



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:55 PM EDT

PDB ID : 2QPD / pdb_00002qpd
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

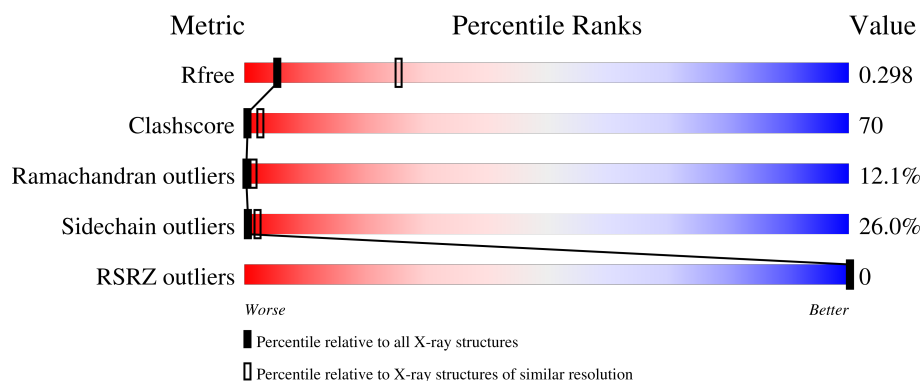
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

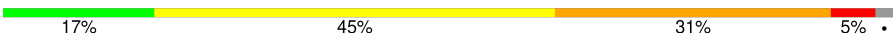
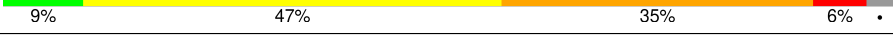
The reported resolution of this entry is 3.25 Å.

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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 ≥ 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	
2	B	168	
3	C	34	

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	-	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			

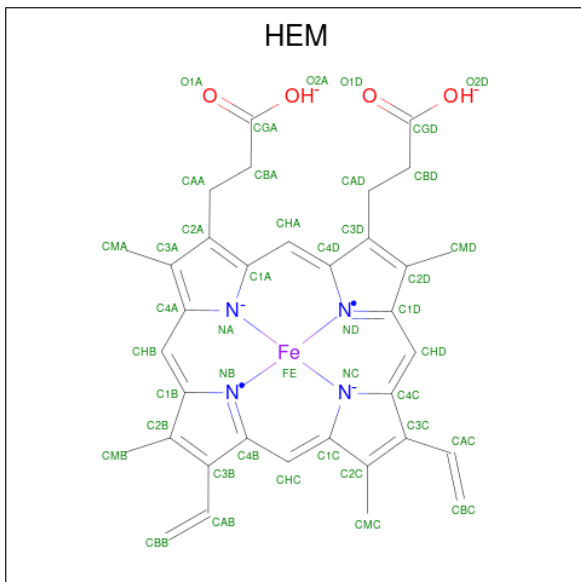
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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 (CCD ID: CU1) (formula: Cu).

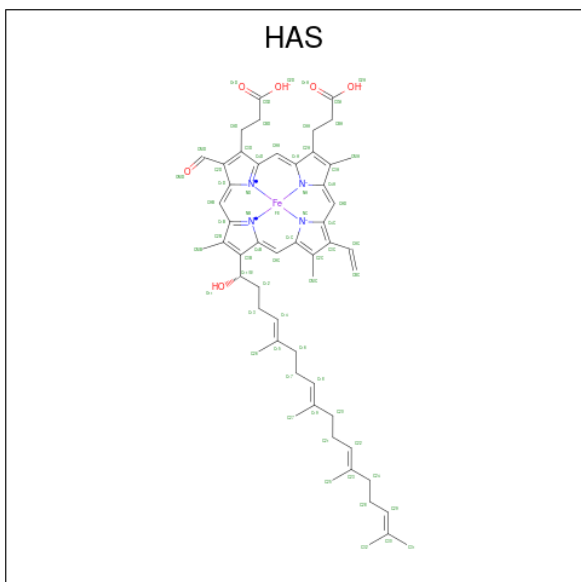
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



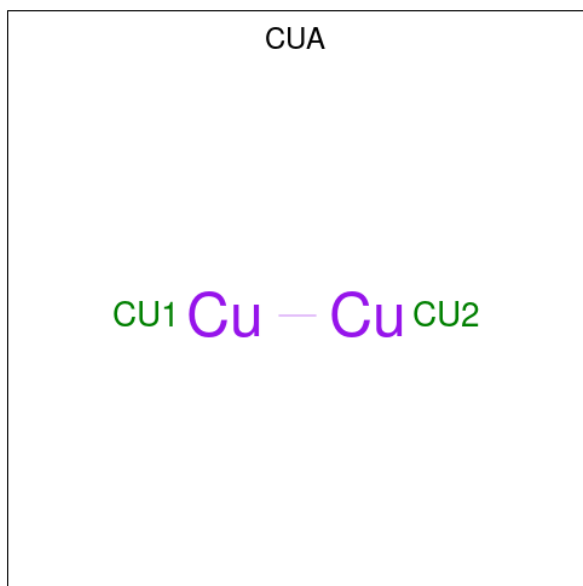
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (CCD ID: 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 (CCD ID: CUA) (formula: Cu₂).

