Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:55 AM EDT

PDB ID	:	1FFT / pdb_00001fft
Title	:	The structure of ubiquinol oxidase from Escherichia coli
Authors	:	Abramson, J.; Riistama, S.; Larsson, G.; Jasaitis, A.; Svensson-Ek, M.; Puustinen, A.; Iwata, S.; Wikstrom, M.
Deposited on	:	2000-07-26
Resolution	:	3.50 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:

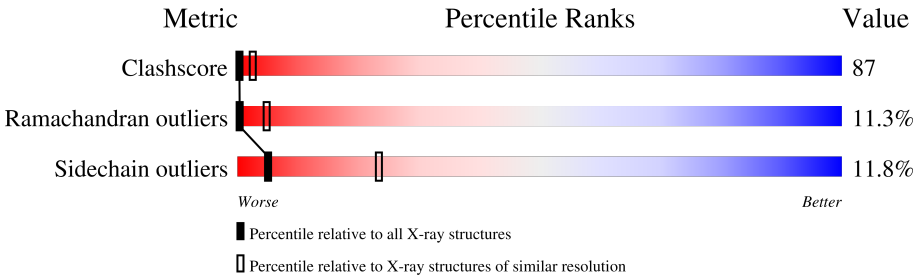
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	663	14% 47% 14% • 24%
1	F	663	15% 46% 13% • 24%
2	B	315	14% 52% 15% • 18%
2	G	315	13% 52% 15% • 18%
3	C	204	18% 53% 18% • 9%
3	H	204	16% 55% 19% • 9%
4	D	109	69% 31%
4	I	109	70% 30%

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
7	HEO	A	1002	X	-	-	-
7	HEO	F	1002	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16136 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 UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	312	0	0
			3954	2654	630	639	31			
1	F	501	Total	C	N	O	S	312	0	0
			3954	2654	630	639	31			

- Molecule 2 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	155	0	0
			2015	1320	324	361	10			
2	G	257	Total	C	N	O	S	155	0	0
			2015	1320	324	361	10			

- Molecule 3 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	185	Total	C	N	O	S	157	0	0
			1451	970	229	240	12			
3	H	185	Total	C	N	O	S	157	0	0
			1451	970	229	240	12			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	cloning artifact	UNP P0ABJ3
C	2	ALA	-	cloning artifact	UNP P0ABJ3
C	3	THR	-	cloning artifact	UNP P0ABJ3
C	4	ASP	-	cloning artifact	UNP P0ABJ3
C	5	THR	-	cloning artifact	UNP P0ABJ3
C	6	LEU	-	cloning artifact	UNP P0ABJ3
C	7	THR	-	cloning artifact	UNP P0ABJ3
C	8	HIS	-	cloning artifact	UNP P0ABJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	9	ALA	-	cloning artifact	UNP P0ABJ3
C	10	THR	-	cloning artifact	UNP P0ABJ3
C	11	ALA	-	cloning artifact	UNP P0ABJ3
C	12	HIS	-	cloning artifact	UNP P0ABJ3
C	13	ALA	-	cloning artifact	UNP P0ABJ3
C	14	HIS	-	cloning artifact	UNP P0ABJ3
C	15	GLU	-	cloning artifact	UNP P0ABJ3
C	16	HIS	-	cloning artifact	UNP P0ABJ3
C	17	GLY	-	cloning artifact	UNP P0ABJ3
C	18	HIS	-	cloning artifact	UNP P0ABJ3
C	19	HIS	-	cloning artifact	UNP P0ABJ3
C	20	ASP	-	cloning artifact	UNP P0ABJ3
C	21	ALA	-	cloning artifact	UNP P0ABJ3
C	22	GLY	-	cloning artifact	UNP P0ABJ3
C	23	GLY	-	cloning artifact	UNP P0ABJ3
C	24	THR	-	cloning artifact	UNP P0ABJ3
H	1	MET	-	cloning artifact	UNP P0ABJ3
H	2	ALA	-	cloning artifact	UNP P0ABJ3
H	3	THR	-	cloning artifact	UNP P0ABJ3
H	4	ASP	-	cloning artifact	UNP P0ABJ3
H	5	THR	-	cloning artifact	UNP P0ABJ3
H	6	LEU	-	cloning artifact	UNP P0ABJ3
H	7	THR	-	cloning artifact	UNP P0ABJ3
H	8	HIS	-	cloning artifact	UNP P0ABJ3
H	9	ALA	-	cloning artifact	UNP P0ABJ3
H	10	THR	-	cloning artifact	UNP P0ABJ3
H	11	ALA	-	cloning artifact	UNP P0ABJ3
H	12	HIS	-	cloning artifact	UNP P0ABJ3
H	13	ALA	-	cloning artifact	UNP P0ABJ3
H	14	HIS	-	cloning artifact	UNP P0ABJ3
H	15	GLU	-	cloning artifact	UNP P0ABJ3
H	16	HIS	-	cloning artifact	UNP P0ABJ3
H	17	GLY	-	cloning artifact	UNP P0ABJ3
H	18	HIS	-	cloning artifact	UNP P0ABJ3
H	19	HIS	-	cloning artifact	UNP P0ABJ3
H	20	ASP	-	cloning artifact	UNP P0ABJ3
H	21	ALA	-	cloning artifact	UNP P0ABJ3
H	22	GLY	-	cloning artifact	UNP P0ABJ3
H	23	GLY	-	cloning artifact	UNP P0ABJ3
H	24	THR	-	cloning artifact	UNP P0ABJ3

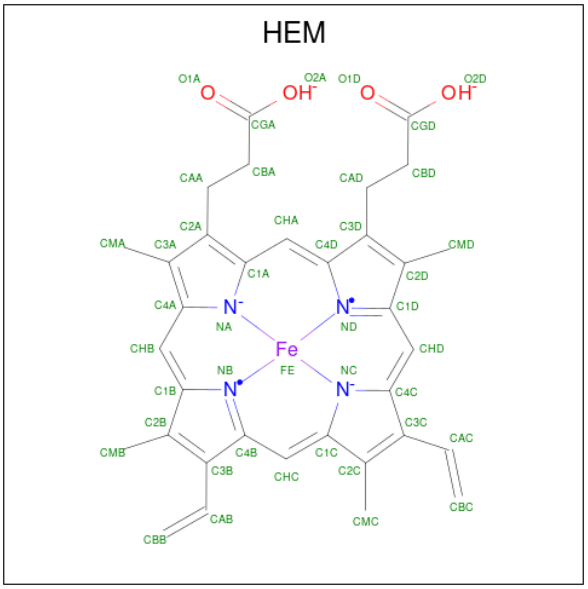
- Molecule 4 is a protein called UBIQUINOL OXIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	109	Total	C	N	O	0	0	0
			545	327	109	109			
4	I	109	Total	C	N	O	0	0	0
			545	327	109	109			

- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cu	0	0
			1	1		
5	F	1	Total	Cu	0	0
			1	1		

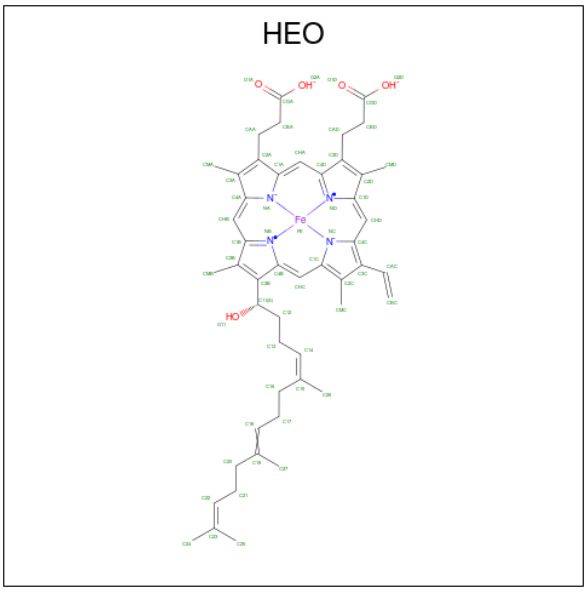
- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 7 is HEME O (CCD ID: HEO) (formula: $C_{49}H_{58}FeN_4O_5$).

HEO



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	0	0
			59	49	1	4	5		
7	F	1	Total	C	Fe	N	O	0	0
			59	49	1	4	5		

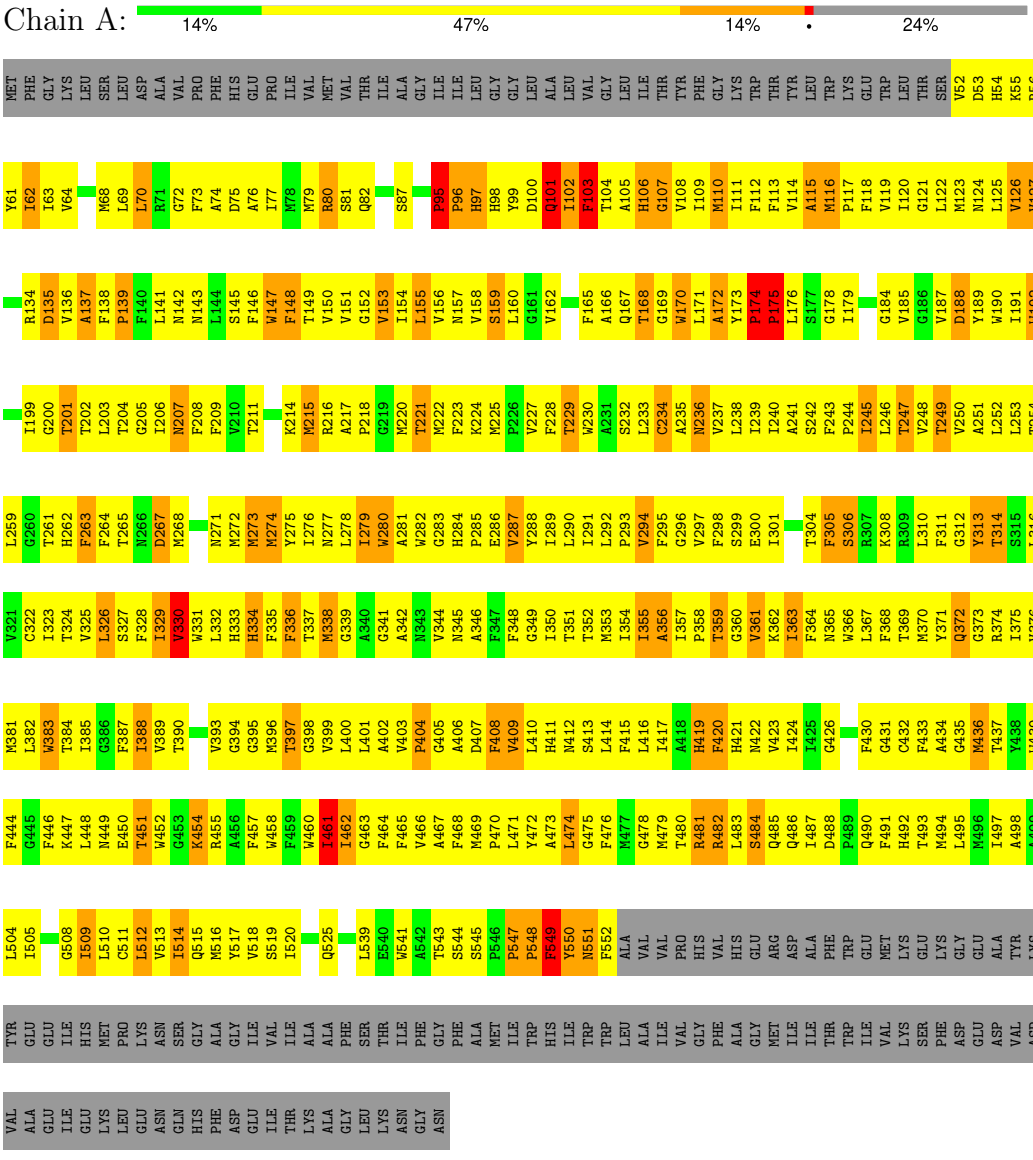
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

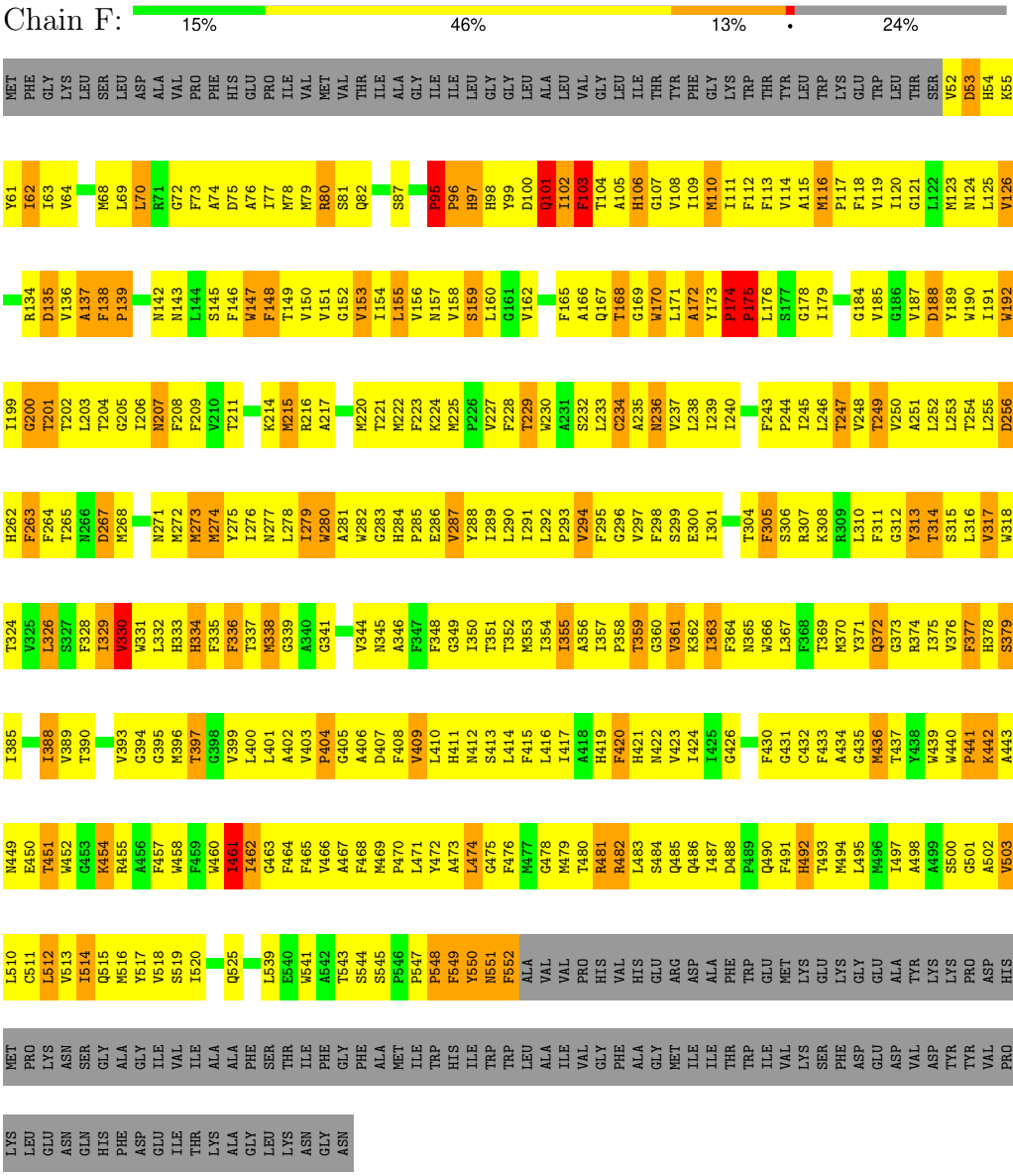
• Molecule 1: UBIQUINOL OXIDASE

Chain A:



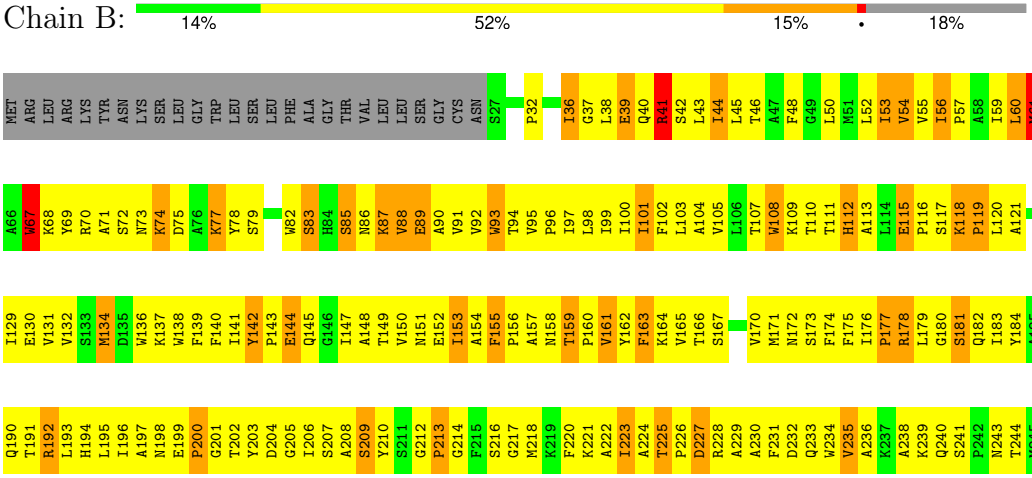
• Molecule 1: UBIQUINOL OXIDASE

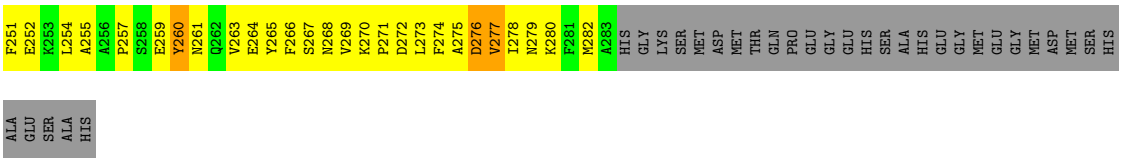
Chain F:



• Molecule 2: UBIQUINOL OXIDASE

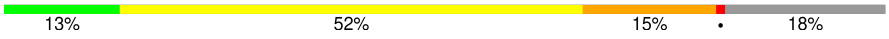
Chain B:

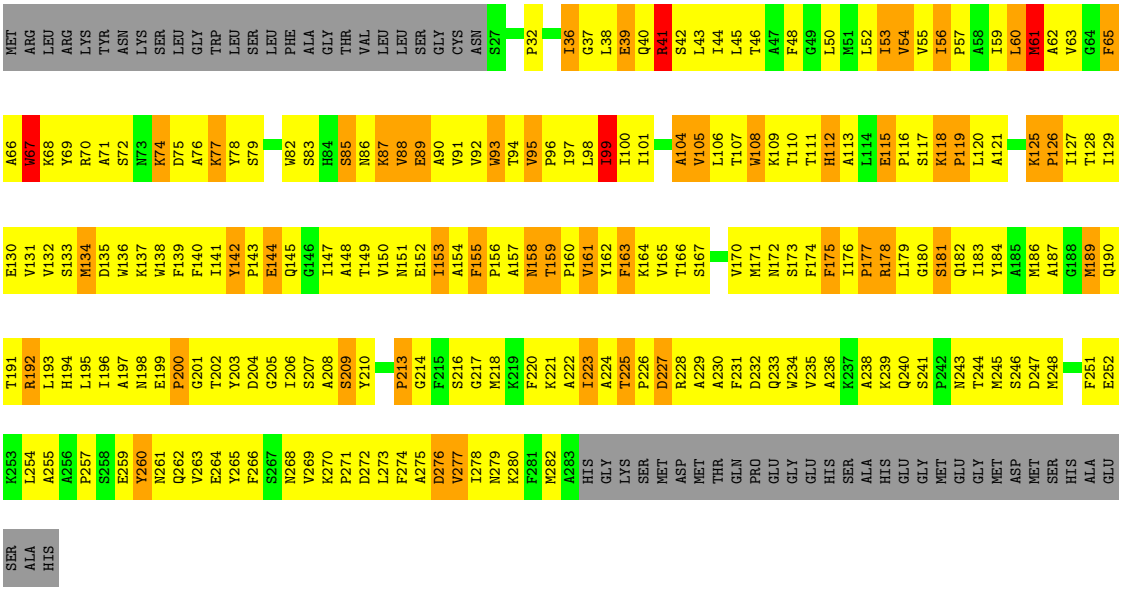




• Molecule 2: UBIQUINOL OXIDASE

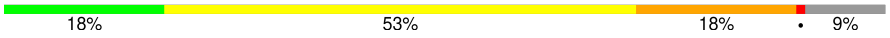
Chain G:

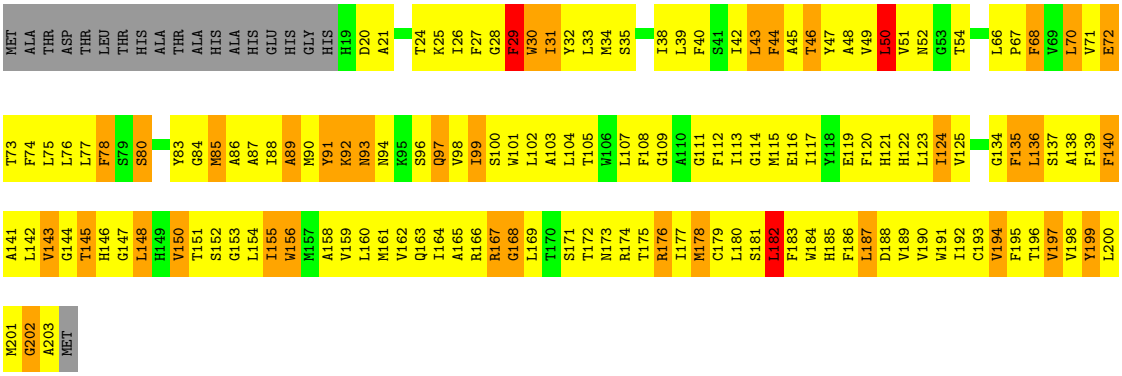




• Molecule 3: UBIQUINOL OXIDASE

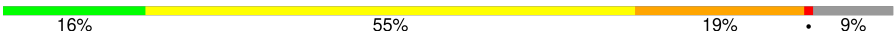
Chain C:





• Molecule 3: UBIQUINOL OXIDASE

Chain H:



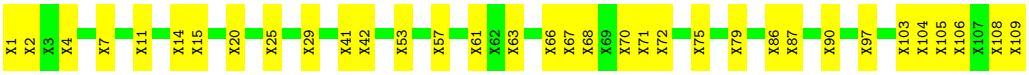




• Molecule 4: UBIQUINOL OXIDASE

Chain D:

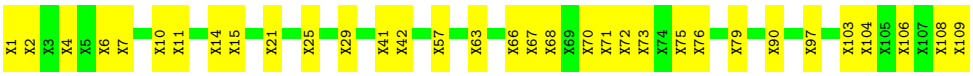




• Molecule 4: UBIQUINOL OXIDASE

Chain I:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	92.10Å 372.50Å 232.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16136	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.55	1/4086 (0.0%)	1.12	44/5573 (0.8%)
1	F	0.54	0/4086	1.08	29/5573 (0.5%)
2	B	0.48	0/2074	1.06	19/2825 (0.7%)
2	G	0.51	0/2074	1.09	22/2825 (0.8%)
3	C	0.57	0/1494	1.10	14/2030 (0.7%)
3	H	0.49	0/1494	1.09	13/2030 (0.6%)
All	All	0.53	1/15308 (0.0%)	1.09	141/20856 (0.7%)

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	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	PRO	C-N	-7.33	1.16	1.33

