



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:56 PM UTC

PDB ID : 4FXB / pdb_00004fxb
Title : Crystal structure of CYP105N1 from *Streptomyces coelicolor*: a cytochrome P450 oxidase in the coelibactin siderophore biosynthetic pathway
Authors : Hong, M.K.; Lim, Y.R.; Kim, J.K.; Kim, D.H.; Kang, L.W.
Deposited on : 2012-07-03
Resolution : 2.90 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

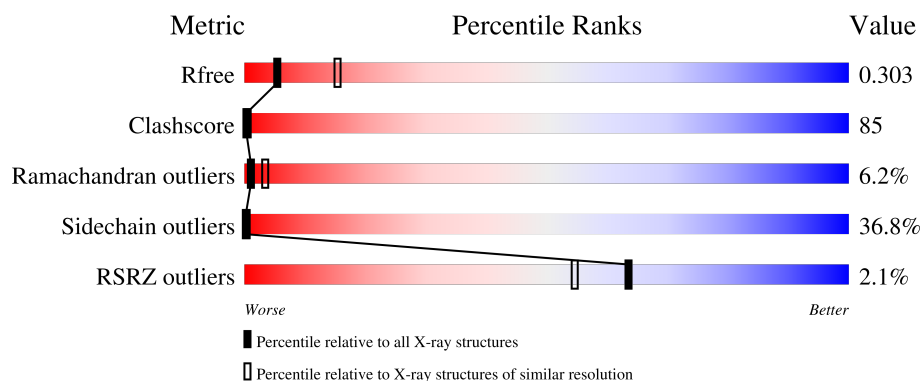
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	417	
1	B	417	

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
2	HEM	B	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6021 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.

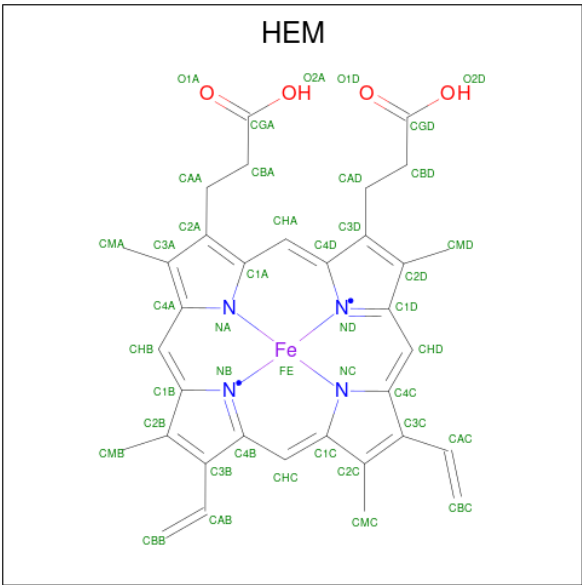
- Molecule 1 is a protein called Putative cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3020	1886	553	572	9			
1	B	370	Total	C	N	O	S	0	0	0
			2858	1790	523	537	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	HIS	-	expression tag	UNP Q9EWP1
A	413	HIS	-	expression tag	UNP Q9EWP1
A	414	HIS	-	expression tag	UNP Q9EWP1
A	415	HIS	-	expression tag	UNP Q9EWP1
A	416	HIS	-	expression tag	UNP Q9EWP1
A	417	HIS	-	expression tag	UNP Q9EWP1
B	412	HIS	-	expression tag	UNP Q9EWP1
B	413	HIS	-	expression tag	UNP Q9EWP1
B	414	HIS	-	expression tag	UNP Q9EWP1
B	415	HIS	-	expression tag	UNP Q9EWP1
B	416	HIS	-	expression tag	UNP Q9EWP1
B	417	HIS	-	expression tag	UNP Q9EWP1

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

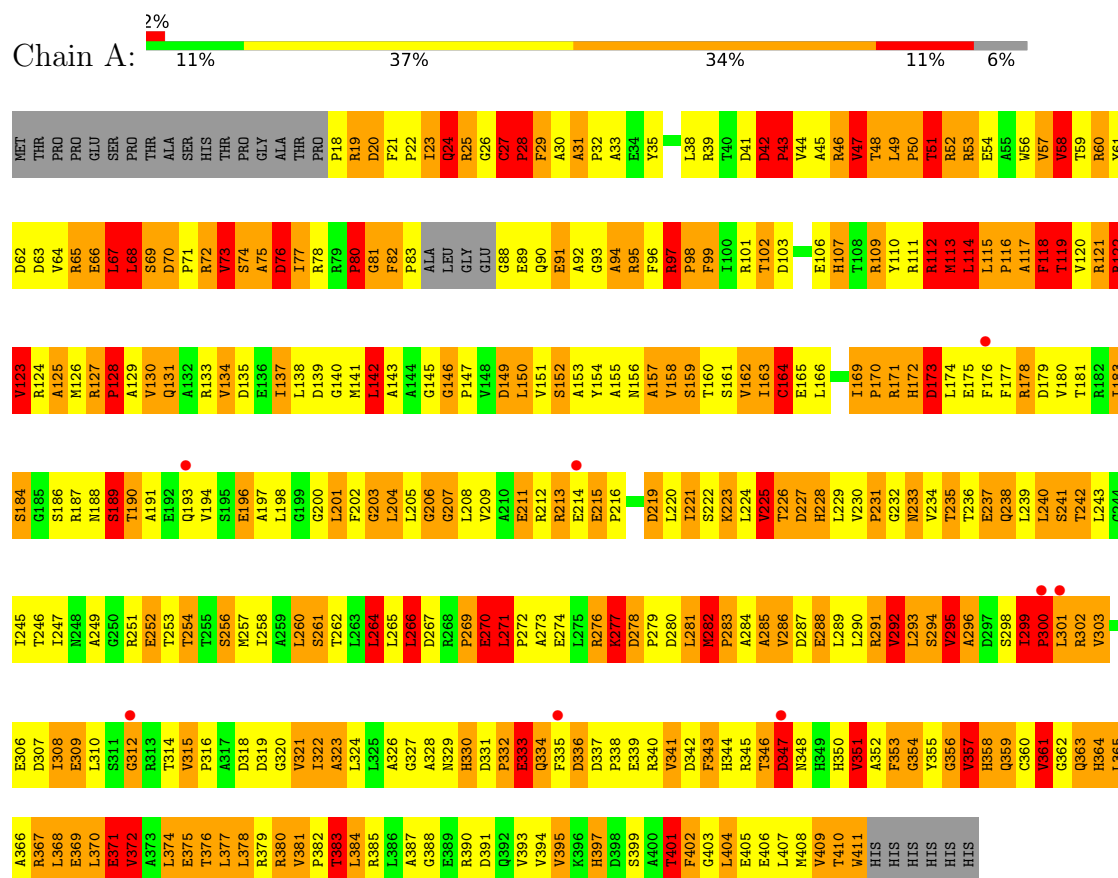
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	22	Total	O	0	0
			22	22		

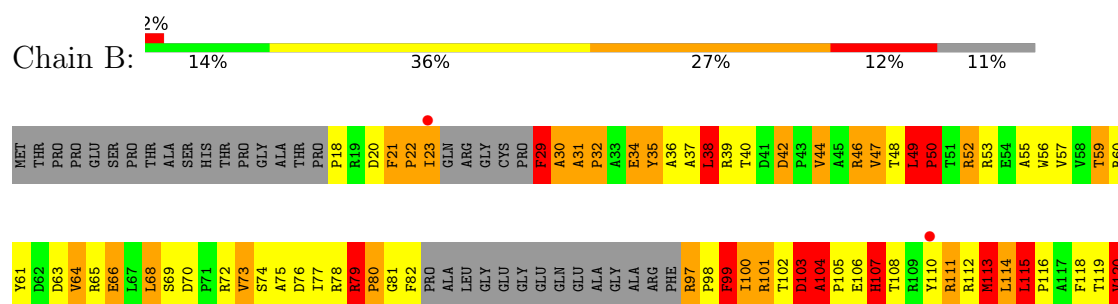
3 Residue-property plots

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: Putative cytochrome P450



• Molecule 1: Putative cytochrome P450





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	133.09Å 133.09Å 227.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.9 (19.93-2.90) 98.8 (19.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.281 , 0.302 0.284 , 0.303	Depositor DCC
R_{free} test set	4974 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6021	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.84	57/3076 (1.9%)	2.15	135/4186 (3.2%)
1	B	1.69	46/2905 (1.6%)	2.07	123/3951 (3.1%)
All	All	1.77	103/5981 (1.7%)	2.11	258/8137 (3.2%)

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	9
1	B	0	9
All	All	0	18

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	LEU	CA-C	-8.57	1.43	1.52
1	A	166	LEU	CA-C	8.40	1.63	1.52
1	A	67	LEU	CA-C	-8.11	1.42	1.52
1	A	118	PHE	CA-C	-7.95	1.44	1.53
1	A	299	ILE	CA-C	-7.87	1.44	1.52
1	B	247	ILE	C-O	-7.86	1.14	1.24
1	A	228	HIS	CA-C	-7.84	1.43	1.53
1	A	281	LEU	N-CA	-7.80	1.37	1.46
1	A	75	ALA	CA-C	7.74	1.64	1.53
1	A	76	ASP	CA-C	7.32	1.62	1.52
1	A	301	LEU	CA-C	-7.21	1.43	1.52
1	B	285	ALA	N-CA	-6.93	1.37	1.46
1	A	115	LEU	CA-C	-6.92	1.44	1.52
1	A	125	ALA	C-O	-6.82	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	356	GLY	N-CA	6.81	1.52	1.45
1	A	292	VAL	N-CA	-6.75	1.38	1.46
1	A	189	SER	CA-C	6.74	1.61	1.52
1	B	341	VAL	CA-C	-6.62	1.46	1.53
1	A	76	ASP	N-CA	6.61	1.54	1.46
1	A	276	ARG	CA-C	6.60	1.61	1.52
1	B	380	ARG	N-CA	6.51	1.54	1.46
1	B	195	SER	N-CA	-6.43	1.38	1.46
1	B	205	LEU	CA-C	-6.42	1.45	1.52
1	A	164	CYS	N-CA	-6.38	1.38	1.46
1	B	349	HIS	CB-CG	6.35	1.59	1.50
1	A	118	PHE	C-O	-6.34	1.17	1.23
1	B	107	HIS	CA-C	-6.25	1.46	1.52
1	B	134	VAL	C-O	6.15	1.32	1.24
1	B	318	ASP	CA-C	6.15	1.60	1.53
1	A	184	SER	CA-C	-6.14	1.45	1.52
1	B	349	HIS	CG-CD2	6.12	1.42	1.35
1	A	364	HIS	CG-ND1	-6.11	1.31	1.38
1	A	333	GLU	CA-C	6.10	1.61	1.52
1	B	148	VAL	CA-C	6.03	1.60	1.52
1	B	30	ALA	N-CA	6.03	1.53	1.46
1	A	344	HIS	CG-CD2	6.01	1.42	1.35
1	B	170	PRO	N-CA	-6.00	1.39	1.47
1	B	304	ALA	N-CA	6.00	1.54	1.46
1	B	247	ILE	CA-C	-5.97	1.45	1.53
1	A	118	PHE	CA-CB	-5.96	1.46	1.53
1	A	74	SER	N-CA	5.93	1.53	1.46
1	A	344	HIS	CE1-NE2	5.93	1.38	1.32
1	B	126	MET	CA-C	5.89	1.60	1.52
1	B	249	ALA	N-CA	5.89	1.53	1.46
1	A	261	SER	CA-C	-5.87	1.44	1.52
1	A	293	LEU	CA-C	-5.85	1.44	1.52
1	B	124	ARG	CA-C	5.82	1.60	1.52
1	A	350	HIS	CE1-NE2	5.79	1.38	1.32
1	A	277	LYS	CA-C	-5.78	1.45	1.52
1	B	392	GLN	CA-C	5.77	1.60	1.53
1	B	384	LEU	CA-C	-5.75	1.45	1.52
1	B	159	SER	CA-C	-5.74	1.45	1.52
1	B	179	ASP	CA-C	5.70	1.60	1.52
1	A	365	LEU	N-CA	-5.63	1.39	1.46
1	B	249	ALA	CA-C	5.61	1.60	1.52
1	A	358	HIS	N-CA	-5.61	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	LEU	C-O	-5.58	1.17	1.24
1	A	354	GLY	N-CA	5.55	1.52	1.45
1	A	128	PRO	CA-C	-5.54	1.44	1.52
1	A	69	SER	N-CA	-5.53	1.38	1.46
1	B	287	ASP	CA-C	5.50	1.60	1.52
1	B	123	VAL	CA-CB	5.50	1.60	1.54
1	B	344	HIS	CB-CG	5.49	1.57	1.50
1	A	117	ALA	N-CA	5.48	1.53	1.46
1	B	383	THR	CA-C	-5.44	1.45	1.52
1	B	304	ALA	C-O	-5.44	1.17	1.23
1	B	325	LEU	CA-C	5.40	1.59	1.52
1	A	353	PHE	CA-C	-5.39	1.46	1.53
1	B	158	VAL	N-CA	5.39	1.52	1.46
1	B	184	SER	N-CA	-5.38	1.39	1.46
1	B	34	GLU	CA-C	5.37	1.59	1.52
1	A	323	ALA	CA-C	-5.37	1.47	1.53
1	B	368	LEU	C-O	-5.34	1.18	1.24
1	A	354	GLY	C-O	-5.34	1.15	1.23
1	B	164	CYS	CA-C	-5.34	1.45	1.52
1	A	376	THR	CA-CB	-5.33	1.45	1.53
1	A	333	GLU	N-CA	5.29	1.53	1.46
1	B	228	HIS	CB-CG	5.28	1.57	1.50
1	A	364	HIS	CD2-NE2	-5.28	1.32	1.37
1	A	27	CYS	N-CA	-5.27	1.38	1.46
1	A	364	HIS	CG-CD2	5.26	1.41	1.35
1	A	371	GLU	CA-C	-5.26	1.45	1.52
1	B	349	HIS	ND1-CE1	5.24	1.37	1.32
1	A	81	GLY	CA-C	-5.20	1.44	1.51
1	B	30	ALA	CA-C	-5.19	1.46	1.52
1	A	58	VAL	C-O	5.18	1.29	1.24
1	A	403	GLY	N-CA	5.17	1.52	1.45
1	A	131	GLN	C-O	5.16	1.30	1.24
1	B	325	LEU	C-O	5.16	1.30	1.24
1	A	119	THR	CB-CG2	5.16	1.69	1.52
1	A	330	HIS	CD2-NE2	-5.14	1.32	1.37
1	A	346	THR	N-CA	5.10	1.52	1.46
1	A	225	VAL	C-O	-5.10	1.18	1.24
1	B	384	LEU	C-O	-5.09	1.18	1.23
1	A	332	PRO	CA-C	5.09	1.59	1.52
1	A	295	VAL	CA-C	-5.08	1.46	1.52
1	B	367	ARG	C-O	-5.08	1.17	1.24
1	B	30	ALA	C-O	-5.06	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	SER	CA-C	5.05	1.59	1.52
1	B	347	ASP	N-CA	5.05	1.52	1.46
1	B	241	SER	CA-C	-5.05	1.46	1.52
1	B	341	VAL	N-CA	-5.04	1.40	1.46
1	A	215	GLU	CA-CB	5.01	1.59	1.53

