	0.43
1:A:69:LEU:HD11	5:A:800:HEM:CGA	2.49	0.43
1:A:351:LEU:HD21	1:A:426:TRP:CZ3	2.53	0.43
1:A:385:PHE:CD2	6:A:801:HAS:CAA	3.02	0.43
1:A:390:ALA:O	1:A:394:THR:HB	2.19	0.43
1:A:445:LEU:HA	1:A:445:LEU:HD23	1.62	0.43
2:B:8:HIS:ND1	2:B:11:ILE:HG21	2.33	0.43
2:B:83:VAL:CG1	2:B:84:LEU:N	2.81	0.43
2:B:92:PRO:HG2	2:B:95:ILE:HG12	2.00	0.43
1:A:95:ARG:HH11	1:A:504:ALA:HB3	1.84	0.43
1:A:192:MET:HG3	1:A:273:LEU:HA	2.01	0.43
1:A:233:HIS:O	1:A:234:PRO:C	2.55	0.43
1:A:522:LEU:HD12	1:A:522:LEU:HA	1.87	0.43
6:A:801:HAS:H281	6:A:801:HAS:H251	1.58	0.43
1:A:184:TYR:O	1:A:188:VAL:HG22	2.19	0.42
1:A:192:MET:HB2	1:A:273:LEU:HB2	2.00	0.42
2:B:122:ASN:HD21	3:C:33:ARG:HB2	1.83	0.42
1:A:546:LEU:HD22	1:A:550:PHE:HE1	1.83	0.42
1:A:66:TYR:O	1:A:70:THR:N	2.48	0.42
1:A:202:LEU:HB2	1:A:227:LEU:HD13	2.01	0.42
1:A:340:PRO:O	1:A:343:ASN:N	2.49	0.42
1:A:506:LEU:HD12	1:A:508:PHE:CE1	2.54	0.42
1:A:385:PHE:HD2	6:A:801:HAS:HAA2	1.84	0.42
1:A:482:LEU:HA	1:A:485:ILE:CD1	2.50	0.42
1:A:20:ALA:HB3	1:A:106:MET:HE3	2.01	0.42
1:A:151:VAL:HB	1:A:152:PHE:H	1.54	0.42
1:A:331:GLY:H	1:A:334:GLY:HA3	1.84	0.42
1:A:393:VAL:O	1:A:396:THR:HB	2.20	0.42
1:A:481:LEU:O	1:A:484:PHE:HB3	2.19	0.42
1:A:533:VAL:O	1:A:537:LEU:HG	2.19	0.42
1:A:545:THR:HG22	1:A:546:LEU:N	2.34	0.42
2:B:55:PRO:HB2	2:B:110:PRO:HA	2.00	0.42
2:B:59:ARG:HH21	2:B:59:ARG:HD3	1.66	0.42
1:A:16:PRO:HD2	1:A:100:ARG:NE	2.34	0.42
1:A:25:LEU:HD22	1:A:29:PHE:CE1	2.55	0.42
1:A:445:LEU:O	1:A:446:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLY:HA2	1:A:515:PRO:HD3	1.80	0.42
1:A:546:LEU:HD23	1:A:546:LEU:HA	1.76	0.42
1:A:42:GLN:NE2	1:A:72:HIS:CD2	2.87	0.42
1:A:220:ASP:N	1:A:555:PRO:HA	2.34	0.42
1:A:248:TYR:CD2	1:A:265:ALA:HB2	2.54	0.42
2:B:27:PHE:N	2:B:27:PHE:HD2	2.18	0.42
2:B:104:VAL:O	2:B:104:VAL:HG12	2.18	0.42
1:A:137:PRO:HA	1:A:138:PRO:HA	1.77	0.42
1:A:251:LEU:HD13	1:A:349:PRO:HG3	2.01	0.42
1:A:381:VAL:HB	1:A:382:PRO:HD3	2.02	0.42
1:A:402:TYR:CD1	1:A:413:ILE:HG21	2.55	0.42
1:A:562:TRP:HA	2:B:155:LEU:CD1	2.50	0.42
2:B:27:PHE:N	2:B:27:PHE:CD2	2.87	0.42
1:A:38:PHE:HA	1:A:41:PHE:CD1	2.50	0.42
1:A:229:TRP:CE3	1:A:283:HIS:CG	3.07	0.42
1:A:300:VAL:O	1:A:301:LEU:C	2.58	0.42
2:B:109:SER:HB3	2:B:129:PRO:CD	2.50	0.42
2:B:167:LYS:H	2:B:167:LYS:HG3	1.70	0.42
1:A:229:TRP:CZ3	1:A:283:HIS:CE1	3.08	0.42
1:A:250:ILE:HG22	1:A:251:LEU:N	2.35	0.42
1:A:379:ALA:HB3	1:A:443:GLY:CA	2.50	0.42
1:A:410:GLY:O	1:A:501:LEU:HD12	2.20	0.42
1:A:52:TYR:CZ	1:A:65:TYR:HD1	2.38	0.41
1:A:236:VAL:O	1:A:239:TRP:N	2.53	0.41
1:A:354:LEU:O	1:A:358:PRO:HD2	2.19	0.41
1:A:374:VAL:O	1:A:374:VAL:CG1	2.68	0.41
1:A:463:ALA:HB3	1:A:467:MET:SD	2.60	0.41
2:B:81:VAL:HG11	2:B:95:ILE:HD13	2.02	0.41
3:C:24:LEU:O	3:C:25:GLY:C	2.58	0.41
1:A:240:LEU:HB2	6:A:801:HAS:HBC1	2.01	0.41
1:A:562:TRP:CD1	1:A:562:TRP:C	2.92	0.41
2:B:93:ASN:HA	2:B:94:PRO:HA	1.85	0.41
2:B:114:HIS:CE1	2:B:153:CYS:HB2	2.54	0.41
2:B:163:THR:HG22	2:B:164:ILE:N	2.35	0.41