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	PRO	CA-C-N	14.04	137.38	119.84
1	A	174	PRO	C-N-CA	14.04	137.38	119.84
1	A	175	PRO	CB-CA-C	12.07	131.48	111.56
1	F	175	PRO	CB-CA-C	11.52	130.56	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	174	PRO	CA-C-N	11.09	133.71	119.84
1	F	174	PRO	C-N-CA	11.09	133.71	119.84
1	F	167	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	A	372	GLN	OE1-CD-NE2	-9.96	112.64	122.60
3	H	31	ILE	N-CA-C	-9.95	103.01	112.96
1	F	372	GLN	OE1-CD-NE2	-9.57	113.03	122.60
3	H	136	LEU	N-CA-C	-8.92	99.25	111.56
1	A	167	GLN	OE1-CD-NE2	-8.90	113.70	122.60
3	H	68	PHE	N-CA-C	-8.56	104.86	114.62
3	C	68	PHE	N-CA-C	-8.15	105.33	114.62
1	A	174	PRO	C-N-CD	-7.66	93.59	125.00
3	H	27	PHE	N-CA-C	-7.65	103.83	113.01
2	G	53	ILE	N-CA-C	-7.65	105.70	111.90
2	G	61	MET	N-CA-C	-7.45	104.64	113.21
1	F	167	GLN	CG-CD-NE2	7.39	127.49	116.40
3	C	125	VAL	N-CA-C	-7.19	103.96	111.58
2	G	225	THR	CA-C-N	7.19	126.71	119.24
2	G	225	THR	C-N-CA	7.19	126.71	119.24
1	F	95	PRO	CA-C-N	7.18	128.82	119.84
1	F	95	PRO	C-N-CA	7.18	128.82	119.84
1	A	95	PRO	CA-C-N	7.10	128.72	119.84
1	A	95	PRO	C-N-CA	7.10	128.72	119.84
3	H	182	LEU	N-CA-C	-7.03	106.61	114.62
1	A	549	PHE	CA-C-N	-6.97	112.10	122.83
1	A	549	PHE	C-N-CA	-6.97	112.10	122.83
3	H	125	VAL	N-CA-C	-6.95	104.21	111.58
1	A	372	GLN	CG-CD-NE2	6.88	126.72	116.40
2	B	225	THR	CA-C-N	6.85	126.37	119.24
2	B	225	THR	C-N-CA	6.85	126.37	119.24
1	F	372	GLN	CG-CD-NE2	6.85	126.68	116.40
2	B	61	MET	N-CA-C	-6.85	105.33	113.21
2	B	53	ILE	N-CA-C	-6.84	105.68	111.56
3	C	148	LEU	N-CA-C	-6.74	104.09	112.72
3	C	136	LEU	N-CA-C	-6.66	103.24	112.30
3	H	80	SER	N-CA-C	-6.65	104.74	112.92
2	B	89	GLU	N-CA-C	-6.65	103.96	111.14
3	C	29	PHE	N-CA-C	-6.64	107.05	114.62
1	A	419	HIS	CA-CB-CG	-6.63	107.17	113.80
1	A	547	PRO	CA-N-CD	-6.63	102.72	112.00
3	H	148	LEU	N-CA-C	-6.52	104.38	112.72
1	F	420	PHE	N-CA-C	6.48	119.66	111.69
1	A	173	TYR	CA-C-N	6.42	126.99	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	TYR	C-N-CA	6.42	126.99	120.38
2	B	115	GLU	CA-C-N	6.40	127.83	119.84
2	B	115	GLU	C-N-CA	6.40	127.83	119.84
2	G	115	GLU	CA-C-N	6.38	127.81	119.84
2	G	115	GLU	C-N-CA	6.38	127.81	119.84
2	G	87	LYS	N-CA-C	-6.37	104.66	112.88
2	B	87	LYS	N-CA-C	-6.37	104.67	112.88
1	A	547	PRO	N-CA-C	6.33	118.42	110.70
1	A	167	GLN	CG-CD-NE2	6.28	125.81	116.40
3	H	153	GLY	N-CA-C	-6.26	107.54	115.31
2	G	105	VAL	N-CA-C	-6.20	103.84	110.36
1	A	334	HIS	N-CA-C	-6.18	104.34	113.61
1	A	70	LEU	N-CA-C	-6.16	105.03	112.54
2	G	89	GLU	N-CA-C	-6.09	103.97	111.40
1	F	334	HIS	N-CA-C	-6.06	104.53	113.61
1	F	305	PHE	N-CA-C	6.04	118.65	111.71
1	F	70	LEU	N-CA-C	-5.98	105.24	112.54
2	G	247	ASP	N-CA-C	5.95	118.01	109.14
2	B	102	PHE	N-CA-C	-5.87	104.58	110.97
1	F	215	MET	N-CA-C	5.85	119.55	111.71
2	B	247	ASP	N-CA-C	5.83	117.82	109.14
1	A	215	MET	N-CA-C	5.80	119.48	111.71
3	C	30	TRP	N-CA-C	-5.80	104.96	111.28
3	C	176	ARG	N-CA-C	5.78	117.25	111.07
2	B	88	VAL	N-CA-C	-5.76	104.22	112.35
1	A	218	PRO	CB-CA-C	5.75	118.86	111.56
3	C	153	GLY	N-CA-C	-5.73	108.20	115.31
1	F	173	TYR	CA-C-N	5.73	126.28	120.38
1	F	173	TYR	C-N-CA	5.73	126.28	120.38
1	A	550	TYR	CB-CA-C	5.72	119.92	111.06
2	G	88	VAL	N-CA-C	-5.69	104.33	112.35
3	C	145	THR	N-CA-C	-5.69	104.77	110.97
1	A	548	PRO	CB-CA-C	5.68	118.85	111.64
3	C	80	SER	N-CA-C	-5.67	105.95	112.92
1	A	484	SER	N-CA-C	-5.63	107.06	114.04
1	A	126	VAL	N-CA-C	5.61	119.03	113.53
1	A	174	PRO	O-C-N	-5.61	114.84	121.46
1	A	305	PHE	N-CA-C	5.53	118.83	111.75
2	B	142	TYR	CA-C-N	5.51	124.70	118.97
2	B	142	TYR	C-N-CA	5.51	124.70	118.97
1	F	126	VAL	N-CA-C	5.49	118.91	113.53
3	H	102	LEU	N-CA-C	-5.48	104.53	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	145	THR	N-CA-C	-5.48	104.99	110.97
3	C	91	TYR	N-CA-C	-5.47	102.78	110.50
1	A	319	ALA	N-CA-C	-5.47	104.35	111.02
1	F	319	ALA	N-CA-C	-5.46	104.36	111.02
1	F	173	TYR	N-CA-C	5.43	117.89	110.01
1	F	461	ILE	N-CA-C	-5.43	105.56	110.82
1	A	547	PRO	CA-C-N	-5.42	114.14	119.93
1	A	547	PRO	C-N-CA	-5.42	114.14	119.93
1	A	454	LYS	N-CA-C	-5.41	106.18	112.89
3	C	182	LEU	N-CA-C	-5.41	108.46	114.62
1	A	173	TYR	N-CA-C	5.39	117.83	110.01
1	A	383	TRP	N-CA-C	-5.39	105.30	111.07
1	A	356	ALA	N-CA-C	-5.38	104.84	111.40
1	A	461	ILE	N-CA-C	-5.31	105.91	110.74
1	F	484	SER	N-CA-C	-5.30	107.46	114.04
1	F	57	LEU	N-CA-C	-5.29	105.51	111.28
2	G	104	ALA	CA-C-N	-5.26	113.82	120.60
2	G	104	ALA	C-N-CA	-5.26	113.82	120.60
2	G	135	ASP	N-CA-C	5.26	117.04	108.63
2	G	163	PHE	N-CA-C	5.25	117.29	108.73
1	F	454	LYS	N-CA-C	-5.25	106.38	112.89
1	A	185	VAL	N-CA-C	-5.25	107.64	112.83
2	B	44	ILE	N-CA-C	-5.22	105.29	110.62
1	A	306	SER	N-CA-C	-5.22	106.42	112.89
2	B	235	VAL	N-CA-C	-5.22	105.45	110.72
2	G	60	LEU	N-CA-C	-5.22	105.27	111.69
1	A	420	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	550	TYR	CA-CB-CG	-5.19	104.56	113.90
3	C	70	LEU	N-CA-C	-5.18	105.54	111.14
1	A	87	SER	CB-CA-C	-5.17	109.64	115.79
2	B	60	LEU	N-CA-C	-5.17	105.27	112.45
2	G	99	ILE	CA-C-N	-5.15	113.27	120.53
2	G	99	ILE	C-N-CA	-5.15	113.27	120.53
3	C	178	MET	N-CA-C	-5.15	107.05	113.38
2	G	175	PHE	N-CA-C	5.15	117.74	108.48
1	F	87	SER	CB-CA-C	-5.13	109.69	115.79
1	A	127	VAL	CB-CA-C	-5.12	108.92	114.35
2	G	142	TYR	CA-C-N	5.12	124.74	119.05
2	G	142	TYR	C-N-CA	5.12	124.74	119.05
3	H	185	HIS	CA-CB-CG	-5.12	108.68	113.80
1	F	185	VAL	N-CA-C	-5.11	107.77	112.83
1	F	550	TYR	CA-C-N	5.11	131.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	550	TYR	C-N-CA	5.11	131.29	121.54
2	G	115	GLU	N-CA-C	5.08	115.44	109.60
1	A	221	THR	N-CA-C	-5.08	103.01	110.52
2	B	83	SER	N-CA-C	5.05	119.06	112.13
2	B	115	GLU	N-CA-C	5.05	115.41	109.60
2	B	163	PHE	N-CA-C	5.05	116.97	108.73
3	H	35	SER	N-CA-C	-5.05	107.19	113.55
1	A	57	LEU	N-CA-C	-5.04	105.78	111.28
1	F	127	VAL	CB-CA-C	-5.03	109.02	114.35
1	A	115	ALA	N-CA-C	-5.01	107.21	113.72
1	F	174	PRO	O-C-N	-5.00	115.56	121.46

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	PRO	Mainchain
1	F	174	PRO	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3954	0	3975	695	0
1	F	3954	0	3975	697	0
2	B	2015	0	2016	333	0
2	G	2015	0	2016	367	0
3	C	1451	0	1458	265	0
3	H	1451	0	1458	276	0
4	D	545	0	114	56	0
4	I	545	0	115	53	0
5	A	1	0	0	0	0
5	F	1	0	0	0	0
6	A	43	0	30	18	0
6	F	43	0	30	18	0
7	A	59	0	56	14	0
7	F	59	0	56	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16136	0	15299	2538	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 87.