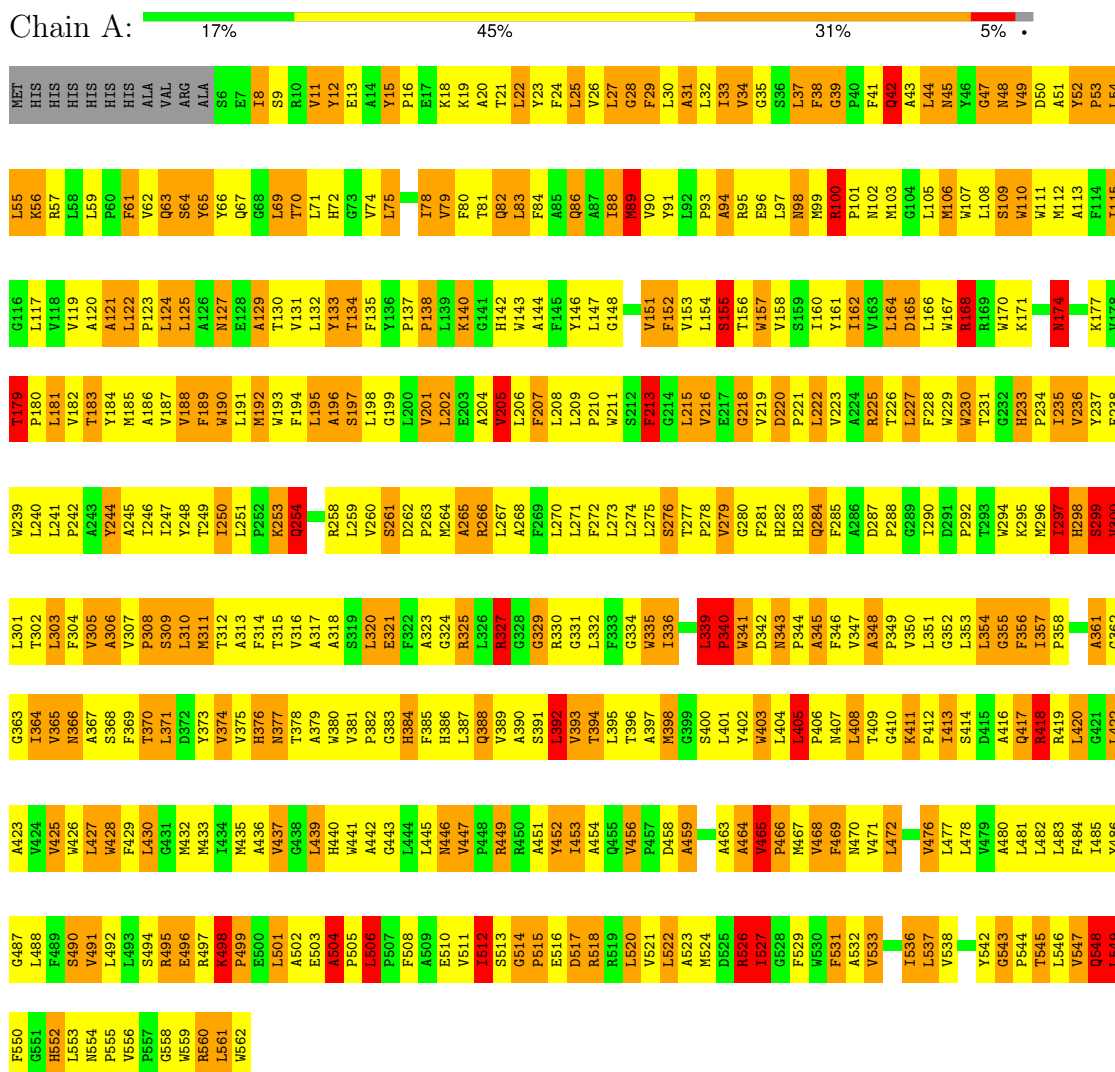


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			2	2		

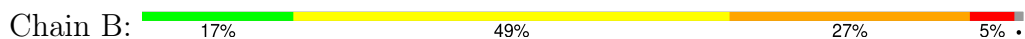
3 Residue-property plots

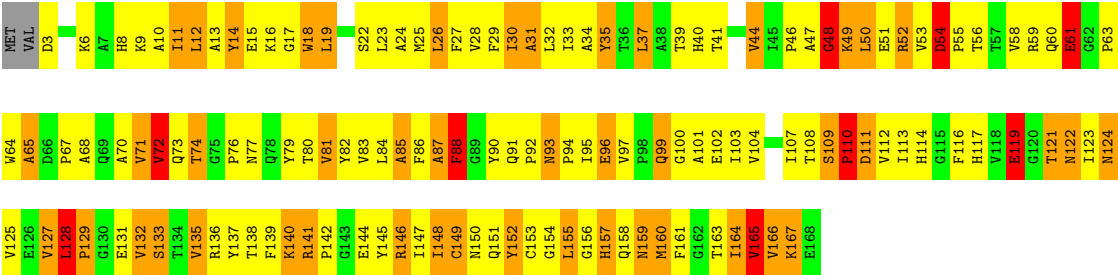
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

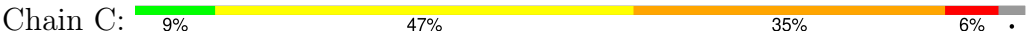


• Molecule 2: Cytochrome c oxidase subunit 2





● 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, α , β , γ	115.19Å 115.19Å 149.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.25 19.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	77.2 (19.98-3.25) 82.2 (19.98-3.25)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6077	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CUA, HEM, CU1, HAS

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	1.32	21/4566 (0.5%)	1.60	83/6266 (1.3%)
2	B	1.38	12/1335 (0.9%)	1.67	30/1822 (1.6%)
3	C	1.43	2/265 (0.8%)	1.45	3/359 (0.8%)
All	All	1.34	35/6166 (0.6%)	1.61	116/8447 (1.4%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	VAL	CA-CB	7.35	1.64	1.54
1	A	447	VAL	CA-CB	6.67	1.62	1.54
2	B	73	GLN	CA-C	6.49	1.61	1.52
2	B	52	ARG	CA-C	6.31	1.60	1.52
1	A	205	VAL	CA-CB	6.28	1.60	1.54
2	B	73	GLN	N-CA	6.13	1.54	1.46
1	A	62	VAL	CA-CB	6.03	1.60	1.53
2	B	121	THR	CA-C	6.03	1.59	1.53
3	C	21	VAL	CA-CB	5.97	1.62	1.54
1	A	447	VAL	CA-C	5.91	1.57	1.53
1	A	250	ILE	CA-CB	-5.87	1.49	1.55
1	A	8	ILE	CA-CB	5.85	1.63	1.54
2	B	127	VAL	CA-CB	5.81	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	VAL	CA-CB	5.80	1.62	1.54
1	A	300	VAL	CA-CB	-5.76	1.47	1.54
1	A	209	LEU	CA-C	5.74	1.60	1.52
1	A	305	VAL	CA-CB	5.61	1.60	1.54
2	B	35	TYR	N-CA	-5.60	1.39	1.46
1	A	213	PHE	N-CA	5.60	1.53	1.46
1	A	207	PHE	CA-C	-5.53	1.48	1.52
1	A	83	LEU	N-CA	-5.52	1.39	1.46
2	B	125	VAL	CA-CB	5.50	1.61	1.54
1	A	459	ALA	CA-CB	-5.43	1.45	1.53
2	B	148	ILE	CA-CB	-5.32	1.47	1.54
1	A	361	ALA	CA-C	5.29	1.60	1.52
1	A	547	VAL	CA-CB	5.29	1.61	1.54
1	A	527	ILE	CA-CB	5.27	1.61	1.54
2	B	93	ASN	N-CA	-5.25	1.41	1.46
1	A	310	LEU	CA-C	-5.16	1.46	1.52
2	B	80	THR	CA-CB	5.12	1.60	1.53
3	C	4	LYS	CA-C	5.08	1.58	1.52
1	A	391	SER	N-CA	5.07	1.52	1.46
2	B	81	VAL	CA-CB	5.06	1.59	1.53
1	A	49	VAL	N-CA	-5.01	1.40	1.46
1	A	303	LEU	N-CA	-5.00	1.40	1.46