1:A:45:ASN:HD21	1:A:452:TYR:HA	1.85	0.41
1:A:79:VAL:HG13	1:A:152:PHE:HE1	1.85	0.41
1:A:371:LEU:HD23	3:C:26:VAL:CG1	2.50	0.41
1:A:15:TYR:HD1	1:A:100:ARG:HH11	1.67	0.41
1:A:288:PRO:HB3	2:B:133:SER:HA	2.02	0.41
2:B:29:PHE:O	2:B:30:ILE:C	2.58	0.41
1:A:48:ASN:C	1:A:48:ASN:HD22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:LEU:HG	1:A:261:SER:H	1.86	0.41
1:A:271:LEU:O	1:A:275:LEU:HB2	2.20	0.41
1:A:320:LEU:H	1:A:320:LEU:HG	1.63	0.41
1:A:346:PHE:C	1:A:349:PRO:HD2	2.39	0.41
1:A:514:GLY:O	1:A:517:ASP:HB2	2.21	0.41
2:B:44:VAL:HG11	2:B:122:ASN:CB	2.44	0.41
2:B:140:LYS:C	2:B:141:ARG:HG3	2.41	0.41
2:B:155:LEU:C	2:B:157:HIS:H	2.24	0.41
1:A:179:THR:CG2	1:A:183:THR:HB	2.51	0.41
1:A:267:LEU:N	1:A:524:MET:SD	2.93	0.41
1:A:365:VAL:C	1:A:367:ALA:N	2.74	0.41
1:A:491:VAL:HG13	1:A:491:VAL:O	2.21	0.41
1:A:546:LEU:O	1:A:550:PHE:CD1	2.71	0.41
2:B:122:ASN:ND2	3:C:33:ARG:HB2	2.35	0.41
3:C:18:THR:C	3:C:20:LEU:N	2.74	0.41
3:C:18:THR:O	3:C:20:LEU:N	2.54	0.41
1:A:21:THR:HB	1:A:408:LEU:HD11	2.03	0.41
1:A:22:LEU:HA	1:A:22:LEU:HD12	1.23	0.41
1:A:41:PHE:O	1:A:42:GLN:C	2.59	0.41
1:A:192:MET:SD	1:A:193:TRP:N	2.94	0.41
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.56	0.41
1:A:297:ILE:C	1:A:299:SER:H	2.23	0.41
1:A:350:VAL:O	1:A:354:LEU:CD2	2.60	0.41
1:A:353:LEU:HB3	6:A:801:HAS:H22	2.03	0.41
1:A:497:ARG:NH2	1:A:499:PRO:HG2	2.31	0.41
1:A:514:GLY:HA3	2:B:8:HIS:CD2	2.55	0.41
2:B:41:THR:HG23	2:B:41:THR:H	1.61	0.41
2:B:49:LYS:HG3	2:B:50:LEU:O	2.20	0.41
2:B:84:LEU:HD12	2:B:84:LEU:HA	1.75	0.41
2:B:123:ILE:HG23	2:B:135:VAL:HG21	2.02	0.41
2:B:139:PHE:CG	2:B:166:VAL:HG11	2.55	0.41
2:B:154:GLY:O	2:B:157:HIS:CB	2.64	0.41
3:C:13:LEU:O	3:C:14:VAL:C	2.59	0.41
1:A:410:GLY:HA3	1:A:499:PRO:CB	2.49	0.41
1:A:481:LEU:HD12	1:A:481:LEU:C	2.41	0.41
1:A:514:GLY:HA2	2:B:8:HIS:CD2	2.56	0.41
1:A:521:VAL:O	1:A:521:VAL:HG12	2.20	0.41
1:A:550:PHE:HA	1:A:553:LEU:HD23	1.99	0.41
2:B:145:TYR:CE1	2:B:166:VAL:HG22	2.55	0.41
1:A:89:MET:HE1	1:A:245:ALA:HB2	2.02	0.40
1:A:184:TYR:HE2	1:A:266:ARG:CB	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD12	1:A:222:LEU:C	2.42	0.40
1:A:314:PHE:CD2	3:C:12:ILE:HD12	2.54	0.40
3:C:18:THR:HG22	3:C:22:PHE:CD1	2.56	0.40
1:A:187:VAL:O	1:A:191:LEU:HB2	2.21	0.40
1:A:191:LEU:HD22	1:A:531:PHE:CE2	2.56	0.40
1:A:306:ALA:O	1:A:307:VAL:C	2.60	0.40
1:A:392:LEU:O	1:A:393:VAL:C	2.58	0.40
1:A:435:MET:O	1:A:436:ALA:C	2.59	0.40
3:C:15:LEU:C	3:C:15:LEU:HD12	2.42	0.40
1:A:170:TRP:O	1:A:174:ASN:HB2	2.21	0.40
1:A:504:ALA:C	1:A:506:LEU:H	2.25	0.40
1:A:485:ILE:C	1:A:487:GLY:N	2.74	0.40
1:A:548:GLN:O	1:A:550:PHE:N	2.54	0.40
2:B:32:LEU:HB3	3:C:27:TYR:OH	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/568 (98%)	359 (65%)	126 (23%)	70 (13%)	0	2
2	B	164/168 (98%)	109 (66%)	40 (24%)	15 (9%)	1	4
3	C	31/34 (91%)	15 (48%)	10 (32%)	6 (19%)	0	0
All	All	750/770 (97%)	483 (64%)	176 (24%)	91 (12%)	0	2

