



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4FXB  
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](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

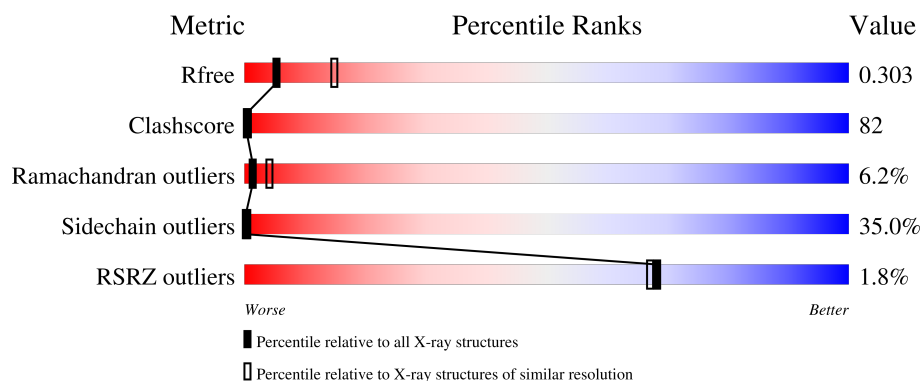
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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 (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

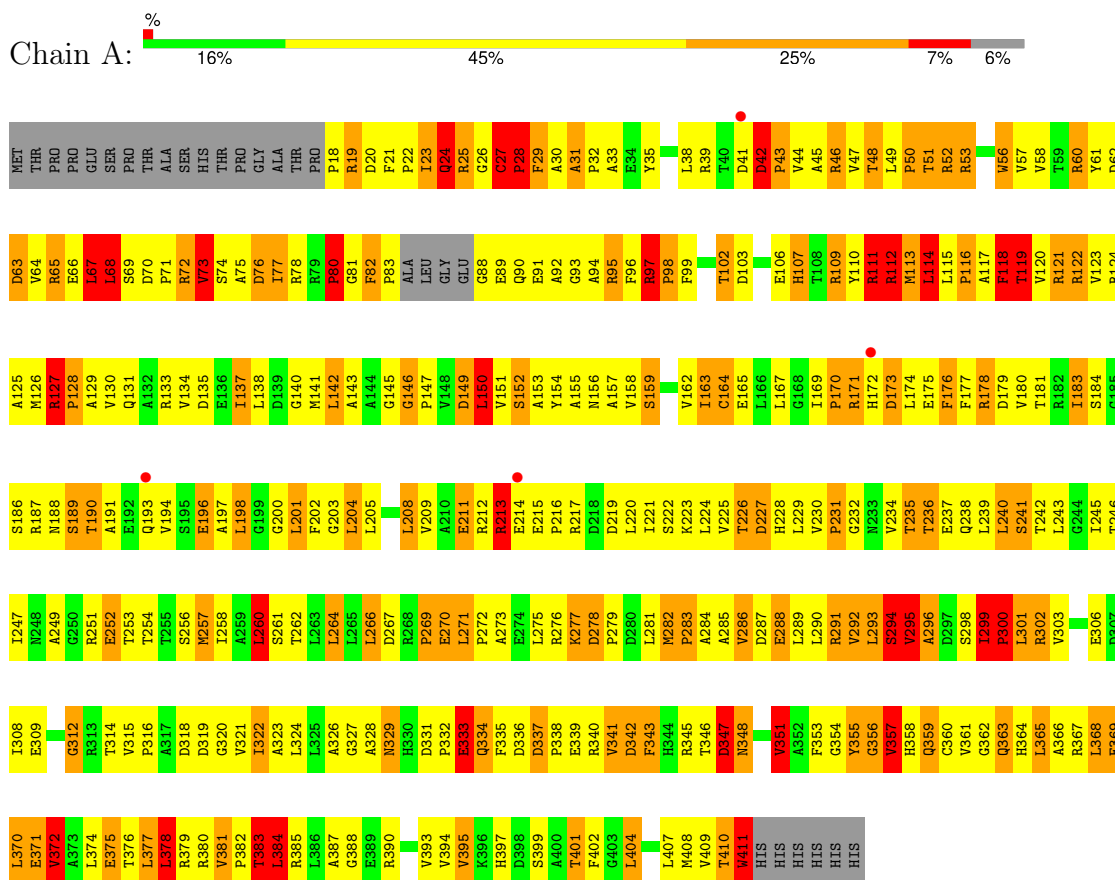
- Molecule 3 is water.

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

### 3 Residue-property plots

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

#### • Molecule 1: Putative cytochrome P450



A373	L374	E375	T376	L377	L378	R379	R380	V381	P382	T383	L384	R385	L386	A387	GLY	E389	R390	D391	Q392	V393	V394	V395	K396	H397	D398	F402	G403	L404	E405	E406	L407	M408	V409	T410	TRP	HIS	HIS	HIS	HIS	HIS																	
L310	R313	T314	V315	P316	A317	D318	D319	G320	V321	T322	A323	L324	L325	A326	G327	D331	P332	E333	Q334	F335	D336	D337	F338	E339	V341	D342	F343	H344	R345	T346	N348	H349	H350	V351	F353	G354	Y355	G356	V357	H358	Q359	C360	V361	G362	Q363	H364	L365	A366	R367	L368	E369	L370	E371	V372			
N248	A249	G250	R251	E252	T253	T254	T255	S256	M257	L258	A259	L260	S261	T262	L263	L264	D267	R268	P269	E270	L271	P272	A273	E274	L275	R276	A277	D278	P279	D280	L281	M282	P283	A284	A285	V286	L289	L290	R291	V292	L293	S294	V295	A296	D297	S298	L299	P300	L301	R302	V303	A304	L305	E306	D307	L308	E309
R122	V123	R124	A125	M126	R127	P128	A129	V130	Q131	A132	R133	V134	D135	E136	I137	L138	D139	G140	M141	L142	A143	G146	P147	V148	D149	L150	V151	S152	A153	Y154	A155	N156	A157	V158	S159	V162	I163	C164	E165	L166	L167	G168	I169	F170	R171	H172	D173	L174	E175	F176	F177	R178	D179	V180	T181	R182	I183
S186	R187	ASN	THR	A191	E192	Q193	V194	S195	E196	A197	L198	G199	G200	L201	L204	L205	G206	G207	L208	E211	R212	R213	E214	E215	P216	R217	D218	D219	L220	I221	S222	K223	L224	V225	T226	D227	H228	L229	V230	P231	G232	M233	V234	T235	Q236	L239	L240	S241	T242	L243	G244	L245	T246	I247			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.2 (19.93-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	4608 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	6021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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