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	LEU	CA-C-N	11.37	134.06	119.84
1	A	339	LEU	C-N-CA	11.37	134.06	119.84
1	A	44	LEU	N-CA-C	-10.52	100.58	113.41
1	A	514	GLY	CA-C-N	10.36	132.79	119.84
1	A	514	GLY	C-N-CA	10.36	132.79	119.84
1	A	220	ASP	CA-C-N	10.24	130.54	119.28
1	A	220	ASP	C-N-CA	10.24	130.54	119.28
1	A	437	VAL	CB-CA-C	-9.20	99.99	112.04
1	A	348	ALA	CA-C-N	-9.10	109.27	119.28
1	A	348	ALA	C-N-CA	-9.10	109.27	119.28
2	B	155	LEU	N-CA-C	9.02	122.28	111.82
2	B	121	THR	N-CA-C	8.50	119.80	108.07
3	C	10	ALA	N-CA-C	-8.43	101.13	111.33
2	B	54	ASP	CA-C-N	7.95	127.61	119.82
2	B	54	ASP	C-N-CA	7.95	127.61	119.82
1	A	336	ILE	N-CA-C	7.60	118.19	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	ARG	CA-C-N	-7.55	112.55	120.03
2	B	141	ARG	C-N-CA	-7.55	112.55	120.03
1	A	343	ASN	CA-C-N	7.37	126.63	118.97
1	A	343	ASN	C-N-CA	7.37	126.63	118.97
1	A	506	LEU	CA-C-N	-7.36	110.64	119.84
1	A	506	LEU	C-N-CA	-7.36	110.64	119.84
1	A	266	ARG	N-CA-C	-7.31	102.69	111.69
1	A	261	SER	N-CA-C	7.15	119.35	107.20
2	B	146	ARG	CB-CG-CD	-7.12	94.92	111.30
1	A	274	LEU	N-CA-C	7.08	118.64	111.07
2	B	109	SER	CA-C-N	7.02	128.61	119.84
2	B	109	SER	C-N-CA	7.02	128.61	119.84
1	A	306	ALA	N-CA-C	-7.00	103.41	112.23
1	A	446	ASN	CA-C-N	-6.96	115.78	123.02
1	A	446	ASN	C-N-CA	-6.96	115.78	123.02
2	B	132	VAL	CA-C-N	6.93	130.59	120.82
2	B	132	VAL	C-N-CA	6.93	130.59	120.82
1	A	247	ILE	N-CA-C	6.84	116.99	110.42
1	A	254	GLN	N-CA-C	-6.73	103.87	111.07
2	B	61	GLU	N-CA-C	6.72	119.16	109.14
2	B	52	ARG	N-CA-C	6.70	119.95	110.23
1	A	29	PHE	N-CA-C	6.68	118.22	111.07
1	A	393	VAL	CB-CA-C	-6.66	103.17	111.70
1	A	471	VAL	CB-CA-C	-6.66	103.35	111.88
1	A	218	GLY	N-CA-C	6.64	122.15	110.80
2	B	79	TYR	CB-CA-C	-6.62	102.46	110.94
1	A	140	LYS	N-CA-C	6.61	120.64	107.62
1	A	174	ASN	CA-C-N	6.61	127.60	120.13
1	A	174	ASN	C-N-CA	6.61	127.60	120.13
1	A	124	LEU	N-CA-C	6.55	118.50	111.36
2	B	85	ALA	N-CA-C	-6.50	100.86	110.48
1	A	504	ALA	N-CA-C	6.39	123.92	109.81
1	A	15	TYR	CA-C-N	6.38	127.82	119.84
1	A	15	TYR	C-N-CA	6.38	127.82	119.84
1	A	498	LYS	CA-C-N	6.32	127.74	119.84
1	A	498	LYS	C-N-CA	6.32	127.74	119.84
1	A	297	ILE	N-CA-C	6.32	116.36	110.42
2	B	128	LEU	CA-C-N	6.23	127.63	119.84
2	B	128	LEU	C-N-CA	6.23	127.63	119.84
2	B	65	ALA	N-CA-C	-6.20	103.25	111.24
3	C	31	PHE	N-CA-C	6.12	117.64	110.97
1	A	179	THR	CA-C-N	-6.08	113.70	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	THR	C-N-CA	-6.08	113.70	119.85
1	A	215	LEU	N-CA-C	5.99	120.77	112.45
1	A	310	LEU	N-CA-C	-5.99	104.45	110.97
1	A	265	ALA	N-CA-C	-5.97	106.32	113.97
1	A	466	PRO	N-CA-C	-5.97	104.86	113.75
1	A	22	LEU	CA-CB-CG	-5.96	95.43	116.30
1	A	225	ARG	NE-CZ-NH2	5.89	124.50	119.20
1	A	393	VAL	N-CA-CB	5.85	116.76	110.62
1	A	447	VAL	CB-CA-C	5.82	117.47	110.78
2	B	68	ALA	N-CA-C	-5.80	104.15	111.11
1	A	249	THR	CB-CA-C	-5.79	99.34	109.07
1	A	527	ILE	CA-C-N	5.79	126.51	120.03
1	A	527	ILE	C-N-CA	5.79	126.51	120.03
1	A	45	ASN	N-CA-C	-5.79	104.17	111.11
2	B	122	ASN	N-CA-C	-5.77	104.78	113.89
2	B	156	GLY	N-CA-C	-5.77	106.26	115.66
1	A	427	LEU	N-CA-C	-5.71	106.08	113.16
1	A	247	ILE	CA-C-N	5.67	127.81	120.44
1	A	247	ILE	C-N-CA	5.67	127.81	120.44
1	A	52	TYR	CA-C-N	5.66	124.85	118.97
1	A	52	TYR	C-N-CA	5.66	124.85	118.97
1	A	284	GLN	N-CA-C	-5.63	103.92	112.99
2	B	164	ILE	N-CA-C	-5.62	99.40	107.78
1	A	341	TRP	CA-CB-CG	-5.62	102.93	113.60
1	A	297	ILE	CB-CA-C	-5.61	104.63	111.87
1	A	298	HIS	N-CA-C	-5.60	106.15	112.87
1	A	465	VAL	CA-C-N	-5.55	112.99	119.32
1	A	465	VAL	C-N-CA	-5.55	112.99	119.32
1	A	512	ILE	N-CA-C	-5.55	97.80	109.34
1	A	205	VAL	N-CA-CB	5.50	116.39	110.62
2	B	50	LEU	CA-CB-CG	5.43	135.32	116.30
2	B	165	VAL	CB-CA-C	-5.42	103.46	110.84
1	A	413	ILE	N-CA-CB	5.42	116.84	110.82
2	B	132	VAL	N-CA-C	5.40	115.30	106.72
1	A	340	PRO	N-CA-C	5.39	123.58	112.47
2	B	125	VAL	CA-C-N	-5.38	114.61	122.19
2	B	125	VAL	C-N-CA	-5.38	114.61	122.19
2	B	53	VAL	CB-CA-C	-5.37	103.07	110.91
1	A	476	VAL	N-CA-C	5.33	115.55	110.53
1	A	374	VAL	N-CA-C	5.32	119.49	112.04
1	A	447	VAL	CA-C-O	5.31	123.08	119.20
1	A	53	PRO	N-CA-C	-5.22	106.00	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	N-CA-C	-5.20	105.31	110.97
1	A	327	ARG	CA-C-N	-5.19	117.80	123.30
1	A	327	ARG	C-N-CA	-5.19	117.80	123.30
1	A	299	SER	N-CA-C	-5.17	105.29	111.03
2	B	128	LEU	CA-CB-CG	5.16	134.36	116.30
1	A	418	ARG	N-CA-C	-5.13	104.95	111.11
3	C	22	PHE	N-CA-C	5.10	117.96	111.69
1	A	100	ARG	N-CA-C	5.09	116.77	109.04
2	B	88	PHE	CB-CA-C	5.08	120.52	110.42
1	A	230	TRP	CA-C-N	5.07	127.34	120.44
1	A	230	TRP	C-N-CA	5.07	127.34	120.44
1	A	47	GLY	N-CA-C	-5.07	106.28	112.77
1	A	138	PRO	N-CA-C	5.03	125.17	112.10
1	A	411	LYS	CA-C-N	5.01	126.10	119.84
1	A	411	LYS	C-N-CA	5.01	126.10	119.84
1	A	56	LYS	N-CA-C	-5.01	105.90	111.36

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	684	0
2	B	1298	0	1280	166	0
3	C	259	0	279	45	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	43	0	30	9	0
6	A	65	0	61	31	0
7	B	2	0	0	0	0
All	All	6077	0	6166	858	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 70.