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	12	TYR
1	A	48	ASN

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Mol	Chain	Res	Type
1	A	151	VAL
1	A	152	PHE
1	A	189	PHE
1	A	197	SER
1	A	335	TRP
1	A	340	PRO
1	A	341	TRP
1	A	464	ALA
1	A	483	LEU
1	A	496	GLU
1	A	506	LEU
1	A	517	ASP
1	A	548	GLN
2	B	11	ILE
2	B	44	VAL
2	B	47	ALA
2	B	49	LYS
2	B	88	PHE
2	B	111	ASP
2	B	152	TYR
3	C	19	ILE
1	A	31	ALA
1	A	39	GLY
1	A	42	GLN
1	A	61	PHE
1	A	79	VAL
1	A	86	GLN
1	A	88	ILE
1	A	89	MET
1	A	94	ALA
1	A	130	THR
1	A	168	ARG
1	A	196	ALA
1	A	213	PHE
1	A	345	ALA
1	A	365	VAL
1	A	366	ASN
1	A	377	ASN
1	A	515	PRO
1	A	549	LEU
2	B	119	GLU
2	B	124	ASN

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Mol	Chain	Res	Type
3	C	14	VAL
3	C	27	TYR
1	A	110	TRP
1	A	142	HIS
1	A	308	PRO
1	A	403	TRP
1	A	452	TYR
1	A	469	PHE
2	B	76	PRO
3	C	13	LEU
3	C	15	LEU
1	A	121	ALA
1	A	129	ALA
1	A	181	LEU
1	A	190	TRP
1	A	376	HIS
1	A	384	HIS
1	A	392	LEU
1	A	531	PHE
2	B	72	VAL
3	C	16	THR
1	A	65	TYR
1	A	109	SER
1	A	355	GLY
1	A	499	PRO
1	A	526	ARG
2	B	31	ALA
2	B	87	ALA
1	A	127	ASN
1	A	155	SER
1	A	279	VAL
1	A	280	GLY
1	A	356	PHE
1	A	383	GLY
1	A	405	LEU
1	A	465	VAL
1	A	491	VAL
2	B	48	GLY
2	B	110	PRO
1	A	329	GLY
1	A	543	GLY
1	A	115	ILE

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Mol	Chain	Res	Type
1	A	233	HIS
1	A	504	ALA
1	A	28	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	453/462 (98%)	350 (77%)	103 (23%)	1	3
2	B	136/138 (99%)	104 (76%)	32 (24%)	1	3
3	C	26/27 (96%)	19 (73%)	7 (27%)	0	1
All	All	615/627 (98%)	473 (77%)	142 (23%)	1	3

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	15	TYR
1	A	23	TYR
1	A	25	LEU
1	A	27	LEU
1	A	37	LEU
1	A	38	PHE
1	A	42	GLN
1	A	48	ASN
1	A	49	VAL
1	A	54	LEU
1	A	55	LEU
1	A	63	GLN
1	A	64	SER
1	A	69	LEU
1	A	70	THR
1	A	82	GLN
1	A	89	MET