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



## 5 Model quality [i](#)

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

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

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	1.33	8/3076 (0.3%)	1.70	57/4186 (1.4%)
1	B	1.22	2/2905 (0.1%)	1.64	51/3951 (1.3%)
All	All	1.28	10/5981 (0.2%)	1.67	108/8137 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
All	All	0	18

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	GLU	CG-CD	7.48	1.63	1.51
1	A	288	GLU	CD-OE1	6.29	1.32	1.25
1	A	56	TRP	CD2-CE2	6.21	1.48	1.41
1	B	99	PHE	CB-CG	-5.86	1.41	1.51
1	A	411	TRP	CD2-CE2	5.81	1.48	1.41
1	A	355	TYR	CG-CD1	5.68	1.46	1.39
1	A	118	PHE	CB-CG	-5.57	1.41	1.51
1	A	119	THR	CB-CG2	5.22	1.69	1.52
1	B	391	ASP	CB-CG	5.17	1.62	1.51
1	A	288	GLU	CD-OE2	5.07	1.31	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	SER	N-CA-C	13.04	146.20	111.00
1	A	53	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	114	LEU	CA-CB-CG	11.17	140.99	115.30
1	B	186	SER	CB-CA-C	-10.91	89.36	110.10
1	A	53	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	B	303	VAL	CB-CA-C	10.64	131.62	111.40
1	B	112	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	B	304	ALA	N-CA-CB	-9.64	96.61	110.10
1	A	68	LEU	CA-CB-CG	-9.38	93.74	115.30
1	A	114	LEU	N-CA-CB	-9.09	92.23	110.40
1	B	397	HIS	CB-CA-C	-8.81	92.77	110.40
1	B	302	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	98	PRO	N-CA-C	-8.42	90.21	112.10
1	A	240	LEU	CA-CB-CG	-8.26	96.30	115.30
1	A	276	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	A	127	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	97	ARG	N-CA-C	-8.07	89.22	111.00
1	A	368	LEU	CB-CG-CD1	-8.06	97.30	111.00
1	A	301	LEU	N-CA-C	-7.90	89.66	111.00
1	A	60	ARG	NE-CZ-NH2	7.89	124.24	120.30
1	B	99	PHE	CB-CA-C	-7.73	94.93	110.40
1	B	229	LEU	N-CA-C	7.67	131.71	111.00
1	A	291	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	A	63	ASP	CB-CG-OD2	7.54	125.08	118.30
1	A	337	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	357	VAL	CB-CA-C	-7.50	97.15	111.40
1	A	260	LEU	CB-CG-CD2	7.43	123.64	111.00
1	B	395	VAL	CB-CA-C	7.41	125.48	111.40
1	B	260	LEU	CA-CB-CG	-7.35	98.40	115.30
1	B	198	LEU	CB-CG-CD2	-7.30	98.60	111.00
1	B	245	ILE	CB-CA-C	-7.27	97.06	111.60
1	A	60	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	293	LEU	CB-CG-CD1	-7.14	98.87	111.00
1	B	167	LEU	CB-CG-CD2	7.13	123.12	111.00
1	B	66	GLU	CB-CA-C	-7.11	96.18	110.40
1	B	232	GLY	N-CA-C	-7.03	95.52	113.10
1	A	150	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	275	LEU	CB-CG-CD2	-6.92	99.24	111.00
1	B	243	LEU	CA-CB-CG	-6.91	99.42	115.30
1	A	301	LEU	CB-CG-CD1	6.83	122.62	111.00
1	A	188	ASN	N-CA-C	6.76	129.24	111.00
1	B	289	LEU	CA-CB-CG	-6.74	99.79	115.30
1	A	365	LEU	CA-CB-CG	-6.68	99.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	B	286	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	24	GLN	N-CA-C	-6.51	93.43	111.00
1	A	213	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	245	ILE	CG1-CB-CG2	6.40	125.49	111.40
1	B	142	LEU	CA-CB-CG	6.34	129.89	115.30
1	A	384	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	295	VAL	CB-CA-C	-6.31	99.42	111.40
1	B	299	ILE	N-CA-C	6.26	127.90	111.00
1	B	385	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	208	LEU	CB-CG-CD1	6.25	121.62	111.00
1	B	187	ARG	N-CA-C	-6.22	94.21	111.00
1	B	386	LEU	CA-CB-CG	-6.22	101.00	115.30
1	A	63	ASP	CB-CG-OD1	-6.21	112.72	118.30
1	B	337	ASP	N-CA-CB	6.11	121.59	110.60
1	B	115	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	A	375	GLU	N-CA-CB	-6.07	99.68	110.60
1	B	378	LEU	CA-CB-CG	-6.01	101.47	115.30
1	A	257	MET	CG-SD-CE	5.99	109.79	100.20
1	A	260	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	193	GLN	N-CA-CB	-5.93	99.92	110.60
1	A	112	ARG	CG-CD-NE	5.90	124.19	111.80
1	B	396	LYS	N-CA-C	-5.89	95.08	111.00
1	B	280	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	234	VAL	CB-CA-C	-5.84	100.30	111.40
1	A	68	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	A	187	ARG	N-CA-C	5.81	126.69	111.00
1	B	61	TYR	CB-CG-CD1	5.77	124.46	121.00
1	B	192	GLU	CB-CA-C	-5.76	98.88	110.40
1	A	111	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	B	365	LEU	CB-CG-CD2	-5.66	101.37	111.00
1	A	378	LEU	CA-CB-CG	-5.66	102.28	115.30
1	B	176	PHE	CB-CA-C	-5.66	99.09	110.40
1	A	383	THR	CA-C-N	-5.65	104.78	117.20
1	A	291	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	236	THR	CA-CB-CG2	-5.56	104.62	112.40
1	A	25	ARG	N-CA-C	-5.52	96.09	111.00
1	A	318	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	312	GLY	N-CA-C	5.50	126.86	113.10
1	B	286	VAL	CA-CB-CG1	-5.49	102.67	110.90
1	B	282	MET	CG-SD-CE	5.47	108.96	100.20
1	A	198	LEU	CB-CG-CD2	-5.40	101.82	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CA-CB-CG	5.39	127.69	115.30
1	A	277	LYS	CB-CA-C	-5.37	99.66	110.40
1	A	167	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	B	304	ALA	N-CA-C	5.35	125.45	111.00
1	B	290	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	215	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	B	340	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	299	ILE	N-CA-C	-5.29	96.71	111.00
1	B	296	ALA	N-CA-C	-5.27	96.78	111.00
1	A	294	SER	CB-CA-C	5.22	120.02	110.10
1	A	343	PHE	CB-CA-C	-5.21	99.98	110.40
1	B	138	LEU	CB-CG-CD2	5.19	119.82	111.00
1	A	67	LEU	CB-CG-CD1	5.18	119.80	111.00
1	B	303	VAL	N-CA-C	-5.17	97.04	111.00
1	B	163	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	A	372	VAL	CB-CA-C	-5.13	101.64	111.40
1	B	112	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	276	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	340	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	150	LEU	CB-CG-CD1	5.07	119.62	111.00
1	B	121	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	347	ASP	N-CA-C	5.02	124.54	111.00
1	B	369	GLU	CA-CB-CG	5.01	124.42	113.40