All (858) 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: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: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:20:ALA:HB3	1:A:106:MET:HE3	1.45	0.99
1:A:518:ARG:HH21	1:A:518:ARG:HG3	1.26	0.98
1:A:385:PHE:CG	6:A:801:HAS:HMA1	1.98	0.97
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
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:385:PHE:CD2	6:A:801:HAS:HMA1	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:385:PHE:HB2	6:A:801:HAS:HMA3	1.56	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:54:LEU:C	1:A:54:LEU:HD22	2.00	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:81:THR:HG1	1:A:239:TRP:CD1	1.93	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: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:89:MET:HE1	1:A:245:ALA:HB2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:497:ARG:C	1:A:499:PRO:HD3	2.09	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:264:MET:HA	1:A:264:MET:HE2	1.65	0.76
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
2:B:109:SER:HB3	2:B:129:PRO:HG3	1.69	0.75
1:A:389:VAL:HG22	5:A:800:HEM:CBC	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:52:TYR:N	1:A:53:PRO:CD	2.51	0.72
1:A:385:PHE:CG	6:A:801:HAS:CMA	2.73	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:472:LEU:HD22	1:A:472:LEU:C	2.16	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:236:VAL:HG23	1:A:237:TYR:N	2.05	0.70
1:A:389:VAL:HG22	5:A:800:HEM:HBC1	1.74	0.70
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:38:PHE:O	1:A:39:GLY:C	2.35	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:PRO:O	1:A:506:LEU:C	2.35	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:385:PHE:CB	6:A:801:HAS:HMA1	2.21	0.69
1:A:89:MET:HE1	1:A:245:ALA:CB	2.23	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: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:30:LEU:O	1:A:31:ALA:C	2.37	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: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: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
3:C:26:VAL:O	3:C:27:TYR:C	2.39	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:220:ASP:HB2	1:A:554:ASN:C	2.21	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
1:A:122:LEU:O	1:A:123:PRO:C	2.37	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:405:LEU:O	1:A:406:PRO:C	2.37	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:364:ILE:O	1:A:365:VAL:C	2.38	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:385:PHE:HB2	6:A:801:HAS:CMA	2.25	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: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: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:511:VAL:HG12	1:A:512:ILE:C	2.23	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: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:472:LEU:C	1:A:472:LEU:CD2	2.73	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
1:A:390:ALA:HA	5:A:800:HEM:HBC2	1.81	0.61
1:A:267:LEU:O	1:A:268:ALA:C	2.41	0.61
1:A:347:VAL:CG1	1:A:351:LEU:HD11	2.29	0.61
1:A:453:ILE:HD13	1:A:453:ILE:C	2.26	0.61
1:A:94:ALA:O	1:A:97:LEU:N	2.30	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:385:PHE:CB	6:A:801:HAS:HMA3	2.22	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: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:44:LEU:C	1:A:47:GLY:H	2.10	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:550:PHE:HA	1:A:553:LEU:HD21	1.83	0.59
2:B:11:ILE:O	2:B:12:LEU:C	2.46	0.59
1:A:244:TYR:O	1:A:248:TYR:HB2	2.02	0.59
1:A:81:THR:OG1	1:A:239:TRP:CD1	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TRP:O	1:A:339:LEU:HD22	2.03	0.59
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:153:VAL:O	1:A:154:LEU:C	2.44	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:64:SER:O	1:A:65:TYR:C	2.44	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
2:B:157:HIS:ND1	2:B:157:HIS:C	2.59	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: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:375:VAL:O	1:A:376:HIS:C	2.47	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:297:ILE:C	1:A:299:SER:N	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ALA:O	2:B:25:MET:C	2.49	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
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:151:VAL:O	1:A:152:PHE:C	2.48	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:428:TRP:CD1	1:A:428:TRP:C	2.84	0.55
1:A:467:MET:HA	1:A:470:ASN:HD22	1.71	0.55
2:B:54:ASP:OD1	2:B:54:ASP:C	2.49	0.55
1:A:340:PRO:C	1:A:342:ASP:H	2.15	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: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:465:VAL:O	1:A:466:PRO:C	2.50	0.55
2:B:35:TYR:C	2:B:35:TYR:CD1	2.76	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:184:TYR:CE2	1:A:266:ARG:HB3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:157:HIS:C	2:B:159:ASN:H	2.15	0.54
1:A:233:HIS:CD2	1:A:233:HIS:C	2.86	0.54
1:A:285:PHE:CE1	1:A:369:PHE:HA	2.43	0.54
1:A:23:TYR:O	1:A:24:PHE:C	2.51	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: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:23:TYR:C	1:A:25:LEU:N	2.63	0.53
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
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
3:C:9:LEU:O	3:C:10:ALA:C	2.51	0.53
1:A:206:LEU:HB2	1:A:207:PHE:CD2	2.44	0.53
2:B:32:LEU:O	2:B:33:ILE:C	2.52	0.53
2:B:86:PHE:CD1	2:B:86:PHE:C	2.86	0.53
1:A:27:LEU:O	1:A:28:GLY:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:189:PHE:O	1:A:190:TRP:C	2.52	0.52
1:A:262:ASP:HB3	1:A:263:PRO:CD	2.40	0.52
1:A:41:PHE:C	1:A:43:ALA:N	2.66	0.52
1:A:410:GLY:HA3	1:A:499:PRO:HG3	1.92	0.52
2:B:10:ALA:O	2:B:11:ILE:C	2.53	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:316:VAL:O	1:A:317:ALA:C	2.52	0.51
1:A:27:LEU:HD23	1:A:83:LEU:HD22	1.91	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:439:LEU:O	1:A:440:HIS:C	2.52	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
1:A:487:GLY:O	1:A:488:LEU:C	2.52	0.51
2:B:84:LEU:HG	2:B:110:PRO:HD3	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLN:CD	1:A:152:PHE:HE2	2.19	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:23:TYR:C	1:A:110:TRP:HE1	2.19	0.51
2:B:55:PRO:HB3	2:B:109:SER:O	2.11	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
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:348:ALA:O	1:A:349:PRO:C	2.50	0.50
1:A:129:ALA:O	1:A:131:VAL:HG22	2.11	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:16:LYS:O	2:B:17:GLY:C	2.54	0.50
1:A:520:LEU:HG	1:A:521:VAL:N	2.25	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
1:A:409:THR:C	1:A:411:LYS:H	2.20	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
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:192:MET:SD	1:A:192:MET:C	2.96	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:228:PHE:C	1:A:228:PHE:CD2	2.90	0.49
1:A:357:ILE:HG22	1:A:358:PRO:CD	2.43	0.49
1:A:97:LEU:O	1:A:98:ASN:C	2.56	0.49
1:A:154:LEU:O	1:A:157:TRP:CB	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:O	1:A:205:VAL:HG23	2.12	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: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:233:HIS:CB	1:A:234:PRO:CD	2.89	0.49
1:A:302:THR:O	1:A:303:LEU:C	2.54	0.49
2:B:90:TYR:CZ	2:B:147:ILE:CG2	2.96	0.48
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
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:20:ALA:HB3	1:A:106:MET:CE	2.32	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:127:ASN:CG	1:A:127:ASN:O	2.57	0.48
1:A:379:ALA:O	1:A:380:TRP:C	2.55	0.48
1:A:386:HIS:C	1:A:390:ALA:HB3	2.38	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
3:C:11:VAL:C	3:C:13:LEU:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:233:HIS:O	1:A:234:PRO:C	2.55	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: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: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:542:TYR:N	1:A:542:TYR:CD2	2.83	0.47
1:A:264:MET:HE2	1:A:264:MET:CA	2.41	0.47
1:A:346:PHE:C	1:A:349:PRO:HD2	2.39	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:297:ILE:C	1:A:299:SER:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:LEU:C	1:A:54:LEU:CD2	2.76	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
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
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: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
3:C:24:LEU:O	3:C:25:GLY:C	2.58	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
1:A:562:TRP:C	1:A:562:TRP:CD1	2.92	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
2:B:155:LEU:C	2:B:157:HIS:H	2.24	0.46
1:A:346:PHE:CZ	1:A:350:VAL:HG21	2.51	0.46
2:B:29:PHE:O	2:B:30:ILE:C	2.58	0.46
2:B:140:LYS:C	2:B:141:ARG:HG3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:TRP:CE3	1:A:213:PHE:HE2	2.33	0.46
1:A:365:VAL:C	1:A:367:ALA:N	2.74	0.46
3:C:18:THR:C	3:C:20:LEU:N	2.74	0.46
1:A:35:GLY:N	1:A:75:LEU:HD12	2.30	0.45
1:A:41:PHE:O	1:A:42:GLN:C	2.59	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
3:C:13:LEU:O	3:C:14:VAL:C	2.59	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
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
1:A:481:LEU:HD12	1:A:481:LEU:C	2.41	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:222:LEU:HD12	1:A:222:LEU:C	2.42	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: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:392:LEU:O	1:A:393:VAL:C	2.58	0.45
1:A:405:LEU:HB3	1:A:406:PRO:CD	2.46	0.45
1:A:435:MET:O	1:A:436:ALA:C	2.59	0.45
3:C:15:LEU:HD12	3:C:15:LEU:C	2.42	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
1:A:504:ALA:C	1:A:506:LEU:H	2.25	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:398:MET:HE2	1:A:484:PHE:CD1	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:ASN:C	1:A:48:ASN:HD22	2.24	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: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:306:ALA:O	1:A:307:VAL:C	2.60	0.44
1:A:547:VAL:O	1:A:548:GLN:C	2.60	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
3:C:9:LEU:C	3:C:11:VAL:N	2.70	0.44
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:18:TRP:O	2:B:19:LEU:C	2.61	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:300:VAL:O	1:A:301:LEU:C	2.58	0.44
1:A:404:LEU:HD12	1:A:404:LEU:HA	1.70	0.44
1:A:67:GLN:CD	1:A:127:ASN:HB2	2.43	0.44
1:A:284:GLN:HG3	1:A:287:ASP:CG	2.43	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:485:ILE:C	1:A:487:GLY:N	2.74	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:344:PRO:C	1:A:346:PHE:N	2.76	0.44
1:A:362:GLY:O	1:A:363:GLY:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:O	1:A:527:ILE:C	2.61	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:189:PHE:C	1:A:191:LEU:N	2.75	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: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
2:B:64:TRP:CD1	2:B:83:VAL:O	2.71	0.43
1:A:80:PHE:CD2	1:A:80:PHE:C	2.95	0.43
1:A:96:GLU:CD	1:A:180:PRO:HB2	2.42	0.43
1:A:161:TYR:O	1:A:162:ILE:C	2.61	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:25:MET:O	2:B:26:LEU:C	2.59	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
1:A:258:ARG:O	1:A:259:LEU:C	2.61	0.43
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:334:GLY:C	1:A:336:ILE:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:LEU:C	1:A:124:LEU:N	2.77	0.43
1:A:192:MET:HG3	1:A:273:LEU:HA	2.01	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: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:439:LEU:C	1:A:441:TRP:N	2.76	0.42
1:A:445:LEU:O	1:A:446:ASN:HB2	2.19	0.42
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
1:A:250:ILE:O	1:A:251:LEU:C	2.62	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:312:THR:C	1:A:314:PHE:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:441:TRP:CD1	1:A:441:TRP:C	2.94	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
3:C:7:GLY:O	3:C:8:ALA:C	2.63	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:365:VAL:O	1:A:366:ASN:C	2.63	0.42
1:A:495:ARG:O	1:A:496:GLU:C	2.61	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:295:LYS:O	1:A:296:MET:C	2.61	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:334:GLY:C	1:A:336:ILE:H	2.28	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
1:A:11:VAL:C	1:A:13:GLU:N	2.77	0.41
1:A:240:LEU:HB2	6:A:801:HAS:HBC1	2.01	0.41
1:A:451:ALA:C	1:A:453:ILE:N	2.77	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:29:PHE:O	1:A:30:LEU:C	2.61	0.41
1:A:45:ASN:HD21	1:A:452:TYR:HA	1.85	0.41
1:A:181:LEU:HG	1:A:185:MET:HE3	2.02	0.41
1:A:387:LEU:C	1:A:388:GLN:HE21	2.29	0.41
1:A:537:LEU:O	1:A:538:VAL:C	2.62	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:20:ALA:CB	1:A:106:MET:HE3	2.33	0.41
1:A:288:PRO:HB3	2:B:133:SER:HA	2.02	0.41
1:A:354:LEU:O	1:A:355:GLY:C	2.63	0.41
1:A:259:LEU:HG	1:A:261:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:365:VAL:C	1:A:367:ALA:H	2.29	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
3:C:11:VAL:O	3:C:12:ILE:C	2.60	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:344:PRO:O	1:A:345:ALA:C	2.64	0.41
1:A:81:THR:HG1	1:A:239:TRP:HD1	1.59	0.41
1:A:112:MET:HB3	1:A:112:MET:HE2	1.69	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: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: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: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:71:VAL:C	2:B:72:VAL:CG1	2.94	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:144:GLU:C	2:B:145:TYR:CD1	2.99	0.41
2:B:154:GLY:O	2:B:157:HIS:CB	2.64	0.41
3:C:31:PHE:C	3:C:33:ARG:N	2.78	0.41
1:A:410:GLY:HA3	1:A:499:PRO:CB	2.49	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:184:TYR:HE2	1:A:266:ARG:CB	2.33	0.40
1:A:314:PHE:CD2	3:C:12:ILE:HD12	2.54	0.40
3:C:15:LEU:O	3:C:16:THR:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HD22	1:A:531:PHE:CE2	2.56	0.40
1:A:264:MET:HA	1:A:264:MET:CE	2.45	0.40
2:B:157:HIS:C	2:B:159:ASN:N	2.77	0.40
1:A:170:TRP:O	1:A:174:ASN:HB2	2.21	0.40
1:A:278:PRO:C	1:A:279:VAL:HG13	2.47	0.40
1:A:548:GLN:O	1:A:550:PHE:N	2.54	0.40
1:A:16:PRO:C	1:A:18:LYS:N	2.79	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	1
2	B	164/168 (98%)	109 (66%)	40 (24%)	15 (9%)	0	3
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	1