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Mol	Chain	Res	Type
1	A	98	ASN
1	A	100	ARG
1	A	106	MET
1	A	122	LEU
1	A	125	LEU
1	A	133	TYR
1	A	134	THR
1	A	155	SER
1	A	157	TRP
1	A	162	ILE
1	A	164	LEU
1	A	168	ARG
1	A	179	THR
1	A	183	THR
1	A	188	VAL
1	A	192	MET
1	A	195	LEU
1	A	201	VAL
1	A	205	VAL
1	A	213	PHE
1	A	215	LEU
1	A	216	VAL
1	A	217	GLU
1	A	222	LEU
1	A	225	ARG
1	A	230	TRP
1	A	244	TYR
1	A	253	LYS
1	A	254	GLN
1	A	276	SER
1	A	287	ASP
1	A	299	SER
1	A	300	VAL
1	A	311	MET
1	A	315	THR
1	A	320	LEU
1	A	321	GLU
1	A	327	ARG
1	A	330	ARG
1	A	339	LEU
1	A	342	ASP
1	A	354	LEU

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Mol	Chain	Res	Type
1	A	364	ILE
1	A	368	SER
1	A	369	PHE
1	A	370	THR
1	A	371	LEU
1	A	388	GLN
1	A	394	THR
1	A	405	LEU
1	A	408	LEU
1	A	418	ARG
1	A	419	ARG
1	A	425	VAL
1	A	428	TRP
1	A	430	LEU
1	A	439	LEU
1	A	449	ARG
1	A	452	TYR
1	A	453	ILE
1	A	456	VAL
1	A	465	VAL
1	A	468	VAL
1	A	472	LEU
1	A	478	LEU
1	A	490	SER
1	A	492	LEU
1	A	494	SER
1	A	495	ARG
1	A	498	LYS
1	A	501	LEU
1	A	513	SER
1	A	518	ARG
1	A	520	LEU
1	A	522	LEU
1	A	526	ARG
1	A	527	ILE
1	A	533	VAL
1	A	536	ILE
1	A	537	LEU
1	A	545	THR
1	A	548	GLN
1	A	552	HIS
1	A	560	ARG

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Mol	Chain	Res	Type
1	A	561	LEU
2	B	3	ASP
2	B	12	LEU
2	B	14	TYR
2	B	15	GLU
2	B	18	TRP
2	B	19	LEU
2	B	22	SER
2	B	23	LEU
2	B	26	LEU
2	B	37	LEU
2	B	39	THR
2	B	52	ARG
2	B	54	ASP
2	B	61	GLU
2	B	74	THR
2	B	77	ASN
2	B	96	GLU
2	B	99	GLN
2	B	107	ILE
2	B	110	PRO
2	B	119	GLU
2	B	128	LEU
2	B	129	PRO
2	B	133	SER
2	B	136	ARG
2	B	140	LYS
2	B	149	CYS
2	B	157	HIS
2	B	160	MET
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	12	ILE
3	C	13	LEU
3	C	21	VAL
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	63	GLN
1	A	76	ASN
1	A	388	GLN
1	A	446	ASN
1	A	554	ASN
2	B	8	HIS
2	B	40	HIS
2	B	60	GLN
2	B	77	ASN
2	B	99	GLN
2	B	117	HIS
2	B	122	ASN

### 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	$\# Z  > 2$
7	CUA	B	802	2	0,1,1	-	-	-		
5	HEM	A	800	1	27,50,50	2.40	9 (33%)	17,82,82	2.76	7 (41%)

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	4.44	20 (35%)	50,109,109	5.70	22 (44%)