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	SER	N-CA-C	16.62	146.20	110.80
1	B	303	VAL	CB-CA-C	14.59	131.62	111.49
1	A	98	PRO	N-CA-C	-12.80	90.21	110.95
1	A	301	LEU	N-CA-C	-12.45	89.66	108.46
1	A	67	LEU	N-CA-C	-12.37	97.83	111.07
1	A	187	ARG	N-CA-C	11.67	126.69	111.75
1	A	188	ASN	N-CA-C	11.45	129.24	113.21
1	B	245	ILE	CB-CA-C	-11.27	97.06	111.94
1	A	114	LEU	N-CA-CB	-10.81	92.23	110.49
1	A	70	ASP	CA-C-N	10.73	133.25	119.84
1	A	70	ASP	C-N-CA	10.73	133.25	119.84
1	B	186	SER	CB-CA-C	-10.58	89.36	110.42
1	B	304	ALA	N-CA-C	10.51	125.45	108.63
1	A	130	VAL	N-CA-C	-10.17	99.92	111.00
1	B	115	LEU	CA-C-N	-9.85	110.79	120.83
1	B	115	LEU	C-N-CA	-9.85	110.79	120.83
1	A	402	PHE	N-CA-C	9.84	123.93	111.24
1	B	229	LEU	N-CA-C	9.82	131.71	110.80
1	B	286	VAL	CB-CA-C	-9.79	98.92	112.14
1	A	391	ASP	N-CA-C	9.74	124.41	113.21
1	A	66	GLU	N-CA-C	-9.70	100.19	112.90
1	B	284	ALA	N-CA-C	-9.68	101.47	113.18
1	B	99	PHE	CB-CA-C	-9.65	94.93	110.86
1	B	381	VAL	CA-C-N	9.55	131.78	119.84
1	B	381	VAL	C-N-CA	9.55	131.78	119.84
1	A	173	ASP	N-CA-C	-9.44	102.36	112.93
1	A	276	ARG	N-CA-C	9.43	121.32	111.14
1	B	66	GLU	CB-CA-C	-9.36	96.18	110.88
1	A	97	ARG	N-CA-C	-9.32	89.22	109.81
1	B	331	ASP	CA-C-N	9.30	131.46	119.84
1	B	331	ASP	C-N-CA	9.30	131.46	119.84
1	B	280	ASP	N-CA-C	-9.26	103.08	114.75
1	B	193	GLN	N-CA-C	-9.17	103.25	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	THR	N-CA-C	-9.09	101.12	113.30
1	A	280	ASP	N-CA-C	-9.01	98.42	111.30
1	B	303	VAL	N-CA-C	-8.93	97.04	109.45
1	B	397	HIS	CB-CA-C	-8.87	92.77	110.42
1	A	347	ASP	N-CA-C	8.86	124.54	107.44
1	B	35	TYR	N-CA-C	8.81	120.57	110.97
1	B	299	ILE	N-CA-C	8.81	127.90	108.88
1	A	97	ARG	CA-C-N	8.77	130.16	119.98
1	A	97	ARG	C-N-CA	8.77	130.16	119.98
1	B	395	VAL	CB-CA-C	8.65	125.48	111.29
1	A	357	VAL	CB-CA-C	-8.62	97.15	111.29
1	A	27	CYS	CA-C-N	8.42	130.37	119.84
1	A	27	CYS	C-N-CA	8.42	130.37	119.84
1	B	304	ALA	N-CA-CB	-8.40	96.61	109.88
1	A	94	ALA	N-CA-C	-8.34	101.86	113.20
1	A	99	PHE	N-CA-C	-8.32	103.13	113.28
1	A	233	ASN	N-CA-C	-8.32	104.15	112.97
1	A	358	HIS	N-CA-C	-8.28	104.32	114.75
1	A	123	VAL	N-CA-C	8.25	119.03	110.36
1	A	162	VAL	N-CA-C	-8.19	102.83	110.53
1	B	245	ILE	N-CA-C	8.17	118.17	110.74
1	A	397	HIS	N-CA-C	8.05	122.80	113.38
1	B	364	HIS	N-CA-C	7.98	119.61	111.07
1	B	176	PHE	N-CA-C	-7.93	101.34	111.02
1	B	394	VAL	N-CA-C	7.93	121.07	108.85
1	B	260	LEU	N-CA-C	7.91	120.90	111.33
1	A	238	GLN	N-CA-C	7.83	120.90	111.82
1	B	158	VAL	N-CA-C	7.82	119.54	110.62
1	A	375	GLU	CA-C-N	7.77	130.69	120.28
1	A	375	GLU	C-N-CA	7.77	130.69	120.28
1	B	177	PHE	N-CA-C	-7.74	102.92	111.36
1	B	257	MET	N-CA-C	7.65	120.29	111.11
1	A	160	THR	N-CA-C	-7.61	103.07	111.36
1	A	161	SER	N-CA-C	-7.57	103.50	112.89
1	B	193	GLN	N-CA-CB	-7.56	99.92	110.65
1	B	176	PHE	CB-CA-C	-7.44	99.09	110.92
1	A	142	LEU	N-CA-C	-7.43	104.35	113.50
1	B	396	LYS	N-CA-C	-7.38	95.08	110.80
1	A	225	VAL	N-CA-C	7.34	117.43	110.53
1	A	352	ALA	N-CA-C	-7.32	103.45	112.38
1	B	205	LEU	N-CA-C	-7.32	102.91	111.03
1	A	169	ILE	N-CA-C	7.29	116.91	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	SER	N-CA-C	7.20	122.82	114.62
1	B	57	VAL	N-CA-C	7.17	119.06	108.45
1	B	357	VAL	N-CA-C	-7.15	102.03	112.04
1	A	265	LEU	N-CA-C	-7.12	102.57	111.11
1	A	49	LEU	CA-C-N	7.10	128.71	119.84
1	A	49	LEU	C-N-CA	7.10	128.71	119.84
1	A	114	LEU	CA-CB-CG	7.05	140.99	116.30
1	A	261	SER	N-CA-C	-7.04	102.81	111.33
1	B	237	GLU	N-CA-C	-7.02	103.70	112.90
1	A	374	LEU	N-CA-C	6.96	118.87	111.28
1	A	91	GLU	N-CA-C	-6.92	102.96	111.33
1	A	49	LEU	N-CA-C	-6.90	101.42	110.39
1	B	49	LEU	CA-C-N	6.89	128.45	119.84
1	B	49	LEU	C-N-CA	6.89	128.45	119.84
1	B	278	ASP	N-CA-C	6.84	124.11	108.93
1	A	43	PRO	N-CA-C	-6.82	104.44	113.65
1	A	203	GLY	N-CA-C	-6.76	104.65	112.50
1	B	126	MET	N-CA-C	6.75	120.39	111.75
1	A	277	LYS	CB-CA-C	-6.74	99.66	110.84
1	B	234	VAL	CB-CA-C	-6.70	100.30	111.29
1	B	52	ARG	N-CA-C	6.62	120.21	111.28
1	A	315	VAL	N-CA-C	6.60	115.16	107.77
1	A	59	THR	N-CA-C	6.59	122.84	113.02
1	B	111	ARG	N-CA-C	6.59	118.46	111.28
1	A	301	LEU	CA-C-N	-6.58	113.39	122.93
1	A	301	LEU	C-N-CA	-6.58	113.39	122.93
1	B	296	ALA	N-CA-C	-6.58	96.78	110.80
1	A	277	LYS	CA-C-N	-6.54	114.47	122.64
1	A	277	LYS	C-N-CA	-6.54	114.47	122.64
1	A	274	GLU	N-CA-C	-6.54	104.24	111.82
1	A	68	LEU	CA-CB-CG	-6.45	93.74	116.30
1	A	409	VAL	N-CA-C	6.41	117.39	108.23
1	A	375	GLU	N-CA-CB	-6.40	99.68	110.49
1	B	245	ILE	N-CA-CB	6.35	118.26	110.64
1	A	346	THR	CB-CA-C	-6.34	100.26	110.79
1	B	192	GLU	CB-CA-C	-6.32	98.88	109.75
1	A	254	THR	N-CA-C	-6.32	102.94	112.04
1	B	103	ASP	N-CA-C	-6.32	100.22	109.63
1	A	270	GLU	CA-C-N	6.31	126.83	119.83
1	A	270	GLU	C-N-CA	6.31	126.83	119.83
1	B	337	ASP	N-CA-CB	6.30	121.59	110.37
1	A	221	ILE	CB-CA-C	-6.29	103.80	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	N-CA-C	6.28	120.29	111.30
1	A	24	GLN	N-CA-C	-6.28	93.43	111.00
1	B	113	MET	N-CA-C	-6.26	104.34	112.23
1	B	341	VAL	N-CA-C	-6.25	98.49	107.37
1	B	263	LEU	N-CA-C	-6.22	103.80	111.33
1	B	222	SER	N-CA-C	6.18	117.68	111.07
1	B	228	HIS	N-CA-C	-6.17	105.23	112.89
1	B	221	ILE	N-CA-CB	6.17	119.83	110.58
1	B	99	PHE	N-CA-C	6.16	119.18	111.24
1	A	266	LEU	CA-C-N	-6.15	111.62	122.26
1	A	266	LEU	C-N-CA	-6.15	111.62	122.26
1	B	232	GLY	N-CA-C	-6.13	95.52	113.30
1	A	67	LEU	N-CA-CB	6.10	118.86	110.01
1	A	164	CYS	N-CA-C	-6.10	104.32	110.97
1	A	219	ASP	CB-CA-C	-6.07	106.82	114.40
1	B	291	ARG	N-CA-C	-6.05	104.61	111.14
1	A	336	ASP	N-CA-C	6.05	118.77	110.24
1	B	187	ARG	N-CA-C	-6.00	94.21	111.00
1	A	237	GLU	N-CA-C	-5.98	104.45	110.97
1	A	206	GLY	N-CA-C	-5.97	105.41	113.24
1	B	249	ALA	N-CA-C	5.96	123.50	110.80
1	A	383	THR	CB-CA-C	5.95	123.25	112.30
1	B	313	ARG	N-CA-C	5.92	118.39	110.35
1	B	267	ASP	N-CA-C	5.91	121.12	111.37
1	B	163	ILE	N-CA-C	-5.89	104.77	110.42
1	A	372	VAL	CB-CA-C	-5.88	101.64	111.29
1	B	355	TYR	CB-CA-C	-5.86	101.73	114.10
1	B	285	ALA	N-CA-C	-5.86	104.25	111.40
1	A	113	MET	N-CA-C	-5.86	105.84	112.87
1	B	255	THR	N-CA-CB	5.85	118.56	110.07
1	B	318	ASP	N-CA-C	5.85	118.33	111.02
1	A	397	HIS	CB-CA-C	-5.82	101.74	111.23
1	B	234	VAL	N-CA-C	5.82	121.45	109.34
1	A	285	ALA	N-CA-C	5.79	120.93	111.37
1	B	371	GLU	CA-C-N	-5.77	113.35	121.55
1	B	371	GLU	C-N-CA	-5.77	113.35	121.55
1	A	312	GLY	N-CA-C	5.77	126.86	113.18
1	B	398	ASP	N-CA-C	-5.75	106.12	114.12
1	A	307	ASP	N-CA-C	-5.73	101.36	109.96
1	A	240	LEU	CA-CB-CG	-5.71	96.30	116.30
1	A	282	MET	CA-C-N	-5.71	112.70	119.84
1	A	282	MET	C-N-CA	-5.71	112.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	CA-C-N	-5.71	111.56	122.13
1	A	380	ARG	C-N-CA	-5.71	111.56	122.13
1	B	165	GLU	N-CA-C	-5.71	105.14	111.36
1	A	122	ARG	CB-CA-C	5.70	119.73	110.96
1	B	194	VAL	CB-CA-C	-5.70	101.95	111.29
1	A	291	ARG	CA-C-O	5.68	126.96	121.00
1	B	196	GLU	N-CA-C	-5.68	105.09	111.28
1	A	20	ASP	N-CA-C	5.67	118.31	109.52
1	A	299	ILE	N-CA-C	-5.63	96.71	108.88
1	A	271	LEU	CA-C-N	-5.62	112.81	119.84
1	A	271	LEU	C-N-CA	-5.62	112.81	119.84
1	A	60	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	A	368	LEU	N-CA-CB	5.58	118.42	110.16
1	A	358	HIS	CB-CA-C	5.57	116.34	109.16
1	A	49	LEU	CB-CA-C	5.56	117.12	108.61
1	A	308	ILE	N-CA-C	5.56	116.06	107.78
1	A	343	PHE	CB-CA-C	-5.56	99.98	109.65
1	A	112	ARG	CG-CD-NE	5.54	124.19	112.00
1	A	368	LEU	CB-CA-C	-5.50	101.50	110.85
1	A	321	VAL	CB-CA-C	-5.48	104.17	110.41
1	A	315	VAL	CA-C-N	5.45	125.45	119.89
1	A	315	VAL	C-N-CA	5.45	125.45	119.89
1	B	74	SER	N-CA-C	5.45	118.11	109.50
1	A	213	ARG	N-CA-C	-5.45	105.24	111.07
1	B	66	GLU	N-CA-C	5.43	116.88	111.07
1	B	303	VAL	CA-C-N	5.43	131.30	122.07
1	B	303	VAL	C-N-CA	5.43	131.30	122.07
1	B	64	VAL	CB-CA-C	-5.42	104.94	112.04
1	A	318	ASP	N-CA-C	5.41	118.71	111.24
1	B	120	VAL	CA-C-N	5.41	131.86	121.54
1	B	120	VAL	C-N-CA	5.41	131.86	121.54
1	A	323	ALA	CA-C-N	-5.40	113.23	121.66
1	A	323	ALA	C-N-CA	-5.40	113.23	121.66
1	A	169	ILE	CA-C-N	-5.39	113.10	119.84
1	A	169	ILE	C-N-CA	-5.39	113.10	119.84
1	A	47	VAL	N-CA-C	5.39	114.95	108.06
1	B	66	GLU	O-C-N	5.39	127.62	122.07
1	B	130	VAL	N-CA-CB	5.38	116.73	110.65
1	B	164	CYS	CB-CA-C	-5.36	101.89	110.79
1	A	288	GLU	N-CA-C	5.36	116.81	110.97
1	A	54	GLU	N-CA-C	-5.34	103.34	110.55
1	A	25	ARG	N-CA-C	-5.33	96.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	B	29	PHE	CA-C-N	5.31	127.85	120.63
1	B	29	PHE	C-N-CA	5.31	127.85	120.63
1	A	376	THR	CA-CB-OG1	-5.30	101.65	109.60
1	B	134	VAL	CA-C-N	5.29	127.32	120.44
1	B	134	VAL	C-N-CA	5.29	127.32	120.44
1	A	405	GLU	N-CA-CB	5.28	117.73	110.07
1	B	382	PRO	N-CA-C	5.28	123.34	112.47
1	B	44	VAL	CB-CA-C	-5.25	105.92	111.23
1	B	243	LEU	CA-C-N	5.25	125.91	120.03
1	B	243	LEU	C-N-CA	5.25	125.91	120.03
1	A	347	ASP	CB-CA-C	-5.25	103.78	111.23
1	B	104	ALA	CA-C-N	-5.24	114.41	127.00
1	B	104	ALA	C-N-CA	-5.24	114.41	127.00
1	A	361	VAL	CA-C-N	5.23	130.11	120.79
1	A	361	VAL	C-N-CA	5.23	130.11	120.79
1	A	367	ARG	N-CA-C	5.23	117.78	111.40
1	A	309	GLU	CB-CA-C	-5.22	101.76	109.90
1	A	53	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	B	149	ASP	N-CA-C	-5.21	101.67	109.95
1	B	172	HIS	CA-C-N	5.20	131.07	121.70
1	B	172	HIS	C-N-CA	5.20	131.07	121.70
1	B	294	SER	CA-C-N	-5.20	113.17	121.02
1	B	294	SER	C-N-CA	-5.20	113.17	121.02
1	A	157	ALA	N-CA-C	-5.19	104.69	111.02
1	B	298	SER	CA-CB-OG	-5.17	100.75	111.10
1	A	131	GLN	O-C-N	5.17	127.61	122.03
1	B	21	PHE	CA-C-N	5.17	126.30	119.84
1	B	21	PHE	C-N-CA	5.17	126.30	119.84
1	B	369	GLU	CA-CB-CG	5.16	124.42	114.10
1	A	357	VAL	N-CA-CB	5.16	119.74	111.23
1	B	79	ARG	N-CA-C	-5.15	98.43	109.81
1	B	174	LEU	N-CA-C	-5.15	103.06	111.04
1	A	134	VAL	N-CA-C	-5.15	105.37	110.62
1	A	401	THR	CB-CA-C	5.15	118.12	109.89
1	B	383	THR	O-C-N	5.14	129.43	122.59
1	B	129	ALA	CA-C-N	-5.13	114.46	120.72
1	B	129	ALA	C-N-CA	-5.13	114.46	120.72
1	B	187	ARG	N-CA-CB	5.13	119.21	110.50
1	B	201	LEU	CD1-CG-CD2	-5.12	99.53	110.80
1	A	376	THR	N-CA-CB	-5.12	102.60	110.12
1	B	38	LEU	CB-CA-C	-5.12	102.79	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	LEU	CA-CB-CG	-5.12	98.40	116.30
1	A	409	VAL	CA-C-N	5.09	130.55	122.10
1	A	409	VAL	C-N-CA	5.09	130.55	122.10
1	A	207	GLY	N-CA-C	-5.07	101.17	113.18
1	B	136	GLU	CA-C-N	5.07	126.94	120.56
1	B	136	GLU	C-N-CA	5.07	126.94	120.56
1	A	264	LEU	O-C-N	5.06	127.50	122.03
1	B	42	ASP	CA-C-N	5.05	124.84	119.28
1	B	42	ASP	C-N-CA	5.05	124.84	119.28
1	B	100	ILE	CB-CA-C	-5.05	103.01	111.29
1	A	172	HIS	CB-CA-C	5.04	120.12	111.45
1	A	242	THR	N-CA-C	-5.03	105.50	111.69
1	B	251	ARG	N-CA-C	5.03	121.52	110.80
1	B	158	VAL	CB-CA-C	-5.02	105.47	112.04
1	B	64	VAL	N-CA-C	5.01	116.33	110.62

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	PRO	Peptide
1	A	186	SER	Peptide
1	A	23	ILE	Peptide
1	A	27	CYS	Peptide
1	A	296	ALA	Peptide
1	A	383	THR	Peptide
1	A	401	THR	Peptide
1	A	80	PRO	Peptide
1	A	97	ARG	Peptide
1	B	104	ALA	Peptide
1	B	146	GLY	Peptide
1	B	186	SER	Peptide
1	B	193	GLN	Peptide
1	B	248	ASN	Peptide
1	B	279	PRO	Peptide
1	B	303	VAL	Peptide
1	B	318	ASP	Peptide
1	B	381	VAL	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	3020	0	3005	547	0
1	B	2858	0	2870	481	0
2	A	43	0	30	18	0
2	B	43	0	30	26	0
3	A	35	0	0	11	0
3	B	22	0	0	2	0
All	All	6021	0	5935	1017	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 85.