All (2538) 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)
3:H:86:ALA:HB1	3:H:91:TYR:CD1	1.43	1.53
3:C:78:PHE:HZ	4:D:57:UNK:CB	1.44	1.30
3:H:83:TYR:HE1	4:I:14:UNK:CB	1.44	1.30
1:A:55:LYS:NZ	1:A:551:ASN:HA	1.44	1.29
3:C:78:PHE:CZ	4:D:57:UNK:CB	2.20	1.24
3:H:78:PHE:CZ	4:I:57:UNK:CB	2.21	1.24
3:H:83:TYR:CE1	4:I:14:UNK:CB	2.21	1.23
3:H:78:PHE:HZ	4:I:57:UNK:CB	1.54	1.20
3:C:30:TRP:CH2	4:D:79:UNK:HA	1.79	1.17
2:G:95:VAL:HG23	2:G:96:PRO:CD	1.73	1.16
3:H:86:ALA:CB	3:H:91:TYR:CD1	2.28	1.14
2:G:148:ALA:HB3	2:G:266:PHE:HB2	1.14	1.14
2:G:95:VAL:HG23	2:G:96:PRO:HD2	1.31	1.13
2:G:244:THR:HB	2:G:268:ASN:HB3	1.26	1.12
3:H:90:MET:HE1	4:I:67:UNK:C	1.79	1.12
2:B:95:VAL:HG23	2:B:96:PRO:HD3	1.27	1.12
2:B:147:ILE:HG23	2:B:239:LYS:HE3	1.28	1.12
2:B:244:THR:HB	2:B:268:ASN:HB3	1.26	1.12
2:G:147:ILE:HG23	2:G:239:LYS:HE3	1.32	1.12
3:H:86:ALA:HB1	3:H:91:TYR:CG	1.86	1.11
2:B:148:ALA:HB3	2:B:266:PHE:HB2	1.13	1.10
1:A:551:ASN:O	1:A:552:PHE:O	1.69	1.08
3:C:30:TRP:CH2	4:D:79:UNK:CA	2.37	1.07
1:A:513:VAL:HA	1:A:516:MET:HE2	1.33	1.06
1:F:513:VAL:HA	1:F:516:MET:HE2	1.34	1.05
1:F:373:GLY:HA2	2:G:71:ALA:HB1	1.39	1.03
1:F:357:ILE:HG13	2:G:100:ILE:CD1	1.89	1.03
1:F:308:LYS:HZ2	1:F:372:GLN:H	1.06	1.01
1:A:174:PRO:CB	1:A:175:PRO:HD3	1.87	1.01
1:F:195:GLN:HE22	1:F:247:THR:HG22	1.26	1.00
1:F:474:LEU:HD21	1:F:494:MET:HB2	1.45	0.99
1:F:57:LEU:O	1:F:60:MET:HB2	1.63	0.99
1:A:57:LEU:O	1:A:60:MET:HB2	1.63	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:89:ALA:HB2	3:C:174:ARG:HD2	1.41	0.98
3:C:70:LEU:HD21	3:C:115:MET:HB2	1.44	0.98
3:H:86:ALA:HB1	3:H:91:TYR:CE1	1.98	0.98
1:F:357:ILE:HG13	2:G:100:ILE:HD11	1.46	0.97
1:A:195:GLN:HE22	1:A:247:THR:HG22	1.28	0.97
3:H:89:ALA:HB2	3:H:174:ARG:HD2	1.45	0.97
1:F:284:HIS:O	1:F:287:VAL:HG22	1.63	0.97
3:C:88:ILE:HG12	3:C:98:VAL:HG13	1.44	0.97
3:C:90:MET:HE1	4:D:68:UNK:CA	1.96	0.96
1:A:308:LYS:NZ	1:A:372:GLN:H	1.63	0.96
2:G:176:ILE:HG21	2:G:179:LEU:HD12	1.46	0.96
1:A:308:LYS:HZ2	1:A:372:GLN:H	1.04	0.96
2:B:176:ILE:HG21	2:B:179:LEU:HD12	1.46	0.95
1:F:331:TRP:CZ2	4:I:97:UNK:CB	2.49	0.95
1:A:373:GLY:HA2	2:B:71:ALA:HB1	1.47	0.95
1:A:284:HIS:O	1:A:287:VAL:HG22	1.64	0.95
1:A:474:LEU:HD21	1:A:494:MET:HB2	1.49	0.95
2:B:203:TYR:HB2	2:B:222:ALA:HB3	1.46	0.95
3:H:86:ALA:CB	3:H:91:TYR:CE1	2.48	0.95
2:G:203:TYR:HB2	2:G:222:ALA:HB3	1.46	0.94
3:C:90:MET:HE1	4:D:68:UNK:N	1.82	0.94
3:H:70:LEU:HD21	3:H:115:MET:HB2	1.47	0.94
3:H:104:LEU:HA	3:H:107:LEU:HD12	1.49	0.93
4:I:1:UNK:H	4:I:4:UNK:CB	1.80	0.93
4:D:1:UNK:H	4:D:4:UNK:CB	1.80	0.93
1:A:55:LYS:HZ1	1:A:551:ASN:HA	1.21	0.93
1:A:159:SER:HA	1:A:189:TYR:HD1	1.32	0.93
4:I:1:UNK:N	4:I:4:UNK:CB	2.32	0.92
4:D:1:UNK:N	4:D:4:UNK:CB	2.32	0.92
2:G:95:VAL:HG23	2:G:96:PRO:HD3	1.51	0.92
1:A:55:LYS:HZ3	1:A:551:ASN:HA	1.16	0.92
3:C:169:LEU:HD23	3:C:174:ARG:HA	1.52	0.91
1:F:55:LYS:NZ	1:F:551:ASN:HA	1.85	0.91
1:F:308:LYS:NZ	1:F:372:GLN:H	1.67	0.91
3:C:30:TRP:HH2	4:D:79:UNK:HA	1.32	0.91
2:G:162:TYR:HA	2:G:194:HIS:CD2	2.06	0.91
1:F:234:CYS:SG	1:F:320:THR:HG22	2.11	0.90
2:G:97:ILE:O	2:G:101:ILE:HG13	1.71	0.90
1:A:119:VAL:HG22	1:A:123:MET:HE2	1.52	0.90
1:A:424:ILE:HG21	6:A:1001:HEM:HAC	1.54	0.90
1:F:399:VAL:HG11	7:F:1002:HEO:H252	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:ILE:HG21	6:F:1001:HEM:HAC	1.54	0.90
2:B:162:TYR:HA	2:B:194:HIS:CD2	2.07	0.89
3:C:109:GLY:O	3:C:113:ILE:HD13	1.73	0.89
7:F:1002:HEO:H201	2:G:56:ILE:HG21	1.53	0.89
3:H:40:PHE:CD1	3:H:190:VAL:HG11	2.08	0.89
1:A:374:ARG:HB3	2:B:79:SER:HB3	1.53	0.89
3:C:40:PHE:CD1	3:C:190:VAL:HG11	2.08	0.88
1:A:214:LYS:NZ	3:C:24:THR:HA	1.88	0.88
2:G:244:THR:CB	2:G:268:ASN:HB3	2.03	0.88
2:B:244:THR:CB	2:B:268:ASN:HB3	2.03	0.88
3:H:169:LEU:HD23	3:H:174:ARG:HA	1.55	0.88
3:C:160:LEU:HD13	3:C:176:ARG:HD3	1.53	0.88
1:A:237:VAL:HA	1:A:240:ILE:HD12	1.54	0.87
3:C:104:LEU:HA	3:C:107:LEU:HD12	1.54	0.87
1:F:159:SER:HA	1:F:189:TYR:HD1	1.37	0.87
1:A:174:PRO:HB2	1:A:175:PRO:HD3	1.56	0.87
3:H:88:ILE:HA	3:H:98:VAL:HG22	1.56	0.87
1:A:515:GLN:HG3	1:A:516:MET:N	1.89	0.87
2:B:147:ILE:CG2	2:B:239:LYS:HE3	2.04	0.87
3:H:160:LEU:HD13	3:H:176:ARG:HD3	1.53	0.87
2:B:100:ILE:O	2:B:101:ILE:HG13	1.73	0.87
3:C:88:ILE:HA	3:C:98:VAL:HG22	1.56	0.87
1:A:178:GLY:HA2	1:A:257:ARG:HG2	1.57	0.87
3:H:88:ILE:HG12	3:H:98:VAL:HG13	1.57	0.86
1:A:205:GLY:HA2	1:A:236:ASN:OD1	1.76	0.86
1:F:119:VAL:HG22	1:F:123:MET:HE2	1.55	0.86
1:A:108:VAL:HG22	1:A:170:TRP:HA	1.57	0.86
1:F:395:GLY:HA3	7:F:1002:HEO:H162	1.57	0.86
1:F:205:GLY:HA2	1:F:236:ASN:OD1	1.76	0.86
3:H:90:MET:HE1	4:I:68:UNK:N	1.91	0.86
1:F:515:GLN:HG3	1:F:516:MET:N	1.90	0.86
1:A:331:TRP:CZ2	4:D:97:UNK:CB	2.59	0.85
1:F:237:VAL:HA	1:F:240:ILE:HD12	1.57	0.85
1:F:108:VAL:HG22	1:F:170:TRP:HA	1.58	0.85
1:F:178:GLY:HA2	1:F:257:ARG:HG2	1.58	0.85
1:F:308:LYS:HZ2	1:F:372:GLN:N	1.75	0.85
1:F:225:MET:HE1	1:F:233:LEU:HD11	1.56	0.85
1:A:159:SER:HA	1:A:189:TYR:CD1	2.12	0.85
1:A:225:MET:HE1	1:A:233:LEU:HD11	1.56	0.85
1:A:248:VAL:HG22	3:C:39:LEU:HD12	1.59	0.85
2:G:264:GLU:HG2	2:G:265:TYR:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ILE:HD11	1:A:435:GLY:HA2	1.58	0.85
1:A:55:LYS:NZ	1:A:551:ASN:CA	2.36	0.84
1:A:216:ARG:NH1	1:A:222:MET:HA	1.92	0.84
3:C:45:ALA:O	3:C:49:VAL:HG23	1.76	0.84
1:F:174:PRO:CB	1:F:175:PRO:HD3	2.07	0.84
2:G:147:ILE:CG2	2:G:239:LYS:HE3	2.06	0.84
1:A:98:HIS:O	1:A:102:ILE:HG13	1.78	0.83
2:B:126:PRO:HB3	2:B:160:PRO:HB2	1.60	0.83
1:F:168:THR:HB	1:F:172:ALA:HA	1.60	0.83
2:B:195:LEU:HD23	2:B:196:ILE:N	1.93	0.83
1:A:306:SER:HA	1:A:375:ILE:HA	1.59	0.83
2:B:264:GLU:HG2	2:B:265:TYR:H	1.43	0.83
1:F:157:ASN:HA	1:F:160:LEU:HD12	1.58	0.83
1:F:195:GLN:HE22	1:F:247:THR:CG2	1.91	0.83
1:F:55:LYS:HZ3	1:F:551:ASN:HA	1.42	0.83
1:F:301:ILE:HD11	1:F:435:GLY:HA2	1.58	0.83
2:B:93:TRP:O	2:B:96:PRO:HD2	1.79	0.83
1:F:306:SER:HA	1:F:375:ILE:HA	1.59	0.83
2:G:142:TYR:HB3	2:G:145:GLN:HB2	1.60	0.83
1:A:376:VAL:O	1:A:381:MET:HG2	1.79	0.83
1:F:357:ILE:HD11	2:G:100:ILE:HD12	1.59	0.82
1:F:137:ALA:O	1:F:139:PRO:HD3	1.78	0.82
1:A:69:LEU:HG	1:A:114:VAL:HG11	1.61	0.82
1:A:195:GLN:HE22	1:A:247:THR:CG2	1.91	0.82
2:G:195:LEU:HD23	2:G:196:ILE:N	1.94	0.82
1:A:157:ASN:HA	1:A:160:LEU:HD12	1.58	0.82
1:A:228:PHE:HA	1:A:296:GLY:HA3	1.61	0.82
3:H:72:GLU:OE1	3:H:75:LEU:HD23	1.80	0.82
3:H:156:TRP:NE1	3:H:180:LEU:HD22	1.94	0.82
2:B:41:ARG:H	2:B:41:ARG:HD2	1.42	0.82
1:F:350:ILE:HA	1:F:353:MET:HE2	1.60	0.82
3:H:45:ALA:O	3:H:49:VAL:HG23	1.79	0.82
1:A:367:LEU:HA	1:A:370:MET:HE3	1.60	0.82
1:F:232:SER:O	1:F:236:ASN:HB2	1.80	0.82
2:B:142:TYR:HB3	2:B:145:GLN:HB2	1.60	0.82
3:H:159:VAL:O	3:H:162:VAL:HG12	1.79	0.82
2:B:90:ALA:HA	2:B:93:TRP:HB2	1.62	0.81
1:F:159:SER:HA	1:F:189:TYR:CD1	2.15	0.81
1:F:216:ARG:NH1	1:F:222:MET:HA	1.95	0.81
1:F:228:PHE:HA	1:F:296:GLY:HA3	1.62	0.81
3:H:90:MET:CE	4:I:67:UNK:CB	2.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:TRP:CZ2	1:F:171:LEU:HD21	2.15	0.81
1:F:373:GLY:HA2	2:G:71:ALA:CB	2.10	0.81
3:C:96:SER:HA	3:C:99:ILE:HD13	1.60	0.81
1:A:234:CYS:SG	1:A:320:THR:HG22	2.21	0.81
1:F:353:MET:HG2	1:F:402:ALA:HB1	1.62	0.81
1:A:395:GLY:HA3	7:A:1002:HEO:H162	1.63	0.81
1:A:480:THR:O	1:A:483:LEU:HG	1.81	0.81
2:G:90:ALA:HA	2:G:93:TRP:HB2	1.64	0.80
2:B:192:ARG:NH1	2:B:192:ARG:HB2	1.96	0.80
1:F:69:LEU:HG	1:F:114:VAL:HG11	1.63	0.80
1:F:357:ILE:CD1	2:G:100:ILE:HD12	2.11	0.80
1:A:175:PRO:O	1:A:179:ILE:HD12	1.81	0.80
1:A:232:SER:O	1:A:236:ASN:HB2	1.81	0.80
1:F:276:ILE:HD13	1:F:338:MET:SD	2.21	0.80
2:G:41:ARG:H	2:G:41:ARG:HD2	1.44	0.80
1:F:357:ILE:CG1	2:G:100:ILE:HD12	2.11	0.80
2:G:192:ARG:NH1	2:G:192:ARG:HB2	1.96	0.80
3:H:78:PHE:CE1	4:I:57:UNK:CB	2.65	0.80
3:H:189:VAL:O	3:H:192:ILE:HG22	1.81	0.80
1:A:55:LYS:HZ1	1:A:551:ASN:CA	1.93	0.80
1:F:249:THR:HG23	1:F:278:LEU:HD12	1.62	0.80
1:F:331:TRP:HZ2	4:I:97:UNK:CB	1.95	0.80
3:H:96:SER:HA	3:H:99:ILE:HD13	1.62	0.80
2:G:126:PRO:HB3	2:G:160:PRO:HB2	1.64	0.80
3:C:159:VAL:O	3:C:162:VAL:HG12	1.82	0.79
3:C:185:HIS:CE1	4:D:61:UNK:CB	2.64	0.79
1:F:98:HIS:O	1:F:102:ILE:HG13	1.82	0.79
2:G:254:LEU:HD13	2:G:254:LEU:O	1.82	0.79
1:A:399:VAL:HG11	7:A:1002:HEO:H252	1.65	0.79
1:F:104:THR:O	1:F:108:VAL:HG23	1.82	0.79
3:H:75:LEU:HD21	4:I:21:UNK:CB	2.13	0.79
2:G:67:TRP:C	2:G:69:TYR:H	1.89	0.79
1:A:308:LYS:HZ2	1:A:372:GLN:N	1.79	0.79
3:C:90:MET:HE1	4:D:68:UNK:HA	1.61	0.79
2:B:95:VAL:CG2	2:B:96:PRO:HD3	2.09	0.79
2:G:36:ILE:HD11	2:G:38:LEU:HB2	1.64	0.79
1:A:126:VAL:HG11	1:A:439:TRP:CZ2	2.16	0.78
1:A:452:TRP:HA	1:A:455:ARG:HD2	1.64	0.78
2:B:67:TRP:C	2:B:69:TYR:H	1.89	0.78
2:G:217:GLY:HA3	2:G:260:TYR:CZ	2.18	0.78
1:A:104:THR:O	1:A:108:VAL:HG23	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ILE:HD11	2:B:38:LEU:HB2	1.64	0.78
1:A:249:THR:HG23	1:A:278:LEU:HD12	1.63	0.78
3:C:89:ALA:CB	3:C:174:ARG:HD2	2.13	0.78
3:H:89:ALA:CB	3:H:174:ARG:HD2	2.14	0.78
1:A:159:SER:HB2	1:A:165:PHE:HD1	1.47	0.78
1:A:353:MET:HG2	1:A:402:ALA:HB1	1.64	0.78
1:F:214:LYS:HE3	3:H:24:THR:HG23	1.66	0.78
3:H:174:ARG:HB3	3:H:177:ILE:HD11	1.66	0.78
2:B:217:GLY:HA3	2:B:260:TYR:CZ	2.18	0.78
3:C:72:GLU:OE1	3:C:75:LEU:HD23	1.84	0.78
2:G:270:LYS:HE3	2:G:276:ASP:OD1	1.83	0.78
3:H:91:TYR:OH	4:I:7:UNK:HA	1.83	0.78
3:C:30:TRP:CH2	4:D:79:UNK:O	2.36	0.78
1:F:214:LYS:NZ	3:H:24:THR:HA	1.99	0.78
1:A:137:ALA:O	1:A:139:PRO:HD3	1.82	0.77
1:A:441:PRO:HG3	1:A:447:LYS:HA	1.64	0.77
2:G:87:LYS:O	2:G:91:VAL:HG23	1.83	0.77
1:A:409:VAL:HG13	2:B:180:GLY:HA2	1.66	0.77
1:A:206:ILE:HG23	3:C:31:ILE:CG2	2.14	0.77
3:H:156:TRP:HE1	3:H:180:LEU:HD22	1.50	0.77
1:F:58:GLY:HA2	1:F:124:ASN:HD22	1.49	0.77
1:F:446:PHE:HZ	1:F:520:ILE:HG12	1.48	0.77
1:A:168:THR:HB	1:A:172:ALA:HA	1.65	0.77
1:A:316:LEU:HD23	1:A:361:VAL:HG12	1.66	0.77
2:B:165:VAL:HB	2:B:191:THR:OG1	1.84	0.77
1:A:214:LYS:HE3	3:C:24:THR:HG23	1.65	0.77
1:F:126:VAL:HG11	1:F:439:TRP:CZ2	2.18	0.77
1:F:357:ILE:CG1	2:G:100:ILE:CD1	2.63	0.77
1:F:409:VAL:HG13	2:G:180:GLY:HA2	1.65	0.77
1:A:339:GLY:O	4:D:104:UNK:CB	2.33	0.77
2:B:175:PHE:CD1	2:B:182:GLN:HB2	2.20	0.77
3:C:189:VAL:O	3:C:192:ILE:HG22	1.84	0.77
1:A:446:PHE:HZ	1:A:520:ILE:HG12	1.48	0.77
1:F:137:ALA:N	1:F:215:MET:HE1	2.00	0.77
1:F:159:SER:CA	1:F:189:TYR:HD1	1.97	0.77
2:B:87:LYS:O	2:B:91:VAL:HG23	1.84	0.76
1:F:480:THR:O	1:F:483:LEU:HG	1.85	0.76
1:F:110:MET:HB3	6:F:1001:HEM:HBC2	1.67	0.76
2:G:36:ILE:HG23	2:G:39:GLU:CD	2.10	0.76
1:A:350:ILE:HA	1:A:353:MET:HE2	1.65	0.76
1:F:316:LEU:HD23	1:F:361:VAL:HG12	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:SER:O	1:A:547:PRO:HD3	1.85	0.76
1:A:58:GLY:HA2	1:A:124:ASN:HD22	1.49	0.76
1:F:308:LYS:NZ	1:F:372:GLN:HB2	2.00	0.76
3:C:156:TRP:NE1	3:C:180:LEU:HD22	2.00	0.76
2:G:36:ILE:HG12	2:G:39:GLU:H	1.50	0.76
1:A:308:LYS:NZ	1:A:372:GLN:HB2	2.00	0.76
2:B:270:LYS:HE3	2:B:276:ASP:OD1	1.84	0.76
3:C:77:LEU:HD21	3:C:108:PHE:HB2	1.66	0.76
1:F:376:VAL:O	1:F:381:MET:HG2	1.85	0.76
1:F:400:LEU:HD22	2:G:50:LEU:HD21	1.68	0.76
3:H:77:LEU:HA	3:H:80:SER:HB3	1.67	0.76
1:F:57:LEU:HD23	1:F:60:MET:HG3	1.67	0.75
1:F:110:MET:CB	6:F:1001:HEM:HBC2	2.16	0.75
1:F:452:TRP:HA	1:F:455:ARG:HD2	1.67	0.75
1:A:57:LEU:HD23	1:A:60:MET:HG3	1.67	0.75
3:C:30:TRP:CH2	4:D:79:UNK:C	2.69	0.75
1:F:222:MET:HE1	1:F:225:MET:HE1	1.68	0.75
1:A:214:LYS:CE	3:C:24:THR:HG23	2.16	0.75
2:G:175:PHE:CD1	2:G:182:GLN:HB2	2.22	0.75
3:H:50:LEU:HD11	3:H:134:GLY:HA3	1.68	0.75
1:F:246:LEU:HD22	1:F:282:TRP:CH2	2.22	0.75
1:A:112:PHE:HD2	1:A:194:LEU:HD22	1.51	0.74
1:A:159:SER:CA	1:A:189:TYR:HD1	1.98	0.74
2:G:138:TRP:HZ3	2:G:174:PHE:HD1	1.33	0.74
2:B:254:LEU:O	2:B:254:LEU:HD13	1.87	0.74
2:B:36:ILE:HG23	2:B:39:GLU:CD	2.12	0.74
2:B:193:LEU:HD23	2:B:194:HIS:N	2.02	0.74
3:C:30:TRP:CH2	4:D:79:UNK:CB	2.69	0.74
3:C:85:MET:HE1	3:C:178:MET:HG3	1.67	0.74
3:C:197:VAL:O	3:C:201:MET:HB3	1.87	0.74
1:F:168:THR:HG23	1:F:176:LEU:HB3	1.68	0.74
2:G:173:SER:N	2:G:208:ALA:HB2	2.02	0.74
3:C:34:MET:N	3:C:34:MET:HE2	2.03	0.74
1:F:70:LEU:HD23	1:F:70:LEU:O	1.87	0.74
1:A:405:GLY:HA2	1:A:408:PHE:CD1	2.23	0.74
1:A:551:ASN:O	1:A:552:PHE:C	2.30	0.74
3:C:50:LEU:HD11	3:C:134:GLY:HA3	1.69	0.74
1:F:367:LEU:HA	1:F:370:MET:HE3	1.70	0.74
1:F:441:PRO:HG3	1:F:447:LYS:HA	1.67	0.74
3:H:99:ILE:HD12	3:H:99:ILE:N	2.03	0.74
1:A:110:MET:CB	6:A:1001:HEM:HBC2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:PHE:HA	2:B:181:SER:O	1.87	0.74
2:G:161:VAL:HG23	2:G:195:LEU:O	1.87	0.74
1:A:211:THR:HG23	1:A:215:MET:HE3	1.69	0.74
2:B:184:TYR:CE2	2:B:186:MET:HB2	2.23	0.74
2:G:162:TYR:HA	2:G:194:HIS:HD2	1.50	0.74
1:A:137:ALA:N	1:A:215:MET:HE1	2.03	0.74
2:B:36:ILE:HG12	2:B:39:GLU:H	1.52	0.73
3:H:30:TRP:CH2	4:I:79:UNK:HA	2.23	0.73
1:A:331:TRP:HZ2	4:D:97:UNK:CB	2.00	0.73
1:F:73:PHE:HB3	1:F:77:ILE:HD11	1.69	0.73
3:H:98:VAL:C	3:H:99:ILE:HD12	2.13	0.73
3:C:77:LEU:HA	3:C:80:SER:HB3	1.70	0.73
2:G:95:VAL:CG2	2:G:96:PRO:HD2	2.15	0.73
2:G:184:TYR:CE2	2:G:186:MET:HB2	2.23	0.73
2:G:193:LEU:HD23	2:G:194:HIS:N	2.02	0.73
1:A:246:LEU:HD22	1:A:282:TRP:CH2	2.24	0.73
2:B:138:TRP:HZ3	2:B:174:PHE:HD1	1.34	0.73
1:A:110:MET:HB3	6:A:1001:HEM:HBC2	1.70	0.73
1:A:397:THR:HB	1:A:419:HIS:HD1	1.54	0.73
1:F:112:PHE:HD2	1:F:194:LEU:HD22	1.52	0.73
1:F:211:THR:HG23	1:F:215:MET:HE3	1.68	0.73
3:H:40:PHE:HD1	3:H:190:VAL:HG11	1.50	0.73
3:C:174:ARG:HB3	3:C:177:ILE:HD11	1.71	0.73
1:F:405:GLY:HA2	1:F:408:PHE:CD1	2.23	0.73
2:G:175:PHE:HA	2:G:181:SER:O	1.88	0.73
3:H:78:PHE:HZ	4:I:57:UNK:CA	2.01	0.73
3:H:90:MET:HE2	4:I:67:UNK:CB	2.17	0.73
1:A:276:ILE:HD13	1:A:338:MET:SD	2.28	0.73
3:H:75:LEU:CD2	4:I:21:UNK:CB	2.66	0.73
1:A:349:GLY:O	1:A:353:MET:HG3	1.88	0.73
1:A:221:THR:HG23	1:A:224:LYS:HE3	1.71	0.73
2:B:54:VAL:HA	2:B:57:PRO:CG	2.19	0.73
3:C:90:MET:HE1	4:D:67:UNK:C	2.19	0.73
3:H:197:VAL:O	3:H:201:MET:HB3	1.88	0.73
3:C:40:PHE:HD1	3:C:190:VAL:HG11	1.53	0.73
3:C:78:PHE:CE1	4:D:57:UNK:CB	2.72	0.73
3:C:196:THR:HA	3:C:200:LEU:HD21	1.69	0.73
1:A:111:ILE:HD12	1:A:170:TRP:CE3	2.24	0.72
1:A:482:ARG:NE	6:A:1001:HEM:O1D	2.22	0.72
3:C:197:VAL:HG13	3:C:198:VAL:N	2.04	0.72
2:G:54:VAL:HA	2:G:57:PRO:CG	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:132:VAL:HG12	2:G:134:MET:SD	2.29	0.72
3:C:30:TRP:HH2	4:D:79:UNK:CA	1.92	0.72
2:G:165:VAL:HB	2:G:191:THR:OG1	1.89	0.72
1:A:201:THR:O	1:A:239:ILE:HG21	1.89	0.72
7:A:1002:HEO:H273	7:A:1002:HEO:C26	2.19	0.72
3:C:144:GLY:O	3:C:148:LEU:HG	1.90	0.72
2:G:95:VAL:CG2	2:G:96:PRO:CD	2.63	0.72
1:A:174:PRO:CB	1:A:175:PRO:CD	2.65	0.72
2:B:173:SER:N	2:B:208:ALA:HB2	2.05	0.72
1:F:367:LEU:HD13	2:G:63:VAL:HG11	1.70	0.72
1:F:227:VAL:HG11	1:F:299:SER:OG	1.89	0.72
3:H:197:VAL:HG13	3:H:198:VAL:N	2.05	0.72
2:B:101:ILE:O	2:B:105:VAL:HG23	1.90	0.72
3:C:99:ILE:HD12	3:C:99:ILE:N	2.05	0.72
1:F:406:ALA:HB2	2:G:45:LEU:HD22	1.72	0.72
1:F:482:ARG:NE	6:F:1001:HEM:O1D	2.22	0.72
1:A:70:LEU:HD23	1:A:70:LEU:O	1.90	0.72
1:F:446:PHE:CZ	1:F:520:ILE:HG12	2.24	0.72
1:A:214:LYS:HZ2	3:C:24:THR:HA	1.53	0.71
1:A:222:MET:HE1	1:A:225:MET:CE	2.20	0.71
1:A:308:LYS:CE	1:A:372:GLN:HB2	2.20	0.71
1:F:58:GLY:CA	1:F:124:ASN:HD22	2.02	0.71
1:F:138:PHE:HZ	3:H:28:GLY:HA3	1.55	0.71
1:A:222:MET:HE1	1:A:225:MET:HE1	1.72	0.71
3:H:77:LEU:HD21	3:H:108:PHE:HB2	1.72	0.71
1:A:355:ILE:C	1:A:358:PRO:HD2	2.15	0.71
3:C:156:TRP:HE1	3:C:180:LEU:HD13	1.55	0.71
3:C:164:ILE:O	3:C:168:GLY:HA2	1.90	0.71
1:F:308:LYS:CE	1:F:372:GLN:HB2	2.21	0.71
7:F:1002:HEO:C26	7:F:1002:HEO:H273	2.20	0.71
3:H:34:MET:HE2	3:H:34:MET:N	2.06	0.71
2:B:161:VAL:HG23	2:B:195:LEU:O	1.90	0.71
2:G:246:SER:OG	2:G:268:ASN:ND2	2.24	0.71
3:H:30:TRP:CZ2	4:I:79:UNK:O	2.43	0.71
3:H:78:PHE:CE2	3:H:185:HIS:HE1	2.08	0.71
1:A:58:GLY:CA	1:A:124:ASN:HD22	2.03	0.71
1:F:201:THR:O	1:F:239:ILE:HG21	1.90	0.71
3:H:196:THR:HA	3:H:200:LEU:HD21	1.73	0.71
2:B:235:VAL:O	2:B:239:LYS:HG2	1.90	0.71
1:F:292:LEU:HB2	1:F:293:PRO:HD3	1.73	0.71
1:A:211:THR:HA	1:A:215:MET:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:SER:HB2	1:F:165:PHE:HD1	1.56	0.71
2:G:97:ILE:O	2:G:101:ILE:CG1	2.39	0.71