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
5	HEM	A	800	1	-	0/6/54/54	-
6	HAS	A	801	1	-	10/35/122/122	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C1D-ND	-12.38	1.32	1.49
6	A	801	HAS	C4D-ND	-11.36	1.34	1.49
6	A	801	HAS	C4A-C3A	10.78	1.52	1.38
6	A	801	HAS	C4B-NB	-10.58	1.35	1.49
6	A	801	HAS	C1B-NB	-10.22	1.35	1.49
6	A	801	HAS	C1A-C2A	8.91	1.50	1.38
6	A	801	HAS	C3D-C2D	8.57	1.44	1.34
6	A	801	HAS	C1C-C2C	8.19	1.49	1.38
6	A	801	HAS	C2B-C3B	7.96	1.41	1.34
6	A	801	HAS	C3C-CAC	-7.01	1.33	1.47
6	A	801	HAS	CHD-C4C	-5.33	1.45	1.51
5	A	800	HEM	C3D-C2D	5.31	1.53	1.37
5	A	800	HEM	C3B-C2B	-5.02	1.33	1.40
6	A	801	HAS	CHA-C4D	-4.84	1.44	1.53
5	A	800	HEM	C3C-CAC	4.73	1.57	1.47
5	A	800	HEM	C3C-C2C	-4.45	1.34	1.40
6	A	801	HAS	C2A-C3A	4.23	1.50	1.37
5	A	800	HEM	C3B-CAB	3.95	1.56	1.47
6	A	801	HAS	CAD-C3D	3.56	1.56	1.51
6	A	801	HAS	C1D-C2D	-3.16	1.46	1.51
6	A	801	HAS	C3C-C2C	3.14	1.44	1.40
5	A	800	HEM	CMA-C3A	3.08	1.58	1.51
6	A	801	HAS	C16-C15	2.78	1.57	1.51
6	A	801	HAS	CAA-C2A	2.76	1.56	1.52
5	A	800	HEM	CAD-C3D	2.59	1.56	1.52
6	A	801	HAS	C14-C15	2.53	1.39	1.33
6	A	801	HAS	CHA-C1A	-2.43	1.45	1.51
5	A	800	HEM	C4D-C3D	2.22	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C1D-CHD	-2.19	1.34	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CHB-C1D-ND	16.96	132.03	110.94
6	A	801	HAS	CAA-C2A-C1A	-16.65	115.60	127.30
6	A	801	HAS	CHB-C1B-NB	16.42	131.36	110.94
6	A	801	HAS	CHC-C1C-C2C	-11.07	110.29	129.45
6	A	801	HAS	CHD-C4A-C3A	-9.87	113.03	129.53
6	A	801	HAS	CHC-C4B-NB	9.58	128.82	110.75
6	A	801	HAS	C4C-C3C-C2C	8.95	118.14	104.41
6	A	801	HAS	OMD-CMD-C2D	-8.37	113.80	124.39
6	A	801	HAS	CHA-C4D-ND	8.28	126.37	110.75
5	A	800	HEM	CAA-CBA-CGA	-6.96	100.99	112.67
6	A	801	HAS	C1A-C2A-C3A	-6.57	96.14	105.93
6	A	801	HAS	CMC-C2C-C3C	-6.01	113.44	124.68
6	A	801	HAS	CMA-C3A-C2A	-5.96	113.70	124.94
6	A	801	HAS	CBD-CAD-C3D	-4.85	105.76	114.35
5	A	800	HEM	CAD-CBD-CGD	-4.79	104.63	112.67
6	A	801	HAS	C17-C18-C19	-3.97	118.09	127.66
6	A	801	HAS	C28-C24-C23	-3.87	100.25	112.98
5	A	800	HEM	C1D-C2D-C3D	-3.86	104.31	107.00
6	A	801	HAS	C4A-C3A-C2A	-3.81	101.75	105.81
6	A	801	HAS	C21-C22-C23	-3.56	119.09	127.66
5	A	800	HEM	CMA-C3A-C2A	3.33	131.23	124.94
5	A	800	HEM	C4A-C3A-C2A	-3.03	104.89	107.00
5	A	800	HEM	CMA-C3A-C4A	-2.98	123.88	128.46
6	A	801	HAS	C25-C23-C24	2.90	120.14	115.27
6	A	801	HAS	C27-C19-C20	2.57	119.59	115.27
6	A	801	HAS	C31-C30-C29	-2.56	115.26	122.65
6	A	801	HAS	C20-C21-C22	-2.26	104.44	111.88
6	A	801	HAS	C13-C12-C11	-2.18	111.07	114.35
5	A	800	HEM	C3B-C4B-NB	-2.17	106.41	109.21

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	801	HAS	C3A-C2A-CAA-CBA
6	A	801	HAS	C2A-CAA-CBA-CGA
6	A	801	HAS	C1D-C2D-CMD-OMD