All (1017) 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:229:LEU:HA	1:A:234:VAL:CB	1.07	1.52
1:A:24:GLN:HG2	1:A:33:ALA:CB	1.42	1.49
1:A:229:LEU:CA	1:A:234:VAL:CB	1.97	1.39
1:A:24:GLN:CG	1:A:33:ALA:HB1	1.57	1.33
1:A:80:PRO:O	1:A:301:LEU:HD13	1.28	1.33
1:B:172:HIS:CB	1:B:173:ASP:HB2	1.57	1.31
1:A:358:HIS:HB3	2:A:501:HEM:O1A	1.16	1.30
1:A:26:GLY:C	1:A:28:PRO:HD3	1.56	1.27
1:B:172:HIS:HB2	1:B:173:ASP:CB	1.64	1.25
1:A:235:THR:HG23	1:A:238:GLN:NE2	1.53	1.23
1:B:113:MET:SD	1:B:229:LEU:HD11	1.85	1.17
1:B:230:VAL:HG12	1:B:234:VAL:HG23	1.24	1.17
1:A:24:GLN:CG	1:A:33:ALA:CB	2.17	1.16
1:A:119:THR:HB	1:B:333:GLU:OE2	1.48	1.14
1:A:96:PHE:HD1	1:A:97:ARG:NH2	1.44	1.14
1:A:42:ASP:CB	1:A:45:ALA:HB2	1.79	1.12
1:A:221:ILE:O	1:A:225:VAL:HG13	1.49	1.13
1:A:19:ARG:HB2	1:A:47:VAL:HG22	1.25	1.12
1:B:231:PRO:HB3	1:B:232:GLY:HA3	1.33	1.10
1:B:23:ILE:HG23	1:B:32:PRO:HB3	1.12	1.09
1:A:97:ARG:NH1	1:A:97:ARG:HB2	1.69	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ALA:H	1:A:32:PRO:CD	1.61	1.07
1:B:158:VAL:HG11	1:B:258:ILE:HD13	1.31	1.07
1:B:137:ILE:O	1:B:141:MET:HG2	1.54	1.07
1:B:231:PRO:CB	1:B:232:GLY:HA3	1.78	1.07
1:A:127:ARG:HB3	1:A:128:PRO:HD3	1.32	1.06
1:A:24:GLN:HB2	1:A:33:ALA:HB2	1.39	1.04
1:A:42:ASP:HB2	1:A:45:ALA:CB	1.88	1.04
1:A:96:PHE:CD1	1:A:97:ARG:NH2	2.25	1.03
1:A:358:HIS:CB	2:A:501:HEM:O1A	2.07	1.03
1:A:97:ARG:HB2	1:A:97:ARG:CZ	1.86	1.02
1:A:189:SER:HB3	1:A:190:THR:C	1.84	1.01
1:B:179:ASP:O	1:B:183:ILE:HG12	1.59	1.01
1:A:181:THR:CG2	1:A:251:ARG:HD3	1.90	1.01
1:A:31:ALA:N	1:A:32:PRO:CD	2.19	1.01
1:B:335:PHE:HE1	1:B:348:ASN:HB2	1.24	1.01
1:A:74:SER:HB2	1:A:103:ASP:HB3	1.40	1.00
1:A:179:ASP:O	1:A:183:ILE:HG13	1.61	1.00
1:B:23:ILE:CG2	1:B:32:PRO:HB3	1.91	1.00
1:B:335:PHE:HZ	1:B:346:THR:HB	1.23	0.99
1:A:96:PHE:O	1:A:98:PRO:HD3	1.61	0.99
1:B:230:VAL:HA	1:B:231:PRO:O	1.63	0.99
1:A:19:ARG:HB2	1:A:47:VAL:CG2	1.91	0.98
1:A:235:THR:CG2	1:A:238:GLN:NE2	2.25	0.98
2:A:501:HEM:HH A	2:A:501:HEM:HBA1	1.43	0.97
1:A:96:PHE:HD1	1:A:97:ARG:HH21	1.07	0.97
1:B:230:VAL:HG12	1:B:234:VAL:CG2	1.95	0.97
1:A:31:ALA:H	1:A:32:PRO:HD3	1.29	0.96
1:A:19:ARG:HG3	1:A:47:VAL:HA	1.45	0.96
1:A:335:PHE:CE1	1:A:345:ARG:HG2	1.99	0.95
1:A:42:ASP:HB2	1:A:45:ALA:HB2	0.96	0.95
1:B:22:PRO:C	1:B:23:ILE:HG12	1.91	0.95
1:B:369:GLU:O	1:B:373:ALA:HB2	1.65	0.95
1:B:335:PHE:CZ	1:B:346:THR:HB	2.02	0.94
1:B:212:ARG:NH1	1:B:217:ARG:NH2	2.15	0.94
1:A:24:GLN:HA	1:A:24:GLN:OE1	1.67	0.94
1:A:74:SER:CB	1:A:103:ASP:HB3	1.97	0.93
1:B:175:GLU:HA	1:B:178:ARG:HB2	1.47	0.93
1:A:383:THR:OG1	1:A:385:ARG:NH2	2.01	0.93
1:B:82:PHE:CB	1:B:301:LEU:HD13	1.98	0.93
1:A:189:SER:HA	1:A:194:VAL:HG23	1.50	0.93
1:A:89:GLU:HA	1:A:90:GLN:HE21	1.31	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PRO:HA	1:A:410:THR:HG23	1.50	0.93
1:A:19:ARG:O	1:A:48:THR:OG1	1.84	0.93
1:A:368:LEU:O	1:A:372:VAL:HG22	1.69	0.92
1:A:97:ARG:HG2	1:A:245:ILE:HD11	1.51	0.92
1:A:117:ALA:O	1:A:122:ARG:HG2	1.68	0.92
1:A:43:PRO:HB3	1:A:60:ARG:HH21	1.33	0.92
1:A:229:LEU:C	1:A:229:LEU:HD23	1.93	0.92
1:B:385:ARG:O	1:B:409:VAL:HG12	1.70	0.92
1:A:19:ARG:CG	1:A:47:VAL:HA	1.99	0.92
1:A:80:PRO:O	1:A:301:LEU:CD1	2.18	0.92
1:A:113:MET:HG3	1:A:228:HIS:ND1	1.85	0.91
1:B:253:THR:HG22	2:B:501:HEM:HBB2	1.51	0.91
1:A:235:THR:HG23	1:A:238:GLN:HE21	1.33	0.91
1:A:270:GLU:O	1:A:273:ALA:HB3	1.70	0.91
1:A:82:PHE:O	1:A:83:PRO:C	2.11	0.91
1:A:96:PHE:O	1:A:97:ARG:C	2.15	0.90
1:A:335:PHE:CZ	1:A:345:ARG:HG2	2.07	0.90
1:A:354:GLY:HA3	1:A:359:GLN:HA	1.54	0.90
1:B:296:ALA:C	1:B:298:SER:H	1.79	0.90
1:B:383:THR:C	1:B:384:LEU:HD13	1.97	0.89
1:A:162:VAL:HG11	1:A:369:GLU:HG2	1.54	0.89
1:B:98:PRO:HD2	1:B:101:ARG:HB3	1.55	0.89
1:B:225:VAL:HG12	1:B:239:LEU:CD1	2.03	0.89
1:A:75:ALA:O	1:A:76:ASP:HB2	1.68	0.89
1:A:291:ARG:NH2	1:A:292:VAL:HG23	1.88	0.89
1:A:282:MET:HA	1:A:285:ALA:HB3	1.54	0.88
1:A:124:ARG:O	1:A:127:ARG:HB2	1.72	0.88
1:A:25:ARG:C	1:A:27:CYS:H	1.81	0.88
1:B:358:HIS:O	2:B:501:HEM:HAA1	1.73	0.88
1:A:21:PHE:HE1	1:A:50:PRO:CD	1.86	0.88
1:A:138:LEU:O	1:A:142:LEU:HD12	1.74	0.88
1:A:223:LYS:NZ	1:A:227:ASP:OD1	2.07	0.88
1:B:158:VAL:HG11	1:B:258:ILE:CD1	2.03	0.87
1:A:24:GLN:CB	1:A:33:ALA:HB2	2.02	0.87
1:B:363:GLN:HG3	1:B:364:HIS:N	1.85	0.87
1:A:58:VAL:HG21	1:A:67:LEU:CD2	2.04	0.86
1:A:189:SER:HB3	1:A:190:THR:CA	2.04	0.86
1:A:291:ARG:O	1:A:294:SER:HB3	1.75	0.86
1:A:82:PHE:O	1:A:83:PRO:O	1.95	0.85
1:B:23:ILE:HG23	1:B:32:PRO:CB	2.02	0.85
1:A:32:PRO:O	1:A:35:TYR:CD2	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PHE:CZ	1:A:362:GLY:HA2	2.11	0.85
1:A:180:VAL:O	1:A:184:SER:HB2	1.75	0.85
1:B:107:HIS:ND1	1:B:107:HIS:C	2.34	0.84
1:B:80:PRO:CB	1:B:303:VAL:HG23	2.07	0.84
1:A:90:GLN:HB3	1:A:92:ALA:O	1.78	0.84
1:B:196:GLU:O	1:B:200:GLY:N	2.10	0.84
1:A:149:ASP:OD2	1:A:152:SER:HB3	1.77	0.83
1:A:240:LEU:HD12	1:A:240:LEU:H	1.39	0.83
1:A:335:PHE:CD1	1:A:345:ARG:HD3	2.13	0.83
1:B:243:LEU:CD1	1:B:243:LEU:N	2.41	0.83
1:A:264:LEU:HD12	1:A:264:LEU:O	1.78	0.83
1:B:231:PRO:CB	1:B:232:GLY:CA	2.56	0.83
1:A:26:GLY:O	1:A:28:PRO:HD3	1.79	0.83
1:A:96:PHE:O	1:A:98:PRO:CD	2.26	0.83
1:A:367:ARG:O	1:A:371:GLU:HG2	1.79	0.83
1:B:20:ASP:CB	1:B:50:PRO:HD3	2.07	0.83
1:A:70:ASP:HB3	1:A:73:VAL:CG2	2.09	0.82
1:B:224:LEU:O	1:B:229:LEU:HB2	1.80	0.81
1:B:76:ASP:HA	1:B:101:ARG:O	1.81	0.81
1:B:350:HIS:CG	1:B:350:HIS:O	2.32	0.81
1:A:229:LEU:HD23	1:A:229:LEU:O	1.78	0.81
1:A:58:VAL:HG21	1:A:67:LEU:HD22	1.60	0.81
1:A:19:ARG:H	1:A:19:ARG:HD2	1.44	0.81
1:B:231:PRO:HB3	1:B:232:GLY:CA	2.10	0.81
1:A:295:VAL:HG12	1:A:402:PHE:HD2	1.45	0.81
1:B:230:VAL:HA	1:B:231:PRO:C	2.06	0.80
1:A:118:PHE:CE1	1:A:362:GLY:HA2	2.16	0.80
1:B:369:GLU:O	1:B:373:ALA:CB	2.28	0.80
1:A:31:ALA:N	1:A:32:PRO:HD2	1.97	0.80
1:A:21:PHE:HE1	1:A:50:PRO:HD2	1.44	0.80
1:B:260:LEU:HG	1:B:404:LEU:HD21	1.62	0.80
1:B:118:PHE:HE2	2:B:501:HEM:HBC2	1.47	0.79
1:A:41:ASP:O	1:A:43:PRO:HD3	1.83	0.79
1:B:335:PHE:CE1	1:B:348:ASN:HB2	2.15	0.79
1:A:113:MET:HG3	1:A:228:HIS:CE1	2.17	0.79
1:A:97:ARG:NH1	1:A:97:ARG:CB	2.46	0.79
1:A:164:CYS:SG	1:A:169:ILE:HB	2.23	0.79
1:B:119:THR:O	1:B:123:VAL:CG1	2.31	0.79
1:A:93:GLY:C	1:A:95:ARG:H	1.92	0.78
1:A:112:ARG:HB2	1:A:112:ARG:HH11	1.48	0.78
1:B:18:PRO:HB3	1:B:48:THR:HG23	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:O	1:B:158:VAL:CG1	2.31	0.78
1:B:155:ALA:HA	1:B:158:VAL:HG12	1.65	0.78
1:B:80:PRO:HA	1:B:303:VAL:CG2	2.13	0.78
1:B:158:VAL:CG1	1:B:258:ILE:HD13	2.13	0.78
1:A:138:LEU:HD23	1:A:141:MET:HG3	1.66	0.77
1:A:31:ALA:HB2	3:A:601:HOH:O	1.84	0.77
1:B:156:ASN:HA	1:B:255:THR:CG2	2.14	0.77
1:A:316:PRO:HB2	1:A:319:ASP:OD1	1.84	0.77
1:B:72:ARG:HH21	1:B:308:ILE:HA	1.48	0.77
1:A:112:ARG:HH11	1:A:112:ARG:CB	1.97	0.77
1:A:68:LEU:HD23	1:A:355:TYR:O	1.85	0.77
1:B:225:VAL:CG2	1:B:226:THR:N	2.47	0.77
1:B:229:LEU:HD23	1:B:234:VAL:HG11	1.66	0.77
1:B:158:VAL:CG1	1:B:258:ILE:CD1	2.63	0.77
1:B:76:ASP:CA	1:B:101:ARG:O	2.34	0.76
1:A:266:LEU:HD21	1:A:384:LEU:HD23	1.67	0.76
1:B:155:ALA:O	1:B:158:VAL:HG12	1.85	0.76
1:A:151:VAL:HA	1:A:155:ALA:HB3	1.66	0.76
1:B:316:PRO:HD2	1:B:319:ASP:OD2	1.84	0.76
1:A:235:THR:O	1:A:238:GLN:N	2.17	0.76
1:B:97:ARG:N	1:B:98:PRO:HD3	2.01	0.76
1:B:243:LEU:HD13	1:B:243:LEU:H	1.51	0.76
1:A:117:ALA:O	1:A:122:ARG:HD2	1.85	0.76
1:A:229:LEU:C	1:A:229:LEU:CD2	2.59	0.75
1:B:76:ASP:N	1:B:101:ARG:O	2.18	0.75
1:A:229:LEU:HD12	1:A:239:LEU:HD22	1.68	0.75
1:B:120:VAL:O	1:B:124:ARG:HB2	1.85	0.75
1:B:204:LEU:O	1:B:208:LEU:HG	1.86	0.75
1:A:117:ALA:O	1:A:122:ARG:CG	2.34	0.75
1:B:113:MET:CE	1:B:229:LEU:HD11	2.17	0.75
1:A:333:GLU:N	1:B:121:ARG:HE	1.84	0.75
1:A:181:THR:HG22	1:A:251:ARG:HD3	1.67	0.75
1:B:194:VAL:CG1	1:B:195:SER:N	2.49	0.75
1:B:260:LEU:HD23	1:B:263:LEU:HD23	1.66	0.74
1:A:368:LEU:O	1:A:372:VAL:CG2	2.34	0.74
1:A:235:THR:OG1	1:A:238:GLN:HG3	1.87	0.74
1:B:35:TYR:O	1:B:38:LEU:HB2	1.85	0.74
1:B:82:PHE:CB	1:B:301:LEU:CD1	2.65	0.74
1:A:147:PRO:CA	1:A:410:THR:HG23	2.17	0.74
1:B:123:VAL:HB	1:B:365:LEU:HD12	1.69	0.74
1:A:357:VAL:HG13	1:B:69:SER:OG	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PRO:HD2	1:B:101:ARG:CB	2.17	0.74
1:B:102:THR:O	1:B:107:HIS:HB3	1.87	0.74
1:B:363:GLN:CG	1:B:364:HIS:N	2.50	0.74
1:B:175:GLU:O	1:B:179:ASP:HB2	1.87	0.74
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.53	0.74
1:B:107:HIS:C	1:B:107:HIS:HD1	1.96	0.73
1:B:214:GLU:O	1:B:216:PRO:HD3	1.87	0.73
1:A:410:THR:C	1:A:411:TRP:CD1	2.66	0.73
1:B:119:THR:O	1:B:123:VAL:HG13	1.87	0.73
1:A:362:GLY:HA3	2:A:501:HEM:C4C	2.24	0.73
1:B:386:LEU:HD12	1:B:386:LEU:N	2.04	0.73
1:A:264:LEU:HD12	1:A:264:LEU:C	2.12	0.73
1:B:212:ARG:HH12	1:B:217:ARG:NH2	1.84	0.73
1:A:19:ARG:HD2	1:A:19:ARG:N	2.03	0.73
1:A:295:VAL:HG12	1:A:402:PHE:CD2	2.24	0.73
1:B:22:PRO:O	1:B:23:ILE:HG12	1.87	0.73
1:A:118:PHE:O	1:A:119:THR:O	2.06	0.72
1:A:147:PRO:HA	1:A:410:THR:CG2	2.19	0.72
1:A:53:ARG:HH22	1:A:82:PHE:HA	1.53	0.72
2:A:501:HEM:HHA	2:A:501:HEM:CBA	2.17	0.72
1:B:230:VAL:CA	1:B:231:PRO:O	2.35	0.72
1:A:141:MET:HE2	1:A:141:MET:HA	1.71	0.72
1:A:370:LEU:HD23	1:A:374:LEU:HD12	1.71	0.72
1:B:212:ARG:NH1	1:B:217:ARG:HH22	1.86	0.72
1:B:347:ASP:OD2	1:B:350:HIS:HB3	1.90	0.72
1:B:383:THR:O	1:B:384:LEU:HD13	1.90	0.72
1:A:299:ILE:O	1:A:300:PRO:O	2.06	0.72
1:A:351:VAL:O	1:A:353:PHE:O	2.07	0.72
1:B:164:CYS:SG	1:B:169:ILE:HB	2.29	0.72
1:B:149:ASP:OD1	1:B:406:GLU:HB2	1.90	0.72
1:B:111:ARG:NH1	1:B:357:VAL:O	2.23	0.71
1:B:340:ARG:HG2	1:B:342:ASP:HB2	1.71	0.71
1:A:164:CYS:SG	1:A:174:LEU:HD22	2.30	0.71
1:A:123:VAL:HG22	1:A:365:LEU:HD13	1.71	0.71
1:B:300:PRO:HA	2:B:501:HEM:O1A	1.89	0.71
1:A:229:LEU:HD11	1:A:236:THR:HG22	1.72	0.71
1:A:309:GLU:HA	1:A:314:THR:HG22	1.71	0.71
1:A:117:ALA:O	1:A:122:ARG:CD	2.39	0.71
1:B:80:PRO:HB3	1:B:303:VAL:CG2	2.21	0.70
1:B:149:ASP:HB2	1:B:408:MET:HG3	1.71	0.70
1:B:381:VAL:CG1	1:B:384:LEU:HD11	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:CG	1:A:33:ALA:HB2	2.11	0.70
1:A:254:THR:HG22	2:A:501:HEM:CAB	2.21	0.70
1:B:78:ARG:HD2	1:B:303:VAL:HG11	1.72	0.70
1:A:230:VAL:HB	1:A:231:PRO:HD3	1.73	0.70
1:B:34:GLU:O	1:B:37:ALA:HB3	1.91	0.70
1:B:132:ALA:O	1:B:135:ASP:HB2	1.90	0.70
1:B:148:VAL:O	1:B:408:MET:HB3	1.91	0.70
1:A:374:LEU:O	1:A:378:LEU:HG	1.91	0.70
1:B:353:PHE:HE1	2:B:501:HEM:C3B	2.09	0.70
1:A:254:THR:O	1:A:257:MET:N	2.24	0.70
1:A:126:MET:HA	3:A:620:HOH:O	1.92	0.70
1:A:240:LEU:HD12	1:A:240:LEU:N	2.05	0.69
1:B:300:PRO:O	1:B:322:ILE:HG23	1.92	0.69
1:B:76:ASP:HA	1:B:101:ARG:C	2.16	0.69
1:B:260:LEU:HD21	1:B:404:LEU:HD11	1.74	0.69
1:A:281:LEU:O	1:A:282:MET:C	2.35	0.69
1:A:358:HIS:ND1	2:A:501:HEM:O1D	2.22	0.69
1:B:271:LEU:HA	1:B:274:GLU:OE2	1.92	0.69
1:A:25:ARG:NE	1:A:402:PHE:CE2	2.54	0.69
1:A:25:ARG:HD2	3:A:601:HOH:O	1.92	0.69
1:B:18:PRO:O	1:B:48:THR:OG1	2.08	0.69
1:B:68:LEU:HD22	1:B:355:TYR:O	1.91	0.69
1:B:229:LEU:HB3	1:B:234:VAL:CG2	2.22	0.69
1:B:238:GLN:HA	1:B:241:SER:OG	1.92	0.69
1:B:167:LEU:N	1:B:167:LEU:CD1	2.56	0.69
1:B:231:PRO:HB2	1:B:232:GLY:HA3	1.72	0.69
1:B:278:ASP:OD2	1:B:280:ASP:HB2	1.92	0.69
1:A:24:GLN:HB3	1:A:25:ARG:C	2.17	0.68
1:A:21:PHE:CE1	1:A:50:PRO:HD2	2.27	0.68
1:A:25:ARG:C	1:A:27:CYS:N	2.44	0.68
1:A:173:ASP:OD1	3:A:626:HOH:O	2.10	0.68
1:B:149:ASP:HB2	1:B:408:MET:CG	2.22	0.68
1:A:19:ARG:HG2	1:A:48:THR:H	1.59	0.68
1:A:286:VAL:HG23	1:A:370:LEU:CD2	2.22	0.68
1:A:49:LEU:O	1:A:52:ARG:N	2.27	0.68
1:B:395:VAL:O	1:B:405:GLU:HG2	1.94	0.68
1:B:138:LEU:HD23	1:B:141:MET:HB2	1.74	0.68
1:B:304:ALA:HB2	1:B:315:VAL:CG1	2.24	0.68
1:A:65:ARG:NH1	1:A:355:TYR:CE2	2.61	0.68
1:B:259:ALA:HB1	1:B:404:LEU:HD23	1.76	0.68
1:A:43:PRO:CD	1:A:44:VAL:H	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:PRO:C	1:B:121:ARG:HE	2.02	0.67
1:B:29:PHE:CD1	1:B:30:ALA:N	2.59	0.67
1:A:25:ARG:HH21	1:A:30:ALA:HA	1.59	0.67
1:A:164:CYS:HA	1:A:169:ILE:HD12	1.76	0.67
1:B:156:ASN:HA	1:B:255:THR:HG21	1.75	0.67
1:A:150:LEU:N	1:A:407:LEU:O	2.25	0.67
1:B:149:ASP:C	1:B:149:ASP:OD2	2.37	0.67
1:B:195:SER:O	1:B:199:GLY:N	2.24	0.67
1:B:225:VAL:HG23	1:B:226:THR:N	2.08	0.67
1:B:80:PRO:HB3	1:B:303:VAL:HG23	1.76	0.67
1:B:179:ASP:O	1:B:182:ARG:HB3	1.95	0.67
1:B:172:HIS:CA	1:B:173:ASP:HB2	2.25	0.67
1:A:62:ASP:HA	1:A:65:ARG:HG2	1.75	0.67
1:B:150:LEU:O	1:B:155:ALA:N	2.24	0.67
1:B:164:CYS:SG	1:B:177:PHE:CD1	2.89	0.66
1:A:25:ARG:O	1:A:27:CYS:N	2.27	0.66
1:B:99:PHE:HE2	1:B:110:TYR:CB	2.09	0.66
1:B:282:MET:O	1:B:285:ALA:HB3	1.95	0.66
1:A:56:TRP:O	1:A:321:VAL:HA	1.95	0.66
1:A:363:GLN:HA	1:A:366:ALA:HB3	1.78	0.66
1:A:89:GLU:HA	1:A:90:GLN:NE2	2.09	0.66
1:A:205:LEU:O	1:A:209:VAL:HG23	1.95	0.66
1:A:80:PRO:HA	1:A:301:LEU:HD22	1.76	0.66
1:B:260:LEU:HG	1:B:404:LEU:CD2	2.25	0.66
1:B:346:THR:C	1:B:348:ASN:H	2.02	0.66
1:A:18:PRO:N	1:A:19:ARG:HH11	1.94	0.66
1:A:88:GLY:C	1:A:89:GLU:HG2	2.21	0.66
1:B:18:PRO:HB3	1:B:48:THR:CG2	2.25	0.66
1:B:194:VAL:HG13	1:B:195:SER:N	2.10	0.66
1:A:270:GLU:H	1:A:270:GLU:CD	2.02	0.66
1:B:80:PRO:CB	1:B:303:VAL:CG2	2.74	0.66
1:B:105:PRO:C	1:B:107:HIS:N	2.52	0.66
1:B:186:SER:OG	1:B:187:ARG:N	2.17	0.66
1:A:254:THR:HG22	2:A:501:HEM:HAB	1.78	0.65
1:B:358:HIS:O	2:B:501:HEM:CAA	2.44	0.65
1:B:38:LEU:O	1:B:42:ASP:O	2.13	0.65
1:B:383:THR:CG2	1:B:384:LEU:N	2.58	0.65
1:A:112:ARG:CB	1:A:112:ARG:NH1	2.59	0.65
1:B:295:VAL:O	1:B:295:VAL:HG13	1.95	0.65
1:A:18:PRO:CD	1:A:19:ARG:NH1	2.60	0.65
1:B:243:LEU:N	1:B:243:LEU:HD12	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:CZ	1:A:97:ARG:CB	2.70	0.65
1:B:296:ALA:O	1:B:297:ASP:HB3	1.96	0.65
1:A:229:LEU:C	1:A:234:VAL:CB	2.68	0.65
1:A:387:ALA:N	1:A:408:MET:O	2.30	0.65
1:B:80:PRO:CA	1:B:303:VAL:CG2	2.75	0.65
1:B:171:ARG:HA	1:B:174:LEU:HB2	1.77	0.65
1:A:30:ALA:HB1	1:A:31:ALA:HB2	1.77	0.65
1:A:21:PHE:CE1	1:A:50:PRO:CD	2.76	0.64
1:A:25:ARG:NH2	1:A:30:ALA:HA	2.11	0.64
1:A:269:PRO:HA	1:A:272:PRO:HG2	1.80	0.64
1:A:301:LEU:HD23	1:A:302:ARG:C	2.21	0.64
1:B:155:ALA:CA	1:B:158:VAL:HG12	2.27	0.64
1:B:167:LEU:O	1:B:219:ASP:HB2	1.97	0.64
1:A:74:SER:HB3	1:A:103:ASP:HB3	1.80	0.64
1:A:385:ARG:HG2	3:A:604:HOH:O	1.97	0.64
1:A:96:PHE:O	1:A:98:PRO:N	2.31	0.64
1:A:96:PHE:CG	1:A:97:ARG:N	2.65	0.64
1:B:296:ALA:C	1:B:298:SER:N	2.48	0.64
1:A:49:LEU:HG	1:A:82:PHE:HD2	1.63	0.64
1:A:366:ALA:O	1:A:370:LEU:HB2	1.98	0.64
1:A:72:ARG:NH1	1:B:104:ALA:HB3	2.13	0.64
1:B:271:LEU:O	1:B:274:GLU:HB2	1.98	0.64
1:B:343:PHE:HD1	1:B:343:PHE:N	1.95	0.64
1:B:243:LEU:N	1:B:243:LEU:HD13	2.11	0.63
1:B:343:PHE:N	1:B:343:PHE:CD1	2.66	0.63
1:B:80:PRO:HA	1:B:303:VAL:HG21	1.79	0.63
1:B:306:GLU:OE1	1:B:307:ASP:N	2.30	0.63
1:A:286:VAL:CG1	1:A:287:ASP:N	2.60	0.63
1:B:39:ARG:O	1:B:60:ARG:NH2	2.31	0.63
1:A:286:VAL:HG23	1:A:370:LEU:HD22	1.78	0.63
1:A:335:PHE:CE1	1:A:345:ARG:CG	2.80	0.63