2:G:235:VAL:O	2:G:239:LYS:HG2	1.90	0.71
1:A:447:LYS:HG3	1:A:448:LEU:H	1.55	0.71
2:B:139:PHE:CE1	2:B:148:ALA:HB1	2.26	0.71
1:F:397:THR:HB	1:F:419:HIS:HD1	1.56	0.71
2:G:203:TYR:O	2:G:221:LYS:HA	1.91	0.71
1:A:168:THR:HG23	1:A:176:LEU:HB3	1.72	0.70
1:A:227:VAL:HG12	1:A:296:GLY:HA2	1.73	0.70
1:A:292:LEU:HB2	1:A:293:PRO:HD3	1.73	0.70
2:B:147:ILE:HD13	2:B:235:VAL:HA	1.73	0.70
1:F:221:THR:HG23	1:F:224:LYS:HE3	1.73	0.70
1:F:481:ARG:HG2	1:F:482:ARG:HG3	1.72	0.70
3:H:156:TRP:HE1	3:H:180:LEU:HD13	1.56	0.70
1:A:73:PHE:HB3	1:A:77:ILE:HD11	1.73	0.70
2:B:203:TYR:O	2:B:221:LYS:HA	1.91	0.70
1:A:446:PHE:CZ	1:A:520:ILE:HG12	2.25	0.70
1:F:276:ILE:HG22	1:F:335:PHE:CZ	2.27	0.70
2:G:147:ILE:HD13	2:G:235:VAL:HA	1.74	0.70
2:B:45:LEU:HD12	2:B:110:THR:HG21	1.74	0.70
1:F:274:MET:HA	1:F:274:MET:HE2	1.74	0.70
3:H:158:ALA:O	3:H:161:MET:HB3	1.91	0.70
1:A:276:ILE:HG22	1:A:335:PHE:CZ	2.27	0.70
2:B:148:ALA:HB3	2:B:266:PHE:CB	2.07	0.70
3:C:78:PHE:HZ	4:D:57:UNK:CA	2.05	0.70
2:G:61:MET:HA	2:G:61:MET:HE3	1.73	0.70
2:G:125:LYS:H	2:G:126:PRO:CD	2.03	0.70
1:A:227:VAL:HG11	1:A:299:SER:OG	1.91	0.70
1:A:414:LEU:HD12	1:A:471:LEU:HB3	1.74	0.70
3:C:158:ALA:O	3:C:161:MET:HB3	1.91	0.70
1:F:257:ARG:CB	1:F:257:ARG:HH11	2.04	0.70
3:C:30:TRP:CZ2	4:D:79:UNK:O	2.45	0.69
1:F:414:LEU:HD12	1:F:471:LEU:HB3	1.74	0.69
2:G:45:LEU:HD12	2:G:110:THR:HG21	1.74	0.69
1:A:227:VAL:HG21	1:A:310:LEU:HD22	1.74	0.69
2:B:162:TYR:HA	2:B:194:HIS:HD2	1.53	0.69
3:C:156:TRP:HE1	3:C:180:LEU:HD22	1.56	0.69
1:A:274:MET:HA	1:A:274:MET:HE2	1.74	0.69
1:F:239:ILE:CG1	1:F:289:ILE:HD13	2.22	0.69
2:G:184:TYR:HE2	2:G:189:MET:HE2	1.57	0.69
2:B:125:LYS:H	2:B:126:PRO:CD	2.03	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:TYR:O	1:F:317:VAL:HG23	1.93	0.69
1:A:62:ILE:H	1:A:62:ILE:HD12	1.57	0.69
1:F:329:ILE:O	1:F:330:VAL:HG13	1.91	0.69
3:H:90:MET:CE	4:I:67:UNK:C	2.65	0.69
1:A:220:MET:HG3	1:A:224:LYS:HB2	1.75	0.69
1:A:382:LEU:HD23	1:A:385:ILE:HD12	1.74	0.69
1:F:174:PRO:C	1:F:176:LEU:H	1.99	0.69
1:F:227:VAL:HG12	1:F:296:GLY:HA2	1.75	0.69
1:F:227:VAL:HG21	1:F:310:LEU:HD22	1.74	0.69
1:F:355:ILE:C	1:F:358:PRO:HD2	2.17	0.69
2:G:67:TRP:C	2:G:69:TYR:N	2.50	0.69
3:C:70:LEU:HD23	3:C:115:MET:HE3	1.74	0.69
3:C:98:VAL:C	3:C:99:ILE:HD12	2.18	0.69
1:F:239:ILE:HG13	1:F:289:ILE:HD13	1.74	0.69
2:G:148:ALA:HB3	2:G:266:PHE:CB	2.08	0.69
3:H:144:GLY:O	3:H:148:LEU:HG	1.93	0.69
2:B:90:ALA:CA	2:B:93:TRP:HB2	2.22	0.69
2:B:205:GLY:HA3	2:B:220:PHE:CE1	2.28	0.69
3:C:77:LEU:HD13	3:C:184:TRP:HZ2	1.56	0.69
1:F:62:ILE:HD12	1:F:62:ILE:H	1.57	0.69
1:F:216:ARG:HH12	1:F:221:THR:C	2.01	0.69
1:F:308:LYS:HZ2	1:F:372:GLN:HB2	1.58	0.69
1:A:209:PHE:HE2	3:C:31:ILE:CD1	2.06	0.69
1:A:332:LEU:HB2	1:A:348:PHE:CB	2.23	0.69
3:C:86:ALA:HB1	3:C:91:TYR:CG	2.28	0.69
1:A:257:ARG:CB	1:A:257:ARG:HH11	2.05	0.69
1:F:440:TRP:HE1	1:F:446:PHE:HE1	1.41	0.69
2:G:139:PHE:CE1	2:G:148:ALA:HB1	2.28	0.69
3:H:164:ILE:O	3:H:168:GLY:HA2	1.93	0.69
4:I:66:UNK:O	4:I:67:UNK:C	2.41	0.69
2:B:199:GLU:OE2	2:B:200:PRO:HD2	1.92	0.68
4:D:66:UNK:O	4:D:67:UNK:C	2.41	0.68
1:F:137:ALA:H	1:F:215:MET:HE1	1.57	0.68
1:F:220:MET:HG3	1:F:224:LYS:HB2	1.75	0.68
1:F:227:VAL:HG11	1:F:299:SER:CB	2.23	0.68
1:A:216:ARG:HH12	1:A:221:THR:C	2.01	0.68
2:G:90:ALA:CA	2:G:93:TRP:HB2	2.22	0.68
1:A:239:ILE:CG1	1:A:289:ILE:HD13	2.23	0.68
1:A:308:LYS:NZ	1:A:372:GLN:N	2.37	0.68
1:A:152:GLY:O	1:A:156:VAL:HG23	1.94	0.68
1:F:175:PRO:O	1:F:179:ILE:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:GLY:O	1:F:353:MET:HG3	1.94	0.68
1:F:447:LYS:HG3	1:F:448:LEU:H	1.57	0.68
1:F:543:THR:HG22	1:F:544:SER:N	2.08	0.68
1:F:551:ASN:O	1:F:552:PHE:HB2	1.93	0.68
3:H:104:LEU:O	3:H:107:LEU:HB2	1.93	0.68
1:F:225:MET:HE1	1:F:233:LEU:CD1	2.24	0.68
1:A:403:VAL:HG13	2:B:107:THR:HG23	1.74	0.68
1:A:481:ARG:HG2	1:A:482:ARG:HG3	1.75	0.68
2:G:140:PHE:HB2	2:G:149:THR:OG1	1.94	0.68
1:A:96:PRO:O	1:A:97:HIS:C	2.35	0.68
1:A:400:LEU:HD22	2:B:50:LEU:HD21	1.75	0.68
2:B:67:TRP:C	2:B:69:TYR:N	2.52	0.68
1:F:111:ILE:HD11	6:F:1001:HEM:CMD	2.24	0.68
2:G:199:GLU:OE2	2:G:200:PRO:HD2	1.92	0.68
2:G:205:GLY:HA3	2:G:220:PHE:CE1	2.29	0.68
1:A:252:LEU:HD22	1:A:263:PHE:CZ	2.28	0.68
1:F:152:GLY:O	1:F:156:VAL:HG23	1.94	0.68
1:F:174:PRO:CB	1:F:175:PRO:CD	2.72	0.68
1:A:154:ILE:O	1:A:158:VAL:HG23	1.93	0.67
1:A:332:LEU:HB2	1:A:348:PHE:HB3	1.76	0.67
7:A:1002:HEO:H273	7:A:1002:HEO:H262	1.76	0.67
1:F:382:LEU:HD23	1:F:385:ILE:HD12	1.75	0.67
2:G:204:ASP:HA	2:G:220:PHE:O	1.94	0.67
3:H:102:LEU:HD23	3:H:161:MET:HE3	1.74	0.67
1:F:175:PRO:O	2:G:170:VAL:HG12	1.95	0.67
2:G:50:LEU:O	2:G:54:VAL:HG13	1.94	0.67
2:B:246:SER:OG	2:B:268:ASN:ND2	2.28	0.67
3:H:77:LEU:HD13	3:H:184:TRP:HZ2	1.58	0.67
2:B:61:MET:HA	2:B:61:MET:HE3	1.75	0.67
2:B:175:PHE:HB2	2:B:182:GLN:HG3	1.77	0.67
2:B:204:ASP:HA	2:B:220:PHE:O	1.94	0.67
3:H:96:SER:C	3:H:98:VAL:H	2.01	0.67
1:A:58:GLY:HA3	1:A:125:LEU:HB2	1.77	0.67
1:A:220:MET:HA	1:A:224:LYS:HD2	1.75	0.67
1:A:227:VAL:HG11	1:A:299:SER:CB	2.24	0.67
1:A:329:ILE:O	1:A:330:VAL:HG13	1.93	0.67
7:A:1002:HEO:H241	2:B:100:ILE:HG12	1.77	0.67
1:F:174:PRO:HB3	1:F:175:PRO:HD3	1.77	0.67
1:F:257:ARG:HH11	1:F:257:ARG:HB3	1.57	0.67
1:F:373:GLY:CA	2:G:71:ALA:HB1	2.21	0.67
1:F:466:VAL:C	1:F:501:GLY:HA3	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:PHE:HE1	1:A:286:GLU:OE2	1.78	0.67
1:A:284:HIS:HB3	1:A:285:PRO:HD3	1.76	0.67
3:C:94:ASN:HB2	3:C:97:GLN:NE2	2.10	0.67
1:F:96:PRO:O	1:F:97:HIS:C	2.35	0.67
1:F:252:LEU:HD22	1:F:263:PHE:CZ	2.29	0.67
1:F:255:LEU:HD23	1:F:259:LEU:HD12	1.77	0.67
1:A:551:ASN:C	1:A:552:PHE:O	2.38	0.67
1:F:308:LYS:NZ	1:F:372:GLN:N	2.38	0.67
2:G:203:TYR:O	2:G:221:LYS:HG3	1.95	0.67
1:A:174:PRO:C	1:A:176:LEU:H	2.00	0.67
1:A:225:MET:HE1	1:A:233:LEU:CD1	2.26	0.67
2:B:140:PHE:HB2	2:B:149:THR:OG1	1.95	0.67
1:F:211:THR:HA	1:F:215:MET:HE2	1.77	0.67
2:G:141:ILE:HD13	2:G:273:LEU:HB3	1.76	0.67
4:I:70:UNK:O	4:I:71:UNK:CB	2.42	0.67
1:A:117:PRO:O	1:A:121:GLY:N	2.28	0.66
1:F:390:THR:O	1:F:393:VAL:HB	1.94	0.66
3:H:160:LEU:HD22	3:H:176:ARG:NH1	2.10	0.66
1:A:214:LYS:HZ1	3:C:24:THR:HA	1.61	0.66
1:F:58:GLY:HA3	1:F:125:LEU:HB2	1.77	0.66
3:H:84:GLY:O	3:H:88:ILE:HG13	1.94	0.66
3:C:102:LEU:HD23	3:C:161:MET:HE3	1.75	0.66
1:F:316:LEU:HG	1:F:365:ASN:HD22	1.60	0.66
1:A:137:ALA:H	1:A:215:MET:HE1	1.59	0.66
7:F:1002:HEO:H273	7:F:1002:HEO:H262	1.77	0.66
2:G:175:PHE:HB2	2:G:182:GLN:HG3	1.78	0.66
4:I:1:UNK:O	4:I:2:UNK:C	2.41	0.66
1:A:313:TYR:O	1:A:317:VAL:HG23	1.96	0.66
1:A:390:THR:O	1:A:393:VAL:HB	1.94	0.66
1:F:220:MET:HA	1:F:224:LYS:HD2	1.76	0.66
3:H:85:MET:O	3:H:88:ILE:HB	1.96	0.66
1:A:170:TRP:CZ2	1:A:171:LEU:HD21	2.29	0.66
1:A:410:LEU:O	1:A:413:SER:HB3	1.95	0.66
3:C:96:SER:C	3:C:98:VAL:H	2.02	0.66
3:C:134:GLY:HA2	3:C:137:SER:HB3	1.78	0.66
4:D:70:UNK:O	4:D:71:UNK:CB	2.42	0.66
1:F:112:PHE:HE1	1:F:286:GLU:OE2	1.79	0.66
1:F:125:LEU:O	1:F:125:LEU:HD23	1.96	0.66
1:F:332:LEU:HB2	1:F:348:PHE:CB	2.25	0.66
2:G:98:LEU:HA	2:G:101:ILE:HD12	1.77	0.66
2:G:171:MET:HG3	2:G:210:TYR:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:30:TRP:HZ2	4:I:79:UNK:O	1.77	0.66
2:B:150:VAL:HG12	2:B:151:ASN:HD22	1.60	0.66
1:F:80:ARG:HG3	1:F:80:ARG:O	1.95	0.66
1:F:339:GLY:O	4:I:104:UNK:CB	2.43	0.66
2:G:60:LEU:C	2:G:62:ALA:H	2.04	0.66
2:B:50:LEU:O	2:B:54:VAL:HG13	1.96	0.66
1:F:117:PRO:O	1:F:121:GLY:N	2.29	0.66
1:F:367:LEU:HA	1:F:370:MET:CE	2.26	0.66
2:G:131:VAL:HB	2:G:165:VAL:HG13	1.78	0.66
2:B:128:THR:HA	2:B:162:TYR:HB2	1.78	0.65
3:C:90:MET:CE	4:D:68:UNK:N	2.58	0.65
4:D:1:UNK:O	4:D:2:UNK:C	2.41	0.65
3:C:103:ALA:HA	3:C:161:MET:HE1	1.78	0.65
1:F:69:LEU:HD22	1:F:73:PHE:CD1	2.31	0.65
1:F:274:MET:HE3	3:H:49:VAL:HG21	1.78	0.65
1:F:282:TRP:C	1:F:285:PRO:HD2	2.21	0.65
1:F:346:ALA:HB1	1:F:350:ILE:CD1	2.27	0.65
1:F:187:VAL:O	1:F:191:ILE:HG13	1.96	0.65
2:G:36:ILE:CG1	2:G:39:GLU:H	2.09	0.65
1:A:257:ARG:HH11	1:A:257:ARG:HB3	1.59	0.65
2:B:131:VAL:HB	2:B:165:VAL:HG13	1.79	0.65
1:F:54:HIS:CD2	1:F:128:PRO:HG2	2.31	0.65
1:F:257:ARG:HB3	1:F:257:ARG:NH1	2.10	0.65
3:H:193:CYS:O	3:H:196:THR:N	2.29	0.65
1:A:314:THR:O	1:A:317:VAL:HB	1.96	0.65
1:F:69:LEU:HD13	1:F:73:PHE:HE1	1.62	0.65
2:B:132:VAL:HG12	2:B:134:MET:SD	2.36	0.65
1:F:332:LEU:HB2	1:F:348:PHE:HB3	1.79	0.65
1:F:284:HIS:HB3	1:F:285:PRO:HD3	1.78	0.65
2:G:41:ARG:HH11	2:G:41:ARG:N	1.94	0.65
3:H:25:LYS:O	3:H:29:PHE:HB3	1.97	0.65
1:A:277:ASN:HA	1:A:335:PHE:HZ	1.62	0.65
1:A:466:VAL:C	1:A:501:GLY:HA3	2.22	0.65
3:C:160:LEU:HD22	3:C:176:ARG:NH1	2.12	0.65
2:G:128:THR:HA	2:G:162:TYR:HB2	1.79	0.65
1:A:69:LEU:HG	1:A:114:VAL:CG1	2.27	0.65
1:A:203:LEU:HA	1:A:206:ILE:HD12	1.77	0.65
3:H:94:ASN:HB2	3:H:97:GLN:NE2	2.12	0.65
1:F:316:LEU:HG	1:F:365:ASN:ND2	2.12	0.65
1:F:367:LEU:HD23	1:F:370:MET:CE	2.27	0.65
1:A:121:GLY:O	1:A:124:ASN:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ILE:HG13	1:A:289:ILE:HD13	1.78	0.64
1:A:257:ARG:HB3	1:A:257:ARG:NH1	2.11	0.64
3:H:91:TYR:OH	4:I:6:UNK:C	2.45	0.64
1:A:332:LEU:H	1:A:348:PHE:HD2	1.44	0.64
2:B:184:TYR:HE2	2:B:189:MET:HE2	1.62	0.64
2:B:227:ASP:CG	2:B:229:ALA:H	2.06	0.64
1:A:159:SER:OG	1:A:189:TYR:CB	2.46	0.64
1:A:159:SER:OG	1:A:189:TYR:HB3	1.97	0.64
1:F:264:PHE:CE1	1:F:275:TYR:HB2	2.33	0.64
3:H:86:ALA:HA	3:H:90:MET:HB2	1.78	0.64
1:A:481:ARG:HG2	1:A:482:ARG:N	2.12	0.64
3:C:74:PHE:HB2	3:C:112:PHE:CD1	2.31	0.64
3:C:94:ASN:HB2	3:C:97:GLN:HE21	1.62	0.64
1:F:154:ILE:O	1:F:158:VAL:HG23	1.96	0.64
2:G:227:ASP:CG	2:G:229:ALA:H	2.06	0.64
3:H:26:ILE:HD11	3:H:175:THR:HG23	1.79	0.64
1:A:111:ILE:HD11	6:A:1001:HEM:CMD	2.28	0.64
1:A:138:PHE:HB2	1:A:207:ASN:ND2	2.12	0.64
1:A:255:LEU:HD23	1:A:259:LEU:HD12	1.80	0.64
3:C:70:LEU:CD2	3:C:115:MET:HB2	2.22	0.64
1:A:367:LEU:HA	1:A:370:MET:CE	2.27	0.64
2:B:41:ARG:N	2:B:41:ARG:HH11	1.95	0.64
3:C:192:ILE:HG23	3:C:192:ILE:O	1.97	0.64
3:H:88:ILE:HA	3:H:98:VAL:CG2	2.27	0.64
3:H:134:GLY:HA2	3:H:137:SER:HB3	1.80	0.64
1:A:282:TRP:C	1:A:285:PRO:HD2	2.22	0.64
3:C:185:HIS:O	3:C:189:VAL:HG23	1.98	0.64
1:F:541:TRP:HA	1:F:541:TRP:CE3	2.33	0.64
1:A:54:HIS:CD2	1:A:128:PRO:HG2	2.32	0.64
1:A:543:THR:HG22	1:A:544:SER:N	2.12	0.64
1:F:69:LEU:HD22	1:F:73:PHE:CE1	2.33	0.64
2:B:159:THR:HG21	2:B:228:ARG:HH21	1.63	0.64
3:C:88:ILE:HA	3:C:98:VAL:CG2	2.27	0.64
1:F:374:ARG:HB3	2:G:79:SER:HB3	1.78	0.64
1:F:111:ILE:HD12	1:F:170:TRP:CE3	2.33	0.63
1:F:316:LEU:HD21	1:F:365:ASN:HB2	1.80	0.63
1:A:460:TRP:CH2	1:A:509:ILE:HD11	2.33	0.63
3:C:143:VAL:O	3:C:147:GLY:N	2.31	0.63
1:F:406:ALA:HB2	2:G:45:LEU:CD2	2.28	0.63
1:F:214:LYS:HZ1	3:H:24:THR:HA	1.63	0.63
2:B:95:VAL:HG23	2:B:96:PRO:CD	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:HA	1:A:448:LEU:HD12	1.78	0.63
3:C:193:CYS:O	3:C:196:THR:N	2.31	0.63
1:F:255:LEU:CD2	1:F:259:LEU:HD12	2.29	0.63
3:H:185:HIS:O	3:H:189:VAL:HG23	1.99	0.63
1:A:262:HIS:HB3	1:A:265:THR:HB	1.80	0.63
2:B:54:VAL:HA	2:B:57:PRO:HG2	1.81	0.63
1:F:437:THR:HA	1:F:448:LEU:HD12	1.78	0.63
1:F:512:LEU:HD23	1:F:513:VAL:N	2.13	0.63
2:G:184:TYR:CE2	2:G:189:MET:HE2	2.33	0.63
1:A:359:THR:HB	7:A:1002:HEO:H272	1.80	0.63
1:A:481:ARG:NH2	1:A:482:ARG:HH21	1.97	0.63
3:C:30:TRP:HH2	4:D:79:UNK:C	2.07	0.63
3:C:85:MET:CE	3:C:178:MET:HG3	2.28	0.63
1:F:262:HIS:HB3	1:F:265:THR:HB	1.80	0.63
1:F:314:THR:O	1:F:317:VAL:HB	1.99	0.63
2:G:264:GLU:HG2	2:G:265:TYR:N	2.12	0.63
1:A:277:ASN:HA	1:A:335:PHE:CZ	2.33	0.63
3:C:83:TYR:HE1	4:D:14:UNK:CB	2.11	0.63
3:C:197:VAL:HG13	3:C:198:VAL:HG23	1.80	0.63
1:F:121:GLY:O	1:F:124:ASN:HB3	1.99	0.63
1:F:277:ASN:HA	1:F:335:PHE:HZ	1.64	0.63
1:A:336:PHE:HE2	1:A:404:PRO:HG3	1.63	0.62
1:A:541:TRP:HA	1:A:541:TRP:CE3	2.34	0.62
7:A:1002:HEO:H201	2:B:56:ILE:HG21	1.80	0.62
2:B:36:ILE:CG1	2:B:39:GLU:H	2.12	0.62
2:B:203:TYR:O	2:B:221:LYS:HG3	1.99	0.62
1:F:57:LEU:HA	1:F:60:MET:CG	2.29	0.62
1:F:280:TRP:HA	1:F:280:TRP:CE3	2.34	0.62
2:G:56:ILE:H	2:G:57:PRO:HD2	1.65	0.62
2:G:57:PRO:O	2:G:61:MET:N	2.26	0.62
2:G:59:ILE:O	2:G:63:VAL:HG23	1.98	0.62
3:H:160:LEU:O	3:H:164:ILE:HG13	1.99	0.62
1:A:248:VAL:CG2	3:C:39:LEU:HD12	2.27	0.62
2:B:56:ILE:H	2:B:57:PRO:HD2	1.65	0.62
3:C:160:LEU:O	3:C:164:ILE:HG13	1.99	0.62
3:C:197:VAL:CG1	3:C:198:VAL:N	2.62	0.62
1:F:335:PHE:HA	1:F:338:MET:HE3	1.80	0.62
2:G:184:TYR:HE2	2:G:186:MET:HB2	1.63	0.62
3:H:33:LEU:HB2	3:H:34:MET:HE2	1.80	0.62
3:H:185:HIS:NE2	4:I:57:UNK:O	2.32	0.62
1:A:407:ASP:OD2	1:A:411:HIS:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:PRO:C	2:B:179:LEU:H	2.08	0.62
1:F:203:LEU:HA	1:F:206:ILE:HD12	1.80	0.62
1:F:359:THR:HB	7:F:1002:HEO:H272	1.80	0.62
1:F:367:LEU:HD13	2:G:63:VAL:CG1	2.29	0.62
2:G:104:ALA:HA	2:G:107:THR:OG1	2.00	0.62
1:A:367:LEU:HD23	1:A:370:MET:CE	2.29	0.62
2:B:184:TYR:HE2	2:B:186:MET:HB2	1.64	0.62
1:F:469:MET:N	1:F:470:PRO:CD	2.62	0.62
1:F:481:ARG:HG2	1:F:482:ARG:N	2.14	0.62
2:G:108:TRP:HZ3	2:G:109:LYS:HE2	1.65	0.62
1:A:174:PRO:HB2	1:A:175:PRO:CD	2.28	0.62
1:A:346:ALA:HB1	1:A:350:ILE:CD1	2.30	0.62
1:A:487:ILE:HA	1:A:492:HIS:CE1	2.34	0.62
1:A:512:LEU:HD23	1:A:513:VAL:N	2.14	0.62
1:F:222:MET:HE1	1:F:225:MET:CE	2.29	0.62
2:G:104:ALA:O	2:G:105:VAL:C	2.38	0.62
2:B:50:LEU:C	2:B:53:ILE:HG22	2.25	0.62
1:F:54:HIS:CE1	1:F:55:LYS:HG3	2.35	0.62
1:F:487:ILE:HA	1:F:492:HIS:CE1	2.35	0.62
2:G:147:ILE:CD1	2:G:235:VAL:HG13	2.29	0.62
2:B:59:ILE:O	2:B:63:VAL:HG23	1.99	0.62
3:C:74:PHE:CZ	3:C:187:LEU:HD22	2.34	0.62
3:C:148:LEU:HA	3:C:151:THR:OG1	1.98	0.62
1:F:79:MET:SD	1:F:102:ILE:HG22	2.39	0.62
1:F:138:PHE:HB2	1:F:207:ASN:ND2	2.14	0.62
1:F:330:VAL:O	1:F:333:HIS:ND1	2.32	0.62
2:G:149:THR:HG22	2:G:265:TYR:HE1	1.64	0.62
3:H:74:PHE:HA	3:H:77:LEU:HD12	1.82	0.62
3:H:103:ALA:HA	3:H:161:MET:HE1	1.82	0.62
1:A:255:LEU:CD2	1:A:259:LEU:HD12	2.30	0.62
2:B:136:TRP:CE3	2:B:259:GLU:HG2	2.35	0.62
1:F:123:MET:HA	1:F:127:VAL:HG23	1.80	0.62
1:F:159:SER:OG	1:F:189:TYR:HB3	2.00	0.62
1:F:277:ASN:HA	1:F:335:PHE:CZ	2.34	0.62
1:F:331:TRP:CH2	4:I:97:UNK:CB	2.82	0.62
3:H:85:MET:N	3:H:88:ILE:HD12	2.14	0.62
3:H:197:VAL:CG1	3:H:198:VAL:N	2.62	0.62
1:A:54:HIS:HD2	1:A:128:PRO:HG2	1.64	0.62
1:A:106:HIS:O	1:A:109:ILE:N	2.32	0.62
1:A:330:VAL:O	1:A:333:HIS:ND1	2.33	0.62
1:A:469:MET:N	1:A:470:PRO:CD	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ARG:NH2	1:A:482:ARG:NH2	2.47	0.62
2:B:148:ALA:CB	2:B:266:PHE:HB2	2.08	0.62
1:F:481:ARG:NH2	1:F:482:ARG:HH21	1.98	0.62
2:B:60:LEU:C	2:B:62:ALA:H	2.08	0.61
3:C:66:LEU:N	3:C:67:PRO:HD2	2.14	0.61
1:F:457:PHE:CE2	1:F:461:ILE:HD11	2.35	0.61
1:A:57:LEU:HA	1:A:60:MET:CG	2.30	0.61
1:A:367:LEU:HD13	2:B:63:VAL:HG11	1.82	0.61
2:B:141:ILE:HD13	2:B:273:LEU:HB3	1.81	0.61
3:C:86:ALA:HA	3:C:90:MET:HB2	1.80	0.61
3:C:183:PHE:O	3:C:186:PHE:HB3	1.99	0.61
1:A:80:ARG:HG3	1:A:80:ARG:O	2.00	0.61
1:A:316:LEU:HG	1:A:365:ASN:ND2	2.16	0.61
1:A:390:THR:HG21	1:A:426:GLY:HA3	1.81	0.61
2:B:171:MET:HG3	2:B:210:TYR:CE2	2.35	0.61
1:F:106:HIS:O	1:F:109:ILE:N	2.33	0.61
1:F:457:PHE:CD2	1:F:461:ILE:HD11	2.35	0.61
3:H:66:LEU:N	3:H:67:PRO:HD2	2.14	0.61
1:F:54:HIS:NE2	1:F:55:LYS:HG3	2.15	0.61
1:F:57:LEU:HA	1:F:60:MET:HG3	1.82	0.61
1:F:159:SER:OG	1:F:189:TYR:CB	2.48	0.61
1:A:252:LEU:HD13	1:A:263:PHE:CE2	2.36	0.61
2:B:264:GLU:HG2	2:B:265:TYR:N	2.15	0.61
1:F:69:LEU:HG	1:F:114:VAL:CG1	2.30	0.61
3:H:70:LEU:CD2	3:H:115:MET:HB2	2.24	0.61
2:G:97:ILE:O	2:G:101:ILE:CD1	2.49	0.61
3:H:86:ALA:C	3:H:88:ILE:H	2.08	0.61
3:H:91:TYR:OH	4:I:7:UNK:CA	2.49	0.61
3:H:94:ASN:HB2	3:H:97:GLN:HE21	1.65	0.61
3:H:143:VAL:O	3:H:147:GLY:N	2.33	0.61
1:A:316:LEU:HD21	1:A:365:ASN:HB2	1.83	0.61
3:C:25:LYS:O	3:C:29:PHE:HB3	2.01	0.61
3:C:102:LEU:O	3:C:105:THR:HB	2.00	0.61
3:H:120:PHE:O	3:H:123:LEU:N	2.32	0.61
1:A:159:SER:HB2	1:A:165:PHE:CD1	2.34	0.61
1:F:333:HIS:HA	1:F:336:PHE:CE1	2.35	0.61
1:F:373:GLY:HA2	2:G:71:ALA:CA	2.30	0.61
1:F:466:VAL:HB	1:F:501:GLY:HA2	1.83	0.61
2:G:136:TRP:CE3	2:G:259:GLU:HG2	2.36	0.61
1:A:305:PHE:HE2	1:A:378:HIS:HB2	1.65	0.61
1:A:441:PRO:O	1:A:443:ALA:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:TRP:HH2	4:D:79:UNK:O	1.79	0.61