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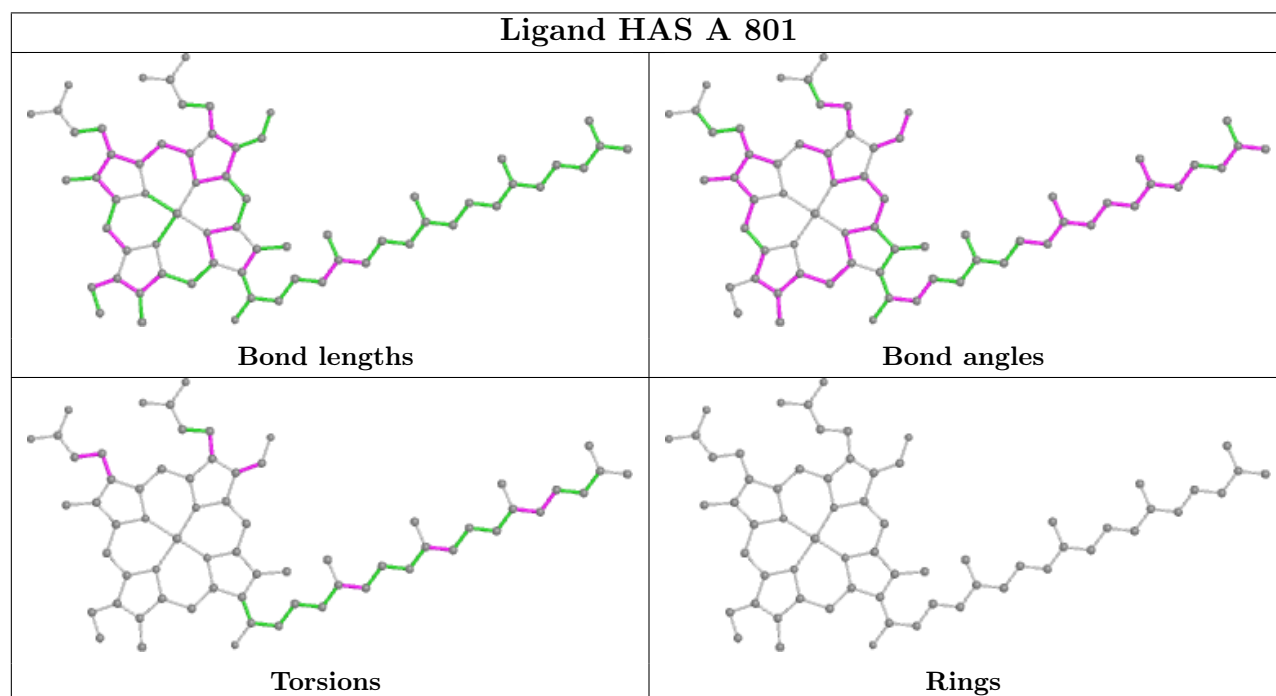
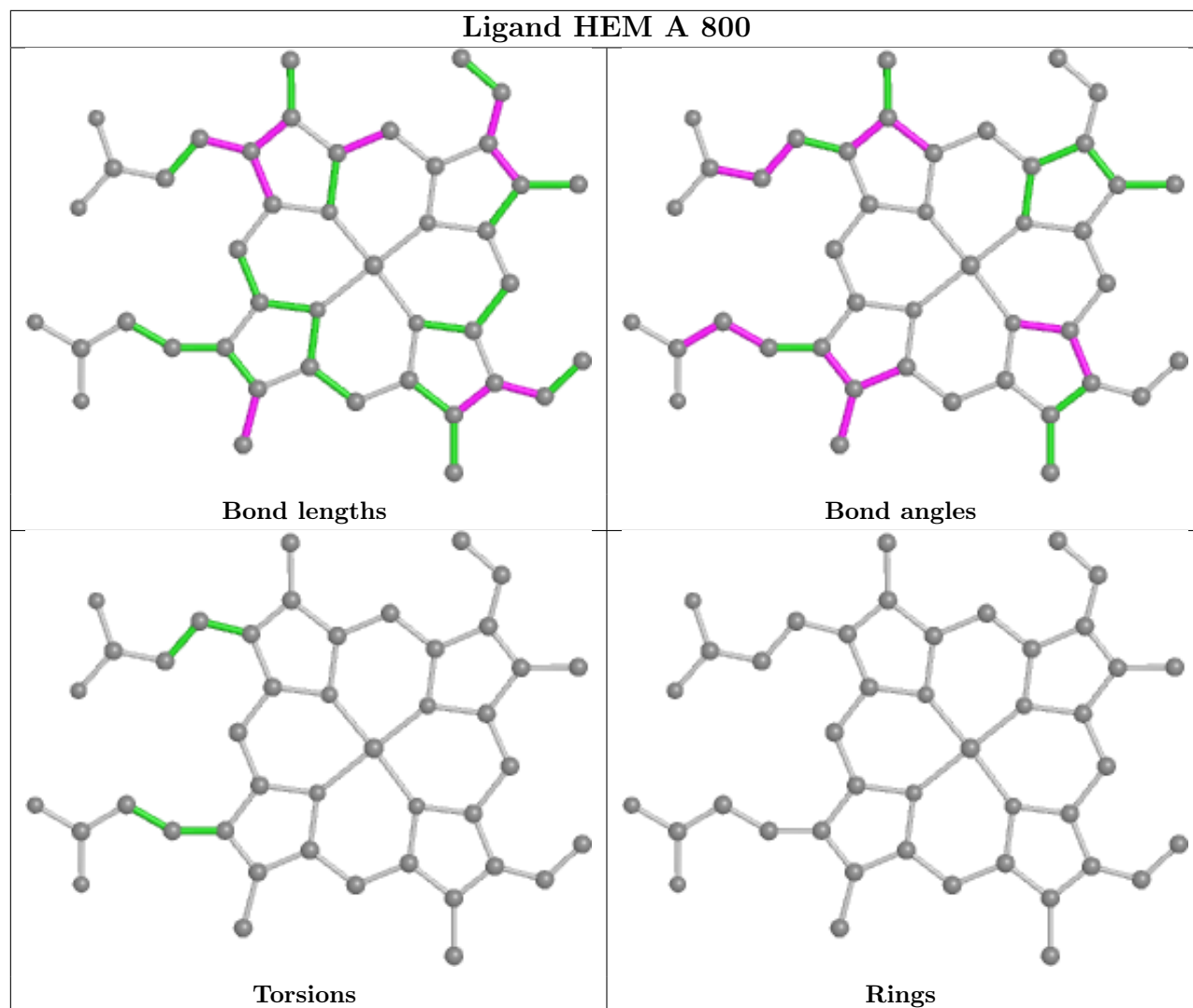
Mol	Chain	Res	Type	Atoms
6	A	801	HAS	C3D-C2D-CMD-OMD
6	A	801	HAS	C26-C15-C16-C17
6	A	801	HAS	C2D-C3D-CAD-CBD
6	A	801	HAS	C25-C23-C24-C28
6	A	801	HAS	C23-C24-C28-C29
6	A	801	HAS	C27-C19-C20-C21
6	A	801	HAS	C14-C15-C16-C17