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	12	TYR
1	A	48	ASN
1	A	151	VAL
1	A	152	PHE
1	A	189	PHE
1	A	197	SER
1	A	335	TRP
1	A	340	PRO

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Mol	Chain	Res	Type
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
3	C	14	VAL
3	C	27	TYR
1	A	110	TRP
1	A	142	HIS
1	A	308	PRO
1	A	403	TRP

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Mol	Chain	Res	Type
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
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%)	338 (75%)	115 (25%)	0	2
2	B	136/138 (99%)	99 (73%)	37 (27%)	0	2
3	C	26/27 (96%)	18 (69%)	8 (31%)	0	1
All	All	615/627 (98%)	455 (74%)	160 (26%)	0	2

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	25	LEU
1	A	27	LEU
1	A	33	ILE
1	A	37	LEU
1	A	38	PHE
1	A	42	GLN
1	A	49	VAL
1	A	54	LEU
1	A	55	LEU
1	A	57	ARG
1	A	63	GLN
1	A	64	SER
1	A	69	LEU
1	A	70	THR
1	A	75	LEU
1	A	78	ILE
1	A	82	GLN
1	A	89	MET
1	A	98	ASN
1	A	100	ARG
1	A	103	MET
1	A	106	MET
1	A	122	LEU
1	A	125	LEU
1	A	133	TYR

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Mol	Chain	Res	Type
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	202	LEU
1	A	205	VAL
1	A	213	PHE
1	A	215	LEU
1	A	216	VAL
1	A	222	LEU
1	A	227	LEU
1	A	235	ILE
1	A	236	VAL
1	A	244	TYR
1	A	253	LYS
1	A	254	GLN
1	A	276	SER
1	A	290	ILE
1	A	297	ILE
1	A	299	SER
1	A	300	VAL
1	A	309	SER
1	A	311	MET
1	A	315	THR
1	A	320	LEU
1	A	321	GLU
1	A	325	ARG
1	A	327	ARG
1	A	330	ARG
1	A	339	LEU
1	A	354	LEU
1	A	357	ILE
1	A	364	ILE
1	A	368	SER

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Mol	Chain	Res	Type
1	A	370	THR
1	A	371	LEU
1	A	388	GLN
1	A	392	LEU
1	A	394	THR
1	A	398	MET
1	A	405	LEU
1	A	408	LEU
1	A	417	GLN
1	A	418	ARG
1	A	419	ARG
1	A	420	LEU
1	A	422	LEU
1	A	425	VAL
1	A	428	TRP
1	A	430	LEU
1	A	439	LEU
1	A	449	ARG
1	A	453	ILE
1	A	456	VAL
1	A	465	VAL
1	A	468	VAL
1	A	472	LEU
1	A	476	VAL
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	512	ILE
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

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Mol	Chain	Res	Type
1	A	548	GLN
1	A	549	LEU
1	A	552	HIS
1	A	560	ARG
1	A	561	LEU
2	B	9	LYS
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	30	ILE
2	B	37	LEU
2	B	39	THR
2	B	54	ASP
2	B	61	GLU
2	B	71	VAL
2	B	72	VAL
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	135	VAL
2	B	136	ARG
2	B	140	LYS
2	B	148	ILE
2	B	149	CYS
2	B	157	HIS
2	B	159	ASN
2	B	160	MET
2	B	165	VAL
2	B	166	VAL
2	B	167	LYS