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

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Mol	Chain	Res	Type	Group
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	523	0
1	B	2858	0	2870	459	0
2	A	43	0	30	18	0
2	B	43	0	30	25	0
3	A	35	0	0	10	0
3	B	22	0	0	2	0
All	All	6021	0	5935	971	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 82.

All (971) 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: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:A:26:GLY:C	1:A:28:PRO:HD3	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HHA	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:189:SER:HB3	1:A:190:THR:C	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:22:PRO:C	1:B:23:ILE:HG12	1.91	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: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: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:A:229:LEU:C	1:A:229:LEU:HD23	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:O	1:A:83:PRO:C	2.11	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
1:A:96:PHE:O	1:A:97:ARG:C	2.15	0.85
1:A:118:PHE:CZ	1:A:362:GLY:HA2	2.11	0.85
1:B:383:THR:C	1:B:384:LEU:HD13	1.97	0.85
1:A:180:VAL:O	1:A:184:SER:HB2	1.75	0.85
1:B:80:PRO:CB	1:B:303:VAL:HG23	2.07	0.84
1:B:296:ALA:C	1:B:298:SER:H	1.79	0.84
1:A:90:GLN:HB3	1:A:92:ALA:O	1.78	0.84
1:A:25:ARG:C	1:A:27:CYS:H	1.81	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: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:B:107:HIS:ND1	1:B:107:HIS:C	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:230:VAL:HA	1:B:231:PRO:C	2.06	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:93:GLY:C	1:A:95:ARG:H	1.92	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:214:GLU:O	1:B:216:PRO:HD3	1.87	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:B:263:LEU:HG	1:B:264:LEU:N	2.04	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:B:383:THR:O	1:B:384:LEU:HD13	1.90	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: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:229:LEU:C	1:A:229:LEU:CD2	2.59	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:264:LEU:HD12	1:A:264:LEU:C	2.12	0.69
1:B:300:PRO:O	1:B:322:ILE:HG23	1.92	0.69
1:B:260:LEU:HD21	1:B:404:LEU:HD11	1.74	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: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:107:HIS:C	1:B:107:HIS:HD1	1.96	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:18:PRO:O	1:B:48:THR:OG1	2.08	0.69
1:A:410:THR:C	1:A:411:TRP:CD1	2.66	0.69
1:B:278:ASP:OD2	1:B:280:ASP:HB2	1.92	0.69
1:A:21:PHE:CE1	1:A:50:PRO:HD2	2.27	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:25:ARG:C	1:A:27:CYS:N	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:296:ALA:C	1:B:298:SER:N	2.48	0.66
1:A:18:PRO:N	1:A:19:ARG:HH11	1.94	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:27:CYS:N	1:A:28:PRO:HD3	1.95	0.66
1:B:80:PRO:CB	1:B:303:VAL:CG2	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LEU:N	1:B:243:LEU:HD12	2.10	0.65
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:387:ALA:N	1:A:408:MET:O	2.30	0.65
1:B:76:ASP:HA	1:B:101:ARG:C	2.16	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:281:LEU:O	1:A:282:MET:C	2.35	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: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:A:24:GLN:HB3	1:A:25:ARG:C	2.17	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:111:ARG:O	1:A:114:LEU:HB3	1.98	0.63
1:A:332:PRO:C	1:B:121:ARG:HE	2.02	0.63
1:A:387:ALA:H	1:A:409:VAL:HA	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:O	1:B:208:LEU:N	2.32	0.63
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:149:ASP:C	1:B:149:ASP:OD2	2.37	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: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: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:B:346:THR:C	1:B:348:ASN:H	2.02	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:88:GLY:C	1:A:89:GLU:HG2	2.21	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:270:GLU:H	1:A:270:GLU:CD	2.02	0.61
1:A:295:VAL:HG12	1:A:402:PHE:HB3	1.82	0.61
1:B:105:PRO:C	1:B:107:HIS:N	2.52	0.61
1:B:149:ASP:OD2	1:B:152:SER:HB2	2.01	0.61
1:A:229:LEU:CB	1:A:234:VAL:CB	2.79	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HD23	1:A:302:ARG:C	2.21	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: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:229:LEU:C	1:A:234:VAL:CB	2.68	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: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: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: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:A:240:LEU:H	1:A:240:LEU:CD1	2.15	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: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:93:GLY:C	1:A:95:ARG:N	2.57	0.58