1:F:316:LEU:HD21	1:F:365:ASN:CB	2.31	0.61
1:F:354:ILE:HA	2:G:100:ILE:HD13	1.82	0.61
3:H:183:PHE:O	3:H:186:PHE:HB3	2.01	0.61
3:H:192:ILE:HG23	3:H:192:ILE:O	2.00	0.61
1:A:54:HIS:CE1	1:A:55:LYS:HG3	2.36	0.61
1:A:125:LEU:O	1:A:125:LEU:HD23	2.01	0.61
1:A:316:LEU:HG	1:A:365:ASN:HD22	1.66	0.61
1:A:333:HIS:HA	1:A:336:PHE:CE1	2.36	0.61
2:B:147:ILE:CD1	2:B:235:VAL:HG13	2.31	0.61
3:C:185:HIS:NE2	4:D:61:UNK:CB	2.64	0.61
1:F:131:ILE:HD12	1:F:216:ARG:HA	1.82	0.61
1:F:364:PHE:HA	1:F:367:LEU:HD12	1.83	0.61
1:A:54:HIS:NE2	1:A:55:LYS:HG3	2.16	0.60
1:A:58:GLY:N	1:A:124:ASN:ND2	2.49	0.60
1:A:131:ILE:HD12	1:A:216:ARG:HA	1.83	0.60
2:B:139:PHE:HE1	2:B:148:ALA:HB1	1.66	0.60
1:F:109:ILE:HG22	1:F:114:VAL:HG23	1.83	0.60
1:F:305:PHE:HE2	1:F:378:HIS:HB2	1.65	0.60
1:F:441:PRO:O	1:F:443:ALA:N	2.34	0.60
1:A:264:PHE:CE1	1:A:275:TYR:HB2	2.37	0.60
1:A:280:TRP:HA	1:A:280:TRP:CE3	2.36	0.60
1:A:450:GLU:OE2	1:A:454:LYS:HE3	2.01	0.60
2:B:127:ILE:H	2:B:127:ILE:HD12	1.67	0.60
2:B:137:LYS:NZ	2:B:261:ASN:HD21	1.99	0.60
3:C:85:MET:N	3:C:88:ILE:HD12	2.16	0.60
2:G:50:LEU:C	2:G:53:ILE:HG22	2.26	0.60
3:H:178:MET:SD	4:I:68:UNK:CB	2.89	0.60
1:A:187:VAL:O	1:A:191:ILE:HG13	2.01	0.60
2:B:228:ARG:HG3	2:B:231:PHE:HD2	1.67	0.60
2:G:36:ILE:N	2:G:39:GLU:OE2	2.29	0.60
1:A:440:TRP:HE1	1:A:446:PHE:HE1	1.50	0.60
2:B:57:PRO:O	2:B:61:MET:N	2.27	0.60
3:C:26:ILE:HG22	3:C:27:PHE:N	2.16	0.60
1:F:235:ALA:O	1:F:238:LEU:HB2	2.01	0.60
1:F:442:LYS:HD3	1:F:541:TRP:CZ3	2.37	0.60
2:G:39:GLU:O	2:G:43:LEU:N	2.33	0.60
3:H:74:PHE:CZ	3:H:187:LEU:HD22	2.36	0.60
3:H:197:VAL:HG13	3:H:198:VAL:HG23	1.82	0.60
2:B:53:ILE:O	2:B:57:PRO:HD2	2.01	0.60
3:C:134:GLY:HA2	3:C:137:SER:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:HIS:HD2	1:F:128:PRO:HG2	1.64	0.60
1:F:252:LEU:HD13	1:F:263:PHE:CE2	2.37	0.60
2:G:54:VAL:HA	2:G:57:PRO:HG2	1.83	0.60
1:A:442:LYS:HD3	1:A:541:TRP:CZ3	2.37	0.60
1:F:336:PHE:HE2	1:F:404:PRO:HG3	1.66	0.60
1:A:73:PHE:O	1:A:74:ALA:C	2.43	0.60
1:A:205:GLY:O	1:A:240:ILE:HD11	2.02	0.60
1:A:457:PHE:CD2	1:A:461:ILE:HD11	2.37	0.60
3:C:38:ILE:HD13	4:D:90:UNK:CB	2.32	0.60
1:F:69:LEU:HD13	1:F:73:PHE:CE1	2.37	0.60
1:F:481:ARG:NH2	1:F:482:ARG:NH2	2.49	0.60
2:G:148:ALA:CB	2:G:266:PHE:HB2	2.09	0.60
2:G:159:THR:HG21	2:G:228:ARG:HH21	1.66	0.60
3:H:96:SER:O	3:H:98:VAL:N	2.35	0.60
1:A:57:LEU:HA	1:A:60:MET:HG3	1.83	0.60
1:A:119:VAL:CG2	1:A:123:MET:HE2	2.30	0.60
1:F:457:PHE:O	1:F:461:ILE:HG13	2.00	0.60
1:F:514:ILE:O	1:F:518:VAL:HG23	2.00	0.60
2:G:56:ILE:N	2:G:56:ILE:HD12	2.16	0.60
2:G:150:VAL:HG12	2:G:151:ASN:HD22	1.65	0.60
2:G:228:ARG:HG3	2:G:231:PHE:HD2	1.67	0.60
2:G:251:PHE:CD2	2:G:273:LEU:HD11	2.37	0.60
1:A:61:TYR:CE1	1:A:146:PHE:HB2	2.37	0.60
1:A:109:ILE:HG22	1:A:114:VAL:HG23	1.84	0.60
1:A:206:ILE:HG23	3:C:31:ILE:HG23	1.83	0.60
3:C:85:MET:O	3:C:88:ILE:HB	2.02	0.60
2:G:243:ASN:ND2	2:G:265:TYR:O	2.34	0.60
1:A:61:TYR:O	1:A:62:ILE:C	2.45	0.60
1:A:123:MET:HA	1:A:127:VAL:HG23	1.83	0.60
1:A:209:PHE:CE2	3:C:31:ILE:CD1	2.85	0.60
2:B:147:ILE:HD13	2:B:235:VAL:HG13	1.84	0.60
2:B:190:GLN:NE2	2:B:192:ARG:HH21	1.99	0.60
3:C:124:ILE:O	3:C:124:ILE:HG22	2.02	0.60
3:C:152:SER:C	3:C:154:LEU:H	2.10	0.60
1:F:541:TRP:HA	1:F:541:TRP:HE3	1.67	0.60
2:G:149:THR:HG22	2:G:265:TYR:CE1	2.36	0.60
3:H:156:TRP:HE1	3:H:180:LEU:CD2	2.15	0.60
1:A:235:ALA:O	1:A:238:LEU:HB2	2.02	0.59
2:B:244:THR:HB	2:B:268:ASN:CB	2.17	0.59
1:F:214:LYS:CE	3:H:24:THR:HG23	2.32	0.59
2:G:39:GLU:HB2	2:G:43:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PHE:HA	1:A:367:LEU:HD12	1.83	0.59
1:A:457:PHE:CE2	1:A:461:ILE:HD11	2.37	0.59
2:B:39:GLU:HB2	2:B:43:LEU:HD12	1.84	0.59
3:C:88:ILE:CG1	3:C:98:VAL:HG13	2.27	0.59
1:F:55:LYS:HZ1	1:F:551:ASN:HA	1.63	0.59
1:F:73:PHE:HB3	1:F:77:ILE:CD1	2.32	0.59
1:F:460:TRP:CH2	1:F:509:ILE:HD11	2.37	0.59
2:G:137:LYS:NZ	2:G:261:ASN:HD21	2.00	0.59
2:G:177:PRO:C	2:G:179:LEU:H	2.11	0.59
1:F:61:TYR:O	1:F:62:ILE:C	2.45	0.59
1:A:69:LEU:HD22	1:A:73:PHE:CD1	2.37	0.59
1:A:312:GLY:HA3	1:A:365:ASN:ND2	2.17	0.59
1:A:449:ASN:OD1	1:A:451:THR:HB	2.03	0.59
2:B:156:PRO:HG2	2:B:228:ARG:HE	1.68	0.59
2:B:243:ASN:ND2	2:B:265:TYR:O	2.35	0.59
3:C:30:TRP:CZ3	4:D:79:UNK:HA	2.35	0.59
3:C:44:PHE:HE1	3:C:142:LEU:HD21	1.67	0.59
2:G:196:ILE:HG22	2:G:198:ASN:HD21	1.67	0.59
3:H:111:GLY:O	3:H:114:GLY:N	2.34	0.59
1:F:58:GLY:N	1:F:124:ASN:ND2	2.51	0.59
3:H:134:GLY:HA2	3:H:137:SER:CB	2.33	0.59
1:A:79:MET:SD	1:A:102:ILE:HG22	2.42	0.59
1:A:105:ALA:O	1:A:109:ILE:HG13	2.02	0.59
1:A:118:PHE:CZ	1:A:294:VAL:HG22	2.37	0.59
1:A:178:GLY:HA2	1:A:257:ARG:CG	2.31	0.59
1:A:464:PHE:HD2	1:A:465:PHE:CE1	2.21	0.59
3:C:74:PHE:HZ	3:C:187:LEU:HD22	1.68	0.59
1:F:73:PHE:O	1:F:74:ALA:C	2.45	0.59
1:F:178:GLY:HA2	1:F:257:ARG:CG	2.30	0.59
1:F:228:PHE:CE1	1:F:297:VAL:HG23	2.37	0.59
2:G:244:THR:HB	2:G:268:ASN:CB	2.18	0.59
1:A:192:TRP:HA	1:A:192:TRP:CE3	2.38	0.59
3:C:77:LEU:HD13	3:C:184:TRP:CZ2	2.37	0.59
1:F:68:MET:HE1	1:F:153:VAL:HG13	1.85	0.59
1:F:332:LEU:H	1:F:348:PHE:HD2	1.50	0.59
3:H:145:THR:C	3:H:147:GLY:H	2.11	0.59
1:A:168:THR:HB	1:A:172:ALA:CA	2.32	0.59
2:B:184:TYR:CE2	2:B:189:MET:HE2	2.38	0.59
1:F:375:ILE:HG12	2:G:67:TRP:HE1	1.67	0.59
2:G:127:ILE:H	2:G:127:ILE:HD12	1.68	0.59
2:G:147:ILE:HD13	2:G:235:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:124:ILE:HG22	3:H:124:ILE:O	2.03	0.59
1:A:389:VAL:HG13	2:B:61:MET:HE1	1.85	0.59
1:A:436:MET:O	1:A:440:TRP:HB2	2.03	0.59
1:F:206:ILE:HG23	3:H:31:ILE:HG23	1.83	0.59
1:F:225:MET:SD	1:F:230:TRP:HA	2.43	0.59
3:H:74:PHE:HZ	3:H:187:LEU:HD22	1.68	0.59
3:H:74:PHE:HB2	3:H:112:PHE:CD1	2.37	0.59
3:H:78:PHE:CE2	3:H:185:HIS:CE1	2.90	0.59
1:A:126:VAL:HG11	1:A:439:TRP:CE2	2.38	0.59
1:A:512:LEU:O	1:A:515:GLN:HG2	2.02	0.59
1:A:541:TRP:HA	1:A:541:TRP:HE3	1.68	0.59
3:C:74:PHE:HA	3:C:77:LEU:HD12	1.85	0.59
1:F:156:VAL:HG12	1:F:160:LEU:HD11	1.85	0.59
2:G:87:LYS:HD2	2:G:87:LYS:N	2.18	0.59
1:A:58:GLY:N	1:A:124:ASN:HD22	2.01	0.58
1:A:280:TRP:O	1:A:331:TRP:HB2	2.03	0.58
2:B:50:LEU:O	2:B:53:ILE:HG22	2.03	0.58
2:B:56:ILE:N	2:B:56:ILE:HD12	2.18	0.58
2:B:159:THR:HG21	2:B:228:ARG:NH2	2.18	0.58
2:B:196:ILE:HG22	2:B:198:ASN:HD21	1.67	0.58
3:C:68:PHE:O	3:C:72:GLU:HB2	2.02	0.58
1:F:55:LYS:HD3	1:F:129:LEU:HD21	1.85	0.58
1:F:168:THR:HB	1:F:172:ALA:CA	2.29	0.58
1:F:272:MET:HE3	2:G:186:MET:HG2	1.84	0.58
1:F:274:MET:HG2	3:H:49:VAL:HG11	1.85	0.58
1:F:390:THR:HG21	1:F:426:GLY:HA3	1.84	0.58
2:G:139:PHE:HE1	2:G:148:ALA:HB1	1.68	0.58
1:A:216:ARG:HH12	1:A:222:MET:HA	1.67	0.58
3:C:26:ILE:HD11	3:C:175:THR:HG23	1.83	0.58
3:C:33:LEU:C	3:C:34:MET:HE2	2.28	0.58
3:C:86:ALA:HB1	3:C:91:TYR:CD1	2.37	0.58
3:C:86:ALA:C	3:C:88:ILE:H	2.11	0.58
1:A:69:LEU:HD22	1:A:73:PHE:CE1	2.38	0.58
2:B:108:TRP:HZ3	2:B:109:LYS:HE2	1.69	0.58
2:B:278:ILE:O	2:B:282:MET:HG2	2.03	0.58
3:C:96:SER:O	3:C:98:VAL:N	2.37	0.58
1:F:79:MET:CE	1:F:102:ILE:HG22	2.32	0.58
1:F:366:TRP:O	1:F:369:THR:HB	2.04	0.58
1:A:373:GLY:HA2	2:B:71:ALA:CB	2.27	0.58
1:A:381:MET:O	1:A:385:ILE:HG13	2.03	0.58
3:C:96:SER:CA	3:C:99:ILE:HD13	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:GLY:N	1:F:124:ASN:HD22	2.01	0.58
1:F:110:MET:HB3	6:F:1001:HEM:CBC	2.33	0.58
1:F:369:THR:O	1:F:369:THR:HG22	2.02	0.58
2:G:196:ILE:HG22	2:G:198:ASN:ND2	2.17	0.58
2:G:197:ALA:C	2:G:198:ASN:HD22	2.11	0.58
1:A:466:VAL:HB	1:A:501:GLY:HA2	1.84	0.58
3:H:113:ILE:HD11	3:H:150:VAL:HG12	1.85	0.58
3:H:152:SER:C	3:H:154:LEU:H	2.11	0.58
1:A:335:PHE:HA	1:A:338:MET:HE3	1.84	0.58
3:H:44:PHE:HE1	3:H:142:LEU:HD21	1.68	0.58
2:B:197:ALA:C	2:B:198:ASN:HD22	2.12	0.58
1:F:192:TRP:HA	1:F:192:TRP:CE3	2.39	0.58
1:F:245:ILE:HD12	1:F:282:TRP:HB2	1.86	0.58
1:F:280:TRP:O	1:F:331:TRP:HB2	2.04	0.58
1:F:373:GLY:HA2	2:G:71:ALA:O	2.03	0.58
1:F:105:ALA:O	1:F:109:ILE:HG13	2.03	0.58
2:G:278:ILE:O	2:G:282:MET:HG2	2.04	0.58
1:A:337:THR:HG22	2:B:184:TYR:HB3	1.85	0.58
2:B:87:LYS:HD2	2:B:87:LYS:N	2.19	0.58
1:F:239:ILE:N	1:F:289:ILE:HD11	2.18	0.58
1:F:449:ASN:OD1	1:F:451:THR:HB	2.04	0.58
2:B:251:PHE:CD2	2:B:273:LEU:HD11	2.39	0.58
3:C:47:TYR:O	3:C:51:VAL:HG13	2.03	0.58
2:G:244:THR:CG2	2:G:268:ASN:HB3	2.33	0.58
1:F:54:HIS:CE1	1:F:135:ASP:HA	2.39	0.57
1:F:111:ILE:HD11	6:F:1001:HEM:HMD2	1.86	0.57
1:F:441:PRO:C	1:F:443:ALA:H	2.12	0.57
1:A:209:PHE:HE2	3:C:31:ILE:HD11	1.68	0.57
2:B:95:VAL:O	2:B:99:ILE:HG12	2.03	0.57
3:C:85:MET:SD	3:C:178:MET:HG3	2.44	0.57
1:F:103:PHE:CZ	6:F:1001:HEM:HMA1	2.39	0.57
1:F:155:LEU:HD13	1:F:193:SER:HA	1.85	0.57
2:G:53:ILE:O	2:G:57:PRO:HD2	2.03	0.57
3:H:38:ILE:HD13	4:I:90:UNK:CB	2.33	0.57
3:H:96:SER:CA	3:H:99:ILE:HD13	2.30	0.57
1:A:54:HIS:CE1	1:A:135:ASP:HA	2.39	0.57
1:A:55:LYS:HD3	1:A:129:LEU:HD21	1.87	0.57
1:A:397:THR:HG21	1:A:472:TYR:OH	2.04	0.57
1:A:441:PRO:C	1:A:443:ALA:H	2.12	0.57
2:B:39:GLU:O	2:B:43:LEU:HB2	2.04	0.57
2:B:196:ILE:HG22	2:B:198:ASN:ND2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:464:PHE:HD2	1:F:465:PHE:CE1	2.23	0.57
1:F:549:PHE:H	1:F:549:PHE:HD1	1.52	0.57
2:G:162:TYR:CG	2:G:194:HIS:NE2	2.72	0.57
2:G:192:ARG:HB2	2:G:192:ARG:HH11	1.68	0.57
1:A:79:MET:CE	1:A:102:ILE:HG22	2.33	0.57
1:A:156:VAL:HG12	1:A:160:LEU:HD11	1.86	0.57
1:A:228:PHE:CE1	1:A:297:VAL:HG23	2.39	0.57
1:A:248:VAL:HG22	3:C:39:LEU:CD1	2.31	0.57
1:A:514:ILE:O	1:A:518:VAL:HG23	2.02	0.57
3:C:29:PHE:HA	3:C:32:TYR:HB2	1.84	0.57
3:C:89:ALA:HB2	3:C:174:ARG:CD	2.25	0.57
3:C:196:THR:HA	3:C:200:LEU:CD2	2.33	0.57
1:F:61:TYR:CE1	1:F:146:PHE:HB2	2.39	0.57
1:F:450:GLU:OE2	1:F:454:LYS:HE3	2.05	0.57
1:A:283:GLY:O	1:A:286:GLU:HB3	2.05	0.57
1:A:492:HIS:HA	1:A:495:LEU:HD12	1.86	0.57
1:A:502:ALA:O	1:A:503:VAL:C	2.47	0.57
2:B:136:TRP:HA	2:B:218:MET:HG2	1.87	0.57
2:B:192:ARG:HB2	2:B:192:ARG:HH11	1.68	0.57
3:C:136:LEU:O	3:C:140:PHE:HB2	2.04	0.57
3:C:193:CYS:O	3:C:194:VAL:C	2.46	0.57
3:C:200:LEU:HD12	3:C:201:MET:N	2.18	0.57
1:F:248:VAL:HG22	3:H:39:LEU:HD12	1.87	0.57
1:F:407:ASP:OD2	1:F:411:HIS:HB2	2.05	0.57
1:F:486:GLN:C	1:F:487:ILE:HG13	2.29	0.57
2:G:179:LEU:HB3	2:G:195:LEU:HD11	1.86	0.57
3:H:88:ILE:HG23	3:H:98:VAL:CG1	2.34	0.57
1:A:79:MET:HG3	1:A:103:PHE:CZ	2.40	0.57
3:C:38:ILE:CD1	4:D:90:UNK:CB	2.82	0.57
2:G:173:SER:HB3	2:G:207:SER:O	2.05	0.57
3:H:38:ILE:CD1	4:I:90:UNK:CB	2.83	0.57
1:A:155:LEU:HD13	1:A:193:SER:HA	1.86	0.57
1:A:239:ILE:N	1:A:289:ILE:HD11	2.20	0.57
1:A:316:LEU:HD21	1:A:365:ASN:CB	2.35	0.57
1:A:549:PHE:HD1	1:A:549:PHE:H	1.53	0.57
1:F:378:HIS:O	1:F:379:SER:C	2.48	0.57
3:H:134:GLY:O	3:H:137:SER:HB3	2.05	0.57
1:A:481:ARG:O	1:A:483:LEU:N	2.38	0.57
2:B:162:TYR:CG	2:B:194:HIS:NE2	2.73	0.57
1:F:79:MET:HG3	1:F:103:PHE:CZ	2.40	0.57
2:G:156:PRO:HG2	2:G:228:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:77:LEU:HD13	3:H:184:TRP:CZ2	2.40	0.57
1:A:437:THR:HA	1:A:448:LEU:CD1	2.34	0.57
1:A:457:PHE:O	1:A:461:ILE:HG13	2.04	0.57
2:B:179:LEU:HB3	2:B:195:LEU:HD11	1.87	0.57
1:A:353:MET:O	2:B:100:ILE:HD12	2.05	0.57
1:F:492:HIS:HA	1:F:495:LEU:HD12	1.87	0.57
2:G:140:PHE:CD2	2:G:153:ILE:HG23	2.40	0.57
3:C:44:PHE:CE1	3:C:142:LEU:HD21	2.40	0.56
3:H:100:SER:O	3:H:103:ALA:HB3	2.05	0.56
1:A:55:LYS:HZ3	1:A:551:ASN:CA	2.04	0.56
2:B:244:THR:CG2	2:B:268:ASN:HB3	2.35	0.56
1:F:548:PRO:N	1:F:552:PHE:O	2.38	0.56
2:G:39:GLU:O	2:G:43:LEU:HB2	2.05	0.56
2:G:136:TRP:HA	2:G:218:MET:HG2	1.87	0.56
3:H:98:VAL:O	3:H:98:VAL:HG12	2.05	0.56
3:H:193:CYS:O	3:H:194:VAL:C	2.47	0.56
1:A:245:ILE:HD12	1:A:282:TRP:HB2	1.87	0.56
1:A:251:ALA:O	1:A:254:THR:HB	2.05	0.56
1:A:414:LEU:HD21	1:A:479:MET:HE2	1.86	0.56
1:A:442:LYS:HD3	1:A:541:TRP:CE3	2.41	0.56
2:B:36:ILE:N	2:B:39:GLU:OE2	2.32	0.56
2:B:149:THR:HG22	2:B:265:TYR:HE1	1.69	0.56
3:C:49:VAL:O	3:C:51:VAL:N	2.31	0.56
3:C:113:ILE:HD11	3:C:150:VAL:HG12	1.87	0.56
3:C:120:PHE:O	3:C:123:LEU:N	2.36	0.56
3:C:145:THR:C	3:C:147:GLY:H	2.12	0.56
1:F:57:LEU:HD11	1:F:143:ASN:HA	1.87	0.56
1:F:381:MET:O	1:F:385:ILE:HG13	2.05	0.56
1:F:426:GLY:HA2	1:F:430:PHE:CD1	2.41	0.56
1:F:436:MET:O	1:F:440:TRP:HB2	2.06	0.56
1:F:474:LEU:HD22	1:F:491:PHE:HA	1.86	0.56
1:F:481:ARG:O	1:F:483:LEU:N	2.39	0.56
2:G:50:LEU:O	2:G:53:ILE:HG22	2.05	0.56
1:A:110:MET:HB3	6:A:1001:HEM:CBC	2.35	0.56
1:A:271:ASN:HD21	1:A:273:MET:HB2	1.71	0.56
1:F:57:LEU:C	1:F:60:MET:HB2	2.29	0.56
1:F:237:VAL:O	1:F:240:ILE:HB	2.05	0.56
1:F:375:ILE:CG1	2:G:67:TRP:HE1	2.19	0.56
1:F:442:LYS:HD3	1:F:541:TRP:CE3	2.41	0.56
3:H:29:PHE:HA	3:H:32:TYR:HB2	1.86	0.56
3:H:145:THR:C	3:H:147:GLY:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:ILE:O	3:C:159:VAL:HG23	2.05	0.56
1:F:126:VAL:HG11	1:F:439:TRP:CE2	2.41	0.56
1:F:159:SER:CA	1:F:189:TYR:CD1	2.81	0.56
1:A:138:PHE:HB2	1:A:207:ASN:HD21	1.69	0.56
1:A:420:PHE:HA	1:A:423:VAL:HG22	1.87	0.56
2:B:93:TRP:C	2:B:96:PRO:HD2	2.30	0.56
3:C:83:TYR:CE1	4:D:14:UNK:CB	2.89	0.56
1:F:311:PHE:HZ	2:G:88:VAL:HG11	1.70	0.56
1:A:68:MET:HE1	1:A:153:VAL:HG13	1.88	0.56
1:A:73:PHE:HB3	1:A:77:ILE:CD1	2.36	0.56
1:A:272:MET:HE3	2:B:186:MET:HG2	1.88	0.56
1:A:366:TRP:O	1:A:369:THR:HB	2.06	0.56
1:F:312:GLY:HA3	1:F:365:ASN:ND2	2.21	0.56
2:G:53:ILE:HG23	2:G:54:VAL:N	2.20	0.56
2:G:248:MET:O	2:G:252:GLU:HG2	2.05	0.56
3:H:77:LEU:HA	3:H:80:SER:CB	2.35	0.56
3:C:180:LEU:C	3:C:182:LEU:H	2.13	0.56
1:F:125:LEU:HD23	1:F:125:LEU:C	2.31	0.56
3:H:155:ILE:O	3:H:159:VAL:HG23	2.05	0.56
1:F:502:ALA:O	1:F:503:VAL:C	2.49	0.56
1:A:69:LEU:HD13	1:A:73:PHE:HE1	1.71	0.56
1:A:431:GLY:O	1:A:432:CYS:C	2.48	0.56
1:F:277:ASN:OD1	1:F:331:TRP:NE1	2.39	0.56
1:F:437:THR:HA	1:F:448:LEU:CD1	2.35	0.56
2:G:95:VAL:O	2:G:98:LEU:HB2	2.06	0.56
2:G:164:LYS:HE3	2:G:274:PHE:CE2	2.40	0.56
1:A:378:HIS:O	1:A:379:SER:C	2.49	0.55
1:F:113:PHE:HE2	1:F:153:VAL:N	2.04	0.55
2:G:41:ARG:H	2:G:41:ARG:HH11	1.54	0.55
3:H:70:LEU:HD23	3:H:115:MET:HE3	1.86	0.55
3:H:180:LEU:C	3:H:182:LEU:H	2.14	0.55
1:A:57:LEU:C	1:A:60:MET:HB2	2.30	0.55
1:A:333:HIS:CD2	1:A:334:HIS:CD2	2.94	0.55
2:B:53:ILE:HG23	2:B:54:VAL:N	2.20	0.55
2:B:175:PHE:HD1	2:B:181:SER:C	2.15	0.55
2:B:248:MET:O	2:B:252:GLU:HG2	2.06	0.55
3:C:98:VAL:O	3:C:98:VAL:HG12	2.06	0.55
3:C:134:GLY:O	3:C:137:SER:HB3	2.06	0.55
1:F:271:ASN:HD21	1:F:273:MET:HB2	1.72	0.55
1:F:419:HIS:HA	1:F:472:TYR:OH	2.06	0.55
3:H:113:ILE:O	3:H:117:ILE:HG13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:HD22	1:A:491:PHE:HA	1.87	0.55
3:H:146:HIS:HE1	3:H:190:VAL:HB	1.71	0.55
1:A:103:PHE:CZ	6:A:1001:HEM:HMA1	2.41	0.55
2:B:136:TRP:HA	2:B:218:MET:SD	2.47	0.55
2:B:165:VAL:HG12	2:B:166:THR:N	2.22	0.55
1:F:199:ILE:O	1:F:202:THR:HB	2.06	0.55
1:F:283:GLY:O	1:F:286:GLU:HB3	2.06	0.55
1:F:330:VAL:HB	1:F:352:THR:OG1	2.06	0.55
1:F:410:LEU:O	1:F:413:SER:HB3	2.06	0.55
3:H:44:PHE:CE1	3:H:142:LEU:HD21	2.41	0.55
1:A:237:VAL:O	1:A:240:ILE:HB	2.06	0.55
1:A:419:HIS:HA	1:A:472:TYR:OH	2.07	0.55
1:A:480:THR:HB	1:A:483:LEU:HD11	1.87	0.55
2:B:149:THR:HG22	2:B:265:TYR:CE1	2.41	0.55
2:B:164:LYS:HE3	2:B:274:PHE:CE2	2.41	0.55
3:C:42:ILE:O	3:C:45:ALA:HB3	2.06	0.55
1:F:102:ILE:O	1:F:104:THR:N	2.39	0.55
1:F:159:SER:HB2	1:F:165:PHE:CD1	2.40	0.55
1:F:288:TYR:OH	1:F:355:ILE:HG21	2.06	0.55
1:F:333:HIS:CD2	1:F:334:HIS:CD2	2.94	0.55
1:F:338:MET:HA	2:G:184:TYR:CG	2.42	0.55
2:G:165:VAL:O	2:G:191:THR:HG23	2.06	0.55
2:G:175:PHE:HD1	2:G:181:SER:C	2.15	0.55
1:A:239:ILE:HG12	1:A:289:ILE:HD13	1.89	0.55
1:A:384:THR:HG22	1:A:388:ILE:HD11	1.89	0.55
2:G:167:SER:HB3	2:G:187:ALA:HA	1.89	0.55
1:A:96:PRO:HB3	1:A:100:ASP:OD1	2.07	0.55
1:A:238:LEU:CB	1:A:289:ILE:HD11	2.35	0.55
1:A:548:PRO:N	1:A:552:PHE:O	2.40	0.55
3:C:113:ILE:O	3:C:117:ILE:HG13	2.06	0.55
1:F:357:ILE:HB	1:F:358:PRO:HD3	1.87	0.55
2:B:143:PRO:HG2	2:B:144:GLU:OE2	2.06	0.55
1:F:106:HIS:CD2	1:F:107:GLY:N	2.75	0.55
1:F:412:ASN:OD1	2:G:209:SER:HB3	2.07	0.55
1:F:512:LEU:O	1:F:515:GLN:HG2	2.06	0.55
3:H:148:LEU:HA	3:H:151:THR:OG1	2.06	0.55
1:A:57:LEU:HD11	1:A:143:ASN:HA	1.89	0.55
1:A:415:PHE:CD1	1:A:472:TYR:HD2	2.25	0.55
2:B:132:VAL:HG12	2:B:132:VAL:O	2.07	0.55
2:B:148:ALA:O	2:B:265:TYR:HD1	1.90	0.55