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Mol	Chain	Res	Type
3	C	2	GLU
3	C	3	GLU
3	C	6	LYS
3	C	12	ILE
3	C	13	LEU
3	C	19	ILE
3	C	21	VAL
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	63	GLN
1	A	76	ASN
1	A	98	ASN
1	A	254	GLN
1	A	388	GLN
1	A	446	ASN
1	A	470	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
2	B	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	72,72,72	2.82	31 (43%)	87,109,109	4.43	45 (51%)
5	HEM	A	800	1	50,50,50	2.14	13 (26%)	67,82,82	1.83	16 (23%)
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	1/1/8/18	12/42/82/82	-
5	HEM	A	800	1	-	6/14/54/54	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3D-C2D	7.71	1.53	1.36
6	A	801	HAS	C4A-NA	-7.65	1.25	1.39
6	A	801	HAS	C1A-NA	-6.50	1.27	1.39
6	A	801	HAS	C2A-C3A	6.23	1.50	1.36
6	A	801	HAS	CHC-C4B	5.92	1.50	1.38
6	A	801	HAS	CHD-C4A	5.75	1.49	1.38
6	A	801	HAS	FE-ND	5.28	2.11	1.94
5	A	800	HEM	FE-ND	5.17	2.10	1.94
6	A	801	HAS	CHB-C1D	5.16	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	CAC-C3C	-5.15	1.33	1.47
5	A	800	HEM	FE-NC	5.13	2.12	1.95
6	A	801	HAS	FE-NB	4.42	2.08	1.94
6	A	801	HAS	C1D-ND	-4.32	1.32	1.40
6	A	801	HAS	CHB-C1B	4.07	1.48	1.39
6	A	801	HAS	C1C-NC	-3.99	1.32	1.39
6	A	801	HAS	CHC-C1C	3.93	1.48	1.39
5	A	800	HEM	CAC-C3C	3.79	1.57	1.47
6	A	801	HAS	C4A-C3A	3.79	1.52	1.45
6	A	801	HAS	C4C-NC	-3.65	1.32	1.39
6	A	801	HAS	CHA-C1A	3.57	1.45	1.38
5	A	800	HEM	CMA-C3A	3.55	1.58	1.50
6	A	801	HAS	O1D-CGD	3.36	1.33	1.22
6	A	801	HAS	C2D-C3D	3.34	1.44	1.37
5	A	800	HEM	CAB-C3B	3.22	1.56	1.47
6	A	801	HAS	C4D-C3D	-3.13	1.39	1.45
5	A	800	HEM	O1D-CGD	3.09	1.32	1.22
6	A	801	HAS	FE-NC	2.97	2.05	1.95
6	A	801	HAS	C1A-C2A	2.90	1.50	1.45
6	A	801	HAS	C4B-NB	-2.88	1.35	1.40
6	A	801	HAS	C16-C15	2.81	1.57	1.51
6	A	801	HAS	CHD-C4C	2.79	1.45	1.39
6	A	801	HAS	C3B-C2B	2.74	1.41	1.34
5	A	800	HEM	FE-NB	2.65	2.03	1.94
6	A	801	HAS	C1C-C2C	2.63	1.49	1.43
5	A	800	HEM	O1A-CGA	2.61	1.30	1.22
6	A	801	HAS	C14-C15	2.60	1.39	1.33
5	A	800	HEM	FE-NA	2.57	2.03	1.95
6	A	801	HAS	CHA-C4D	2.53	1.44	1.39
6	A	801	HAS	CBA-CGA	2.46	1.56	1.50
6	A	801	HAS	C4D-ND	-2.38	1.34	1.38
6	A	801	HAS	C1B-C2B	-2.13	1.40	1.44
5	A	800	HEM	CMB-C2B	2.13	1.55	1.50
5	A	800	HEM	CMD-C2D	2.11	1.55	1.50
5	A	800	HEM	CAD-C3D	2.11	1.56	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C3C-C2C-C1C	-14.49	90.09	107.17
6	A	801	HAS	CHA-C1A-C2A	-12.12	105.73	124.86
6	A	801	HAS	C2D-C3D-C4D	-11.90	97.82	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C2A-C1A-NA	11.37	121.29	110.32
6	A	801	HAS	CBC-CAC-C3C	9.07	172.82	127.53
6	A	801	HAS	C4C-C3C-C2C	8.72	118.14	107.30
6	A	801	HAS	C1A-C2A-C3A	-8.33	96.14	107.11
6	A	801	HAS	C3D-C4D-ND	7.91	117.99	110.35
6	A	801	HAS	CHA-C1A-NA	7.59	132.72	124.45
6	A	801	HAS	CHB-C1B-NB	6.44	131.36	124.42
6	A	801	HAS	CHA-C4D-C3D	-6.31	115.58	124.77
6	A	801	HAS	CHB-C1D-ND	6.20	132.03	124.37
6	A	801	HAS	CHD-C4A-C3A	-5.99	113.03	125.49
6	A	801	HAS	CHC-C1C-C2C	-5.90	110.29	127.43
6	A	801	HAS	CMC-C2C-C3C	-5.58	113.44	126.55
6	A	801	HAS	C2C-C1C-NC	5.54	119.02	110.14
6	A	801	HAS	C1B-CHB-C1D	-5.46	113.88	125.69
6	A	801	HAS	OMD-CMD-C2D	-5.24	113.80	125.62
5	A	800	HEM	C4D-ND-C1D	5.20	111.37	105.21
6	A	801	HAS	CHD-C4A-NA	5.06	129.97	124.45
6	A	801	HAS	C1A-CHA-C4D	-5.01	115.37	126.02
6	A	801	HAS	C3C-C4C-NC	-4.94	105.64	109.80
6	A	801	HAS	CHB-C1B-C2B	-4.87	117.34	125.03
5	A	800	HEM	CAA-CBA-CGA	-4.78	100.99	113.67
6	A	801	HAS	CMA-C3A-C4A	-4.62	116.59	124.73
6	A	801	HAS	CMA-C3A-C2A	-4.60	113.70	126.15
6	A	801	HAS	CAA-C2A-C1A	-4.55	115.60	124.85
6	A	801	HAS	C1C-CHC-C4B	-4.51	115.64	126.25
5	A	800	HEM	C3B-C4B-NB	-4.26	106.41	109.47
6	A	801	HAS	CAD-C3D-C4D	4.17	131.97	124.70
6	A	801	HAS	C17-C18-C19	-4.16	118.09	127.62
6	A	801	HAS	C28-C24-C23	-3.90	100.25	113.19
6	A	801	HAS	C3A-C4A-NA	3.76	116.59	109.64
6	A	801	HAS	C21-C22-C23	-3.73	119.09	127.62
6	A	801	HAS	CHC-C4B-NB	3.60	128.82	124.37
6	A	801	HAS	C4A-C3A-C2A	-3.52	101.75	106.97
5	A	800	HEM	CAD-CBD-CGD	-3.41	104.63	113.67
6	A	801	HAS	C1D-C2D-C3D	3.40	110.41	107.28
6	A	801	HAS	CHC-C1C-NC	3.36	129.95	123.86
5	A	800	HEM	C2A-C1A-NA	-3.33	106.46	110.15
6	A	801	HAS	CMC-C2C-C1C	-3.11	120.69	125.42
5	A	800	HEM	C4B-C3B-C2B	2.99	110.03	107.28
5	A	800	HEM	C3C-C2C-C1C	2.95	109.84	107.05
6	A	801	HAS	O2A-CGA-CBA	2.84	122.97	114.00
6	A	801	HAS	C25-C23-C24	2.83	120.14	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	CMA-C3A-C2A	2.64	131.23	125.62
5	A	800	HEM	CAD-C3D-C4D	2.63	129.28	124.70
5	A	800	HEM	CHA-C1A-C2A	2.63	131.05	125.30
5	A	800	HEM	C1D-C2D-C3D	-2.54	104.31	106.98
6	A	801	HAS	C27-C19-C20	2.51	119.59	115.23
6	A	801	HAS	C31-C30-C29	-2.46	115.26	122.66
6	A	801	HAS	CBD-CAD-C3D	-2.45	105.76	112.53
5	A	800	HEM	C3D-C4D-ND	-2.41	107.52	110.17
6	A	801	HAS	C4C-CHD-C4A	-2.37	117.33	124.66
5	A	800	HEM	CMD-C2D-C1D	2.17	128.43	125.03
6	A	801	HAS	CAA-C2A-C3A	-2.16	123.83	127.87
5	A	800	HEM	CHC-C4B-NB	2.10	126.69	124.42
6	A	801	HAS	C13-C12-C11	-2.08	111.07	114.39
6	A	801	HAS	CHC-C4B-C3B	-2.06	120.60	125.80
5	A	800	HEM	CBC-CAC-C3C	-2.04	117.33	127.53
5	A	800	HEM	CAA-C2A-C3A	-2.02	122.55	127.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	HAS	NA