1:A:335:PHE:HD2	1:A:347:ASP:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:ASP:OD1	1:A:103:ASP:N	2.33	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:A:119:THR:HB	1:B:333:GLU:CD	2.23	0.57
1:A:387:ALA:N	1:A:409:VAL:HA	2.19	0.57
1:B:205:LEU:O	1:B:206:GLY:C	2.42	0.57
1:B:281:LEU:HD13	1:B:343:PHE:CD2	2.39	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:162:VAL:HG11	1:B:369:GLU:CD	2.25	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
1:B:250:GLY:CA	2:B:501:HEM:C2C	2.88	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:97:ARG:HB3	1:A:98:PRO:CA	2.33	0.56
1:A:292:VAL:CG1	1:A:293:LEU:N	2.69	0.56
1:B:155:ALA:C	1:B:158:VAL:HG12	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:PHE:CZ	1:B:166:LEU:HD21	2.40	0.56
1:B:278:ASP:C	1:B:280:ASP:H	2.09	0.56
1:A:65:ARG:HB2	1:A:355:TYR:CD2	2.40	0.56
1:A:41:ASP:O	1:A:43:PRO:CD	2.54	0.56
1:B:29:PHE:CG	1:B:30:ALA:N	2.74	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:A:184:SER:OG	1:A:198:LEU:HD11	2.05	0.55
1:A:286:VAL:HG21	1:A:370:LEU:HB3	1.87	0.55
1:A:381:VAL:CG2	1:A:381:VAL:O	2.54	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:271:LEU:O	1:A:272:PRO:C	2.45	0.55
1:A:303:VAL:HA	1:A:319:ASP:O	2.07	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:380:ARG:C	1:A:382:PRO:HD3	2.27	0.55
1:B:199:GLY:O	1:B:200:GLY:C	2.44	0.55
1:A:74:SER:CB	1:A:103:ASP:CB	2.80	0.55
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:32:PRO:O	1:A:33:ALA:HB3	2.06	0.55
1:A:236:THR:O	1:A:240:LEU:HD13	2.06	0.55
1:B:126:MET:O	1:B:127:ARG:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:281:LEU:O	1:B:282:MET:C	2.45	0.54
1:A:282:MET:O	1:A:283:PRO:C	2.44	0.54
1:A:298:SER:C	1:A:299:ILE:O	2.41	0.54
1:A:97:ARG:CB	1:A:97:ARG:HH11	2.17	0.54
1:A:278:ASP:C	1:A:278:ASP:OD1	2.45	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: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: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
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:255:THR:O	1:B:256:SER:C	2.47	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:326:ALA:O	1:A:327:GLY:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:235:THR:O	1:A:235:THR:OG1	2.27	0.52
1:B:114:LEU:C	1:B:116:PRO:HD2	2.29	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:242:THR:O	1:B:243:LEU:C	2.46	0.52
1:A:49:LEU:C	1:A:51:THR:H	2.13	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:303:VAL:HG11	1:B:318:ASP:OD1	2.10	0.52
1:A:301:LEU:HD12	1:A:322:ILE:HG13	1.91	0.52
1:B:363:GLN:CG	1:B:364:HIS:H	2.22	0.52
1:A:80:PRO:C	1:A:301:LEU:HD13	2.23	0.52
1:A:118:PHE:CE1	1:A:362:GLY:CA	2.92	0.52
1:A:175:GLU:C	1:A:177:PHE:N	2.62	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:B:230:VAL:O	1:B:230:VAL:HG23	2.10	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: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:384:LEU:HB2	1:A:411:TRP:CD1	2.45	0.51
1:A:232:GLY:C	1:A:234:VAL:H	2.13	0.51
1:B:113:MET:SD	1:B:229:LEU:CD1	2.78	0.51
1:B:150:LEU:C	1:B:152:SER:N	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:GLY:HA3	2:B:501:HEM:C3C	2.45	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: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:B:105:PRO:C	1:B:107:HIS:H	2.14	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: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
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: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: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:94:ALA:O	1:A:95:ARG:C	2.50	0.49
1:A:131:GLN:NE2	1:A:135:ASP:OD1	2.44	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:62:ASP:C	1:B:112:ARG:HH22	2.15	0.49
1:A:354:GLY:C	1:A:359:GLN:HB2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:293:LEU:O	1:A:294:SER:C	2.50	0.49
1:B:178:ARG:O	1:B:182:ARG:HB2	2.11	0.49
1:A:82:PHE:C	1:A:83:PRO:O	2.50	0.49
1:B:105:PRO:O	1:B:106:GLU:C	2.50	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:118:PHE:O	1:A:119:THR:C	2.49	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:A:289:LEU:O	1:A:290:LEU:C	2.51	0.49
1:B:102:THR:CG2	1:B:103:ASP:H	2.25	0.49
1:B:194:VAL:HG12	1:B:195:SER:N	2.28	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:356:GLY:C	1:B:358:HIS:N	2.65	0.48
1:A:240:LEU:O	1:A:241:SER:C	2.49	0.48
1:B:120:VAL:HG22	1:B:364:HIS:CE1	2.48	0.48
1:A:172:HIS:C	1:A:174:LEU:H	2.16	0.48
1:A:235:THR:CG2	1:A:238:GLN:CD	2.79	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:120:VAL:O	1:A:121:ARG:C	2.51	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:A:43:PRO:CD	1:A:44:VAL:N	2.72	0.47
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:238:GLN:O	1:B:239:LEU:C	2.48	0.47
1:B:304:ALA:CB	1:B:315:VAL:HG12	2.43	0.47
1:B:326:ALA:O	1:B:327:GLY:C	2.52	0.47
1:A:62:ASP:OD1	1:A:65:ARG:HD2	2.14	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