There are no ring outliers.

2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	9	0
6	A	801	HAS	33	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	557/568 (98%)	-0.70	7 (1%) 77 75	8, 39, 82, 189	0
2	B	166/168 (98%)	-0.82	1 (0%) 89 89	11, 39, 66, 150	0
3	C	33/34 (97%)	-0.86	1 (3%) 50 48	16, 28, 99, 128	0
All	All	756/770 (98%)	-0.74	9 (1%) 79 77	8, 39, 82, 189	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	SER	4.5
1	A	495	ARG	4.3
2	B	3	ASP	3.1
1	A	6	SER	3.1
1	A	173	ALA	2.9
1	A	8	ILE	2.8
1	A	7	GLU	2.1
1	A	215	LEU	2.1
3	C	3	GLU	2.1

### 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](#)

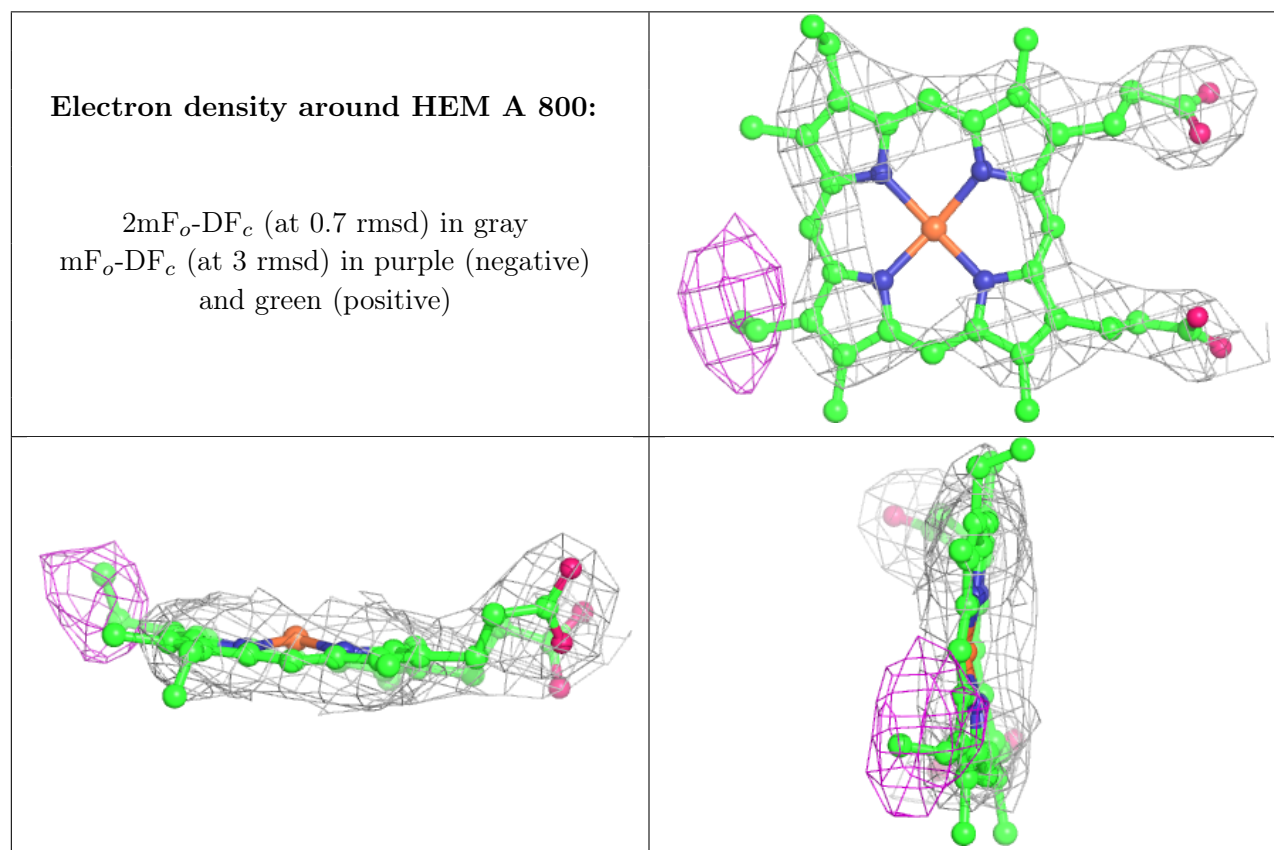
There are no monosaccharides in this entry.