1:B:269:PRO:O	1:B:272:PRO:HD2	1.98	0.63
1:A:130:VAL:O	1:A:134:VAL:HG23	1.98	0.63
1:A:102:THR:HG21	1:A:106:GLU:HG2	1.80	0.63
1:A:257:MET:O	1:A:261:SER:OG	2.11	0.63
1:B:167:LEU:N	1:B:167:LEU:HD13	2.13	0.63
1:B:281:LEU:HD13	1:B:343:PHE:HD2	1.63	0.63
1:A:93:GLY:C	1:A:95:ARG:N	2.57	0.63
1:A:111:ARG:O	1:A:114:LEU:HB3	1.98	0.63
1:A:387:ALA:H	1:A:409:VAL:HA	1.63	0.63
1:B:205:LEU:O	1:B:208:LEU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG12	1:A:56:TRP:CE3	2.35	0.62
1:B:99:PHE:HB2	1:B:245:ILE:HD13	1.81	0.62
1:B:263:LEU:HG	1:B:264:LEU:N	2.04	0.62
1:A:147:PRO:HG3	1:A:410:THR:HG21	1.80	0.62
1:B:107:HIS:NE2	1:B:357:VAL:HG11	2.13	0.62
1:B:133:ARG:O	1:B:137:ILE:HG13	1.97	0.62
1:B:335:PHE:CZ	1:B:346:THR:CB	2.79	0.62
1:B:260:LEU:HD23	1:B:263:LEU:CD2	2.29	0.62
1:A:119:THR:HB	1:B:333:GLU:CD	2.23	0.62
1:A:279:PRO:O	1:A:282:MET:HE1	1.99	0.62
1:B:205:LEU:O	1:B:206:GLY:C	2.42	0.62
1:B:286:VAL:HG11	1:B:370:LEU:HB2	1.80	0.62
1:A:390:ARG:O	1:A:393:VAL:HG12	1.99	0.62
1:B:119:THR:O	1:B:123:VAL:HG12	1.99	0.62
1:A:291:ARG:HD3	1:A:348:ASN:ND2	2.15	0.62
1:B:118:PHE:CE2	2:B:501:HEM:HBC2	2.34	0.62
1:A:18:PRO:HD2	1:A:19:ARG:NH1	2.14	0.62
1:A:64:VAL:HG13	1:A:323:ALA:HB1	1.82	0.62
1:B:65:ARG:HG3	1:B:355:TYR:CD2	2.34	0.62
1:B:102:THR:O	1:B:107:HIS:CB	2.47	0.62
1:B:162:VAL:HG11	1:B:369:GLU:CD	2.25	0.62
1:B:353:PHE:CE1	2:B:501:HEM:C2B	2.88	0.62
1:A:73:VAL:O	1:A:302:ARG:HB3	2.00	0.61
1:A:189:SER:HB3	1:A:190:THR:HA	1.81	0.61
1:B:225:VAL:HG12	1:B:239:LEU:HD13	1.83	0.61
1:A:25:ARG:HH21	1:A:25:ARG:HG2	1.64	0.61
1:A:70:ASP:HB3	1:A:73:VAL:HG21	1.81	0.61
1:B:110:TYR:O	1:B:113:MET:HB2	2.00	0.61
1:B:157:ALA:O	1:B:178:ARG:NH1	2.32	0.61
1:B:99:PHE:HE2	1:B:110:TYR:HB3	1.65	0.61
1:A:131:GLN:OE1	1:A:372:VAL:HG12	2.01	0.61
1:B:155:ALA:HA	1:B:158:VAL:CG1	2.30	0.61
1:A:31:ALA:CB	3:A:601:HOH:O	2.46	0.61
1:B:340:ARG:CG	1:B:342:ASP:HB2	2.29	0.61
1:A:27:CYS:N	1:A:28:PRO:HD3	1.95	0.61
1:A:295:VAL:HG12	1:A:402:PHE:HB3	1.82	0.61
1:B:155:ALA:C	1:B:158:VAL:HG12	2.25	0.61
1:B:149:ASP:OD2	1:B:152:SER:HB2	2.01	0.61
1:B:278:ASP:C	1:B:280:ASP:H	2.09	0.61
1:A:80:PRO:C	1:A:301:LEU:HD13	2.23	0.60
1:A:229:LEU:CB	1:A:234:VAL:CB	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HD2	1:A:91:GLU:HG3	1.83	0.60
1:A:381:VAL:N	1:A:382:PRO:HD3	2.15	0.60
1:B:80:PRO:CA	1:B:303:VAL:HG23	2.31	0.60
1:B:225:VAL:HG12	1:B:239:LEU:HD11	1.83	0.60
1:A:173:ASP:OD1	1:A:173:ASP:N	2.33	0.60
1:B:113:MET:HE2	1:B:229:LEU:HD11	1.83	0.60
1:A:184:SER:OG	1:A:198:LEU:CD1	2.50	0.60
1:B:72:ARG:NH2	1:B:308:ILE:HA	2.17	0.60
1:A:97:ARG:HG2	1:A:245:ILE:CD1	2.27	0.60
1:A:271:LEU:O	1:A:272:PRO:C	2.45	0.60
1:A:127:ARG:CB	1:A:128:PRO:HD3	2.17	0.60
1:B:155:ALA:O	1:B:158:VAL:HG13	1.99	0.60
1:A:380:ARG:C	1:A:382:PRO:HD3	2.27	0.60
1:B:199:GLY:O	1:B:200:GLY:C	2.44	0.60
1:B:230:VAL:CG1	1:B:234:VAL:CG2	2.77	0.60
1:A:189:SER:HB3	1:A:191:ALA:N	2.16	0.60
1:A:286:VAL:CG2	1:A:370:LEU:HB3	2.31	0.60
1:B:107:HIS:CG	1:B:108:THR:N	2.70	0.60
1:B:151:VAL:O	1:B:156:ASN:HB2	2.00	0.60
1:B:271:LEU:HB2	1:B:272:PRO:HD3	1.82	0.60
1:A:74:SER:HB2	1:A:103:ASP:CB	2.23	0.59
1:B:335:PHE:HZ	1:B:346:THR:CB	2.06	0.59
1:B:126:MET:O	1:B:127:ARG:C	2.43	0.59
1:A:181:THR:HG23	1:A:251:ARG:HD3	1.83	0.59
1:B:195:SER:O	1:B:198:LEU:HB3	2.02	0.59
1:A:113:MET:HE1	1:A:233:ASN:HD21	1.67	0.59
1:A:213:ARG:CZ	1:A:230:VAL:HG22	2.32	0.59
1:A:249:ALA:HB3	2:A:501:HEM:CBC	2.33	0.59
1:A:271:LEU:HD12	1:A:343:PHE:CE2	2.38	0.59
1:A:370:LEU:HD23	1:A:374:LEU:CD1	2.31	0.59
1:A:371:GLU:O	1:A:375:GLU:HB2	2.01	0.59
1:B:187:ARG:N	1:B:187:ARG:HD2	2.17	0.59
1:B:225:VAL:HG22	1:B:226:THR:H	1.68	0.59
1:B:281:LEU:O	1:B:282:MET:C	2.45	0.59
1:A:240:LEU:H	1:A:240:LEU:CD1	2.15	0.59
1:A:282:MET:O	1:A:283:PRO:C	2.44	0.59
1:B:122:ARG:O	1:B:125:ALA:HB3	2.03	0.59
1:B:253:THR:CG2	2:B:501:HEM:HBB2	2.30	0.59
1:B:229:LEU:HB3	1:B:234:VAL:HG21	1.83	0.59
1:A:24:GLN:HG2	1:A:33:ALA:HB1	0.65	0.59
1:A:278:ASP:C	1:A:278:ASP:OD1	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:O	1:B:212:ARG:N	2.27	0.59
1:B:228:HIS:O	1:B:229:LEU:HD12	2.01	0.59
1:B:291:ARG:HG2	1:B:291:ARG:NH1	2.17	0.59
1:B:172:HIS:HB2	1:B:173:ASP:HB2	0.69	0.59
1:B:386:LEU:HD12	1:B:386:LEU:H	1.68	0.59
1:A:66:GLU:OE2	1:B:115:LEU:HD11	2.03	0.58
1:A:384:LEU:HA	1:A:410:THR:O	2.03	0.58
1:B:76:ASP:HB3	1:B:102:THR:HA	1.85	0.58
1:A:335:PHE:HD2	1:A:347:ASP:HB3	1.68	0.58
1:B:228:HIS:HB3	1:B:229:LEU:HD13	1.85	0.58
1:B:381:VAL:HG13	1:B:384:LEU:HD11	1.84	0.58
1:A:43:PRO:HB3	1:A:60:ARG:NH2	2.13	0.58
1:B:135:ASP:O	1:B:139:ASP:HB2	2.04	0.58
1:B:126:MET:CE	1:B:365:LEU:HD11	2.33	0.58
1:B:295:VAL:O	1:B:295:VAL:CG1	2.50	0.58
1:A:18:PRO:N	1:A:19:ARG:HD2	2.18	0.58
1:B:346:THR:O	1:B:348:ASN:N	2.21	0.58
1:B:289:LEU:O	1:B:293:LEU:HB2	2.04	0.58
1:A:286:VAL:CG2	1:A:370:LEU:HD22	2.34	0.58
1:A:326:ALA:O	1:A:329:ASN:N	2.36	0.58
1:B:78:ARG:HD2	1:B:303:VAL:CG1	2.32	0.58
1:B:303:VAL:HG22	1:B:319:ASP:O	2.03	0.58
1:A:24:GLN:N	1:A:25:ARG:HA	2.19	0.58
1:A:42:ASP:OD1	1:A:42:ASP:N	2.36	0.58
1:A:379:ARG:HG2	1:A:380:ARG:HG2	1.86	0.58
1:B:31:ALA:HB1	1:B:32:PRO:CD	2.34	0.58
1:A:18:PRO:CD	1:A:19:ARG:HH11	2.17	0.57
1:A:53:ARG:NH1	1:A:91:GLU:OE2	2.37	0.57
1:B:255:THR:O	1:B:256:SER:C	2.47	0.57
1:A:387:ALA:N	1:A:409:VAL:HA	2.19	0.57
1:A:326:ALA:O	1:A:327:GLY:C	2.44	0.57
1:B:281:LEU:HD13	1:B:343:PHE:CD2	2.39	0.57
1:B:114:LEU:C	1:B:116:PRO:HD2	2.29	0.57
1:A:49:LEU:C	1:A:51:THR:H	2.13	0.57
1:B:242:THR:O	1:B:243:LEU:C	2.46	0.57
1:B:381:VAL:HG11	1:B:384:LEU:HD11	1.87	0.57
1:A:43:PRO:HG2	1:A:44:VAL:N	2.19	0.57
1:A:113:MET:HA	1:A:228:HIS:CE1	2.40	0.57
1:B:221:ILE:O	1:B:225:VAL:HG13	2.05	0.57
1:B:211:GLU:O	1:B:214:GLU:N	2.35	0.57
1:B:130:VAL:HG21	1:B:368:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLY:CA	2:B:501:HEM:C2C	2.88	0.57
1:A:175:GLU:C	1:A:177:PHE:N	2.62	0.57
1:B:278:ASP:OD2	1:B:280:ASP:CB	2.52	0.57
1:B:301:LEU:O	1:B:302:ARG:HG3	2.05	0.57
1:A:27:CYS:O	1:A:29:PHE:O	2.24	0.56
1:A:249:ALA:HB1	2:A:501:HEM:C4C	2.39	0.56
1:A:298:SER:C	1:A:299:ILE:O	2.41	0.56
1:A:97:ARG:HB3	1:A:98:PRO:CA	2.33	0.56
1:A:252:GLU:OE1	1:A:401:THR:HG23	2.05	0.56
1:B:99:PHE:HZ	1:B:111:ARG:HA	1.70	0.56
1:B:118:PHE:CZ	1:B:166:LEU:HD21	2.40	0.56
1:A:65:ARG:HB2	1:A:355:TYR:CD2	2.40	0.56
1:B:150:LEU:C	1:B:152:SER:N	2.61	0.56
1:A:232:GLY:C	1:A:234:VAL:H	2.13	0.56
1:A:41:ASP:O	1:A:43:PRO:CD	2.54	0.56
1:A:103:ASP:OD1	1:A:103:ASP:N	2.33	0.56
1:B:252:GLU:O	1:B:252:GLU:HG3	2.05	0.56
1:A:270:GLU:O	1:A:273:ALA:CB	2.47	0.56
1:B:229:LEU:HB3	1:B:234:VAL:HG22	1.88	0.56
1:B:105:PRO:C	1:B:107:HIS:H	2.14	0.55
1:A:184:SER:OG	1:A:198:LEU:HD11	2.05	0.55
1:A:235:THR:CG2	1:A:238:GLN:CD	2.79	0.55
1:A:286:VAL:HG21	1:A:370:LEU:HB3	1.87	0.55
2:A:501:HEM:HBA1	2:A:501:HEM:CHA	2.23	0.55
1:A:133:ARG:O	1:A:137:ILE:HG23	2.07	0.55
1:A:303:VAL:HA	1:A:319:ASP:O	2.07	0.55
1:A:381:VAL:CG2	1:A:381:VAL:O	2.54	0.55
1:B:279:PRO:O	1:B:282:MET:HE2	2.06	0.55
1:B:281:LEU:O	1:B:285:ALA:HB2	2.06	0.55
1:A:24:GLN:N	1:A:25:ARG:CA	2.64	0.55
1:A:291:ARG:HD3	1:A:348:ASN:HD21	1.72	0.55
1:A:384:LEU:HB2	1:A:411:TRP:HD1	1.70	0.55
1:A:230:VAL:CB	1:A:231:PRO:HD3	2.32	0.55
1:B:44:VAL:CG2	1:B:310:LEU:HD23	2.36	0.55
1:B:149:ASP:HA	1:B:408:MET:HA	1.88	0.55
1:B:167:LEU:HD13	1:B:167:LEU:H	1.70	0.55
1:A:24:GLN:CB	1:A:33:ALA:CB	2.69	0.55
1:A:24:GLN:HB3	1:A:26:GLY:N	2.21	0.55
1:A:25:ARG:NE	1:A:402:PHE:CZ	2.74	0.55
1:A:266:LEU:HD21	1:A:384:LEU:CD2	2.36	0.55
1:A:74:SER:CB	1:A:103:ASP:CB	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:O	1:A:184:SER:CB	2.51	0.55
1:A:189:SER:CB	1:A:190:THR:CA	2.82	0.55
1:A:301:LEU:HD21	1:A:320:GLY:HA2	1.89	0.55
1:B:297:ASP:OD1	1:B:326:ALA:HB3	2.06	0.55
1:A:109:ARG:O	1:A:113:MET:HB2	2.07	0.55
1:B:250:GLY:HA2	2:B:501:HEM:C2C	2.42	0.55
1:A:236:THR:O	1:A:240:LEU:HD13	2.06	0.55
1:A:43:PRO:CG	1:A:44:VAL:N	2.69	0.55
1:B:23:ILE:HD12	1:B:32:PRO:HG3	1.87	0.55
1:B:243:LEU:CD1	1:B:243:LEU:H	2.10	0.55
1:A:24:GLN:CB	1:A:25:ARG:CA	2.85	0.54
1:A:43:PRO:CG	1:A:44:VAL:H	2.19	0.54
1:A:56:TRP:N	1:A:320:GLY:O	2.22	0.54
1:B:78:ARG:O	1:B:79:ARG:HG3	2.07	0.54
1:A:94:ALA:O	1:A:95:ARG:C	2.50	0.54
1:A:150:LEU:HD21	1:A:262:THR:HG21	1.89	0.54
1:A:286:VAL:CG1	1:A:287:ASP:H	2.20	0.54
1:A:62:ASP:C	1:B:112:ARG:HH22	2.15	0.54
1:A:97:ARG:CB	1:A:97:ARG:HH11	2.17	0.54
1:A:354:GLY:C	1:A:359:GLN:HB2	2.33	0.54
1:A:286:VAL:HG12	1:A:287:ASP:H	1.72	0.54
1:A:147:PRO:CB	1:A:410:THR:HG23	2.38	0.54
1:B:177:PHE:HA	1:B:180:VAL:HG22	1.90	0.54
1:A:82:PHE:C	1:A:83:PRO:O	2.50	0.54
1:A:293:LEU:O	1:A:294:SER:C	2.50	0.54
1:B:105:PRO:O	1:B:106:GLU:C	2.50	0.54
1:B:296:ALA:HB1	1:B:299:ILE:HG22	1.90	0.54
1:B:383:THR:HG22	1:B:384:LEU:N	2.21	0.54
1:B:394:VAL:HG13	1:B:395:VAL:O	2.07	0.54
1:B:47:VAL:HG13	1:B:55:ALA:O	2.08	0.54
1:A:25:ARG:NH2	1:A:30:ALA:CA	2.71	0.54
1:A:118:PHE:O	1:A:119:THR:C	2.49	0.54
1:A:257:MET:SD	1:A:293:LEU:HD12	2.47	0.54
1:B:140:GLY:O	1:B:143:ALA:N	2.41	0.54
1:B:230:VAL:HB	1:B:231:PRO:O	2.08	0.54
1:A:102:THR:HB	1:A:107:HIS:HB2	1.90	0.53
1:A:145:GLY:O	1:A:146:GLY:O	2.26	0.53
1:B:72:ARG:O	1:B:308:ILE:HD13	2.08	0.53
1:A:122:ARG:HA	3:A:621:HOH:O	2.07	0.53
1:A:286:VAL:HG13	1:A:287:ASP:N	2.21	0.53
1:B:118:PHE:HB3	1:B:361:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:HIS:C	1:A:174:LEU:H	2.16	0.53
1:A:242:THR:O	1:A:246:THR:N	2.39	0.53
1:B:225:VAL:CG2	1:B:226:THR:H	2.19	0.53
1:A:269:PRO:HG2	1:A:270:GLU:OE2	2.08	0.53
1:B:271:LEU:HD22	1:B:343:PHE:CE1	2.43	0.53
1:A:26:GLY:O	1:A:27:CYS:HB3	2.08	0.53
1:B:356:GLY:C	1:B:358:HIS:N	2.65	0.53
1:A:32:PRO:O	1:A:33:ALA:HB3	2.06	0.53
1:B:70:ASP:OD1	1:B:72:ARG:HG3	2.09	0.53
1:A:112:ARG:NH1	1:A:112:ARG:HB3	2.24	0.53
1:A:52:ARG:NH1	3:A:608:HOH:O	2.41	0.53
1:A:112:ARG:HB2	1:A:112:ARG:NH1	2.21	0.53
1:A:336:ASP:OD1	1:A:337:ASP:HB2	2.09	0.53
1:B:35:TYR:O	1:B:38:LEU:N	2.42	0.53
1:A:65:ARG:HB2	1:A:65:ARG:HH11	1.74	0.52
1:A:120:VAL:O	1:A:121:ARG:C	2.51	0.52
1:A:235:THR:O	1:A:235:THR:OG1	2.27	0.52
1:A:25:ARG:NH2	1:A:25:ARG:HG2	2.21	0.52
1:B:238:GLN:O	1:B:242:THR:HG23	2.09	0.52
1:B:165:GLU:HA	1:B:165:GLU:OE1	2.10	0.52
1:A:19:ARG:H	1:A:19:ARG:CD	2.08	0.52
1:A:254:THR:CG2	2:A:501:HEM:HAB	2.39	0.52
1:B:238:GLN:O	1:B:239:LEU:C	2.48	0.52
1:B:303:VAL:HG11	1:B:318:ASP:OD1	2.10	0.52
1:B:326:ALA:O	1:B:327:GLY:C	2.52	0.52
1:B:126:MET:HE2	1:B:365:LEU:HD11	1.90	0.52
1:A:301:LEU:HD12	1:A:322:ILE:HG13	1.91	0.52
1:B:214:GLU:C	1:B:216:PRO:HD3	2.33	0.52
1:B:363:GLN:CG	1:B:364:HIS:H	2.22	0.52
1:A:118:PHE:CE1	1:A:362:GLY:CA	2.92	0.52
1:A:356:GLY:C	1:A:358:HIS:H	2.17	0.52
1:A:53:ARG:NH2	1:A:81:GLY:O	2.42	0.52
1:A:97:ARG:HB3	1:A:98:PRO:HA	1.92	0.52
1:A:240:LEU:O	1:A:241:SER:C	2.49	0.52
1:A:289:LEU:O	1:A:290:LEU:C	2.51	0.52
1:B:361:VAL:CG2	2:B:501:HEM:HMD2	2.40	0.52
1:A:65:ARG:NH1	1:A:65:ARG:HB2	2.25	0.52
1:A:291:ARG:HH22	1:A:292:VAL:HG23	1.73	0.52
1:B:47:VAL:O	1:B:47:VAL:HG22	2.09	0.52
1:B:113:MET:CG	1:B:229:LEU:HD11	2.40	0.52
1:B:359:GLN:OE1	1:B:359:GLN:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HA	1:A:155:ALA:CB	2.39	0.51
1:A:353:PHE:CE2	1:A:363:GLN:HB2	2.44	0.51
1:B:229:LEU:CD2	1:B:234:VAL:HG11	2.39	0.51
1:A:21:PHE:C	1:A:21:PHE:CD2	2.89	0.51
1:A:384:LEU:HB2	1:A:411:TRP:CD1	2.45	0.51
1:A:385:ARG:C	1:A:409:VAL:HG12	2.36	0.51
1:B:113:MET:SD	1:B:229:LEU:CD1	2.78	0.51
1:A:24:GLN:H	1:A:25:ARG:HA	1.75	0.51
1:A:43:PRO:HG2	1:A:44:VAL:H	1.75	0.51
1:B:102:THR:HG22	1:B:103:ASP:H	1.75	0.51
1:B:148:VAL:O	1:B:408:MET:CB	2.58	0.51
1:B:230:VAL:O	1:B:230:VAL:HG23	2.10	0.51
1:A:63:ASP:O	1:A:67:LEU:HB3	2.11	0.51
1:A:173:ASP:HB3	1:A:176:PHE:HD1	1.76	0.51
1:A:257:MET:HB3	1:A:370:LEU:HD11	1.92	0.51
1:B:150:LEU:HB2	1:B:154:TYR:HB3	1.93	0.51
1:B:302:ARG:NH2	1:B:358:HIS:CB	2.74	0.51
1:B:250:GLY:HA3	2:B:501:HEM:C3C	2.45	0.51
1:A:292:VAL:CG1	1:A:293:LEU:N	2.69	0.51
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.23	0.51
1:A:286:VAL:HG23	1:A:370:LEU:HD23	1.92	0.51
1:B:138:LEU:O	1:B:139:ASP:C	2.54	0.51
1:A:122:ARG:O	1:A:125:ALA:HB3	2.11	0.51
1:A:140:GLY:O	1:A:143:ALA:N	2.44	0.51
1:A:147:PRO:CA	1:A:410:THR:CG2	2.84	0.51
1:A:189:SER:CB	1:A:190:THR:HA	2.41	0.51
1:A:239:LEU:O	1:A:242:THR:N	2.42	0.51
1:B:242:THR:O	1:B:245:ILE:HG13	2.10	0.51
1:B:350:HIS:O	1:B:350:HIS:ND1	2.44	0.51
1:A:19:ARG:CB	1:A:47:VAL:HA	2.41	0.50
1:A:61:TYR:HB3	1:A:333:GLU:OE2	2.11	0.50
1:A:90:GLN:HG3	1:A:92:ALA:H	1.77	0.50
1:A:24:GLN:HB3	1:A:25:ARG:CA	2.42	0.50
1:A:261:SER:HB3	1:A:289:LEU:HD13	1.93	0.50
1:A:300:PRO:O	1:A:322:ILE:HG23	2.11	0.50
1:B:159:SER:OG	1:B:255:THR:HG22	2.10	0.50
1:B:100:ILE:HD11	2:B:501:HEM:HAD2	1.94	0.50
1:B:179:ASP:O	1:B:183:ILE:CG1	2.48	0.50
1:B:223:LYS:O	1:B:224:LEU:C	2.54	0.50
1:B:250:GLY:HA3	2:B:501:HEM:C2C	2.47	0.50
1:B:381:VAL:HG13	1:B:381:VAL:O	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PHE:CG	1:B:30:ALA:N	2.74	0.50
1:B:102:THR:HB	1:B:106:GLU:HG2	1.94	0.50
1:B:223:LYS:HA	1:B:227:ASP:HB2	1.92	0.50
1:B:230:VAL:CG1	1:B:234:VAL:HG23	2.17	0.50
1:B:300:PRO:HG3	1:B:325:LEU:CD1	2.42	0.50
1:A:238:GLN:HA	1:A:241:SER:OG	2.11	0.50
1:B:245:ILE:O	1:B:246:THR:C	2.55	0.50
1:A:99:PHE:CD1	1:A:99:PHE:C	2.89	0.50
1:A:177:PHE:C	1:A:179:ASP:H	2.19	0.50
1:B:72:ARG:HB2	1:B:308:ILE:HG23	1.93	0.50
1:B:304:ALA:CB	1:B:315:VAL:CG1	2.89	0.50
1:B:75:ALA:C	1:B:101:ARG:O	2.55	0.50
1:B:229:LEU:HD23	1:B:234:VAL:CG1	2.39	0.50
1:A:26:GLY:O	1:A:27:CYS:CB	2.59	0.49
1:A:131:GLN:NE2	1:A:135:ASP:OD1	2.44	0.49
1:A:177:PHE:C	1:A:179:ASP:N	2.70	0.49
1:A:370:LEU:O	1:A:374:LEU:HD12	2.11	0.49
1:B:118:PHE:HE2	2:B:501:HEM:CBC	2.23	0.49
1:B:353:PHE:CE1	2:B:501:HEM:C3B	2.96	0.49
1:A:205:LEU:C	1:A:209:VAL:HG23	2.37	0.49
1:A:21:PHE:CD2	1:A:21:PHE:O	2.66	0.49
1:A:200:GLY:O	1:A:203:GLY:N	2.46	0.49
1:A:355:TYR:HE1	1:B:355:TYR:HE1	1.60	0.49
1:B:118:PHE:HZ	1:B:166:LEU:HD21	1.76	0.49
1:B:221:ILE:CD1	1:B:243:LEU:HD21	2.42	0.49
1:A:102:THR:HB	1:A:107:HIS:CB	2.43	0.49
1:A:288:GLU:OE2	1:A:345:ARG:NH2	2.45	0.49
1:B:107:HIS:ND1	1:B:108:THR:N	2.60	0.49
1:B:201:LEU:O	1:B:201:LEU:HD23	2.12	0.49
1:B:278:ASP:C	1:B:280:ASP:N	2.68	0.49
1:B:178:ARG:O	1:B:182:ARG:HB2	2.11	0.49
1:B:198:LEU:O	1:B:201:LEU:N	2.40	0.49
1:A:24:GLN:CB	1:A:25:ARG:HA	2.41	0.49
1:A:88:GLY:O	1:A:89:GLU:HG2	2.13	0.49
1:B:212:ARG:HH12	1:B:217:ARG:HH22	1.50	0.49
1:A:113:MET:HE1	1:A:233:ASN:ND2	2.28	0.49
1:B:38:LEU:O	1:B:42:ASP:C	2.55	0.49
1:A:19:ARG:N	1:A:19:ARG:CD	2.69	0.49
1:A:162:VAL:HG21	1:A:369:GLU:OE1	2.12	0.49
1:A:253:THR:O	1:A:256:SER:HB3	2.13	0.49
1:B:102:THR:CG2	1:B:103:ASP:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:VAL:HG12	1:B:195:SER:N	2.28	0.49
1:A:340:ARG:C	1:A:342:ASP:H	2.20	0.49
1:A:347:ASP:OD2	1:B:120:VAL:HG11	2.13	0.49