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:214:GLU:C	1:B:216:PRO:HD3	2.33	0.47
1:B:331:ASP:HA	1:B:332:PRO:HD2	1.51	0.47
1:A:292:VAL:HG12	1:A:293:LEU:N	2.29	0.47
1:A:356:GLY:C	1:A:358:HIS:H	2.17	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: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: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:A:21:PHE:CD2	1:A:21:PHE:C	2.89	0.47
1:A:25:ARG:HE	1:A:402:PHE:HE2	1.46	0.47
1:A:385:ARG:C	1:A:409:VAL:HG12	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:61:TYR:OH	1:B:349:HIS:HB2	2.15	0.46
1:B:256:SER:OG	1:B:402:PHE:O	2.27	0.46
1:B:297:ASP:OD1	1:B:326:ALA:CB	2.64	0.46
1:B:359:GLN:OE1	1:B:359:GLN:C	2.53	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:278:ASP:C	1:B:280:ASP:N	2.68	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:370:LEU:HD21	1:A:374:LEU:HD11	1.98	0.46
1:B:138:LEU:O	1:B:139:ASP:C	2.54	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: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:A:123:VAL:HG11	1:A:364:HIS:HB3	1.97	0.46
1:B:223:LYS:O	1:B:224:LEU:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG13	1:B:258:ILE:CD1	2.45	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:177:PHE:C	1:A:179:ASP:N	2.70	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: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:B:315:VAL:HA	1:B:316:PRO:HD3	1.69	0.45
1:A:99:PHE:CD1	1:A:99:PHE:C	2.89	0.45
1:A:141:MET:HA	1:A:141:MET:CE	2.46	0.45
1:A:290:LEU:HD13	1:A:353:PHE:CE2	2.51	0.45
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:245:ILE:O	1:B:246:THR:C	2.55	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: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:A:177:PHE:C	1:A:179:ASP:H	2.19	0.45
1:B:38:LEU:O	1:B:42:ASP:C	2.55	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:A:340:ARG:C	1:A:342:ASP:H	2.20	0.45
1:B:75:ALA:C	1:B:101:ARG:O	2.55	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:A:205:LEU:C	1:A:209:VAL:HG23	2.37	0.45
1:B:149:ASP:CB	1:B:408:MET:CG	2.95	0.45
1:B:319:ASP:N	1:B:319:ASP:OD1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:376:THR:O	1:A:377:LEU:C	2.55	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
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:260:LEU:HD13	1:A:293:LEU:HD22	1.99	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: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:A:72:ARG:HH11	1:B:104:ALA:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:112:ARG:C	1:A:114:LEU:H	2.20	0.43
1:A:175:GLU:O	1:A:176:PHE:C	2.57	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
1:A:115:LEU:O	1:A:116:PRO:C	2.57	0.43
1:A:301:LEU:HD21	1:A:320:GLY:CA	2.48	0.43
1:A:371:GLU:O	1:A:372:VAL:C	2.57	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: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:B:211:GLU:C	1:B:213:ARG:N	2.72	0.43
1:A:25:ARG:O	1:A:26:GLY:C	2.56	0.42
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:222:SER:O	1:A:223:LYS:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:346:THR:C	1:B:348:ASN:N	2.69	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:262:THR:O	1:B:263:LEU:C	2.55	0.42
1:B:269:PRO:C	1:B:272:PRO:HD2	2.39	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
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: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:275:LEU:C	1:B:278:ASP:H	2.22	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:110:TYR:O	1:A:111:ARG:C	2.58	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:377:LEU:HD22	1:B:377:LEU:O	2.20	0.42
1:A:112:ARG:C	1:A:114:LEU:N	2.73	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: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:356:GLY:C	1:A:358:HIS:N	2.72	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:A:279:PRO:O	1:A:282:MET:HE2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:379:ARG:O	1:A:382:PRO:HG3	2.21	0.41
1:A:27:CYS:C	1:A:29:PHE:O	2.58	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: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:385:ARG:H	1:B:385:ARG:HG2	1.67	0.41
1:B:403:GLY:C	1:B:404:LEU:HD13	2.41	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:A:351:VAL:C	1:A:353:PHE:N	2.67	0.41
1:B:99:PHE:CE2	1:B:110:TYR:HB2	2.56	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:192:GLU:C	1:B:194:VAL:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HG11	1:A:369:GLU:CG	2.38	0.40
1:A:387:ALA:H	1:A:408:MET:C	2.22	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: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: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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/417 (93%)	261 (68%)	96 (25%)	29 (8%)	<b>1</b>	<b>2</b>
1	B	360/417 (86%)	232 (64%)	111 (31%)	17 (5%)	<b>2</b>	<b>8</b>
All	All	746/834 (89%)	493 (66%)	207 (28%)	46 (6%)	<b>1</b>	<b>4</b>