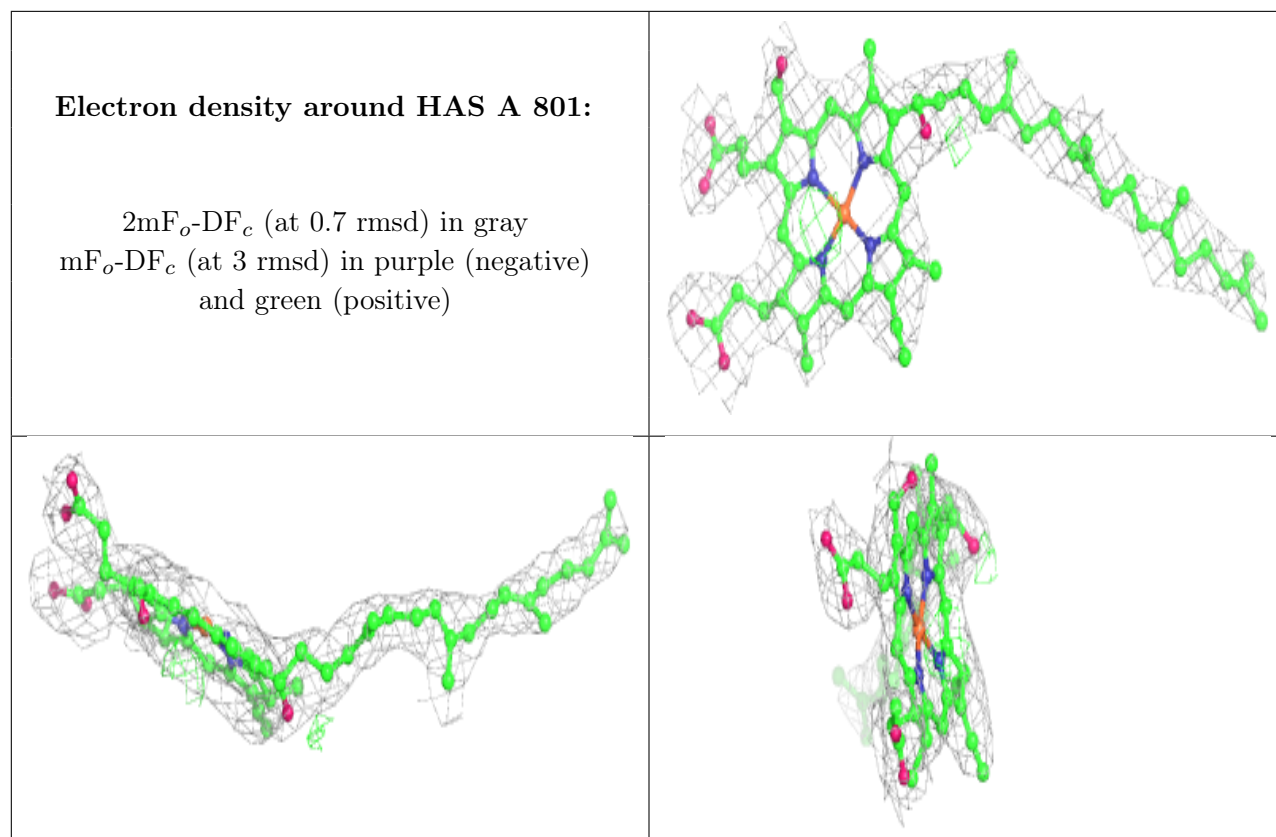
## 6.4 Ligands ⓘ

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
4	CU1	A	803	1/1	0.98	0.10	83,83,83,83	0
5	HEM	A	800	43/43	0.98	0.14	44,71,84,86	0
6	HAS	A	801	65/65	0.98	0.13	17,54,76,85	0
7	CUA	B	802	2/2	1.00	0.06	49,49,49,52	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.