1:B:72:ARG:NE	1:B:307:ASP:O	2.41	0.49
1:B:73:VAL:O	1:B:73:VAL:CG1	2.60	0.49
1:B:72:ARG:HD2	1:B:306:GLU:HB3	1.94	0.48
1:B:353:PHE:HE1	2:B:501:HEM:C2B	2.29	0.48
1:B:49:LEU:O	1:B:52:ARG:N	2.46	0.48
1:A:281:LEU:O	1:A:284:ALA:N	2.47	0.48
1:B:118:PHE:CE2	2:B:501:HEM:CBC	2.96	0.48
1:B:120:VAL:HG22	1:B:364:HIS:CE1	2.48	0.48
1:A:278:ASP:OD1	1:A:278:ASP:O	2.31	0.48
1:A:291:ARG:NH2	1:A:338:PRO:O	2.45	0.48
1:B:224:LEU:HD11	1:B:243:LEU:HD11	1.96	0.48
1:B:229:LEU:O	1:B:231:PRO:HB2	2.13	0.48
1:B:361:VAL:HG21	2:B:501:HEM:HMD2	1.94	0.48
1:A:149:ASP:CG	1:A:152:SER:HB3	2.39	0.48
1:A:301:LEU:HG	1:A:322:ILE:HG13	1.94	0.48
1:B:23:ILE:HD12	1:B:32:PRO:CG	2.44	0.48
1:B:300:PRO:O	1:B:322:ILE:CG2	2.60	0.48
1:B:341:VAL:CG1	1:B:343:PHE:HE1	2.27	0.48
1:A:57:VAL:HG23	1:A:322:ILE:HD12	1.96	0.48
1:A:361:VAL:HG13	2:A:501:HEM:HBD2	1.96	0.48
1:A:112:ARG:C	1:A:114:LEU:H	2.20	0.48
1:A:175:GLU:O	1:A:176:PHE:C	2.57	0.48
1:A:376:THR:O	1:A:377:LEU:C	2.55	0.48
1:A:381:VAL:N	1:A:382:PRO:CD	2.76	0.48
1:B:80:PRO:CA	1:B:303:VAL:HG21	2.42	0.48
1:A:18:PRO:CA	1:A:19:ARG:HH11	2.27	0.48
1:A:301:LEU:HA	1:A:322:ILE:HG23	1.96	0.48
1:B:147:PRO:O	1:B:147:PRO:HG2	2.14	0.47
1:B:166:LEU:HD22	2:B:501:HEM:HBC1	1.95	0.47
1:B:167:LEU:HA	1:B:220:LEU:HB3	1.96	0.47
1:B:353:PHE:CD1	2:B:501:HEM:C2B	3.02	0.47
1:A:257:MET:HG2	1:A:295:VAL:CG2	2.45	0.47
1:B:256:SER:OG	1:B:402:PHE:O	2.27	0.47
1:B:304:ALA:CB	1:B:315:VAL:HG12	2.43	0.47
1:A:62:ASP:OD1	1:A:65:ARG:HD2	2.14	0.47
1:A:25:ARG:O	1:A:26:GLY:C	2.56	0.47
1:A:164:CYS:SG	1:A:169:ILE:CB	2.98	0.47
1:A:184:SER:OG	1:A:198:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HA	1:A:285:ALA:CB	2.34	0.47
1:B:36:ALA:O	1:B:40:THR:HG23	2.15	0.47
1:B:99:PHE:HE2	1:B:110:TYR:HB2	1.79	0.47
1:B:128:PRO:HB2	1:B:129:ALA:H	1.38	0.47
1:B:211:GLU:C	1:B:213:ARG:N	2.72	0.47
1:B:331:ASP:HA	1:B:332:PRO:HD2	1.51	0.47
1:A:222:SER:O	1:A:223:LYS:C	2.57	0.47
1:A:292:VAL:HG12	1:A:293:LEU:N	2.29	0.47
1:A:23:ILE:O	1:A:397:HIS:HE1	1.96	0.47
1:A:115:LEU:N	1:A:116:PRO:HD2	2.29	0.47
1:A:115:LEU:O	1:A:116:PRO:C	2.57	0.47
1:B:22:PRO:C	1:B:23:ILE:CG1	2.77	0.47
1:A:43:PRO:CD	1:A:44:VAL:N	2.72	0.47
1:A:64:VAL:HG21	1:A:328:ALA:HB2	1.97	0.47
1:A:156:ASN:O	1:A:159:SER:HB2	2.15	0.47
1:A:370:LEU:CD2	1:A:374:LEU:CD1	2.92	0.47
1:A:371:GLU:O	1:A:372:VAL:C	2.57	0.47
1:B:262:THR:O	1:B:263:LEU:C	2.55	0.47
1:B:269:PRO:C	1:B:272:PRO:HD2	2.39	0.47
1:B:275:LEU:C	1:B:278:ASP:H	2.22	0.47
1:B:278:ASP:HB3	1:B:281:LEU:HB2	1.97	0.47
1:B:353:PHE:CZ	1:B:363:GLN:HA	2.49	0.47
1:B:113:MET:HE2	1:B:229:LEU:CD1	2.45	0.47
1:A:25:ARG:HE	1:A:402:PHE:HE2	1.46	0.47
1:A:27:CYS:C	1:A:29:PHE:O	2.58	0.47
1:B:261:SER:HA	1:B:289:LEU:HD22	1.96	0.47
1:B:372:VAL:O	1:B:376:THR:OG1	2.32	0.47
1:B:383:THR:HG23	1:B:384:LEU:H	1.80	0.47
1:A:21:PHE:HA	1:A:22:PRO:HD3	1.53	0.47
1:A:43:PRO:HD2	1:A:44:VAL:H	1.78	0.47
1:A:72:ARG:NH1	1:B:104:ALA:CB	2.78	0.47
1:A:110:TYR:O	1:A:111:ARG:C	2.58	0.47
1:B:44:VAL:HG21	1:B:310:LEU:HD23	1.95	0.47
1:B:21:PHE:CD2	1:B:50:PRO:HG2	2.50	0.46
1:B:77:ILE:H	1:B:101:ARG:HE	1.63	0.46
1:A:122:ARG:HE	1:A:122:ARG:HB2	1.66	0.46
1:A:194:VAL:O	1:A:197:ALA:N	2.48	0.46
1:A:383:THR:HG1	1:A:385:ARG:NH2	2.09	0.46
1:A:181:THR:CG2	1:A:251:ARG:CD	2.79	0.46
1:A:211:GLU:HA	1:A:214:GLU:OE1	2.15	0.46
1:A:225:VAL:HG23	1:A:226:THR:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:TYR:OH	1:B:349:HIS:HB2	2.15	0.46
1:B:297:ASP:OD1	1:B:326:ALA:CB	2.64	0.46
1:A:62:ASP:HB2	1:A:333:GLU:OE1	2.16	0.46
1:A:179:ASP:O	1:A:183:ILE:CG1	2.48	0.46
1:A:301:LEU:HD23	1:A:302:ARG:O	2.15	0.46
1:B:304:ALA:HB2	1:B:315:VAL:HG11	1.94	0.46
1:A:19:ARG:HG2	1:A:48:THR:N	2.27	0.46
1:A:42:ASP:O	1:A:45:ALA:N	2.49	0.46
1:A:356:GLY:C	1:A:358:HIS:N	2.72	0.46
1:A:370:LEU:HD21	1:A:374:LEU:HD11	1.98	0.46
1:A:138:LEU:HA	1:A:141:MET:CG	2.46	0.46
1:A:221:ILE:O	1:A:225:VAL:CG1	2.42	0.46
1:A:301:LEU:HD23	1:A:302:ARG:N	2.31	0.46
1:A:381:VAL:O	1:A:381:VAL:HG22	2.14	0.46
1:B:375:GLU:OE2	1:B:379:ARG:NE	2.46	0.46
1:B:385:ARG:C	1:B:386:LEU:HG	2.41	0.46
1:A:46:ARG:HG2	1:A:56:TRP:CZ2	2.50	0.46
1:B:102:THR:HG22	1:B:103:ASP:N	2.30	0.46
1:B:118:PHE:CD2	1:B:361:VAL:O	2.69	0.46
1:B:154:TYR:O	1:B:158:VAL:HG12	2.16	0.46
1:B:403:GLY:C	1:B:404:LEU:HD13	2.41	0.46
1:A:123:VAL:HG11	1:A:364:HIS:HB3	1.97	0.46
1:A:229:LEU:O	1:A:234:VAL:CB	2.63	0.45
1:A:257:MET:HB3	1:A:370:LEU:CD1	2.46	0.45
1:A:283:PRO:O	1:A:286:VAL:HG12	2.15	0.45
1:B:99:PHE:HZ	1:B:111:ARG:CA	2.29	0.45
1:B:158:VAL:HG13	1:B:258:ILE:CD1	2.45	0.45
1:B:346:THR:C	1:B:348:ASN:N	2.69	0.45
1:B:383:THR:CG2	1:B:384:LEU:H	2.27	0.45
1:A:115:LEU:HD21	1:A:361:VAL:HB	1.98	0.45
1:A:261:SER:HB2	1:A:374:LEU:HD21	1.96	0.45
1:B:97:ARG:N	1:B:98:PRO:CD	2.76	0.45
1:B:192:GLU:C	1:B:194:VAL:H	2.23	0.45
1:A:67:LEU:HD12	1:A:67:LEU:O	2.16	0.45
1:A:117:ALA:HB1	1:A:220:LEU:HD13	1.97	0.45
1:A:121:ARG:HA	1:A:124:ARG:HE	1.81	0.45
1:A:377:LEU:HB3	1:A:378:LEU:HD23	1.99	0.45
1:A:378:LEU:HD23	1:A:378:LEU:N	2.32	0.45
1:A:387:ALA:H	1:A:408:MET:C	2.22	0.45
1:B:315:VAL:HA	1:B:316:PRO:HD3	1.69	0.45
1:A:290:LEU:HD13	1:A:353:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LEU:CD2	1:A:374:LEU:HD11	2.46	0.45
1:B:159:SER:O	1:B:162:VAL:HG12	2.17	0.45
1:B:275:LEU:HD23	1:B:281:LEU:HB3	1.98	0.45
1:B:333:GLU:HG3	1:B:334:GLN:N	2.31	0.45
1:A:351:VAL:C	1:A:353:PHE:N	2.67	0.45
1:A:377:LEU:HD22	1:A:377:LEU:HA	1.71	0.45
1:B:46:ARG:HG3	1:B:56:TRP:CD2	2.52	0.45
1:B:230:VAL:O	1:B:230:VAL:CG2	2.65	0.45
1:A:65:ARG:NH1	1:A:355:TYR:CD2	2.85	0.45
1:B:147:PRO:O	1:B:147:PRO:CG	2.64	0.45
1:B:271:LEU:O	1:B:274:GLU:N	2.49	0.45
1:B:270:GLU:O	1:B:274:GLU:N	2.49	0.45
1:B:377:LEU:HD13	1:B:378:LEU:HG	1.99	0.45
1:B:149:ASP:CB	1:B:408:MET:CG	2.95	0.45
1:B:319:ASP:OD1	1:B:319:ASP:N	2.50	0.45
1:B:44:VAL:HG22	1:B:310:LEU:HD23	1.99	0.45
1:B:194:VAL:HG13	1:B:195:SER:CA	2.47	0.45
1:A:26:GLY:O	1:A:28:PRO:CD	2.57	0.45
1:A:149:ASP:OD2	1:A:149:ASP:C	2.60	0.45
1:A:150:LEU:HD13	1:A:154:TYR:HB3	2.00	0.45
1:B:149:ASP:CB	1:B:408:MET:HG2	2.47	0.45
1:A:70:ASP:HA	1:A:71:PRO:HD2	1.43	0.44
1:A:137:ILE:O	1:A:137:ILE:HD12	2.17	0.44
1:A:151:VAL:CA	1:A:155:ALA:HB3	2.41	0.44
1:A:159:SER:O	1:A:163:ILE:HG13	2.17	0.44
1:A:204:LEU:O	1:A:208:LEU:HD13	2.17	0.44
1:A:279:PRO:O	1:A:282:MET:CE	2.65	0.44
1:B:259:ALA:CB	1:B:404:LEU:HD23	2.44	0.44
1:B:356:GLY:C	1:B:358:HIS:H	2.23	0.44
1:A:153:ALA:O	1:A:157:ALA:HB2	2.17	0.44
1:A:181:THR:HG22	1:A:251:ARG:CD	2.43	0.44
1:A:235:THR:HG1	1:A:238:GLN:HG3	1.82	0.44
1:B:65:ARG:HG3	1:B:355:TYR:CE2	2.52	0.44
1:B:104:ALA:HA	1:B:105:PRO:HA	1.52	0.44
1:B:171:ARG:CA	1:B:174:LEU:HB2	2.47	0.44
1:B:261:SER:O	1:B:264:LEU:HB3	2.17	0.44
1:B:393:VAL:CG2	1:B:394:VAL:N	2.81	0.44
1:A:142:LEU:HA	1:A:411:TRP:CH2	2.52	0.44
1:A:385:ARG:N	1:A:410:THR:O	2.49	0.44
1:B:101:ARG:HG3	1:B:102:THR:N	2.32	0.44
1:B:403:GLY:O	1:B:404:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:O	1:A:118:PHE:N	2.47	0.44
1:A:127:ARG:HB3	1:A:128:PRO:CD	2.23	0.44
1:A:133:ARG:NE	1:A:165:GLU:HB2	2.33	0.44
1:A:140:GLY:O	1:A:141:MET:C	2.60	0.44
1:A:260:LEU:HD13	1:A:293:LEU:HD22	1.99	0.44
1:A:67:LEU:HD12	1:A:67:LEU:C	2.43	0.44
1:A:194:VAL:O	1:A:196:GLU:N	2.51	0.44
1:A:229:LEU:HG	1:A:234:VAL:CB	2.47	0.44
1:A:236:THR:H	1:A:236:THR:HG23	1.40	0.44
1:B:300:PRO:HG3	1:B:325:LEU:HD13	1.99	0.44
1:A:225:VAL:O	1:A:229:LEU:HB3	2.18	0.44
1:A:354:GLY:H	1:A:360:CYS:H	1.65	0.44
1:B:196:GLU:O	1:B:197:ALA:C	2.58	0.44
1:A:112:ARG:C	1:A:114:LEU:N	2.73	0.44
1:A:190:THR:O	1:A:193:GLN:N	2.50	0.44
1:A:358:HIS:O	2:A:501:HEM:HBD1	2.18	0.44
1:B:114:LEU:HD22	1:B:114:LEU:HA	1.70	0.44
1:B:149:ASP:OD2	1:B:150:LEU:N	2.51	0.44
1:B:360:CYS:HB2	2:B:501:HEM:C4A	2.51	0.44
1:A:19:ARG:HG3	1:A:47:VAL:CA	2.31	0.44
1:A:212:ARG:O	1:A:216:PRO:HB3	2.18	0.44
1:B:150:LEU:HB2	1:B:154:TYR:CB	2.48	0.44
1:A:99:PHE:HA	1:A:102:THR:OG1	2.18	0.43
1:A:129:ALA:HB1	1:A:165:GLU:OE2	2.18	0.43
1:B:116:PRO:CB	3:B:619:HOH:O	2.66	0.43
1:B:202:PHE:O	1:B:203:GLY:C	2.61	0.43
1:A:72:ARG:HH11	1:B:104:ALA:HB3	1.83	0.43
1:A:145:GLY:C	1:A:146:GLY:O	2.61	0.43
1:B:61:TYR:HH	1:B:349:HIS:HB2	1.83	0.43
1:B:114:LEU:HD12	1:B:361:VAL:HG21	1.99	0.43
1:B:39:ARG:HG3	1:B:60:ARG:HA	2.00	0.43
1:B:217:ARG:HB2	1:B:217:ARG:CZ	2.47	0.43
1:B:230:VAL:CB	1:B:231:PRO:O	2.65	0.43
1:B:303:VAL:HG13	1:B:318:ASP:HA	2.01	0.43
1:A:30:ALA:C	1:A:32:PRO:HD2	2.43	0.43
1:A:276:ARG:O	1:A:277:LYS:C	2.61	0.43
1:A:368:LEU:O	1:A:369:GLU:C	2.62	0.43
1:B:193:GLN:H	1:B:193:GLN:HG3	1.36	0.43
1:B:235:THR:O	1:B:238:GLN:HB3	2.17	0.43
1:A:19:ARG:HB2	1:A:47:VAL:HA	2.01	0.43
1:A:83:PRO:HB2	1:A:89:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:C	1:A:411:TRP:CG	2.96	0.43
1:A:301:LEU:HD21	1:A:320:GLY:CA	2.48	0.43
1:B:18:PRO:C	1:B:48:THR:H	2.27	0.43
1:B:49:LEU:C	1:B:49:LEU:HD12	2.43	0.43
1:B:72:ARG:HB2	1:B:308:ILE:CG2	2.49	0.43
1:A:72:ARG:CB	3:A:602:HOH:O	2.67	0.43
1:A:205:LEU:O	1:A:206:GLY:C	2.60	0.43
1:A:206:GLY:O	1:A:207:GLY:C	2.62	0.43
1:B:103:ASP:O	1:B:104:ALA:C	2.62	0.43
1:B:111:ARG:C	1:B:113:MET:H	2.26	0.43
1:B:245:ILE:HG13	1:B:245:ILE:H	1.59	0.43
1:A:360:CYS:HB2	2:A:501:HEM:C4A	2.54	0.43
1:B:46:ARG:HG2	1:B:55:ALA:O	2.18	0.43
1:B:63:ASP:O	1:B:66:GLU:HB2	2.18	0.43
1:B:64:VAL:HG13	1:B:323:ALA:HB1	1.99	0.43
1:B:176:PHE:O	1:B:180:VAL:HG13	2.19	0.43
2:B:501:HEM:CBA	2:B:501:HEM:CMA	2.97	0.43
1:A:181:THR:HG23	1:A:251:ARG:HH11	1.84	0.43
1:B:138:LEU:CD2	1:B:141:MET:HB2	2.44	0.43
1:A:25:ARG:NH1	1:A:27:CYS:O	2.51	0.42
1:A:377:LEU:HB3	1:A:378:LEU:CD2	2.48	0.42
1:B:35:TYR:HA	1:B:38:LEU:HD13	2.01	0.42
1:B:59:THR:HG23	1:B:324:LEU:HD12	2.00	0.42
1:A:53:ARG:HE	1:A:53:ARG:HB2	1.63	0.42
1:A:249:ALA:HB3	2:A:501:HEM:HBC2	2.01	0.42
1:A:281:LEU:HA	1:A:281:LEU:HD23	1.76	0.42
1:B:149:ASP:HB2	1:B:408:MET:HG2	1.99	0.42
1:B:302:ARG:HH22	1:B:358:HIS:CB	2.32	0.42
1:A:21:PHE:HE1	1:A:50:PRO:CG	2.31	0.42
1:A:149:ASP:O	1:A:153:ALA:HB3	2.19	0.42
1:A:282:MET:CA	1:A:285:ALA:HB3	2.37	0.42
1:A:315:VAL:HA	1:A:316:PRO:HD3	1.88	0.42
1:A:356:GLY:O	1:A:358:HIS:N	2.52	0.42
1:B:116:PRO:HB2	3:B:619:HOH:O	2.18	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.91	0.42
1:B:150:LEU:HD23	1:B:409:VAL:CG2	2.50	0.42
1:B:174:LEU:HG	1:B:178:ARG:HD3	2.01	0.42
1:B:238:GLN:HA	1:B:241:SER:HG	1.80	0.42
1:B:304:ALA:HB1	1:B:315:VAL:HG12	2.02	0.42
1:B:361:VAL:HG22	2:B:501:HEM:C2D	2.54	0.42
1:B:56:TRP:NE1	1:B:319:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASP:O	1:B:183:ILE:N	2.49	0.42
1:B:212:ARG:NH1	1:B:217:ARG:HH21	2.06	0.42
1:A:49:LEU:O	1:A:51:THR:N	2.52	0.42
1:A:173:ASP:CG	3:A:626:HOH:O	2.62	0.42
1:A:175:GLU:C	1:A:177:PHE:H	2.28	0.42
1:B:46:ARG:HG3	1:B:56:TRP:CE2	2.55	0.42
1:B:113:MET:SD	1:B:229:LEU:HD21	2.60	0.42
1:B:162:VAL:HG11	1:B:369:GLU:CG	2.49	0.42
1:B:282:MET:N	1:B:283:PRO:CD	2.83	0.42
1:B:357:VAL:O	1:B:357:VAL:HG13	2.16	0.42
1:A:296:ALA:HB2	2:A:501:HEM:HMB2	2.01	0.42
1:B:107:HIS:CE1	1:B:108:THR:HA	2.55	0.42
1:B:221:ILE:HA	1:B:224:LEU:HD12	2.02	0.42
1:A:70:ASP:O	1:A:73:VAL:HG23	2.19	0.42
1:A:147:PRO:CB	1:A:410:THR:CG2	2.98	0.42
1:B:46:ARG:HB2	1:B:56:TRP:CZ3	2.55	0.42
1:B:175:GLU:O	1:B:179:ASP:N	2.52	0.42
1:B:342:ASP:C	1:B:344:HIS:H	2.27	0.42
1:B:377:LEU:HD22	1:B:377:LEU:O	2.20	0.42
1:A:164:CYS:SG	1:A:169:ILE:HD12	2.59	0.42
1:A:365:LEU:HA	1:A:365:LEU:HD12	1.34	0.42
1:A:18:PRO:CG	1:A:19:ARG:NH1	2.83	0.41
1:A:141:MET:HE2	1:A:141:MET:CA	2.45	0.41
1:A:331:ASP:O	1:A:334:GLN:HB3	2.20	0.41
1:A:335:PHE:CG	1:A:345:ARG:HD3	2.55	0.41
1:A:395:VAL:HA	1:A:404:LEU:HA	2.02	0.41
1:B:138:LEU:CD1	1:B:377:LEU:HD23	2.50	0.41
1:B:162:VAL:HG11	1:B:369:GLU:HG2	2.02	0.41
1:A:72:ARG:HB2	3:A:602:HOH:O	2.20	0.41
1:A:141:MET:HA	1:A:141:MET:CE	2.46	0.41
1:A:154:TYR:O	1:A:157:ALA:HB3	2.19	0.41
1:A:205:LEU:O	1:A:209:VAL:N	2.39	0.41
1:A:299:ILE:HB	1:A:300:PRO:CD	2.50	0.41
1:B:107:HIS:NE2	1:B:357:VAL:CG1	2.83	0.41
1:A:28:PRO:HA	1:A:29:PHE:HA	1.68	0.41
1:A:219:ASP:H	1:A:222:SER:HB2	1.85	0.41
1:B:39:ARG:HG3	1:B:60:ARG:CA	2.50	0.41
1:B:118:PHE:HD2	1:B:362:GLY:HA2	1.85	0.41
1:A:96:PHE:CD1	1:A:97:ARG:CZ	3.00	0.41
1:A:138:LEU:O	1:A:139:ASP:C	2.63	0.41
1:A:194:VAL:C	1:A:196:GLU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:O	1:A:382:PRO:HG3	2.21	0.41
1:B:390:ARG:C	1:B:392:GLN:N	2.78	0.41
1:A:112:ARG:HH12	1:B:66:GLU:HG3	1.86	0.41
1:A:202:PHE:HD2	1:A:240:LEU:HD23	1.86	0.41
1:A:288:GLU:CD	1:A:345:ARG:HH21	2.28	0.41
1:A:376:THR:HA	1:A:379:ARG:HB3	2.01	0.41
1:B:115:LEU:N	1:B:116:PRO:CD	2.84	0.41
1:B:171:ARG:H	1:B:171:ARG:HG3	1.71	0.41
1:B:286:VAL:O	1:B:286:VAL:HG12	2.19	0.41
1:B:353:PHE:C	2:B:501:HEM:HMA1	2.45	0.41
1:B:385:ARG:H	1:B:385:ARG:HG2	1.67	0.41
1:A:35:TYR:CE1	1:A:324:LEU:HD13	2.56	0.41
1:A:66:GLU:HB3	1:B:112:ARG:NH1	2.36	0.41
1:A:147:PRO:HB3	1:A:410:THR:HG23	2.01	0.41
1:A:149:ASP:OD2	1:A:152:SER:CB	2.59	0.41
1:A:301:LEU:HD21	1:A:321:VAL:N	2.35	0.41
1:B:20:ASP:O	1:B:22:PRO:HD3	2.20	0.41
1:B:282:MET:N	1:B:283:PRO:HD3	2.36	0.41
1:A:46:ARG:HG2	1:A:56:TRP:CE2	2.56	0.41
1:A:198:LEU:HD12	1:A:198:LEU:N	2.36	0.41
1:B:99:PHE:CE2	1:B:110:TYR:HB2	2.56	0.41
1:B:283:PRO:C	1:B:285:ALA:H	2.22	0.41
1:B:406:GLU:O	1:B:406:GLU:HG3	2.21	0.41
1:A:29:PHE:CE2	1:A:264:LEU:HA	2.55	0.41
1:A:72:ARG:HH12	1:B:104:ALA:CB	2.33	0.41
1:A:174:LEU:O	1:A:178:ARG:N	2.39	0.41
1:A:225:VAL:CG2	1:A:226:THR:N	2.83	0.41
1:B:49:LEU:O	1:B:49:LEU:HG	2.20	0.41
1:B:395:VAL:CG2	1:B:396:LYS:N	2.83	0.41
1:A:117:ALA:CB	1:A:220:LEU:HD13	2.51	0.41
1:A:157:ALA:O	1:A:158:VAL:C	2.63	0.41
1:B:233:ASN:O	1:B:234:VAL:HG13	2.21	0.41
1:B:302:ARG:NH2	1:B:358:HIS:HB2	2.36	0.41
1:B:407:LEU:C	1:B:408:MET:HG3	2.46	0.41
1:A:137:ILE:HD12	1:A:137:ILE:C	2.46	0.40
1:A:162:VAL:HG11	1:A:369:GLU:CG	2.38	0.40
1:A:235:THR:HG21	1:A:238:GLN:CD	2.44	0.40
1:B:177:PHE:HE2	1:B:247:ILE:HD13	1.86	0.40
1:B:368:LEU:HD22	1:B:368:LEU:HA	1.83	0.40
1:B:398:ASP:OD1	1:B:398:ASP:C	2.64	0.40
1:A:283:PRO:O	1:A:284:ALA:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:CG	1:B:229:LEU:CD1	2.99	0.40
1:A:23:ILE:CB	1:A:24:GLN:O	2.69	0.40
1:A:24:GLN:CG	1:A:33:ALA:CA	2.95	0.40
1:A:180:VAL:HG21	1:A:201:LEU:HD23	2.02	0.40
1:A:296:ALA:HB2	2:A:501:HEM:CMB	2.51	0.40
1:A:375:GLU:HB3	1:A:376:THR:H	1.61	0.40
1:B:81:GLY:O	1:B:82:PHE:CB	2.69	0.40
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.94	0.40
1:A:122:ARG:HG3	1:A:123:VAL:N	2.35	0.40
1:B:192:GLU:C	1:B:194:VAL:N	2.79	0.40
1:B:302:ARG:HH22	1:B:358:HIS:HB3	1.87	0.40
1:B:367:ARG:HH11	1:B:367:ARG:HB2	1.87	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	386/417 (93%)	261 (68%)	96 (25%)	29 (8%)	1	2
1	B	360/417 (86%)	232 (64%)	111 (31%)	17 (5%)	2	7
All	All	746/834 (89%)	493 (66%)	207 (28%)	46 (6%)	1	3