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	28	PRO
1	A	42	ASP

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Mol	Chain	Res	Type
1	A	50	PRO
1	A	76	ASP
1	A	97	ARG
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

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Mol	Chain	Res	Type
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%)	209 (65%)	113 (35%)	0	0
1	B	306/347 (88%)	199 (65%)	107 (35%)	0	0
All	All	628/694 (90%)	408 (65%)	220 (35%)	0	0

All (220) 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	48	THR
1	A	51	THR
1	A	52	ARG
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

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Mol	Chain	Res	Type
1	A	97	ARG
1	A	102	THR
1	A	107	HIS
1	A	109	ARG
1	A	111	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	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	176	PHE
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	213	ARG
1	A	217	ARG
1	A	224	LEU
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

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	258	ILE
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	306	GLU
1	A	308	ILE
1	A	322	ILE
1	A	329	ASN
1	A	333	GLU
1	A	334	GLN
1	A	339	GLU
1	A	341	VAL
1	A	342	ASP
1	A	346	THR
1	A	347	ASP
1	A	348	ASN
1	A	351	VAL
1	A	357	VAL
1	A	359	GLN
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

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Mol	Chain	Res	Type
1	A	384	LEU
1	A	394	VAL
1	A	395	VAL
1	A	399	SER
1	A	404	LEU
1	A	410	THR
1	A	411	TRP
1	B	23	ILE
1	B	29	PHE
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	74	SER
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	109	ARG
1	B	113	MET
1	B	114	LEU
1	B	120	VAL
1	B	121	ARG
1	B	122	ARG
1	B	123	VAL
1	B	124	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	171	ARG
1	B	172	HIS

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Mol	Chain	Res	Type
1	B	173	ASP
1	B	176	PHE
1	B	178	ARG
1	B	179	ASP
1	B	187	ARG
1	B	198	LEU
1	B	204	LEU
1	B	217	ARG
1	B	218	ASP
1	B	225	VAL
1	B	227	ASP
1	B	228	HIS
1	B	231	PRO
1	B	233	ASN
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	254	THR
1	B	255	THR
1	B	257	MET
1	B	263	LEU
1	B	267	ASP
1	B	270	GLU
1	B	276	ARG
1	B	278	ASP
1	B	280	ASP
1	B	281	LEU
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	313	ARG
1	B	314	THR
1	B	319	ASP
1	B	321	VAL
1	B	322	ILE

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Mol	Chain	Res	Type
1	B	333	GLU
1	B	337	ASP
1	B	339	GLU
1	B	340	ARG
1	B	345	ARG
1	B	347	ASP
1	B	351	VAL
1	B	355	TYR
1	B	357	VAL
1	B	359	GLN
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	384	LEU
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	233	ASN
1	A	238	GLN
1	A	330	HIS
1	A	334	GLN
1	A	344	HIS
1	A	348	ASN
1	A	364	HIS

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Mol	Chain	Res	Type
1	A	397	HIS
1	B	233	ASN
1	B	330	HIS
1	B	364	HIS
1	B	392	GLN
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 monosaccharides 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	42,50,50	1.96	5 (11%)	46,82,82	1.61	6 (13%)
2	HEM	A	501	1	42,50,50	1.95	5 (11%)	46,82,82	1.59	6 (13%)

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	-	9/12/54/54	-
2	HEM	A	501	1	-	8/12/54/54	-

All (10) 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	C3C-C2C	-4.82	1.33	1.40
2	A	501	HEM	C3C-C2C	-4.74	1.34	1.40
2	B	501	HEM	C3C-CAC	3.22	1.54	1.47
2	A	501	HEM	C3C-CAC	3.19	1.54	1.47
2	B	501	HEM	CAB-C3B	2.79	1.54	1.47
2	A	501	HEM	CAB-C3B	2.78	1.54	1.47
2	A	501	HEM	C3C-C4C	2.73	1.45	1.41
2	B	501	HEM	C3C-C4C	2.72	1.45	1.41

All (12) 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	B	501	HEM	C4C-CHD-C1D	3.06	126.60	122.56
2	A	501	HEM	C4C-CHD-C1D	2.79	126.24	122.56
2	B	501	HEM	C4B-CHC-C1C	2.53	125.89	122.56
2	A	501	HEM	C4B-CHC-C1C	2.47	125.82	122.56
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
2	B	501	HEM	C3B-C4B-NB	-2.21	107.88	109.47

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C1A-C2A-CAA-CBA
2	A	501	HEM	C3A-C2A-CAA-CBA
2	A	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C1A-C2A-CAA-CBA
2	B	501	HEM	C3A-C2A-CAA-CBA

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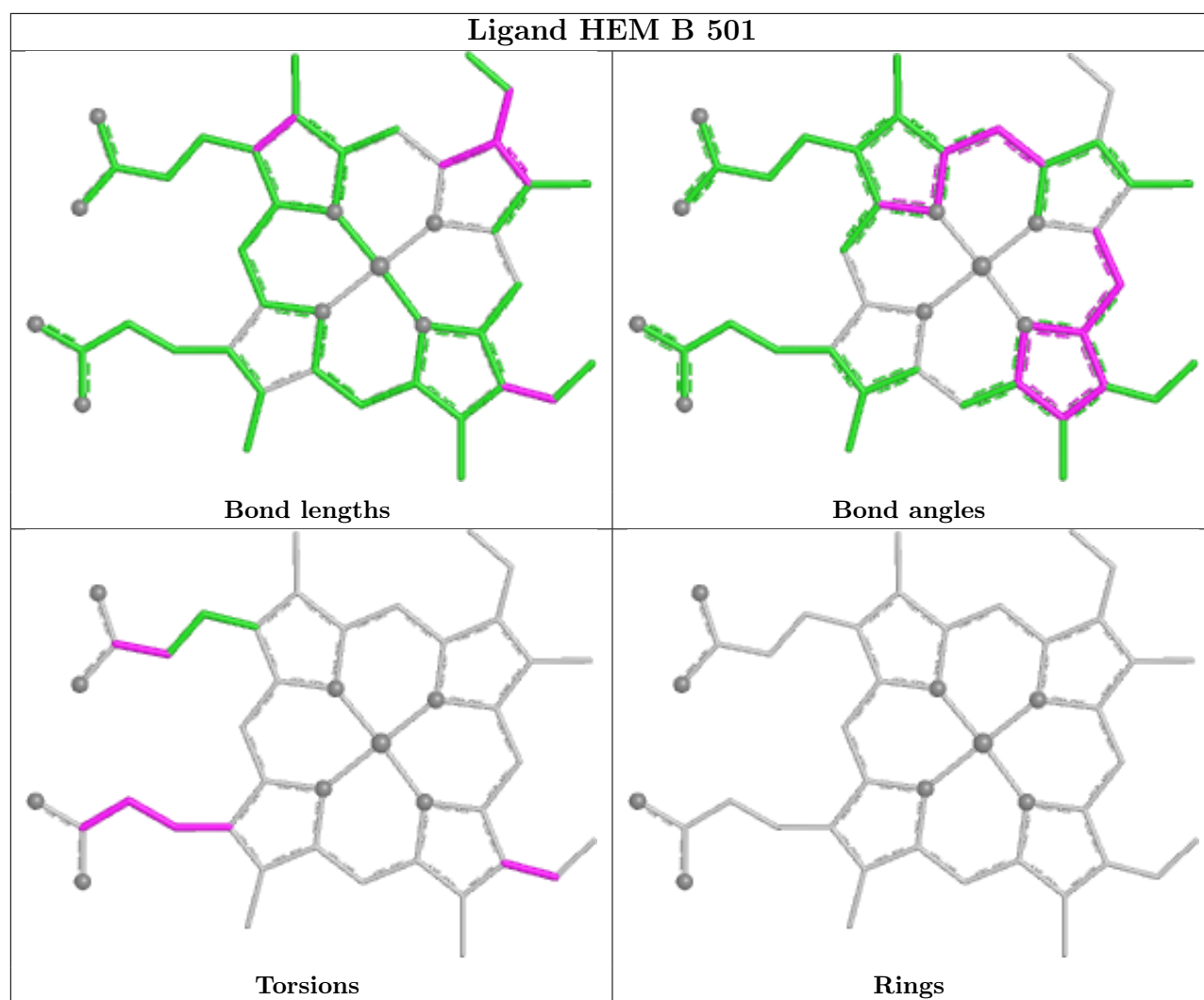
Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C2B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C2A-CAA-CBA-CGA
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	B	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	A	501	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