2:B:173:SER:HB3	2:B:207:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:ASP:OD1	2:B:229:ALA:HB3	2.07	0.55
3:C:77:LEU:HA	3:C:80:SER:CB	2.36	0.55
3:C:195:PHE:CD1	3:C:199:TYR:HB2	2.41	0.55
1:F:384:THR:HG22	1:F:388:ILE:HD11	1.89	0.55
2:G:40:GLN:HB2	2:G:41:ARG:NH1	2.22	0.55
2:G:82:TRP:HE3	2:G:83:SER:H	1.55	0.55
2:G:148:ALA:O	2:G:265:TYR:HD1	1.90	0.55
2:G:156:PRO:HD3	2:G:231:PHE:CE2	2.42	0.55
2:G:163:PHE:CD2	2:G:193:LEU:HD22	2.41	0.55
2:G:228:ARG:O	2:G:232:ASP:OD1	2.25	0.55
2:G:270:LYS:HE3	2:G:276:ASP:CG	2.32	0.55
1:A:102:ILE:O	1:A:104:THR:N	2.40	0.55
1:A:106:HIS:CD2	1:A:107:GLY:N	2.75	0.55
1:A:225:MET:SD	1:A:230:TRP:HA	2.47	0.55
2:B:175:PHE:HD2	2:B:206:ILE:HD11	1.72	0.55
1:F:515:GLN:O	1:F:518:VAL:HB	2.07	0.55
1:F:515:GLN:CG	1:F:516:MET:N	2.68	0.55
3:H:90:MET:CE	4:I:68:UNK:N	2.68	0.55
1:A:308:LYS:HZ2	1:A:372:GLN:HB2	1.72	0.54
1:A:515:GLN:CG	1:A:516:MET:N	2.68	0.54
1:F:96:PRO:HB3	1:F:100:ASP:OD1	2.07	0.54
1:F:104:THR:HG23	6:F:1001:HEM:O2D	2.06	0.54
1:F:394:GLY:HA3	1:F:422:ASN:OD1	2.07	0.54
1:F:431:GLY:O	1:F:432:CYS:C	2.49	0.54
2:G:165:VAL:HG12	2:G:166:THR:N	2.22	0.54
3:H:136:LEU:O	3:H:140:PHE:HB2	2.06	0.54
1:A:110:MET:O	1:A:115:ALA:HB3	2.07	0.54
1:A:159:SER:CA	1:A:189:TYR:CD1	2.81	0.54
1:A:359:THR:HB	7:A:1002:HEO:C27	2.37	0.54
1:A:426:GLY:HA2	1:A:430:PHE:CD1	2.42	0.54
1:A:446:PHE:CZ	1:A:520:ILE:HA	2.42	0.54
2:B:155:PHE:HA	2:B:231:PHE:CE1	2.42	0.54
1:F:466:VAL:O	1:F:501:GLY:HA3	2.07	0.54
1:F:497:ILE:O	1:F:500:SER:HB2	2.07	0.54
2:G:36:ILE:CD1	2:G:39:GLU:H	2.20	0.54
2:G:37:GLY:O	2:G:40:GLN:HG2	2.08	0.54
2:G:159:THR:HG21	2:G:228:ARG:NH2	2.22	0.54
3:H:195:PHE:CD1	3:H:199:TYR:HB2	2.41	0.54
1:A:497:ILE:O	1:A:500:SER:HB2	2.07	0.54
3:C:111:GLY:O	3:C:114:GLY:N	2.39	0.54
3:C:156:TRP:HE1	3:C:180:LEU:CD1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:VAL:HG13	2:G:61:MET:HE1	1.89	0.54
3:C:146:HIS:HE1	3:C:190:VAL:HB	1.73	0.54
1:F:280:TRP:HA	1:F:280:TRP:HE3	1.73	0.54
1:F:414:LEU:HD21	1:F:479:MET:HE2	1.89	0.54
1:A:310:LEU:HD11	1:A:366:TRP:CD1	2.42	0.54
2:B:50:LEU:HA	2:B:53:ILE:CG2	2.38	0.54
3:C:156:TRP:HE1	3:C:180:LEU:CD2	2.20	0.54
1:F:174:PRO:HB2	1:F:175:PRO:HD3	1.87	0.54
1:F:238:LEU:CB	1:F:289:ILE:HD11	2.36	0.54
1:F:306:SER:O	1:F:374:ARG:O	2.26	0.54
1:F:346:ALA:HB1	1:F:350:ILE:HD12	1.89	0.54
3:H:68:PHE:O	3:H:72:GLU:HB2	2.07	0.54
3:H:72:GLU:OE1	3:H:72:GLU:HA	2.07	0.54
3:H:143:VAL:O	3:H:144:GLY:C	2.49	0.54
1:A:174:PRO:HB3	1:A:175:PRO:HD3	1.82	0.54
1:A:205:GLY:O	1:A:209:PHE:HB2	2.08	0.54
2:B:65:PHE:O	2:B:68:LYS:HE2	2.08	0.54
2:B:200:PRO:HA	2:B:224:ALA:O	2.07	0.54
1:A:69:LEU:HD13	1:A:73:PHE:CE1	2.43	0.54
1:A:116:MET:N	1:A:117:PRO:CD	2.70	0.54
1:A:209:PHE:HE2	3:C:31:ILE:HD13	1.72	0.54
1:A:332:LEU:HD22	1:A:335:PHE:CB	2.37	0.54
1:A:515:GLN:O	1:A:518:VAL:HB	2.07	0.54
2:B:40:GLN:HB2	2:B:41:ARG:NH1	2.23	0.54
2:B:273:LEU:O	2:B:276:ASP:HB2	2.08	0.54
3:C:33:LEU:HB2	3:C:34:MET:HE2	1.89	0.54
3:C:145:THR:C	3:C:147:GLY:N	2.63	0.54
1:F:118:PHE:CZ	1:F:294:VAL:HG22	2.42	0.54
1:F:251:ALA:O	1:F:254:THR:HB	2.08	0.54
1:F:446:PHE:CZ	1:F:520:ILE:HA	2.43	0.54
1:F:480:THR:HB	1:F:483:LEU:HD11	1.88	0.54
2:G:132:VAL:HG12	2:G:132:VAL:O	2.08	0.54
1:A:112:PHE:CE1	1:A:286:GLU:OE2	2.58	0.54
1:A:216:ARG:HH12	1:A:222:MET:CA	2.21	0.54
2:B:88:VAL:O	2:B:91:VAL:HB	2.08	0.54
4:D:20:UNK:CB	4:D:53:UNK:CB	2.86	0.54
2:G:39:GLU:HG2	2:G:40:GLN:OE1	2.08	0.54
2:G:155:PHE:HA	2:G:231:PHE:CE1	2.42	0.54
2:G:273:LEU:O	2:G:276:ASP:HB2	2.08	0.54
1:A:187:VAL:O	1:A:190:TRP:HB3	2.08	0.54
2:B:165:VAL:O	2:B:191:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ALA:HA	2:B:233:GLN:NE2	2.22	0.54
3:C:30:TRP:CZ2	4:D:79:UNK:CB	2.91	0.54
1:F:216:ARG:HH12	1:F:222:MET:HA	1.72	0.54
2:G:243:ASN:O	2:G:266:PHE:HA	2.07	0.54
3:H:156:TRP:HE1	3:H:180:LEU:CD1	2.20	0.54
1:A:277:ASN:OD1	1:A:331:TRP:NE1	2.41	0.54
3:C:88:ILE:HG23	3:C:98:VAL:CG1	2.37	0.54
1:F:389:VAL:HA	2:G:61:MET:HE1	1.90	0.54
1:F:397:THR:HG21	1:F:472:TYR:OH	2.07	0.54
3:H:49:VAL:O	3:H:51:VAL:N	2.33	0.54
1:A:192:TRP:HA	1:A:192:TRP:HE3	1.73	0.53
1:A:288:TYR:OH	1:A:355:ILE:HG21	2.08	0.53
1:A:369:THR:O	1:A:369:THR:HG22	2.07	0.53
1:F:253:LEU:O	1:F:256:ASP:N	2.41	0.53
1:F:310:LEU:HD11	1:F:366:TRP:CD1	2.43	0.53
2:G:192:ARG:HB2	2:G:192:ARG:CZ	2.38	0.53
2:G:207:SER:OG	2:G:218:MET:HB2	2.08	0.53
3:C:196:THR:O	3:C:196:THR:HG22	2.08	0.53
1:F:110:MET:O	1:F:115:ALA:HB3	2.08	0.53
1:F:308:LYS:NZ	1:F:372:GLN:CB	2.71	0.53
2:G:157:ALA:O	2:G:158:ASN:C	2.51	0.53
1:A:111:ILE:HD11	6:A:1001:HEM:HMD2	1.91	0.53
1:A:118:PHE:CE2	1:A:294:VAL:HG22	2.43	0.53
1:A:216:ARG:NH1	1:A:222:MET:CA	2.70	0.53
1:A:308:LYS:NZ	1:A:372:GLN:CB	2.71	0.53
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.90	0.53
2:B:50:LEU:HA	2:B:53:ILE:HG22	1.90	0.53
3:C:160:LEU:HD13	3:C:176:ARG:CD	2.33	0.53
1:F:138:PHE:HB2	1:F:207:ASN:HD21	1.72	0.53
1:F:308:LYS:HZ2	1:F:372:GLN:CB	2.21	0.53
2:G:88:VAL:O	2:G:91:VAL:HB	2.09	0.53
2:G:227:ASP:OD1	2:G:229:ALA:HB3	2.09	0.53
1:A:150:VAL:O	1:A:153:VAL:HB	2.08	0.53
7:A:1002:HEO:C24	2:B:100:ILE:HG12	2.38	0.53
2:B:41:ARG:H	2:B:41:ARG:HH11	1.56	0.53
3:C:143:VAL:O	3:C:144:GLY:C	2.50	0.53
1:F:112:PHE:CE1	1:F:286:GLU:OE2	2.59	0.53
2:G:74:LYS:HE2	2:G:75:ASP:OD2	2.08	0.53
2:G:190:GLN:NE2	2:G:192:ARG:HH21	2.06	0.53
1:A:383:TRP:HB3	1:A:434:ALA:HB2	1.91	0.53
2:B:140:PHE:CD2	2:B:153:ILE:HG23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:VAL:O	2:B:151:ASN:HB2	2.09	0.53
2:B:167:SER:HB3	2:B:187:ALA:HA	1.91	0.53
1:F:239:ILE:HG12	1:F:289:ILE:HD13	1.91	0.53
7:F:1002:HEO:H241	2:G:99:ILE:HB	1.90	0.53
1:A:113:PHE:HE2	1:A:153:VAL:N	2.07	0.53
1:A:171:LEU:HD11	1:A:280:TRP:CH2	2.44	0.53
1:A:235:ALA:HB2	1:A:292:LEU:HB2	1.90	0.53
2:B:192:ARG:HB2	2:B:192:ARG:CZ	2.39	0.53
3:C:72:GLU:OE1	3:C:72:GLU:HA	2.08	0.53
3:C:113:ILE:HD11	3:C:150:VAL:CG1	2.38	0.53
3:C:174:ARG:HD3	3:C:177:ILE:HD11	1.91	0.53
1:F:116:MET:N	1:F:117:PRO:CD	2.71	0.53
2:G:143:PRO:HG2	2:G:144:GLU:OE2	2.08	0.53
3:H:89:ALA:HB2	3:H:174:ARG:CD	2.27	0.53
3:H:197:VAL:CG1	3:H:198:VAL:H	2.20	0.53
1:A:502:ALA:O	1:A:504:LEU:N	2.42	0.53
2:B:36:ILE:CD1	2:B:39:GLU:H	2.22	0.53
2:B:90:ALA:HA	2:B:93:TRP:CB	2.35	0.53
2:B:136:TRP:CE2	2:B:213:PRO:O	2.61	0.53
1:A:466:VAL:O	1:A:501:GLY:HA3	2.09	0.53
3:C:33:LEU:HB2	3:C:34:MET:CE	2.39	0.53
1:F:301:ILE:HG23	1:F:380:ALA:HB1	1.90	0.53
1:F:316:LEU:HD11	1:F:365:ASN:HB3	1.91	0.53
1:F:383:TRP:HB3	1:F:434:ALA:HB2	1.91	0.53
1:F:415:PHE:CD1	1:F:472:TYR:HD2	2.27	0.53
3:H:47:TYR:C	3:H:49:VAL:H	2.17	0.53
3:H:113:ILE:HD11	3:H:150:VAL:CG1	2.38	0.53
1:A:125:LEU:HD23	1:A:125:LEU:C	2.34	0.53
1:A:199:ILE:O	1:A:202:THR:HB	2.09	0.53
1:A:311:PHE:CZ	2:B:88:VAL:HG21	2.43	0.53
3:C:197:VAL:CG1	3:C:198:VAL:H	2.20	0.53
1:F:57:LEU:HD12	1:F:142:ASN:HD22	1.74	0.53
1:F:190:TRP:HE3	1:F:191:ILE:HG12	1.74	0.53
1:F:192:TRP:HA	1:F:192:TRP:HE3	1.74	0.53
1:F:279:ILE:HG22	1:F:280:TRP:N	2.24	0.53
2:G:90:ALA:HA	2:G:93:TRP:CB	2.36	0.53
1:A:104:THR:HG23	6:A:1001:HEM:O2D	2.08	0.53
1:A:306:SER:O	1:A:374:ARG:O	2.27	0.53
2:B:39:GLU:HG2	2:B:40:GLN:OE1	2.09	0.53
2:B:228:ARG:O	2:B:232:ASP:OD1	2.27	0.53
1:F:52:VAL:HG12	1:F:52:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:PRO:C	1:F:176:LEU:N	2.66	0.53
1:F:174:PRO:HB2	1:F:175:PRO:CD	2.39	0.53
1:F:288:TYR:HE2	1:F:323:ILE:HG23	1.74	0.53
2:G:39:GLU:HG2	2:G:40:GLN:N	2.24	0.53
2:G:125:LYS:H	2:G:126:PRO:HD2	1.71	0.53
2:G:264:GLU:CG	2:G:265:TYR:H	2.16	0.53
3:H:99:ILE:N	3:H:99:ILE:CD1	2.72	0.53
1:F:187:VAL:O	1:F:190:TRP:HB3	2.09	0.52
1:F:205:GLY:O	1:F:209:PHE:HB2	2.09	0.52
1:F:359:THR:HB	7:F:1002:HEO:C27	2.39	0.52
2:G:136:TRP:CE2	2:G:213:PRO:O	2.61	0.52
3:H:196:THR:HA	3:H:200:LEU:CD2	2.38	0.52
1:A:301:ILE:HG23	1:A:380:ALA:HB1	1.90	0.52
3:C:21:ALA:HA	3:C:24:THR:OG1	2.09	0.52
3:H:102:LEU:O	3:H:105:THR:HB	2.09	0.52
1:A:382:LEU:HD23	1:A:385:ILE:CD1	2.39	0.52
2:B:82:TRP:HE3	2:B:83:SER:H	1.57	0.52
3:C:66:LEU:C	3:C:68:PHE:H	2.18	0.52
1:F:225:MET:HG3	1:F:229:THR:HB	1.90	0.52
1:A:76:ALA:HA	1:A:79:MET:HE3	1.90	0.52
1:A:211:THR:HG23	1:A:215:MET:CE	2.39	0.52
1:A:233:LEU:O	1:A:234:CYS:C	2.52	0.52
1:A:280:TRP:HA	1:A:280:TRP:HE3	1.75	0.52
1:A:394:GLY:HA3	1:A:422:ASN:OD1	2.09	0.52
1:A:548:PRO:O	1:A:550:TYR:N	2.42	0.52
2:B:67:TRP:CG	2:B:68:LYS:N	2.75	0.52
3:C:74:PHE:CE2	3:C:188:ASP:HA	2.44	0.52
1:F:76:ALA:HA	1:F:79:MET:HE3	1.91	0.52
1:F:169:GLY:O	1:F:171:LEU:N	2.43	0.52
1:F:171:LEU:HD11	1:F:280:TRP:CH2	2.44	0.52
1:F:487:ILE:O	1:F:488:ASP:C	2.52	0.52
1:F:502:ALA:O	1:F:504:LEU:N	2.43	0.52
3:H:47:TYR:O	3:H:51:VAL:HG13	2.08	0.52
3:H:174:ARG:HD3	3:H:177:ILE:HD11	1.92	0.52
3:C:47:TYR:C	3:C:49:VAL:H	2.17	0.52
3:C:136:LEU:C	3:C:140:PHE:HB2	2.34	0.52
1:F:206:ILE:HG23	3:H:31:ILE:CG2	2.40	0.52
2:G:270:LYS:HZ2	2:G:272:ASP:H	1.56	0.52
3:H:33:LEU:HB2	3:H:34:MET:CE	2.39	0.52
1:A:336:PHE:CE2	1:A:404:PRO:HG3	2.44	0.52
1:A:486:GLN:C	1:A:487:ILE:HG13	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:PRO:O	2:B:179:LEU:N	2.43	0.52
1:F:233:LEU:O	1:F:234:CYS:C	2.52	0.52
1:F:235:ALA:HB2	1:F:292:LEU:HB2	1.90	0.52
2:G:89:GLU:O	2:G:93:TRP:HB2	2.09	0.52
3:H:66:LEU:C	3:H:68:PHE:H	2.18	0.52
1:A:373:GLY:HA2	2:B:71:ALA:O	2.10	0.52
2:B:101:ILE:CA	2:B:104:ALA:HB3	2.40	0.52
3:C:46:THR:O	3:C:49:VAL:HB	2.10	0.52
1:F:543:THR:CG2	1:F:544:SER:N	2.72	0.52
2:G:95:VAL:CG2	2:G:96:PRO:HD3	2.33	0.52
2:G:200:PRO:HA	2:G:224:ALA:O	2.09	0.52
3:H:83:TYR:CZ	4:I:14:UNK:CB	2.88	0.52
2:B:37:GLY:O	2:B:40:GLN:HG2	2.10	0.52
2:B:207:SER:OG	2:B:218:MET:HB2	2.10	0.52
2:B:225:THR:HB	2:B:226:PRO:HD2	1.92	0.52
2:B:228:ARG:HG3	2:B:231:PHE:CD2	2.44	0.52
3:C:185:HIS:NE2	4:D:57:UNK:O	2.42	0.52
3:H:74:PHE:CE2	3:H:188:ASP:HA	2.44	0.52
3:H:174:ARG:HB3	3:H:177:ILE:CD1	2.39	0.52
1:A:54:HIS:ND1	1:A:135:ASP:OD2	2.43	0.52
1:A:225:MET:HG3	1:A:229:THR:HB	1.92	0.52
1:A:253:LEU:O	1:A:256:ASP:N	2.43	0.52
1:A:312:GLY:O	1:A:316:LEU:HG	2.10	0.52
2:B:138:TRP:CZ3	2:B:174:PHE:HD1	2.23	0.52
1:F:273:MET:SD	2:G:189:MET:HE1	2.49	0.52
1:F:362:LYS:HB3	1:F:366:TRP:CH2	2.45	0.52
2:G:230:ALA:HA	2:G:233:GLN:NE2	2.25	0.52
3:H:120:PHE:O	3:H:121:HIS:C	2.52	0.52
2:B:39:GLU:HG2	2:B:40:GLN:N	2.25	0.52
2:B:125:LYS:H	2:B:126:PRO:HD2	1.72	0.52
4:D:11:UNK:O	4:D:15:UNK:N	2.42	0.52
4:D:86:UNK:O	4:D:87:UNK:C	2.57	0.52
1:F:205:GLY:O	1:F:240:ILE:HD11	2.10	0.52
3:H:21:ALA:HA	3:H:24:THR:OG1	2.10	0.52
1:A:68:MET:CE	1:A:153:VAL:HG13	2.40	0.51
1:A:318:TRP:O	1:A:322:CYS:SG	2.69	0.51
1:A:362:LYS:HB3	1:A:366:TRP:CH2	2.45	0.51
1:A:412:ASN:CG	2:B:209:SER:HB3	2.35	0.51
2:B:157:ALA:O	2:B:158:ASN:C	2.53	0.51
3:C:89:ALA:O	3:C:90:MET:C	2.53	0.51
1:F:248:VAL:O	1:F:252:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:TRP:O	1:F:322:CYS:SG	2.68	0.51
1:F:363:ILE:HG22	1:F:364:PHE:N	2.25	0.51
1:F:420:PHE:HA	1:F:423:VAL:HG22	1.91	0.51
1:F:474:LEU:CD2	1:F:494:MET:HB2	2.31	0.51
2:G:95:VAL:HA	2:G:98:LEU:HD12	1.93	0.51
3:H:42:ILE:O	3:H:45:ALA:HB3	2.10	0.51
1:A:405:GLY:HA2	1:A:408:PHE:HD1	1.73	0.51
3:C:177:ILE:HD12	3:C:177:ILE:C	2.35	0.51
1:F:203:LEU:O	1:F:206:ILE:N	2.42	0.51
1:F:277:ASN:CA	1:F:335:PHE:HZ	2.22	0.51
1:F:307:ARG:O	2:G:79:SER:HB2	2.10	0.51
2:G:50:LEU:HA	2:G:53:ILE:CG2	2.40	0.51
3:H:33:LEU:C	3:H:35:SER:H	2.17	0.51
2:B:177:PRO:C	2:B:179:LEU:N	2.69	0.51
3:C:143:VAL:O	3:C:146:HIS:N	2.44	0.51
1:F:311:PHE:CZ	2:G:88:VAL:HG21	2.45	0.51
2:G:273:LEU:HA	2:G:276:ASP:HB2	1.91	0.51
1:A:52:VAL:O	1:A:52:VAL:HG12	2.10	0.51
2:B:74:LYS:HE2	2:B:75:ASP:OD2	2.09	0.51
3:C:152:SER:C	3:C:154:LEU:N	2.68	0.51
1:F:272:MET:C	1:F:274:MET:H	2.18	0.51
1:F:373:GLY:C	1:F:375:ILE:HD12	2.35	0.51
2:G:101:ILE:O	2:G:105:VAL:HG23	2.10	0.51
3:H:29:PHE:C	3:H:31:ILE:H	2.16	0.51
4:I:11:UNK:O	4:I:15:UNK:N	2.42	0.51
1:A:298:PHE:CE1	1:A:384:THR:HG23	2.45	0.51
1:A:420:PHE:O	1:A:421:HIS:C	2.52	0.51
3:C:97:GLN:O	3:C:97:GLN:HG2	2.10	0.51
1:F:68:MET:CE	1:F:153:VAL:HG13	2.40	0.51
1:F:150:VAL:O	1:F:153:VAL:HB	2.10	0.51
1:F:214:LYS:HZ2	3:H:24:THR:HA	1.73	0.51
1:F:464:PHE:CD1	1:F:468:PHE:HD1	2.27	0.51
2:G:159:THR:O	2:G:196:ILE:HD13	2.10	0.51
3:H:89:ALA:O	3:H:90:MET:C	2.53	0.51
1:A:255:LEU:HB3	1:A:261:THR:HG21	1.92	0.51
1:A:272:MET:C	1:A:274:MET:H	2.18	0.51
1:A:451:THR:HG22	1:A:452:TRP:N	2.24	0.51
2:B:273:LEU:HA	2:B:276:ASP:HB2	1.92	0.51
1:F:54:HIS:ND1	1:F:135:ASP:OD2	2.44	0.51
1:F:442:LYS:HB2	1:F:541:TRP:HZ3	1.75	0.51
3:H:46:THR:O	3:H:49:VAL:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:200:LEU:HD12	3:H:201:MET:N	2.25	0.51
1:A:356:ALA:O	1:A:359:THR:N	2.42	0.51
1:A:441:PRO:C	1:A:443:ALA:N	2.69	0.51
1:A:460:TRP:HZ3	1:A:509:ILE:HG12	1.76	0.51
2:B:163:PHE:CD2	2:B:193:LEU:HD22	2.45	0.51
1:F:73:PHE:O	1:F:77:ILE:HG13	2.11	0.51
1:F:312:GLY:O	1:F:316:LEU:HG	2.10	0.51
1:F:332:LEU:HD22	1:F:335:PHE:CB	2.40	0.51
2:G:99:ILE:HD13	2:G:99:ILE:N	2.26	0.51
1:A:108:VAL:CG2	1:A:170:TRP:HA	2.36	0.51
1:A:277:ASN:CA	1:A:335:PHE:HZ	2.22	0.51
1:A:279:ILE:HG22	1:A:280:TRP:N	2.25	0.51
1:A:346:ALA:HB1	1:A:350:ILE:HD12	1.92	0.51
3:C:120:PHE:O	3:C:121:HIS:C	2.53	0.51
1:F:54:HIS:CG	1:F:55:LYS:N	2.79	0.51
1:F:282:TRP:O	1:F:285:PRO:HD2	2.11	0.51
1:F:356:ALA:O	1:F:359:THR:N	2.42	0.51
1:F:367:LEU:HD23	1:F:370:MET:HE1	1.92	0.51
2:G:50:LEU:HA	2:G:53:ILE:HG22	1.92	0.51
2:G:65:PHE:O	2:G:68:LYS:HE2	2.11	0.51
3:H:91:TYR:OH	4:I:7:UNK:N	2.42	0.51
1:A:316:LEU:HD11	1:A:365:ASN:HB3	1.93	0.51
2:B:85:SER:HB3	2:B:88:VAL:HG13	1.93	0.51
2:B:270:LYS:HE3	2:B:276:ASP:CG	2.36	0.51
3:C:71:VAL:HG22	3:C:191:TRP:HE1	1.76	0.51
1:F:216:ARG:NH1	1:F:222:MET:CA	2.73	0.51
1:F:451:THR:HG22	1:F:452:TRP:N	2.24	0.51
3:H:69:VAL:HG12	3:H:115:MET:SD	2.51	0.51
3:H:171:SER:C	3:H:173:ASN:H	2.18	0.51
1:A:138:PHE:HZ	3:C:28:GLY:HA3	1.76	0.50
1:A:146:PHE:O	1:A:149:THR:N	2.45	0.50
1:A:311:PHE:CG	1:A:312:GLY:N	2.79	0.50
2:B:195:LEU:HD23	2:B:195:LEU:C	2.37	0.50
3:C:47:TYR:C	3:C:49:VAL:N	2.68	0.50
3:C:103:ALA:CA	3:C:161:MET:HE1	2.42	0.50
1:F:108:VAL:CG2	1:F:170:TRP:HA	2.37	0.50
1:F:405:GLY:HA2	1:F:408:PHE:HD1	1.73	0.50
3:H:47:TYR:C	3:H:49:VAL:N	2.68	0.50
3:H:89:ALA:HB1	3:H:171:SER:HA	1.93	0.50
3:C:76:LEU:HB2	3:C:108:PHE:CE2	2.45	0.50
1:F:169:GLY:O	1:F:172:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:36:ILE:HG12	2:G:39:GLU:HB3	1.92	0.50
2:G:138:TRP:CZ3	2:G:174:PHE:HD1	2.22	0.50
3:H:76:LEU:HB2	3:H:108:PHE:CE2	2.45	0.50
3:H:152:SER:C	3:H:154:LEU:N	2.68	0.50
1:A:142:ASN:OD1	1:A:208:PHE:HE1	1.95	0.50
1:A:190:TRP:HE3	1:A:191:ILE:HG12	1.76	0.50
3:C:99:ILE:N	3:C:99:ILE:CD1	2.74	0.50
1:F:134:ARG:O	1:F:135:ASP:CG	2.54	0.50
1:F:159:SER:CB	1:F:189:TYR:HD1	2.24	0.50
1:F:160:LEU:HD23	1:F:165:PHE:HB2	1.92	0.50
1:F:216:ARG:HH12	1:F:222:MET:CA	2.24	0.50
1:F:441:PRO:C	1:F:443:ALA:N	2.70	0.50
3:H:136:LEU:C	3:H:140:PHE:HB2	2.36	0.50
1:A:142:ASN:OD1	1:A:208:PHE:CE1	2.64	0.50
1:A:263:PHE:HE2	3:C:46:THR:HG21	1.75	0.50
1:A:330:VAL:HG12	1:A:351:THR:HB	1.94	0.50
1:A:353:MET:SD	2:B:107:THR:HG21	2.51	0.50
3:C:160:LEU:O	3:C:163:GLN:HB3	2.10	0.50
3:C:171:SER:C	3:C:173:ASN:H	2.19	0.50
1:F:170:TRP:CE2	1:F:171:LEU:HD21	2.45	0.50
2:G:155:PHE:HZ	2:G:222:ALA:HB1	1.76	0.50
2:G:193:LEU:HD23	2:G:193:LEU:C	2.37	0.50
1:A:72:GLY:O	1:A:75:ASP:HB2	2.12	0.50
1:A:209:PHE:CE2	3:C:31:ILE:HD11	2.45	0.50
1:A:239:ILE:O	1:A:239:ILE:HG22	2.11	0.50
1:A:411:HIS:NE2	1:A:412:ASN:OD1	2.44	0.50
2:G:127:ILE:HG22	2:G:128:THR:N	2.26	0.50
2:G:175:PHE:HD2	2:G:206:ILE:HD11	1.77	0.50
2:G:225:THR:HB	2:G:226:PRO:HD2	1.94	0.50
3:H:47:TYR:O	3:H:49:VAL:N	2.45	0.50
3:H:166:ARG:NE	3:H:167:ARG:HH22	2.09	0.50
1:A:156:VAL:HG12	1:A:160:LEU:CD1	2.41	0.50
1:A:209:PHE:CE2	3:C:31:ILE:HD13	2.45	0.50
1:A:295:PHE:HE2	1:A:362:LYS:HG3	1.77	0.50
1:F:374:ARG:N	2:G:71:ALA:O	2.45	0.50
2:G:67:TRP:CG	2:G:68:LYS:N	2.76	0.50
3:H:196:THR:O	3:H:196:THR:HG22	2.12	0.50
1:A:203:LEU:O	1:A:206:ILE:N	2.44	0.50
1:A:406:ALA:HB2	2:B:45:LEU:CD2	2.42	0.50
2:B:95:VAL:HA	2:B:98:LEU:HD12	1.94	0.50
1:F:69:LEU:O	1:F:73:PHE:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:ILE:O	1:F:217:ALA:HB2	2.12	0.50