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	28	PRO
1	A	42	ASP
1	A	50	PRO
1	A	76	ASP
1	A	97	ARG

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Mol	Chain	Res	Type
1	A	119	THR
1	A	171	ARG
1	A	300	PRO
1	B	50	PRO
1	B	80	PRO
1	B	128	PRO
1	B	231	PRO
1	B	347	ASP
1	B	382	PRO
1	A	31	ALA
1	A	80	PRO
1	A	146	GLY
1	A	372	VAL
1	B	32	PRO
1	B	409	VAL
1	A	189	SER
1	A	356	GLY
1	B	194	VAL
1	A	116	PRO
1	B	22	PRO
1	B	31	ALA
1	B	332	PRO
1	B	351	VAL
1	A	269	PRO
1	A	341	VAL
1	A	357	VAL
1	A	388	GLY
1	B	147	PRO
1	A	170	PRO
1	A	312	GLY
1	A	351	VAL
1	B	215	GLU
1	A	82	PHE
1	A	283	PRO
1	B	206	GLY
1	A	73	VAL
1	A	77	ILE
1	A	299	ILE
1	B	283	PRO
1	A	231	PRO

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	322/347 (93%)	204 (63%)	118 (37%)	0	0
1	B	306/347 (88%)	193 (63%)	113 (37%)	0	0
All	All	628/694 (90%)	397 (63%)	231 (37%)	0	0