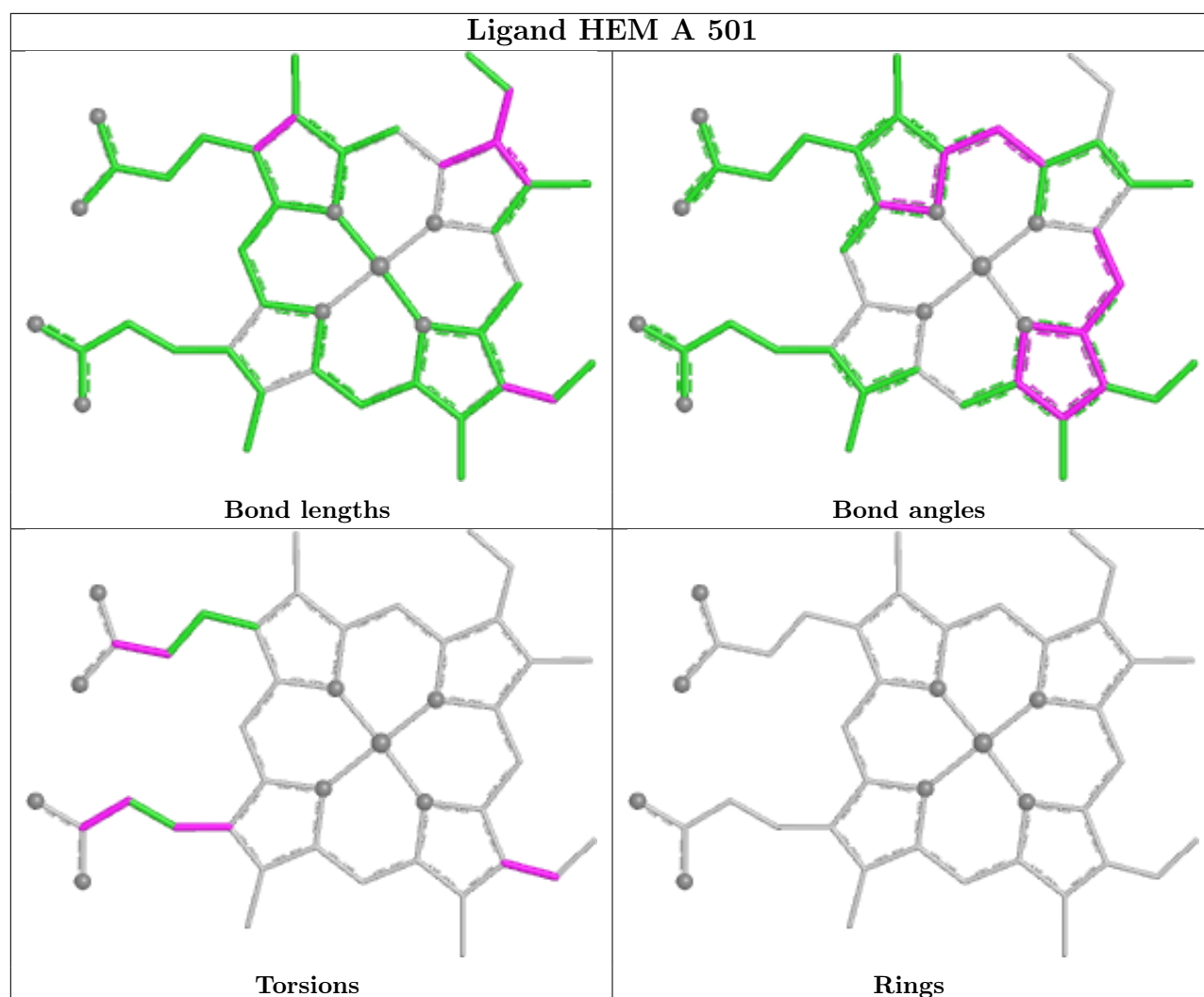
2 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	HEM	25	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	390/417 (93%)	-0.09	4 (1%) 82 82	10, 40, 77, 114	0
1	B	370/417 (88%)	-0.04	10 (2%) 54 50	13, 45, 86, 125	0
All	All	760/834 (91%)	-0.07	14 (1%) 68 67	10, 43, 83, 125	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	HIS	4.4
1	A	214	GLU	3.7
1	A	193	GLN	3.5
1	B	23	ILE	3.0
1	B	52	ARG	2.6
1	B	228	HIS	2.5
1	A	41	ASP	2.5
1	B	193	GLN	2.4
1	B	143	ALA	2.2
1	B	142	LEU	2.1
1	B	101	ARG	2.1
1	B	102	THR	2.1
1	B	110	TYR	2.1
1	B	349	HIS	2.0