1:F:277:ASN:N	1:F:335:PHE:HZ	2.10	0.50
1:F:353:MET:SD	2:G:107:THR:HG21	2.51	0.50
2:G:196:ILE:CG2	2:G:198:ASN:HD21	2.24	0.50
3:H:29:PHE:HZ	3:H:182:LEU:HB3	1.76	0.50
1:A:331:TRP:CH2	4:D:97:UNK:CB	2.95	0.50
2:B:270:LYS:HZ2	2:B:272:ASP:H	1.58	0.50
3:C:84:GLY:C	3:C:88:ILE:HD12	2.37	0.50
3:C:150:VAL:HG12	3:C:150:VAL:O	2.10	0.50
1:F:155:LEU:HD13	1:F:193:SER:CA	2.42	0.50
3:H:96:SER:C	3:H:98:VAL:N	2.67	0.50
1:A:54:HIS:CE1	1:A:135:ASP:OD2	2.65	0.50
1:A:111:ILE:CD1	1:A:170:TRP:CE3	2.95	0.50
1:A:330:VAL:HB	1:A:352:THR:OG1	2.12	0.50
1:A:442:LYS:NZ	1:A:543:THR:O	2.45	0.50
2:B:39:GLU:O	2:B:43:LEU:N	2.37	0.50
2:B:97:ILE:O	2:B:101:ILE:HD12	2.12	0.50
2:B:176:ILE:CG2	2:B:179:LEU:HD12	2.30	0.50
1:F:202:THR:O	1:F:206:ILE:HG13	2.11	0.50
1:F:543:THR:HG22	1:F:544:SER:H	1.77	0.50
1:A:169:GLY:O	1:A:171:LEU:N	2.45	0.49
2:B:89:GLU:O	2:B:93:TRP:HB2	2.11	0.49
4:D:71:UNK:O	4:D:72:UNK:C	2.59	0.49
1:F:54:HIS:CE1	1:F:135:ASP:OD2	2.65	0.49
1:F:298:PHE:CE1	1:F:384:THR:HG23	2.47	0.49
1:F:551:ASN:O	1:F:552:PHE:CB	2.57	0.49
3:H:160:LEU:HD13	3:H:176:ARG:CD	2.33	0.49
1:A:202:THR:O	1:A:206:ILE:HG13	2.11	0.49
1:A:417:ILE:HD13	6:A:1001:HEM:HBA2	1.94	0.49
1:A:442:LYS:HB2	1:A:541:TRP:HZ3	1.76	0.49
3:C:30:TRP:CZ2	4:D:79:UNK:C	2.95	0.49
4:D:108:UNK:O	4:D:109:UNK:CB	2.59	0.49
1:F:118:PHE:CE2	1:F:294:VAL:HG22	2.46	0.49
1:F:146:PHE:O	1:F:149:THR:N	2.46	0.49
2:G:240:GLN:O	2:G:241:SER:C	2.53	0.49
1:A:120:ILE:HG23	1:A:204:THR:HG21	1.94	0.49
1:A:375:ILE:HG21	1:A:381:MET:HE2	1.94	0.49
1:A:452:TRP:HA	1:A:455:ARG:CD	2.37	0.49
1:A:548:PRO:O	1:A:551:ASN:N	2.45	0.49
1:F:295:PHE:HE2	1:F:362:LYS:HG3	1.77	0.49
1:F:311:PHE:CG	1:F:312:GLY:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:HIS:NE2	1:F:412:ASN:OD1	2.45	0.49
2:G:132:VAL:O	2:G:134:MET:SD	2.70	0.49
3:H:199:TYR:N	3:H:199:TYR:CD1	2.79	0.49
1:A:329:ILE:O	1:A:329:ILE:HG22	2.12	0.49
1:A:447:LYS:HG3	1:A:448:LEU:N	2.25	0.49
2:B:240:GLN:O	2:B:241:SER:C	2.53	0.49
3:C:166:ARG:NE	3:C:167:ARG:HH22	2.09	0.49
1:F:136:VAL:HG23	1:F:211:THR:OG1	2.12	0.49
1:F:191:ILE:CG2	1:F:250:VAL:HG13	2.43	0.49
4:I:71:UNK:O	4:I:72:UNK:C	2.59	0.49
1:A:54:HIS:CG	1:A:55:LYS:N	2.81	0.49
1:A:169:GLY:HA2	1:A:482:ARG:NH1	2.28	0.49
1:A:244:PRO:O	1:A:245:ILE:C	2.55	0.49
1:A:465:PHE:O	1:A:470:PRO:HD3	2.13	0.49
2:B:264:GLU:CG	2:B:265:TYR:H	2.19	0.49
1:F:151:VAL:HG11	1:F:196:LEU:HD13	1.93	0.49
1:F:222:MET:HE1	1:F:233:LEU:HD11	1.94	0.49
1:F:482:ARG:NH2	6:F:1001:HEM:CGD	2.76	0.49
2:G:36:ILE:HG12	2:G:39:GLU:N	2.22	0.49
1:A:275:TYR:C	1:A:275:TYR:CD2	2.90	0.49
1:A:363:ILE:HG22	1:A:364:PHE:N	2.27	0.49
1:A:487:ILE:O	1:A:488:ASP:C	2.55	0.49
1:A:502:ALA:C	1:A:504:LEU:N	2.68	0.49
1:F:336:PHE:CE2	1:F:404:PRO:HG3	2.46	0.49
1:F:485:GLN:OE1	1:F:485:GLN:HA	2.12	0.49
1:A:191:ILE:CG2	1:A:250:VAL:HG13	2.43	0.49
1:A:374:ARG:CB	2:B:79:SER:HB3	2.35	0.49
1:F:155:LEU:HD12	1:F:196:LEU:HD12	1.94	0.49
1:F:244:PRO:O	1:F:245:ILE:C	2.56	0.49
1:F:374:ARG:HB2	2:G:78:TYR:O	2.12	0.49
1:A:155:LEU:HD13	1:A:193:SER:CA	2.43	0.49
1:A:169:GLY:O	1:A:172:ALA:N	2.46	0.49
1:A:288:TYR:HE2	1:A:323:ILE:HG23	1.78	0.49
1:A:464:PHE:HA	1:A:505:ILE:HD11	1.94	0.49
1:A:488:ASP:OD1	1:A:490:GLN:HG3	2.13	0.49
2:B:36:ILE:HG12	2:B:39:GLU:HB3	1.94	0.49
3:C:96:SER:C	3:C:98:VAL:N	2.67	0.49
1:F:171:LEU:O	1:F:172:ALA:HB3	2.12	0.49
1:A:155:LEU:HD12	1:A:196:LEU:HD12	1.94	0.49
1:A:373:GLY:CA	2:B:71:ALA:HB1	2.32	0.49
1:A:474:LEU:CD2	1:A:491:PHE:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:THR:OG1	2:B:206:ILE:HB	2.11	0.49
3:C:26:ILE:C	3:C:28:GLY:N	2.69	0.49
3:C:90:MET:CE	4:D:68:UNK:CA	2.82	0.49
1:F:72:GLY:O	1:F:75:ASP:HB2	2.13	0.49
1:F:275:TYR:C	1:F:275:TYR:CD2	2.91	0.49
2:G:85:SER:HB3	2:G:88:VAL:HG13	1.95	0.49
2:G:177:PRO:C	2:G:179:LEU:N	2.71	0.49
3:H:29:PHE:C	3:H:31:ILE:N	2.70	0.49
1:A:136:VAL:HG23	1:A:211:THR:OG1	2.13	0.49
2:B:48:PHE:CE1	2:B:52:LEU:HD11	2.48	0.49
2:B:183:ILE:HG13	2:B:184:TYR:N	2.28	0.49
1:F:98:HIS:O	1:F:99:TYR:C	2.56	0.49
1:F:412:ASN:CG	2:G:209:SER:HB3	2.38	0.49
1:F:476:PHE:C	1:F:478:GLY:H	2.21	0.49
3:H:91:TYR:HE2	4:I:6:UNK:CB	2.26	0.49
1:A:69:LEU:O	1:A:73:PHE:HB2	2.13	0.48
1:A:131:ILE:O	1:A:217:ALA:HB2	2.13	0.48
1:A:169:GLY:C	1:A:171:LEU:N	2.69	0.48
3:C:89:ALA:HB1	3:C:171:SER:HA	1.95	0.48
3:C:174:ARG:HB3	3:C:177:ILE:CD1	2.43	0.48
1:F:411:HIS:ND1	7:F:1002:HEO:O2A	2.45	0.48
2:G:176:ILE:CG2	2:G:179:LEU:HD12	2.30	0.48
2:G:202:THR:HA	2:G:223:ILE:HA	1.95	0.48
3:H:160:LEU:O	3:H:163:GLN:HB3	2.12	0.48
4:I:103:UNK:O	4:I:106:UNK:HA	2.13	0.48
1:A:59:ILE:O	1:A:60:MET:C	2.56	0.48
2:B:202:THR:HA	2:B:223:ILE:HA	1.95	0.48
3:C:66:LEU:N	3:C:67:PRO:CD	2.75	0.48
4:D:25:UNK:O	4:D:29:UNK:N	2.46	0.48
1:F:426:GLY:HA2	1:F:430:PHE:CE1	2.48	0.48
1:F:502:ALA:C	1:F:504:LEU:N	2.68	0.48
2:G:130:GLU:OE1	2:G:141:ILE:O	2.30	0.48
2:G:170:VAL:HG23	2:G:171:MET:O	2.13	0.48
3:H:97:GLN:O	3:H:97:GLN:HG2	2.13	0.48
2:B:50:LEU:CA	2:B:53:ILE:HG22	2.43	0.48
1:F:80:ARG:O	1:F:80:ARG:CG	2.60	0.48
1:F:120:ILE:HG23	1:F:204:THR:HG21	1.95	0.48
1:A:367:LEU:HD23	1:A:370:MET:HE1	1.94	0.48
1:A:476:PHE:C	1:A:478:GLY:H	2.21	0.48
3:C:174:ARG:HH11	3:C:177:ILE:HG12	1.78	0.48
1:F:396:MET:HB3	2:G:53:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:PHE:HE2	6:A:1001:HEM:HAB	1.78	0.48
1:A:466:VAL:O	1:A:466:VAL:HG12	2.13	0.48
3:C:29:PHE:HZ	3:C:182:LEU:HB3	1.78	0.48
1:F:147:TRP:O	1:F:151:VAL:HG23	2.13	0.48
1:F:447:LYS:HG3	1:F:448:LEU:N	2.26	0.48
2:G:195:LEU:HD23	2:G:195:LEU:C	2.39	0.48
2:G:275:ALA:O	2:G:279:ASN:ND2	2.47	0.48
3:H:91:TYR:O	3:H:92:LYS:C	2.54	0.48
1:A:57:LEU:HD12	1:A:142:ASN:HD22	1.78	0.48
1:A:73:PHE:O	1:A:77:ILE:HG13	2.14	0.48
1:A:414:LEU:HD23	1:A:479:MET:HB3	1.96	0.48
2:B:243:ASN:O	2:B:266:PHE:HA	2.13	0.48
3:C:51:VAL:HG12	3:C:135:PHE:CE2	2.48	0.48
3:C:100:SER:O	3:C:103:ALA:HB3	2.14	0.48
3:C:112:PHE:HZ	3:C:191:TRP:CZ3	2.31	0.48
1:F:465:PHE:O	1:F:470:PRO:HD3	2.14	0.48
2:G:136:TRP:HA	2:G:218:MET:SD	2.54	0.48
3:H:66:LEU:N	3:H:67:PRO:CD	2.75	0.48
3:H:71:VAL:HG22	3:H:191:TRP:HE1	1.79	0.48
1:A:105:ALA:O	1:A:108:VAL:HB	2.13	0.48
1:A:134:ARG:O	1:A:135:ASP:CG	2.56	0.48
1:A:382:LEU:HA	1:A:385:ILE:CD1	2.43	0.48
1:A:543:THR:CG2	1:A:544:SER:N	2.75	0.48
3:C:124:ILE:HD11	3:C:140:PHE:HZ	1.79	0.48
1:F:79:MET:C	1:F:81:SER:H	2.20	0.48
1:F:169:GLY:HA2	1:F:482:ARG:NH1	2.29	0.48
1:F:235:ALA:O	1:F:289:ILE:HG12	2.13	0.48
1:F:336:PHE:CE2	1:F:404:PRO:HA	2.48	0.48
4:I:25:UNK:O	4:I:29:UNK:N	2.46	0.48
1:A:235:ALA:O	1:A:289:ILE:HG12	2.13	0.48
1:A:332:LEU:HB2	1:A:348:PHE:CG	2.49	0.48
1:A:498:ALA:C	1:A:500:SER:H	2.22	0.48
2:B:95:VAL:O	2:B:98:LEU:HB2	2.13	0.48
2:B:236:ALA:HA	2:B:239:LYS:HG3	1.96	0.48
1:F:332:LEU:C	1:F:334:HIS:H	2.20	0.48
1:F:483:LEU:HD22	2:G:216:SER:HA	1.96	0.48
1:F:486:GLN:HG2	1:F:492:HIS:NE2	2.29	0.48
3:H:150:VAL:HG12	3:H:150:VAL:O	2.13	0.48
1:A:332:LEU:CD2	1:A:335:PHE:CG	2.96	0.48
1:A:379:SER:O	1:A:382:LEU:HB2	2.14	0.48
1:A:464:PHE:CD1	1:A:468:PHE:HD1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ILE:HG12	2:B:39:GLU:N	2.24	0.48
3:C:139:PHE:C	3:C:141:ALA:H	2.22	0.48
1:F:169:GLY:C	1:F:171:LEU:N	2.70	0.48
1:F:420:PHE:O	1:F:421:HIS:C	2.55	0.48
3:H:83:TYR:C	3:H:101:TRP:CZ3	2.91	0.48
1:A:151:VAL:HG11	1:A:196:LEU:HD13	1.94	0.48
1:A:541:TRP:C	1:A:543:THR:N	2.70	0.48
2:B:196:ILE:CG2	2:B:198:ASN:HD21	2.26	0.48
3:C:47:TYR:O	3:C:49:VAL:N	2.47	0.48
3:C:84:GLY:O	3:C:85:MET:C	2.57	0.48
3:C:166:ARG:HB2	3:C:167:ARG:NH2	2.27	0.48
1:F:59:ILE:O	1:F:60:MET:C	2.56	0.48
1:F:330:VAL:HG12	1:F:351:THR:HB	1.96	0.48
1:F:464:PHE:HA	1:F:505:ILE:HD11	1.95	0.48
2:G:56:ILE:N	2:G:57:PRO:HD2	2.27	0.48
2:G:184:TYR:CD2	2:G:186:MET:HB2	2.48	0.48
1:A:96:PRO:HG2	2:B:213:PRO:HA	1.96	0.47
1:A:253:LEU:O	1:A:256:ASP:HB2	2.14	0.47
1:A:282:TRP:O	1:A:285:PRO:HD2	2.14	0.47
1:A:491:PHE:O	1:A:495:LEU:HG	2.14	0.47
2:B:101:ILE:HA	2:B:104:ALA:HB3	1.96	0.47
2:B:174:PHE:O	2:B:182:GLN:HA	2.14	0.47
2:B:186:MET:HB3	2:B:189:MET:HG3	1.95	0.47
1:F:105:ALA:O	1:F:108:VAL:HB	2.13	0.47
1:F:488:ASP:OD1	1:F:490:GLN:HG3	2.14	0.47
1:F:491:PHE:C	1:F:493:THR:N	2.71	0.47
2:G:177:PRO:O	2:G:179:LEU:N	2.47	0.47
2:G:228:ARG:HG3	2:G:231:PHE:CD2	2.46	0.47
3:H:88:ILE:CG1	3:H:98:VAL:HG13	2.37	0.47
2:B:193:LEU:HD23	2:B:193:LEU:C	2.39	0.47
3:C:90:MET:CE	4:D:67:UNK:C	2.90	0.47
1:F:119:VAL:CG2	1:F:123:MET:HE2	2.34	0.47
1:F:253:LEU:O	1:F:256:ASP:HB2	2.14	0.47
1:F:482:ARG:NH2	6:F:1001:HEM:O2D	2.47	0.47
2:G:95:VAL:O	2:G:99:ILE:HG12	2.14	0.47
2:G:131:VAL:CG2	2:G:165:VAL:HG22	2.44	0.47
2:G:136:TRP:HB2	2:G:259:GLU:HA	1.95	0.47
3:H:143:VAL:O	3:H:146:HIS:N	2.47	0.47
1:A:79:MET:C	1:A:81:SER:H	2.20	0.47
1:A:297:VAL:HG22	1:A:439:TRP:HZ3	1.79	0.47
1:A:330:VAL:HG13	1:A:351:THR:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:HA	1:A:464:PHE:CZ	2.49	0.47
2:B:195:LEU:HD23	2:B:196:ILE:C	2.39	0.47
4:D:103:UNK:O	4:D:106:UNK:HA	2.14	0.47
1:F:385:ILE:HA	1:F:388:ILE:HD12	1.95	0.47
1:F:541:TRP:C	1:F:543:THR:N	2.70	0.47
2:G:175:PHE:HD1	2:G:181:SER:O	1.98	0.47
3:H:84:GLY:O	3:H:85:MET:C	2.57	0.47
3:H:166:ARG:HB2	3:H:167:ARG:NH2	2.27	0.47
1:A:464:PHE:HD2	1:A:465:PHE:CD1	2.33	0.47
3:C:74:PHE:HD1	3:C:77:LEU:HD12	1.79	0.47
1:F:142:ASN:OD1	1:F:208:PHE:CE1	2.67	0.47
1:F:311:PHE:CZ	2:G:88:VAL:HG11	2.48	0.47
3:H:78:PHE:HZ	4:I:57:UNK:HA	1.78	0.47
3:H:85:MET:HA	3:H:88:ILE:HD12	1.95	0.47
3:H:124:ILE:HD11	3:H:140:PHE:HZ	1.80	0.47
1:A:170:TRP:NE1	1:A:171:LEU:HG	2.29	0.47
1:A:389:VAL:HG12	1:A:390:THR:N	2.29	0.47
1:A:474:LEU:CD2	1:A:494:MET:HB2	2.34	0.47
1:A:516:MET:O	1:A:519:SER:N	2.40	0.47
3:C:72:GLU:O	3:C:75:LEU:HB3	2.14	0.47
3:C:195:PHE:CD1	3:C:199:TYR:CB	2.98	0.47
1:F:397:THR:HG23	1:F:415:PHE:CZ	2.49	0.47
1:F:460:TRP:HZ3	1:F:509:ILE:HG12	1.80	0.47
2:G:130:GLU:OE1	2:G:141:ILE:HG22	2.15	0.47
1:A:79:MET:C	1:A:81:SER:N	2.72	0.47
1:A:384:THR:O	1:A:388:ILE:HG13	2.14	0.47
1:A:485:GLN:HA	1:A:485:GLN:OE1	2.13	0.47
2:B:170:VAL:HG23	2:B:171:MET:O	2.15	0.47
3:C:199:TYR:N	3:C:199:TYR:CD1	2.81	0.47
2:G:48:PHE:CE1	2:G:52:LEU:HD11	2.49	0.47
1:A:147:TRP:O	1:A:151:VAL:HG23	2.14	0.47
1:A:512:LEU:O	1:A:516:MET:HG3	2.14	0.47
2:B:56:ILE:N	2:B:57:PRO:HD2	2.28	0.47
1:F:330:VAL:HG13	1:F:351:THR:CG2	2.44	0.47
1:F:375:ILE:HG21	1:F:381:MET:HE2	1.96	0.47
2:G:174:PHE:O	2:G:182:GLN:HA	2.15	0.47
3:H:51:VAL:HG12	3:H:135:PHE:CE2	2.49	0.47
3:H:88:ILE:HG23	3:H:98:VAL:HG11	1.95	0.47
3:H:177:ILE:C	3:H:177:ILE:HD12	2.39	0.47
4:I:73:UNK:O	4:I:75:UNK:N	2.48	0.47
1:A:277:ASN:N	1:A:335:PHE:HZ	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ALA:HB2	2:B:45:LEU:HD22	1.96	0.47
1:F:345:ASN:O	1:F:349:GLY:N	2.46	0.47
2:G:99:ILE:O	2:G:100:ILE:C	2.53	0.47
3:H:33:LEU:C	3:H:34:MET:HE2	2.40	0.47
3:H:174:ARG:CB	3:H:177:ILE:HD11	2.42	0.47
2:B:131:VAL:CG2	2:B:165:VAL:HG22	2.45	0.47
2:B:137:LYS:CE	2:B:261:ASN:ND2	2.78	0.47
2:B:269:VAL:O	2:B:270:LYS:C	2.56	0.47
1:F:112:PHE:C	1:F:113:PHE:CD1	2.93	0.47
1:F:306:SER:HB3	1:F:375:ILE:HG13	1.96	0.47
1:A:354:ILE:C	1:A:356:ALA:H	2.22	0.47
2:B:139:PHE:HA	2:B:149:THR:O	2.15	0.47
3:C:191:TRP:O	3:C:191:TRP:CD1	2.68	0.47
1:F:354:ILE:C	1:F:356:ALA:H	2.22	0.47
1:F:357:ILE:CD1	2:G:100:ILE:CD1	2.89	0.47
1:F:389:VAL:HG12	1:F:390:THR:N	2.30	0.47
1:F:512:LEU:O	1:F:516:MET:HG3	2.15	0.47
3:H:85:MET:CA	3:H:88:ILE:HD12	2.45	0.47
1:A:156:VAL:O	1:A:160:LEU:HD12	2.15	0.46
1:A:332:LEU:HD22	1:A:335:PHE:HB2	1.96	0.46
1:A:491:PHE:H	1:A:491:PHE:HD1	1.62	0.46
1:A:511:CYS:SG	1:A:512:LEU:N	2.88	0.46
2:B:159:THR:O	2:B:196:ILE:HD13	2.15	0.46
3:C:88:ILE:O	3:C:174:ARG:NE	2.48	0.46
4:D:86:UNK:O	4:D:90:UNK:N	2.48	0.46
1:F:168:THR:CB	1:F:172:ALA:HA	2.40	0.46
1:F:332:LEU:CD2	1:F:335:PHE:CG	2.97	0.46
1:F:337:THR:C	1:F:339:GLY:H	2.24	0.46
1:F:491:PHE:C	1:F:493:THR:H	2.22	0.46
2:G:125:LYS:N	2:G:126:PRO:CD	2.71	0.46
2:G:195:LEU:HD23	2:G:196:ILE:C	2.40	0.46
1:A:482:ARG:NH2	6:A:1001:HEM:CGD	2.79	0.46
7:A:1002:HEO:H241	2:B:99:ILE:HB	1.96	0.46
2:B:156:PRO:HD3	2:B:231:PHE:CE2	2.51	0.46
2:B:184:TYR:CD2	2:B:186:MET:HB2	2.49	0.46
1:F:79:MET:C	1:F:81:SER:N	2.72	0.46
1:F:253:LEU:O	1:F:254:THR:C	2.58	0.46
1:F:458:TRP:O	1:F:462:ILE:HG13	2.15	0.46
1:F:498:ALA:C	1:F:500:SER:H	2.24	0.46
3:H:30:TRP:CH2	4:I:79:UNK:CA	2.97	0.46
3:H:119:GLU:O	3:H:120:PHE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:THR:HG23	1:A:415:PHE:CZ	2.50	0.46
2:B:130:GLU:OE1	2:B:141:ILE:HG22	2.15	0.46
2:B:134:MET:CE	2:B:255:ALA:HB2	2.45	0.46
3:C:197:VAL:CG1	3:C:198:VAL:HG23	2.45	0.46
1:F:126:VAL:O	1:F:126:VAL:HG12	2.15	0.46
1:F:238:LEU:HD21	1:F:324:THR:HG23	1.95	0.46
1:F:281:ALA:HA	1:F:331:TRP:CG	2.50	0.46
2:G:130:GLU:OE1	2:G:141:ILE:HB	2.16	0.46
3:H:199:TYR:H	3:H:199:TYR:HD1	1.60	0.46
1:A:295:PHE:CE2	1:A:362:LYS:HG3	2.50	0.46
1:A:452:TRP:O	1:A:455:ARG:HB2	2.15	0.46
1:A:463:GLY:O	1:A:464:PHE:C	2.56	0.46
2:B:54:VAL:C	2:B:56:ILE:N	2.73	0.46
3:C:139:PHE:C	3:C:141:ALA:N	2.74	0.46
1:F:103:PHE:CZ	6:F:1001:HEM:CMA	2.99	0.46
1:F:306:SER:HA	1:F:375:ILE:HG23	1.96	0.46
1:F:474:LEU:CD2	1:F:491:PHE:HA	2.45	0.46
1:A:127:VAL:N	1:A:128:PRO:CD	2.77	0.46
1:A:336:PHE:CE2	1:A:404:PRO:HA	2.50	0.46
1:A:374:ARG:HB2	2:B:78:TYR:O	2.16	0.46
2:B:217:GLY:CA	2:B:260:TYR:CZ	2.95	0.46
3:C:91:TYR:OH	4:D:7:UNK:CB	2.63	0.46
1:F:389:VAL:HG13	2:G:61:MET:CE	2.46	0.46
2:G:67:TRP:O	2:G:69:TYR:N	2.48	0.46
3:H:174:ARG:HH11	3:H:177:ILE:HG12	1.80	0.46
1:A:171:LEU:O	1:A:172:ALA:HB3	2.15	0.46
1:A:426:GLY:HA2	1:A:430:PHE:CE1	2.51	0.46
2:B:134:MET:HE2	2:B:255:ALA:HB2	1.97	0.46
2:B:136:TRP:HA	2:B:218:MET:CG	2.45	0.46
3:C:26:ILE:C	3:C:28:GLY:H	2.24	0.46
2:G:50:LEU:CA	2:G:53:ILE:HG22	2.45	0.46
2:G:152:GLU:OE2	2:G:223:ILE:HG13	2.16	0.46
3:H:84:GLY:C	3:H:88:ILE:HD12	2.41	0.46
3:H:103:ALA:CA	3:H:161:MET:HE1	2.46	0.46
1:A:281:ALA:HA	1:A:331:TRP:CG	2.50	0.46
1:A:337:THR:C	1:A:339:GLY:H	2.24	0.46
1:A:408:PHE:O	2:B:182:GLN:NE2	2.42	0.46
1:A:482:ARG:NH2	6:A:1001:HEM:O2D	2.49	0.46
2:B:88:VAL:HG23	2:B:89:GLU:N	2.31	0.46
2:B:138:TRP:HE1	2:B:218:MET:HE2	1.81	0.46
2:B:238:ALA:O	2:B:241:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:VAL:O	2:B:280:LYS:HG2	2.16	0.46
3:C:134:GLY:CA	3:C:137:SER:HB3	2.45	0.46
1:F:110:MET:HB2	6:F:1001:HEM:HBC2	1.97	0.46
1:F:297:VAL:HG22	1:F:439:TRP:HZ3	1.81	0.46
1:F:384:THR:O	1:F:388:ILE:HG13	2.16	0.46
1:F:403:VAL:HG13	2:G:107:THR:HG23	1.97	0.46
1:F:422:ASN:HA	1:F:464:PHE:CZ	2.50	0.46
1:F:491:PHE:H	1:F:491:PHE:HD1	1.62	0.46
2:G:186:MET:HB3	2:G:189:MET:HG3	1.97	0.46
1:A:238:LEU:HD21	1:A:324:THR:HG23	1.96	0.46
2:B:125:LYS:N	2:B:126:PRO:CD	2.72	0.46
2:B:152:GLU:OE2	2:B:223:ILE:HG13	2.16	0.46
2:B:155:PHE:HZ	2:B:222:ALA:HB1	1.80	0.46
1:F:127:VAL:N	1:F:128:PRO:CD	2.77	0.46
1:F:239:ILE:O	1:F:239:ILE:HG22	2.15	0.46
1:F:395:GLY:CA	7:F:1002:HEO:H162	2.38	0.46
2:G:111:THR:O	2:G:111:THR:HG22	2.16	0.46
2:G:201:GLY:O	2:G:224:ALA:HB3	2.16	0.46
2:G:238:ALA:O	2:G:241:SER:N	2.48	0.46
3:H:72:GLU:O	3:H:75:LEU:HB3	2.15	0.46
3:H:174:ARG:HD3	3:H:177:ILE:CD1	2.46	0.46
1:A:112:PHE:C	1:A:113:PHE:CD1	2.93	0.46
1:A:345:ASN:O	1:A:349:GLY:N	2.48	0.46
1:A:398:GLY:O	7:A:1002:HEO:HMB3	2.15	0.46
2:B:46:THR:O	2:B:50:LEU:HG	2.15	0.46
2:B:214:GLY:O	2:B:218:MET:HG3	2.16	0.46
3:C:92:LYS:HE2	3:C:92:LYS:HB3	1.82	0.46
1:F:272:MET:HE3	2:G:186:MET:CG	2.45	0.46
1:F:452:TRP:HA	1:F:455:ARG:CD	2.41	0.46
3:H:26:ILE:C	3:H:28:GLY:N	2.70	0.46
3:H:102:LEU:HD23	3:H:161:MET:CE	2.45	0.46
1:A:110:MET:HB2	6:A:1001:HEM:HBC2	1.96	0.46
1:A:318:TRP:O	1:A:322:CYS:N	2.36	0.46
2:B:149:THR:HG21	2:B:234:TRP:CH2	2.50	0.46
2:B:175:PHE:HD1	2:B:181:SER:O	1.99	0.46
1:F:255:LEU:HB3	1:F:261:THR:HG21	1.98	0.46
2:G:56:ILE:HD11	2:G:99:ILE:HG13	1.98	0.46
2:G:150:VAL:O	2:G:151:ASN:HB2	2.17	0.46
2:G:217:GLY:CA	2:G:260:TYR:CZ	2.96	0.46
2:G:277:VAL:O	2:G:280:LYS:HG2	2.16	0.46
3:H:86:ALA:C	3:H:88:ILE:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:O	1:A:254:THR:C	2.59	0.45
1:A:332:LEU:C	1:A:334:HIS:H	2.22	0.45
1:A:486:GLN:CD	1:A:486:GLN:N	2.74	0.45
2:B:53:ILE:O	2:B:55:VAL:N	2.49	0.45