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	20	ASP
1	A	24	GLN
1	A	28	PRO
1	A	29	PHE
1	A	38	LEU
1	A	39	ARG
1	A	42	ASP
1	A	43	PRO
1	A	46	ARG
1	A	47	VAL
1	A	48	THR
1	A	51	THR
1	A	52	ARG
1	A	57	VAL
1	A	58	VAL
1	A	65	ARG
1	A	67	LEU
1	A	68	LEU
1	A	69	SER
1	A	72	ARG
1	A	73	VAL
1	A	77	ILE
1	A	78	ARG
1	A	95	ARG
1	A	97	ARG
1	A	102	THR

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Mol	Chain	Res	Type
1	A	107	HIS
1	A	109	ARG
1	A	112	ARG
1	A	113	MET
1	A	114	LEU
1	A	118	PHE
1	A	121	ARG
1	A	122	ARG
1	A	123	VAL
1	A	127	ARG
1	A	128	PRO
1	A	137	ILE
1	A	142	LEU
1	A	149	ASP
1	A	150	LEU
1	A	152	SER
1	A	158	VAL
1	A	159	SER
1	A	163	ILE
1	A	164	CYS
1	A	171	ARG
1	A	173	ASP
1	A	178	ARG
1	A	183	ILE
1	A	190	THR
1	A	196	GLU
1	A	201	LEU
1	A	204	LEU
1	A	211	GLU
1	A	215	GLU
1	A	223	LYS
1	A	224	LEU
1	A	225	VAL
1	A	226	THR
1	A	227	ASP
1	A	235	THR
1	A	237	GLU
1	A	241	SER
1	A	243	LEU
1	A	247	ILE
1	A	252	GLU
1	A	258	ILE

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	264	LEU
1	A	266	LEU
1	A	267	ASP
1	A	270	GLU
1	A	271	LEU
1	A	277	LYS
1	A	278	ASP
1	A	282	MET
1	A	286	VAL
1	A	292	VAL
1	A	294	SER
1	A	295	VAL
1	A	299	ILE
1	A	300	PRO
1	A	302	ARG
1	A	303	VAL
1	A	306	GLU
1	A	308	ILE
1	A	310	LEU
1	A	322	ILE
1	A	330	HIS
1	A	333	GLU
1	A	334	GLN
1	A	339	GLU
1	A	341	VAL
1	A	346	THR
1	A	347	ASP
1	A	351	VAL
1	A	357	VAL
1	A	359	GLN
1	A	361	VAL
1	A	363	GLN
1	A	369	GLU
1	A	370	LEU
1	A	371	GLU
1	A	372	VAL
1	A	377	LEU
1	A	378	LEU
1	A	381	VAL
1	A	383	THR
1	A	384	LEU