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

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

### 6.3 Carbohydrates [i](#)

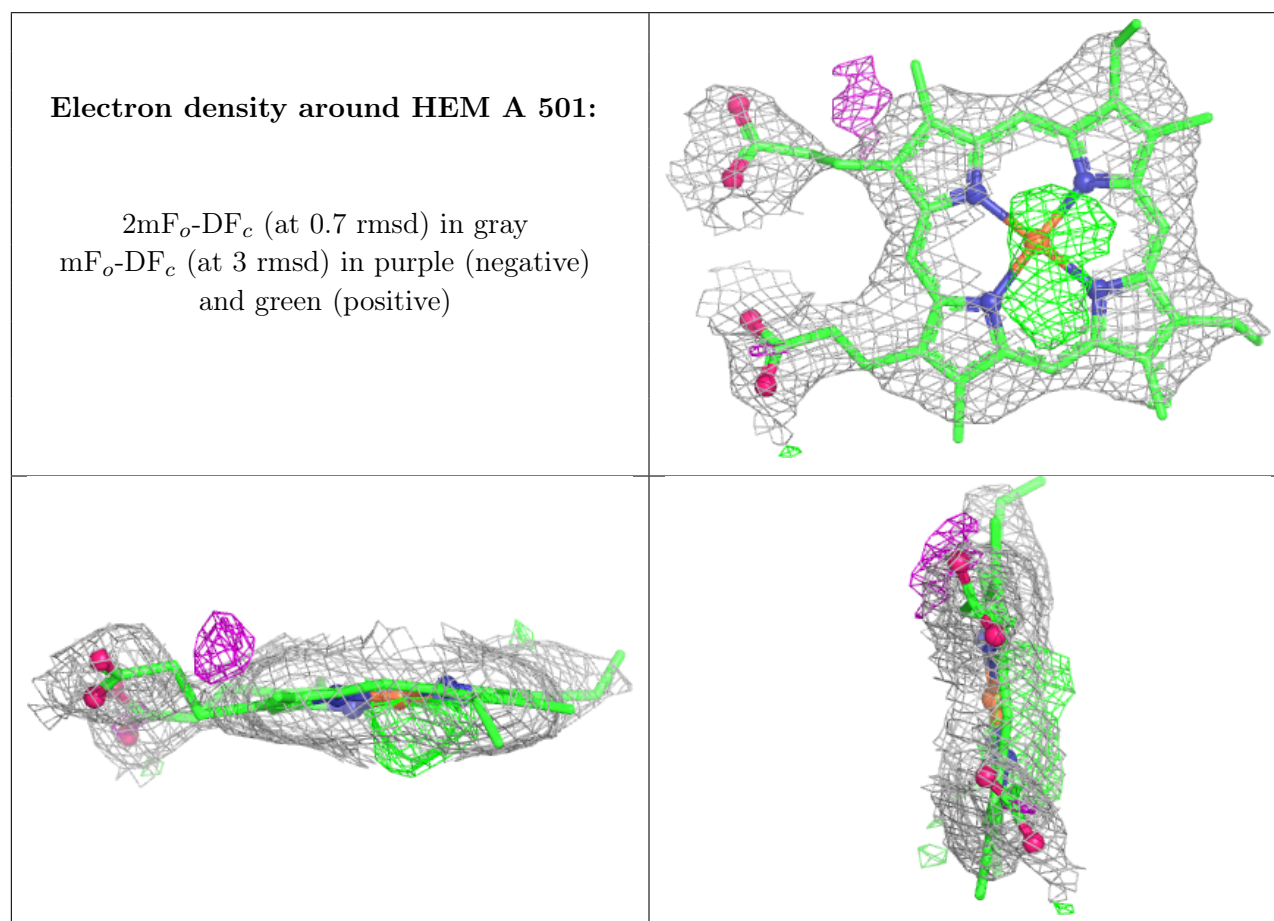
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

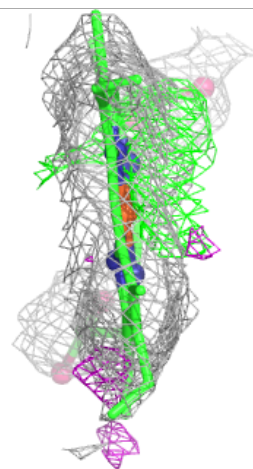
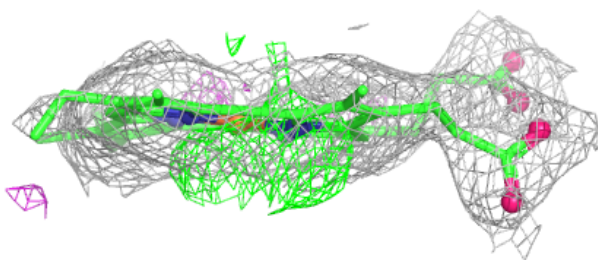
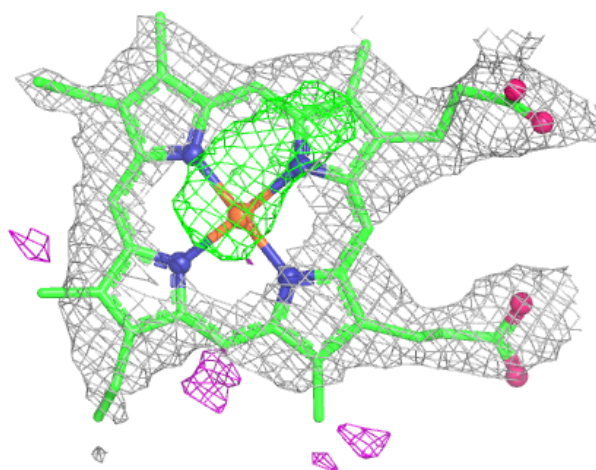
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	A	501	43/43	0.90	0.25	23,31,44,49	0
2	HEM	B	501	43/43	0.92	0.20	21,28,36,46	0

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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.