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800	HEM	C2B-C3B-CAB-CBB
5	A	800	HEM	C2C-C3C-CAC-CBC
5	A	800	HEM	C4C-C3C-CAC-CBC
6	A	801	HAS	C1D-C2D-CMD-OMD
6	A	801	HAS	C3D-C2D-CMD-OMD
6	A	801	HAS	C3A-C2A-CAA-CBA
6	A	801	HAS	C2A-CAA-CBA-CGA
5	A	800	HEM	C4B-C3B-CAB-CBB
6	A	801	HAS	C2D-C3D-CAD-CBD
6	A	801	HAS	C4D-C3D-CAD-CBD
6	A	801	HAS	C26-C15-C16-C17
6	A	801	HAS	C25-C23-C24-C28
6	A	801	HAS	C27-C19-C20-C21
5	A	800	HEM	C2D-C3D-CAD-CBD
6	A	801	HAS	C23-C24-C28-C29
5	A	800	HEM	C4D-C3D-CAD-CBD
6	A	801	HAS	C14-C15-C16-C17

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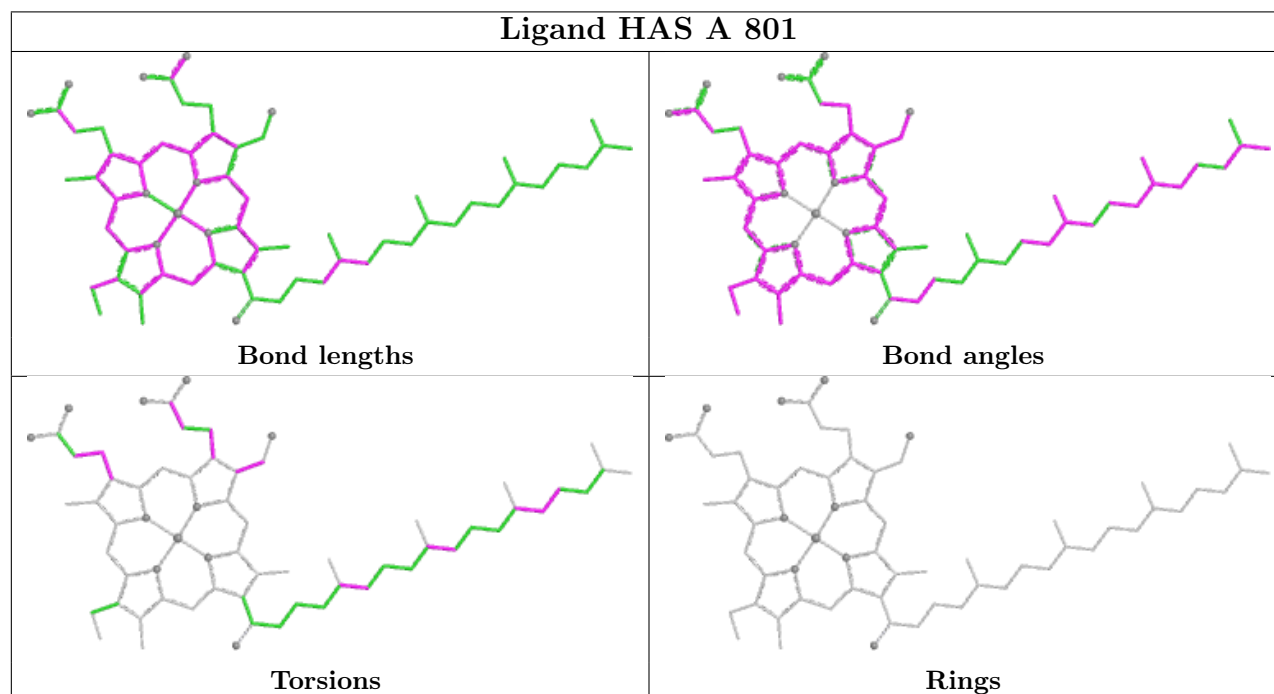
Mol	Chain	Res	Type	Atoms
6	A	801	HAS	CAD-CBD-CGD-O2D

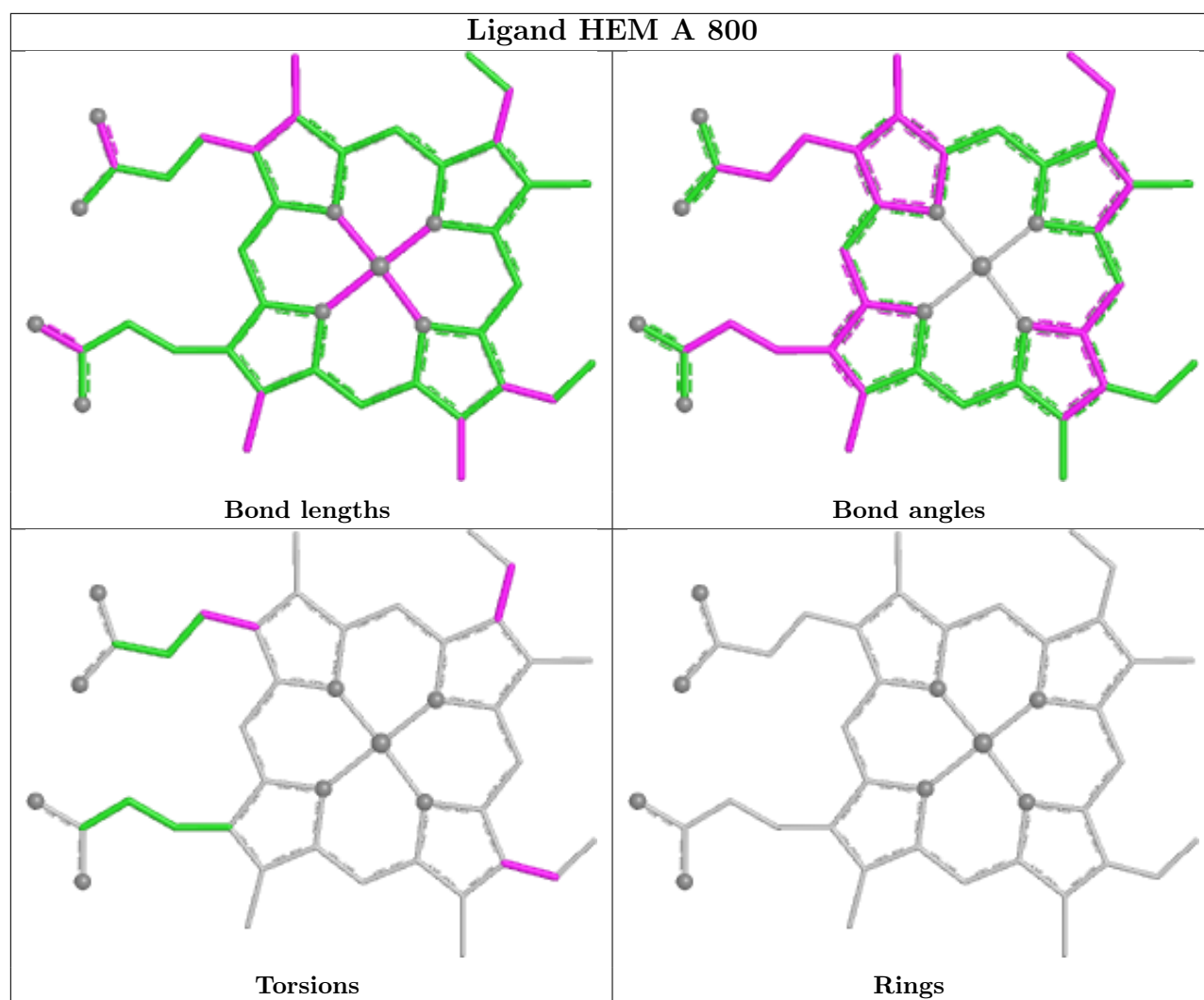
There are no ring outliers.