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Mol	Chain	Res	Type
1	A	394	VAL
1	A	395	VAL
1	A	399	SER
1	A	404	LEU
1	A	406	GLU
1	A	410	THR
1	A	411	TRP
1	B	23	ILE
1	B	29	PHE
1	B	38	LEU
1	B	46	ARG
1	B	47	VAL
1	B	49	LEU
1	B	50	PRO
1	B	53	ARG
1	B	59	THR
1	B	68	LEU
1	B	73	VAL
1	B	79	ARG
1	B	97	ARG
1	B	99	PHE
1	B	101	ARG
1	B	103	ASP
1	B	107	HIS
1	B	113	MET
1	B	114	LEU
1	B	115	LEU
1	B	120	VAL
1	B	121	ARG
1	B	122	ARG
1	B	123	VAL
1	B	126	MET
1	B	127	ARG
1	B	138	LEU
1	B	142	LEU
1	B	147	PRO
1	B	148	VAL
1	B	149	ASP
1	B	152	SER
1	B	164	CYS
1	B	167	LEU
1	B	169	ILE

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Mol	Chain	Res	Type
1	B	171	ARG
1	B	173	ASP
1	B	176	PHE
1	B	178	ARG
1	B	179	ASP
1	B	183	ILE
1	B	198	LEU
1	B	204	LEU
1	B	214	GLU
1	B	217	ARG
1	B	218	ASP
1	B	225	VAL
1	B	227	ASP
1	B	228	HIS
1	B	230	VAL
1	B	231	PRO
1	B	234	VAL
1	B	235	THR
1	B	245	ILE
1	B	246	THR
1	B	247	ILE
1	B	251	ARG
1	B	253	THR
1	B	254	THR
1	B	255	THR
1	B	257	MET
1	B	263	LEU
1	B	270	GLU
1	B	278	ASP
1	B	280	ASP
1	B	281	LEU
1	B	286	VAL
1	B	290	LEU
1	B	294	SER
1	B	295	VAL
1	B	298	SER
1	B	299	ILE
1	B	303	VAL
1	B	308	ILE
1	B	310	LEU
1	B	313	ARG
1	B	314	THR

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Mol	Chain	Res	Type
1	B	315	VAL
1	B	319	ASP
1	B	321	VAL
1	B	322	ILE
1	B	333	GLU
1	B	337	ASP
1	B	339	GLU
1	B	340	ARG
1	B	345	ARG
1	B	346	THR
1	B	347	ASP
1	B	351	VAL
1	B	355	TYR
1	B	357	VAL
1	B	365	LEU
1	B	367	ARG
1	B	368	LEU
1	B	371	GLU
1	B	375	GLU
1	B	376	THR
1	B	377	LEU
1	B	382	PRO
1	B	383	THR
1	B	384	LEU
1	B	385	ARG
1	B	386	LEU
1	B	391	ASP
1	B	392	GLN
1	B	393	VAL
1	B	394	VAL
1	B	395	VAL
1	B	397	HIS
1	B	398	ASP
1	B	404	LEU
1	B	407	LEU
1	B	409	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	107	HIS

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	238	GLN
1	A	248	ASN
1	A	330	HIS
1	A	334	GLN
1	A	348	ASN
1	A	359	GLN
1	A	364	HIS
1	A	397	HIS
1	B	233	ASN
1	B	330	HIS
1	B	364	HIS
1	B	397	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	B	501	1	50,50,50	1.92	8 (16%)	67,82,82	1.32	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	501	1	50,50,50	1.91	8 (16%)	67,82,82	1.31	5 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	11/14/54/54	-
2	HEM	A	501	1	-	10/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3D-C2D	7.97	1.53	1.36
2	B	501	HEM	C3D-C2D	7.94	1.53	1.36
2	B	501	HEM	FE-ND	4.60	2.09	1.94
2	A	501	HEM	FE-ND	4.52	2.08	1.94
2	B	501	HEM	FE-NB	4.15	2.07	1.94
2	A	501	HEM	FE-NB	4.09	2.07	1.94
2	B	501	HEM	FE-NA	3.57	2.06	1.95
2	B	501	HEM	FE-NC	3.57	2.06	1.95
2	A	501	HEM	FE-NC	3.53	2.06	1.95
2	A	501	HEM	FE-NA	3.52	2.06	1.95
2	B	501	HEM	CAC-C3C	2.81	1.54	1.47
2	B	501	HEM	CAB-C3B	2.79	1.54	1.47
2	A	501	HEM	CAC-C3C	2.78	1.54	1.47
2	A	501	HEM	CAB-C3B	2.78	1.54	1.47
2	B	501	HEM	CMC-C2C	2.01	1.54	1.50
2	A	501	HEM	CMA-C3A	2.00	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C4D-ND-C1D	5.52	111.75	105.21
2	A	501	HEM	C4D-ND-C1D	5.50	111.72	105.21
2	A	501	HEM	C1B-NB-C4B	2.35	107.99	105.21
2	B	501	HEM	C1B-NB-C4B	2.28	107.91	105.21
2	B	501	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	A	501	HEM	C3B-C2B-C1B	2.27	108.11	106.41
2	A	501	HEM	C3B-C4B-NB	-2.24	107.86	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	HEM	C3B-C4B-NB	-2.21	107.88	109.47
2	B	501	HEM	C2A-C1A-NA	-2.02	107.91	110.15
2	A	501	HEM	C2A-C1A-NA	-2.02	107.92	110.15

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C3A-C2A-CAA-CBA
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C4C-C3C-CAC-CBC
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	C2C-C3C-CAC-CBC
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	C4C-C3C-CAC-CBC

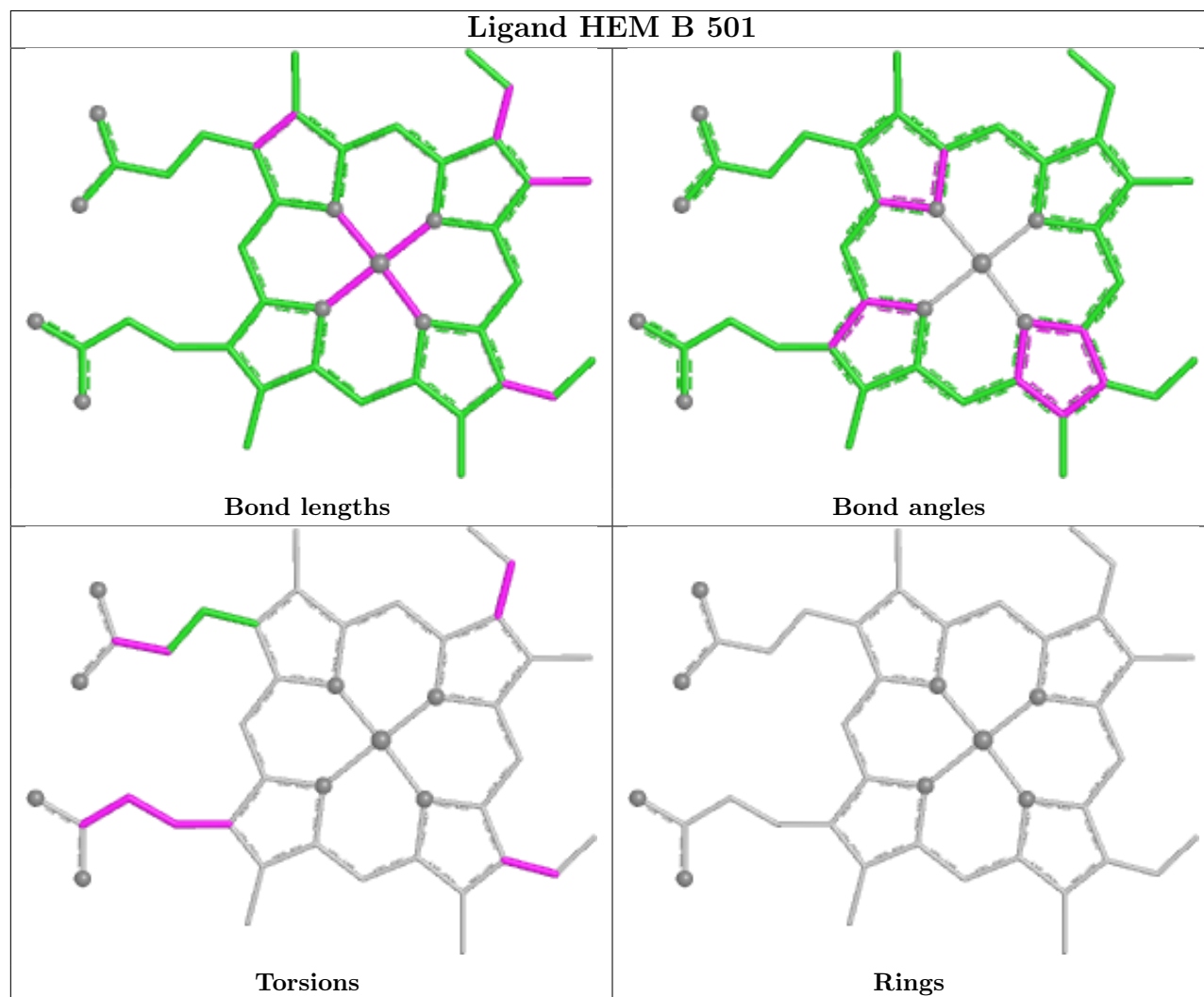
There are no ring outliers.

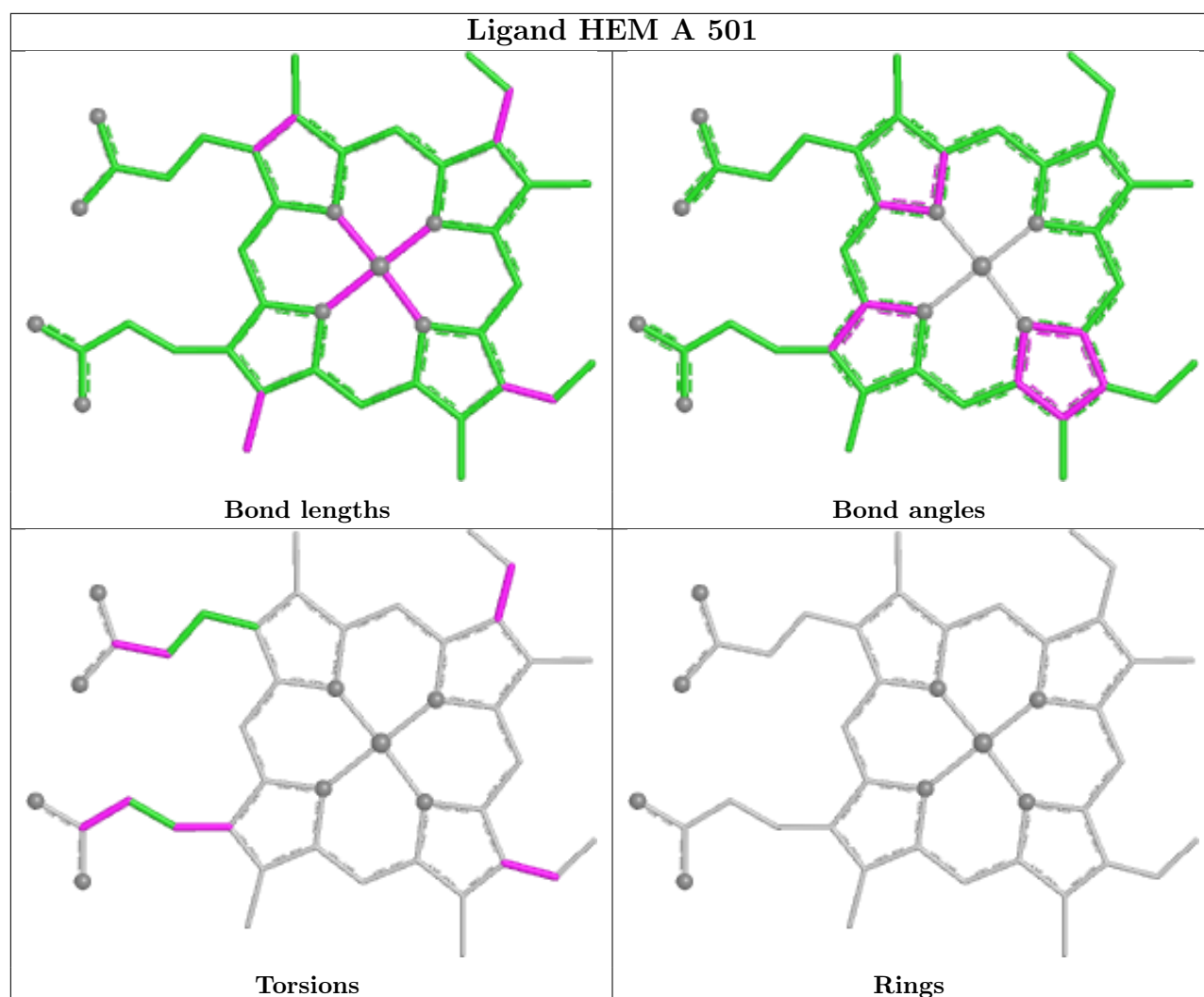
2 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	26	0
2	A	501	HEM	18	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	390/417 (93%)	-0.01	8 (2%) 63 54	10, 40, 77, 114	0
1	B	370/417 (88%)	0.15	8 (2%) 62 53	13, 45, 86, 125	0
All	All	760/834 (91%)	0.07	16 (2%) 63 54	10, 43, 83, 125	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ASP	3.5
1	B	110	TYR	3.5
1	B	349	HIS	3.5
1	B	23	ILE	3.3
1	A	193	GLN	3.1
1	A	176	PHE	3.0
1	B	212	ARG	2.8
1	A	312	GLY	2.8
1	B	228	HIS	2.8
1	A	335	PHE	2.6
1	A	214	GLU	2.5
1	B	410	THR	2.2
1	B	142	LEU	2.2
1	A	301	LEU	2.1
1	B	334	GLN	2.1
1	A	300	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

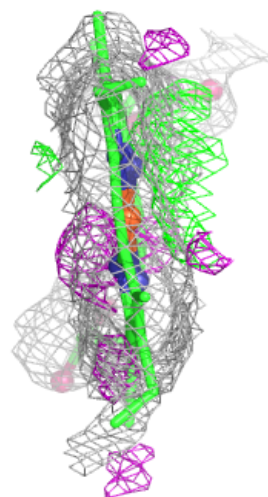
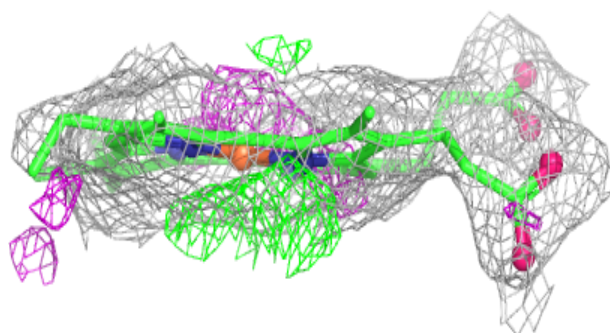
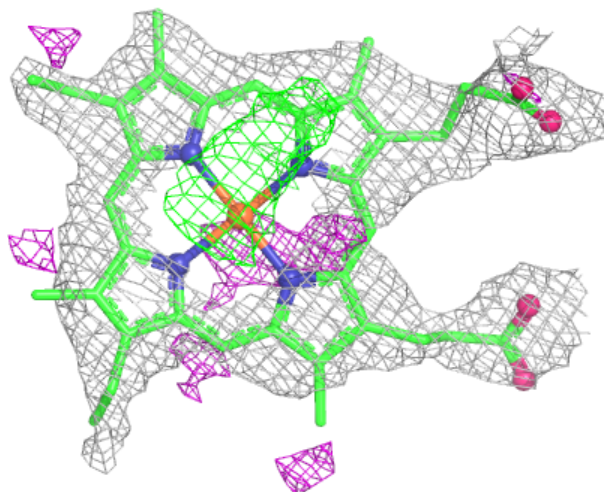
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	501	43/43	0.93	0.12	21,28,36,46	0
2	HEM	A	501	43/43	0.95	0.12	23,31,44,49	0

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

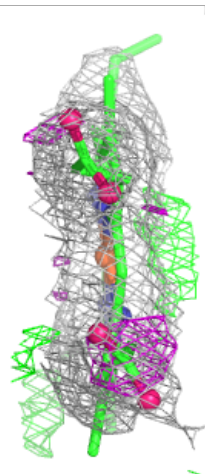
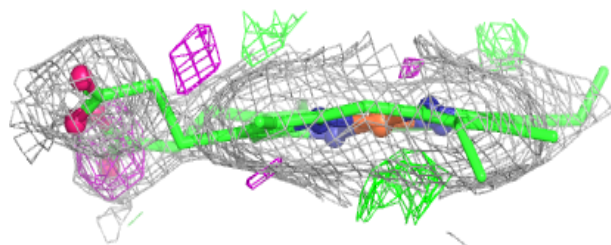
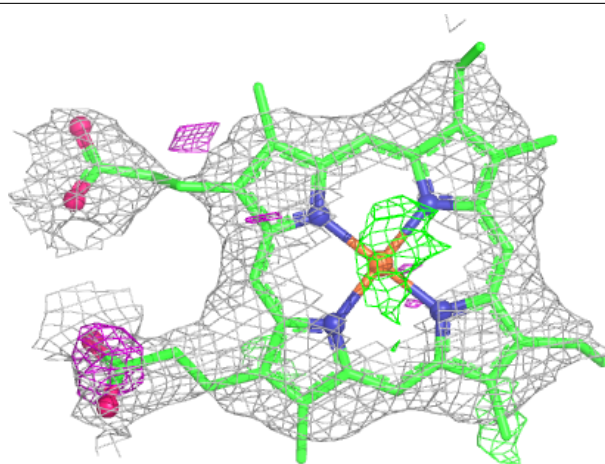
Electron density around HEM B 501:

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



Electron density around HEM A 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.