2 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	801	HAS	31	0
5	A	800	HEM	9	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, 95th 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 ²)	Q<0.9
1	A	557/568 (98%)	-0.84	0 100 100	8, 39, 82, 189	0
2	B	166/168 (98%)	-0.96	0 100 100	11, 39, 66, 150	0
3	C	33/34 (97%)	-0.87	0 100 100	16, 28, 99, 128	0
All	All	756/770 (98%)	-0.86	0 100 100	8, 39, 82, 189	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

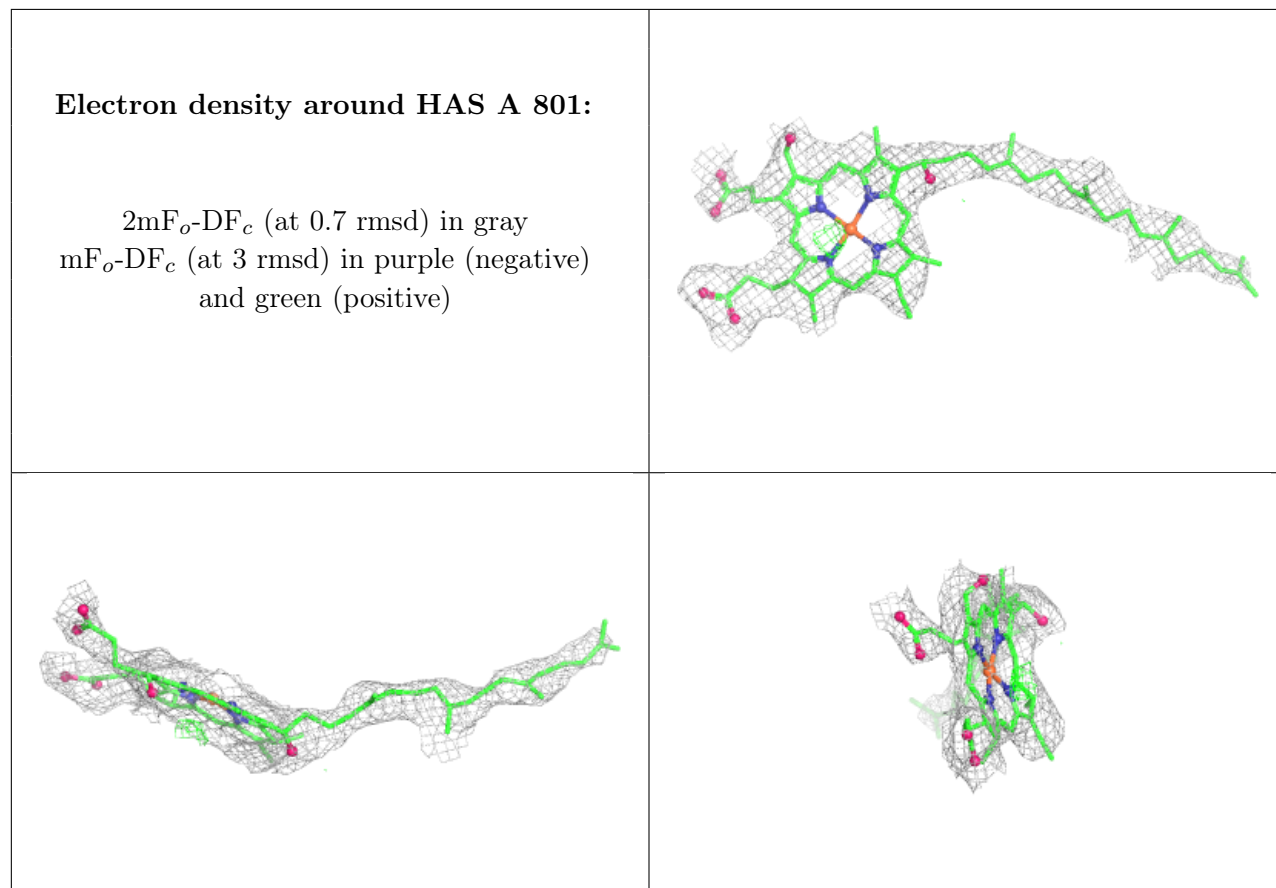
6.4 Ligands [i](#)

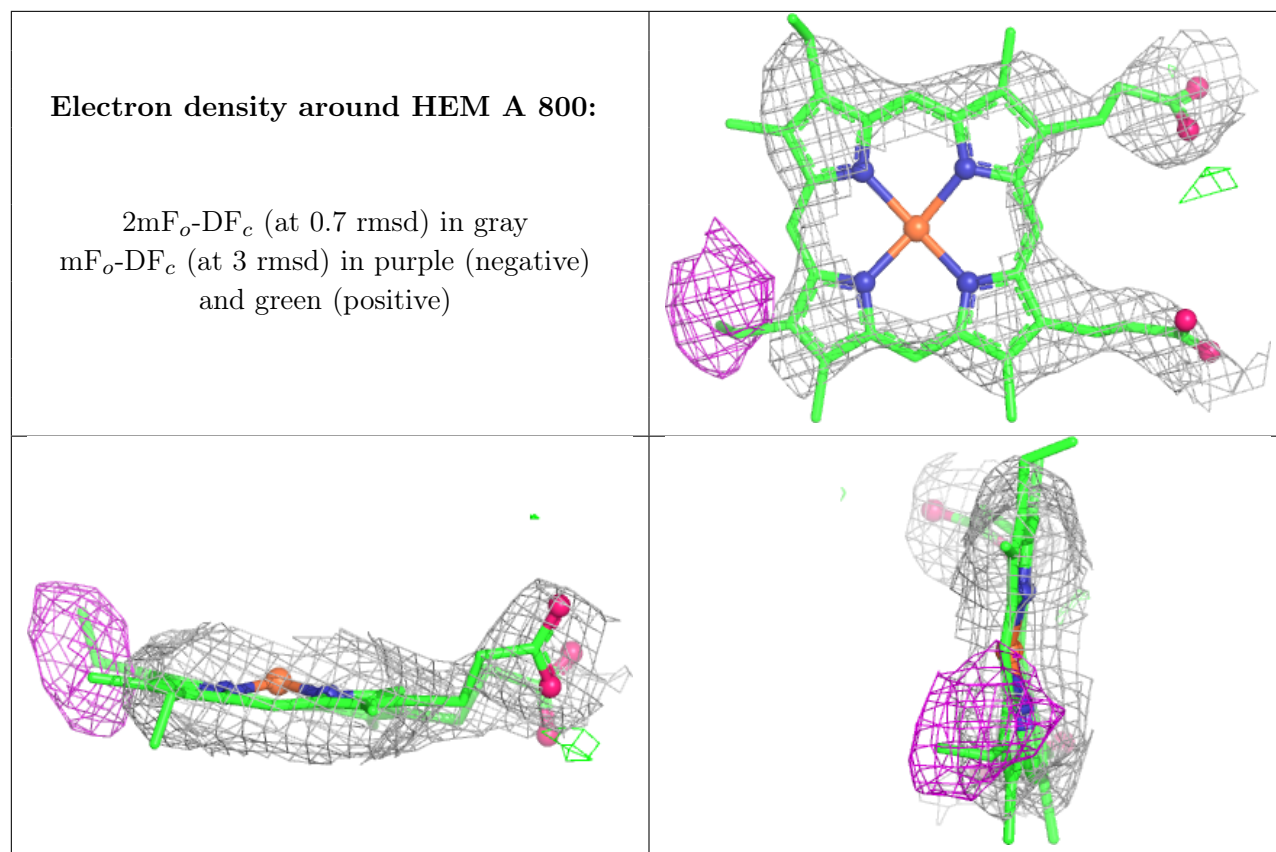
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	HAS	A	801	65/65	0.96	0.08	17,54,76,85	0
5	HEM	A	800	43/43	0.97	0.08	44,71,84,86	0
4	CU1	A	803	1/1	0.97	0.03	83,83,83,83	0
7	CUA	B	802	2/2	0.99	0.03	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.