2:B:137:LYS:CE	2:B:261:ASN:HD21	2.29	0.45
2:B:142:TYR:HE1	2:B:234:TRP:HZ3	1.64	0.45
4:D:63:UNK:O	4:D:67:UNK:N	2.50	0.45
1:F:102:ILE:O	1:F:105:ALA:N	2.49	0.45
1:F:118:PHE:CD2	1:F:119:VAL:N	2.85	0.45
1:F:155:LEU:CD1	1:F:193:SER:HA	2.46	0.45
1:F:292:LEU:CB	1:F:293:PRO:HD3	2.44	0.45
1:F:352:THR:HA	1:F:355:ILE:HG12	1.97	0.45
1:F:414:LEU:HD23	1:F:479:MET:HB3	1.98	0.45
2:G:154:ALA:HB3	2:G:234:TRP:CD2	2.51	0.45
1:A:118:PHE:CD2	1:A:119:VAL:N	2.85	0.45
1:A:146:PHE:O	1:A:148:PHE:N	2.49	0.45
1:A:375:ILE:CG1	2:B:67:TRP:HE1	2.29	0.45
2:B:86:ASN:C	2:B:87:LYS:HD2	2.40	0.45
2:B:127:ILE:HG22	2:B:128:THR:N	2.31	0.45
3:C:102:LEU:HD23	3:C:161:MET:CE	2.45	0.45
1:F:79:MET:HG3	1:F:103:PHE:CE2	2.51	0.45
1:F:277:ASN:O	1:F:281:ALA:HB2	2.16	0.45
1:F:295:PHE:CE2	1:F:362:LYS:HG3	2.51	0.45
3:H:199:TYR:N	3:H:199:TYR:HD1	2.13	0.45
1:A:168:THR:HB	1:A:172:ALA:CB	2.46	0.45
1:A:335:PHE:HA	1:A:338:MET:CE	2.47	0.45
1:A:441:PRO:HG2	1:A:447:LYS:HD2	1.98	0.45
1:A:468:PHE:HA	1:A:471:LEU:HG	1.98	0.45
2:B:233:GLN:O	2:B:236:ALA:HB3	2.17	0.45
1:F:61:TYR:CE1	1:F:146:PHE:CD1	3.05	0.45
1:F:120:ILE:HD13	1:F:201:THR:OG1	2.16	0.45
1:F:463:GLY:O	1:F:464:PHE:C	2.57	0.45
2:G:88:VAL:HG23	2:G:89:GLU:N	2.31	0.45
1:A:126:VAL:O	1:A:126:VAL:HG12	2.16	0.45
1:A:377:PHE:CD1	1:A:377:PHE:N	2.84	0.45
2:B:130:GLU:HA	2:B:164:LYS:HB2	1.99	0.45
3:C:88:ILE:HG23	3:C:98:VAL:HG11	1.97	0.45
1:F:142:ASN:OD1	1:F:208:PHE:HE1	2.00	0.45
1:F:195:GLN:HG2	1:F:250:VAL:HG11	1.97	0.45
1:F:284:HIS:NE2	1:F:288:TYR:CE1	2.84	0.45
2:G:54:VAL:C	2:G:56:ILE:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:97:ILE:HG12	2:G:101:ILE:HD11	1.98	0.45
2:G:162:TYR:CD1	2:G:194:HIS:NE2	2.85	0.45
3:H:33:LEU:C	3:H:35:SER:N	2.74	0.45
3:H:74:PHE:HD1	3:H:77:LEU:HD12	1.81	0.45
3:H:191:TRP:CD1	3:H:191:TRP:O	2.69	0.45
1:A:79:MET:HG3	1:A:103:PHE:CE2	2.52	0.45
1:A:221:THR:H	1:A:224:LYS:HD2	1.81	0.45
1:A:284:HIS:NE2	1:A:288:TYR:CE1	2.84	0.45
3:C:192:ILE:O	3:C:192:ILE:HG12	2.16	0.45
3:C:202:GLY:O	3:C:203:ALA:HB3	2.17	0.45
1:F:57:LEU:HD23	1:F:57:LEU:HA	1.79	0.45
1:F:316:LEU:HD21	1:F:365:ASN:CG	2.41	0.45
1:F:379:SER:O	1:F:382:LEU:HB2	2.17	0.45
2:G:90:ALA:O	2:G:91:VAL:C	2.59	0.45
3:H:139:PHE:C	3:H:141:ALA:N	2.75	0.45
3:H:145:THR:O	3:H:147:GLY:N	2.49	0.45
1:A:385:ILE:HA	1:A:388:ILE:HD12	1.98	0.45
1:A:473:ALA:C	1:A:475:GLY:N	2.75	0.45
2:B:111:THR:O	2:B:111:THR:HG22	2.17	0.45
3:C:50:LEU:HD11	3:C:134:GLY:CA	2.44	0.45
1:F:56:ARG:O	1:F:60:MET:HG2	2.17	0.45
1:F:291:ILE:HA	1:F:294:VAL:HG23	1.99	0.45
1:F:360:GLY:O	1:F:361:VAL:C	2.59	0.45
1:F:377:PHE:CD1	1:F:377:PHE:N	2.84	0.45
1:F:388:ILE:HG13	1:F:388:ILE:H	1.50	0.45
1:F:464:PHE:HD2	1:F:465:PHE:CD1	2.35	0.45
2:G:38:LEU:HA	2:G:41:ARG:HD3	1.98	0.45
2:G:86:ASN:C	2:G:87:LYS:HD2	2.41	0.45
2:G:236:ALA:HA	2:G:239:LYS:HG3	1.99	0.45
2:G:254:LEU:HD13	2:G:254:LEU:C	2.41	0.45
1:A:106:HIS:CD2	1:A:107:GLY:H	2.35	0.45
1:A:277:ASN:O	1:A:281:ALA:HB2	2.17	0.45
1:A:415:PHE:CD1	1:A:472:TYR:CD2	3.04	0.45
1:A:424:ILE:CG2	6:A:1001:HEM:HAC	2.38	0.45
1:A:480:THR:HB	1:A:483:LEU:CG	2.46	0.45
2:B:136:TRP:NE1	2:B:213:PRO:O	2.49	0.45
3:C:119:GLU:O	3:C:120:PHE:C	2.60	0.45
3:C:156:TRP:NE1	3:C:180:LEU:HD13	2.28	0.45
1:F:248:VAL:HG13	3:H:43:LEU:CD2	2.47	0.45
1:F:468:PHE:HA	1:F:471:LEU:HG	1.98	0.45
1:F:491:PHE:O	1:F:493:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:43:LEU:O	2:G:46:THR:OG1	2.31	0.45
1:A:80:ARG:O	1:A:80:ARG:CG	2.64	0.45
1:A:102:ILE:O	1:A:105:ALA:N	2.49	0.45
1:A:292:LEU:CB	1:A:293:PRO:HD3	2.44	0.45
1:A:352:THR:HA	1:A:355:ILE:HG12	1.97	0.45
1:A:367:LEU:HD13	2:B:63:VAL:CG1	2.46	0.45
1:A:491:PHE:C	1:A:493:THR:N	2.74	0.45
2:B:275:ALA:O	2:B:279:ASN:ND2	2.50	0.45
1:F:101:GLN:CG	1:F:165:PHE:O	2.65	0.45
1:F:329:ILE:O	1:F:329:ILE:HG22	2.17	0.45
2:G:60:LEU:C	2:G:62:ALA:N	2.68	0.45
2:G:137:LYS:CE	2:G:261:ASN:ND2	2.79	0.45
2:G:149:THR:HG21	2:G:234:TRP:CH2	2.51	0.45
2:G:156:PRO:HG3	2:G:231:PHE:CD2	2.52	0.45
3:H:102:LEU:CD2	3:H:161:MET:HE3	2.45	0.45
1:A:55:LYS:HZ1	1:A:551:ASN:N	2.15	0.45
1:A:187:VAL:O	1:A:188:ASP:C	2.59	0.45
1:A:248:VAL:O	1:A:252:LEU:HG	2.17	0.45
1:A:417:ILE:HA	1:A:420:PHE:CE2	2.51	0.45
1:A:481:ARG:HG2	1:A:482:ARG:H	1.80	0.45
2:B:137:LYS:HE2	2:B:261:ASN:ND2	2.32	0.45
2:B:193:LEU:HD23	2:B:194:HIS:O	2.17	0.45
3:C:145:THR:OG1	3:C:146:HIS:N	2.50	0.45
3:C:150:VAL:HG22	3:C:187:LEU:CD1	2.47	0.45
1:F:75:ASP:C	1:F:79:MET:HE2	2.42	0.45
1:F:248:VAL:HG21	3:H:42:ILE:CG2	2.47	0.45
1:F:332:LEU:HB2	1:F:348:PHE:CG	2.52	0.45
1:F:417:ILE:HA	1:F:420:PHE:CE2	2.51	0.45
2:G:46:THR:O	2:G:50:LEU:HG	2.16	0.45
2:G:70:ARG:C	2:G:72:SER:H	2.25	0.45
2:G:217:GLY:HA3	2:G:260:TYR:CE1	2.52	0.45
2:G:265:TYR:O	2:G:266:PHE:CD2	2.70	0.45
3:H:137:SER:O	3:H:140:PHE:HB3	2.17	0.45
3:H:191:TRP:C	3:H:193:CYS:H	2.24	0.45
1:A:274:MET:HE3	3:C:49:VAL:HG21	1.99	0.45
1:A:291:ILE:HA	1:A:294:VAL:HG23	1.99	0.45
1:A:311:PHE:HZ	2:B:88:VAL:HG21	1.81	0.45
1:A:332:LEU:HD22	1:A:335:PHE:CG	2.52	0.45
1:A:409:VAL:HG12	2:B:175:PHE:HZ	1.80	0.45
1:F:138:PHE:CZ	3:H:28:GLY:HA3	2.44	0.45
1:F:318:TRP:O	1:F:322:CYS:N	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:THR:O	1:F:369:THR:CG2	2.65	0.45
1:F:374:ARG:HD3	2:G:76:ALA:O	2.17	0.45
1:F:424:ILE:CG2	6:F:1001:HEM:HAC	2.38	0.45
2:G:44:ILE:O	2:G:45:LEU:C	2.60	0.45
2:G:61:MET:HA	2:G:61:MET:CE	2.44	0.45
3:H:134:GLY:CA	3:H:137:SER:HB3	2.46	0.45
3:H:139:PHE:C	3:H:141:ALA:H	2.24	0.45
3:H:197:VAL:CG1	3:H:198:VAL:HG23	2.47	0.45
1:A:155:LEU:CD1	1:A:193:SER:HA	2.47	0.44
1:A:393:VAL:O	1:A:396:MET:HE2	2.17	0.44
2:B:136:TRP:HB2	2:B:259:GLU:HA	1.98	0.44
1:F:187:VAL:O	1:F:188:ASP:C	2.60	0.44
1:F:395:GLY:O	1:F:399:VAL:HG23	2.17	0.44
1:F:466:VAL:O	1:F:466:VAL:HG12	2.16	0.44
2:G:142:TYR:HE1	2:G:234:TRP:HZ3	1.64	0.44
1:A:116:MET:HB3	1:A:117:PRO:HD3	1.98	0.44
1:A:146:PHE:C	1:A:148:PHE:N	2.75	0.44
2:B:56:ILE:O	2:B:60:LEU:N	2.48	0.44
2:B:154:ALA:HB3	2:B:234:TRP:CD2	2.52	0.44
2:B:225:THR:HB	2:B:226:PRO:CD	2.47	0.44
3:C:83:TYR:C	3:C:101:TRP:CZ3	2.95	0.44
1:F:168:THR:CG2	1:F:176:LEU:HB3	2.41	0.44
1:F:211:THR:HG23	1:F:215:MET:CE	2.42	0.44
1:F:463:GLY:HA3	1:F:505:ILE:HG13	1.99	0.44
2:G:74:LYS:HE2	2:G:75:ASP:CG	2.42	0.44
2:G:155:PHE:CZ	2:G:222:ALA:HB1	2.52	0.44
1:A:96:PRO:CG	2:B:213:PRO:HA	2.47	0.44
1:A:115:ALA:O	1:A:290:LEU:HD11	2.17	0.44
2:B:138:TRP:HH2	2:B:174:PHE:HA	1.82	0.44
3:C:190:VAL:O	3:C:194:VAL:HG23	2.17	0.44
1:F:243:PHE:HA	1:F:282:TRP:CD1	2.53	0.44
1:F:246:LEU:CD1	1:F:250:VAL:HG23	2.47	0.44
1:F:389:VAL:O	1:F:393:VAL:HG23	2.16	0.44
1:A:316:LEU:CD2	1:A:362:LYS:HA	2.47	0.44
1:A:458:TRP:O	1:A:462:ILE:HG13	2.18	0.44
2:B:36:ILE:HG23	2:B:39:GLU:HB3	2.00	0.44
2:B:53:ILE:C	2:B:55:VAL:N	2.75	0.44
2:B:90:ALA:O	2:B:91:VAL:C	2.60	0.44
2:B:132:VAL:O	2:B:134:MET:SD	2.76	0.44
2:B:175:PHE:CD2	2:B:206:ILE:HD11	2.51	0.44
3:C:26:ILE:CD1	3:C:175:THR:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:MET:HA	3:C:88:ILE:HD12	1.97	0.44
3:C:137:SER:O	3:C:140:PHE:HB3	2.18	0.44
4:D:41:UNK:O	4:D:42:UNK:C	2.66	0.44
1:F:274:MET:CE	3:H:49:VAL:HG21	2.47	0.44
4:I:41:UNK:O	4:I:42:UNK:C	2.66	0.44
1:A:56:ARG:O	1:A:60:MET:HG2	2.18	0.44
1:A:338:MET:HA	2:B:184:TYR:CG	2.53	0.44
2:B:74:LYS:HE2	2:B:75:ASP:CG	2.42	0.44
3:C:148:LEU:O	3:C:151:THR:N	2.50	0.44
3:C:191:TRP:C	3:C:193:CYS:H	2.25	0.44
1:F:79:MET:SD	1:F:102:ILE:CG2	3.05	0.44
1:F:245:ILE:HB	1:F:282:TRP:HB2	2.00	0.44
1:F:400:LEU:HD11	2:G:46:THR:HA	2.00	0.44
2:G:45:LEU:CD1	2:G:110:THR:HG21	2.45	0.44
2:G:269:VAL:O	2:G:270:LYS:C	2.60	0.44
1:A:61:TYR:CE1	1:A:146:PHE:CD1	3.06	0.44
1:A:484:SER:H	2:B:216:SER:CB	2.30	0.44
2:B:38:LEU:HA	2:B:41:ARG:HD3	1.99	0.44
2:B:67:TRP:O	2:B:69:TYR:N	2.50	0.44
1:F:111:ILE:HD11	6:F:1001:HEM:HMD3	1.98	0.44
1:F:116:MET:HB3	1:F:117:PRO:HD3	1.98	0.44
1:F:127:VAL:HG13	1:F:229:THR:HG23	1.99	0.44
1:F:248:VAL:CG2	3:H:39:LEU:HD12	2.47	0.44
1:F:316:LEU:CD2	1:F:362:LYS:HA	2.48	0.44
1:F:332:LEU:HD22	1:F:335:PHE:CG	2.53	0.44
1:A:105:ALA:O	1:A:106:HIS:O	2.36	0.44
1:A:157:ASN:CA	1:A:160:LEU:HD12	2.37	0.44
1:A:368:PHE:CE1	2:B:88:VAL:HB	2.53	0.44
1:A:466:VAL:HB	1:A:501:GLY:CA	2.48	0.44
2:B:61:MET:HA	2:B:61:MET:CE	2.45	0.44
1:F:105:ALA:O	1:F:106:HIS:O	2.36	0.44
1:F:160:LEU:HD23	1:F:165:PHE:CB	2.48	0.44
1:F:337:THR:HG22	2:G:184:TYR:HB3	2.00	0.44
1:F:382:LEU:HD23	1:F:385:ILE:CD1	2.45	0.44
1:A:57:LEU:CD1	1:A:143:ASN:HA	2.47	0.44
1:A:101:GLN:CG	1:A:165:PHE:O	2.66	0.44
1:A:150:VAL:O	1:A:153:VAL:CB	2.66	0.44
1:A:238:LEU:HB2	1:A:289:ILE:HD11	1.98	0.44
1:A:267:ASP:OD1	1:A:267:ASP:N	2.51	0.44
1:A:437:THR:HG23	1:A:448:LEU:HD12	2.00	0.44
1:A:486:GLN:HG2	1:A:492:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:MET:HB3	2:B:189:MET:CG	2.47	0.44
3:C:67:PRO:HB2	3:C:195:PHE:CD1	2.52	0.44
3:C:86:ALA:C	3:C:88:ILE:N	2.75	0.44
3:C:87:ALA:HB1	3:C:97:GLN:CD	2.43	0.44
1:F:357:ILE:O	1:F:361:VAL:HG23	2.18	0.44
2:G:142:TYR:HA	2:G:143:PRO:HD2	1.87	0.44
3:H:145:THR:OG1	3:H:146:HIS:N	2.51	0.44
4:I:75:UNK:O	4:I:79:UNK:N	2.51	0.44
1:A:159:SER:OG	1:A:189:TYR:HB2	2.16	0.44
1:A:243:PHE:HA	1:A:282:TRP:CD1	2.53	0.44
2:B:41:ARG:H	2:B:41:ARG:CD	2.23	0.44
2:B:147:ILE:CD1	2:B:235:VAL:HA	2.44	0.44
2:B:201:GLY:O	2:B:224:ALA:HB3	2.18	0.44
4:D:75:UNK:O	4:D:79:UNK:N	2.50	0.44
1:F:406:ALA:CB	2:G:45:LEU:HD22	2.45	0.44
3:H:33:LEU:CB	3:H:34:MET:HE2	2.47	0.44
3:H:50:LEU:HD11	3:H:134:GLY:CA	2.43	0.44
3:H:139:PHE:O	3:H:141:ALA:N	2.51	0.44
3:H:197:VAL:HG13	3:H:198:VAL:H	1.81	0.44
1:A:61:TYR:O	1:A:64:VAL:N	2.51	0.43
1:A:74:ALA:O	1:A:75:ASP:C	2.61	0.43
1:A:103:PHE:CZ	6:A:1001:HEM:CMA	3.01	0.43
1:A:360:GLY:O	1:A:361:VAL:C	2.60	0.43
1:A:388:ILE:HG13	1:A:388:ILE:H	1.52	0.43
2:B:45:LEU:CD1	2:B:110:THR:HG21	2.46	0.43
3:C:94:ASN:HB2	3:C:97:GLN:HB3	2.00	0.43
1:F:55:LYS:HD3	1:F:551:ASN:OD1	2.17	0.43
1:F:106:HIS:CD2	1:F:107:GLY:H	2.36	0.43
1:F:238:LEU:HB2	1:F:289:ILE:HD11	1.99	0.43
1:F:267:ASP:OD1	1:F:267:ASP:N	2.50	0.43
1:F:308:LYS:HZ2	1:F:372:GLN:CA	2.31	0.43
1:F:319:ALA:HB1	1:F:362:LYS:HE2	2.00	0.43
1:F:393:VAL:O	1:F:396:MET:HE2	2.18	0.43
1:F:417:ILE:HD13	6:F:1001:HEM:HBA2	2.00	0.43
1:F:486:GLN:CD	1:F:486:GLN:N	2.76	0.43
2:G:36:ILE:HG23	2:G:39:GLU:HB3	2.00	0.43
2:G:136:TRP:NE1	2:G:213:PRO:O	2.51	0.43
2:G:140:PHE:HD2	2:G:149:THR:OG1	2.01	0.43
3:H:67:PRO:HB2	3:H:195:PHE:CD1	2.52	0.43
3:H:93:ASN:CG	3:H:94:ASN:N	2.75	0.43
3:H:116:GLU:OE1	3:H:143:VAL:HG11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ILE:O	2:B:45:LEU:C	2.61	0.43
3:C:84:GLY:O	3:C:88:ILE:HG13	2.18	0.43
1:F:292:LEU:HA	1:F:295:PHE:CD1	2.52	0.43
1:F:316:LEU:HD22	1:F:362:LYS:HA	2.00	0.43
1:F:330:VAL:CG1	1:F:352:THR:OG1	2.66	0.43
1:F:441:PRO:HG2	1:F:447:LYS:HD2	2.00	0.43
2:G:129:ILE:C	2:G:130:GLU:HG3	2.43	0.43
3:H:88:ILE:O	3:H:174:ARG:NE	2.51	0.43
3:H:156:TRP:NE1	3:H:180:LEU:HD13	2.29	0.43
1:A:120:ILE:HD13	1:A:201:THR:OG1	2.18	0.43
1:A:277:ASN:HD21	4:D:97:UNK:CB	2.31	0.43
1:A:473:ALA:O	1:A:475:GLY:N	2.50	0.43
2:B:162:TYR:CD1	2:B:194:HIS:NE2	2.87	0.43
3:C:93:ASN:CG	3:C:94:ASN:N	2.76	0.43
1:F:346:ALA:HA	1:F:350:ILE:HG13	1.99	0.43
1:F:355:ILE:O	1:F:355:ILE:HG22	2.18	0.43
1:F:411:HIS:CE1	1:F:412:ASN:ND2	2.87	0.43
1:F:548:PRO:O	1:F:550:TYR:N	2.51	0.43
2:G:214:GLY:O	2:G:218:MET:HG3	2.19	0.43
2:G:233:GLN:O	2:G:236:ALA:HB3	2.19	0.43
3:H:167:ARG:HH11	3:H:167:ARG:HG3	1.83	0.43
3:H:190:VAL:O	3:H:194:VAL:HG23	2.18	0.43
1:A:57:LEU:HD23	1:A:57:LEU:HA	1.79	0.43
1:A:79:MET:O	1:A:81:SER:N	2.52	0.43
3:C:199:TYR:N	3:C:199:TYR:HD1	2.15	0.43
1:F:148:PHE:HD2	1:F:148:PHE:HA	1.70	0.43
1:F:157:ASN:CA	1:F:160:LEU:HD12	2.40	0.43
1:F:168:THR:O	1:F:172:ALA:HA	2.18	0.43
1:F:328:PHE:O	1:F:331:TRP:HZ3	2.02	0.43
1:F:440:TRP:O	1:F:444:PHE:HB2	2.18	0.43
2:G:89:GLU:HB3	2:G:93:TRP:CD2	2.54	0.43
2:G:239:LYS:HE2	2:G:239:LYS:HA	1.99	0.43
3:H:185:HIS:O	3:H:185:HIS:CG	2.70	0.43
1:A:127:VAL:HG13	1:A:229:THR:HG23	2.00	0.43
1:A:357:ILE:N	1:A:358:PRO:CD	2.81	0.43
1:A:389:VAL:O	1:A:393:VAL:HG23	2.18	0.43
1:A:412:ASN:OD1	2:B:209:SER:HB3	2.18	0.43
2:B:130:GLU:OE1	2:B:141:ILE:HB	2.19	0.43
2:B:271:PRO:O	2:B:272:ASP:OD1	2.36	0.43
3:C:78:PHE:HD2	3:C:78:PHE:O	2.01	0.43
3:C:139:PHE:O	3:C:141:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ARG:HD3	3:C:177:ILE:CD1	2.48	0.43
1:F:57:LEU:CD1	1:F:143:ASN:HA	2.48	0.43
1:F:151:VAL:O	1:F:155:LEU:HB2	2.17	0.43
1:F:221:THR:H	1:F:224:LYS:HD2	1.83	0.43
1:F:415:PHE:CD1	1:F:472:TYR:CD2	3.06	0.43
2:G:136:TRP:HA	2:G:218:MET:CG	2.47	0.43
2:G:137:LYS:HE2	2:G:261:ASN:ND2	2.34	0.43
2:G:158:ASN:O	2:G:159:THR:HG23	2.19	0.43
4:I:63:UNK:O	4:I:67:UNK:N	2.52	0.43
1:A:111:ILE:HD11	6:A:1001:HEM:HMD3	1.99	0.43
1:A:246:LEU:CD1	1:A:250:VAL:HG23	2.49	0.43
1:A:251:ALA:O	1:A:254:THR:CB	2.66	0.43
1:A:325:VAL:O	1:A:327:SER:N	2.47	0.43
1:A:543:THR:HG22	1:A:544:SER:H	1.84	0.43
2:B:130:GLU:OE1	2:B:141:ILE:O	2.36	0.43
2:B:265:TYR:O	2:B:266:PHE:CD2	2.71	0.43
3:C:85:MET:CA	3:C:88:ILE:HD12	2.49	0.43
1:F:367:LEU:HD13	2:G:63:VAL:CB	2.48	0.43
2:G:59:ILE:O	2:G:62:ALA:HB3	2.17	0.43
2:G:137:LYS:CE	2:G:261:ASN:HD21	2.32	0.43
2:G:138:TRP:HH2	2:G:174:PHE:HA	1.82	0.43
3:H:86:ALA:HB2	3:H:91:TYR:CE1	2.46	0.43
1:A:241:ALA:O	1:A:328:PHE:HE2	2.01	0.43
1:A:243:PHE:N	1:A:244:PRO:CD	2.81	0.43
2:B:39:GLU:CB	2:B:43:LEU:HD12	2.48	0.43
1:F:74:ALA:O	1:F:75:ASP:C	2.61	0.43
1:F:404:PRO:HG2	2:G:111:THR:CG2	2.49	0.43
3:H:107:LEU:C	3:H:109:GLY:N	2.73	0.43
3:H:150:VAL:HG22	3:H:187:LEU:CD1	2.48	0.43
1:A:151:VAL:O	1:A:155:LEU:HB2	2.17	0.43
1:A:356:ALA:HA	7:A:1002:HEO:H262	1.99	0.43
1:A:442:LYS:HB2	1:A:541:TRP:CZ3	2.52	0.43
1:A:486:GLN:NE2	1:A:486:GLN:H	2.17	0.43
1:F:73:PHE:HE2	6:F:1001:HEM:HAB	1.83	0.43
1:F:146:PHE:O	1:F:148:PHE:N	2.51	0.43
1:F:239:ILE:O	1:F:243:PHE:HB2	2.18	0.43
2:G:134:MET:HG2	2:G:255:ALA:CB	2.48	0.43
2:G:248:MET:HA	2:G:251:PHE:HB3	2.00	0.43
4:I:73:UNK:O	4:I:76:UNK:N	2.52	0.43
1:A:61:TYR:O	1:A:63:ILE:N	2.52	0.43
1:A:98:HIS:O	1:A:99:TYR:C	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TRP:CE3	1:A:191:ILE:HG12	2.53	0.43
1:A:195:GLN:O	1:A:196:LEU:C	2.62	0.43
1:A:516:MET:O	1:A:517:TYR:C	2.61	0.43
3:C:112:PHE:HZ	3:C:191:TRP:CE3	2.37	0.43
1:F:79:MET:O	1:F:81:SER:N	2.52	0.43
1:F:169:GLY:C	1:F:171:LEU:H	2.26	0.43
1:F:306:SER:HA	1:F:375:ILE:CA	2.40	0.43
2:G:56:ILE:O	2:G:60:LEU:N	2.49	0.43
1:A:80:ARG:NH2	1:A:467:ALA:O	2.52	0.43
1:A:119:VAL:CG2	1:A:293:PRO:HG2	2.48	0.43
1:A:169:GLY:C	1:A:171:LEU:H	2.26	0.43
1:A:319:ALA:HB1	1:A:362:LYS:HE2	2.01	0.43
1:A:498:ALA:C	1:A:500:SER:N	2.77	0.43
1:A:541:TRP:C	1:A:543:THR:H	2.27	0.43
1:A:551:ASN:CG	1:A:552:PHE:H	2.27	0.43
2:B:153:ILE:HD11	2:B:220:PHE:CE2	2.54	0.43
3:C:150:VAL:HG22	3:C:187:LEU:HD11	2.01	0.43
1:F:80:ARG:NH2	1:F:467:ALA:O	2.52	0.43
1:F:115:ALA:O	1:F:290:LEU:HD11	2.19	0.43
1:F:195:GLN:O	1:F:196:LEU:C	2.62	0.43
1:F:375:ILE:HG21	2:G:67:TRP:CZ2	2.54	0.43
1:F:435:GLY:O	1:F:437:THR:N	2.52	0.43
2:G:130:GLU:HA	2:G:164:LYS:HB2	2.01	0.43
2:G:186:MET:HB3	2:G:189:MET:CG	2.48	0.43
3:H:78:PHE:CZ	4:I:57:UNK:CA	2.88	0.43
3:H:92:LYS:HE2	3:H:92:LYS:HB3	1.85	0.43
3:H:166:ARG:NE	3:H:167:ARG:NH2	2.66	0.43
1:A:373:GLY:C	1:A:375:ILE:HD12	2.43	0.42
1:A:396:MET:HB3	2:B:53:ILE:HD13	2.00	0.42
1:A:452:TRP:HA	1:A:455:ARG:HB2	2.01	0.42
1:A:460:TRP:CZ3	1:A:509:ILE:HG12	2.54	0.42
1:A:480:THR:HB	1:A:483:LEU:CD1	2.48	0.42
1:A:508:GLY:C	1:A:510:LEU:N	2.76	0.42
2:B:70:ARG:C	2:B:72:SER:H	2.27	0.42
2:B:201:GLY:O	2:B:203:TYR:CE1	2.72	0.42
3:C:72:GLU:O	3:C:73:THR:C	2.61	0.42
1:F:119:VAL:CG2	1:F:293:PRO:HG2	2.48	0.42
1:F:150:VAL:O	1:F:153:VAL:CB	2.67	0.42
1:F:243:PHE:N	1:F:244:PRO:CD	2.81	0.42
1:F:466:VAL:HB	1:F:501:GLY:CA	2.48	0.42
2:G:39:GLU:CB	2:G:43:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:41:ARG:H	2:G:41:ARG:CD	2.24	0.42
2:G:147:ILE:CD1	2:G:235:VAL:HA	2.45	0.42
3:H:26:ILE:CD1	3:H:175:THR:HG23	2.46	0.42
2:B:134:MET:HG2	2:B:255:ALA:CB	2.48	0.42
2:B:140:PHE:HD2	2:B:149:THR:OG1	2.02	0.42
4:D:66:UNK:C	4:D:68:UNK:N	2.79	0.42
1:F:61:TYR:O	1:F:63:ILE:N	2.52	0.42
1:F:79:MET:SD	1:F:103:PHE:N	2.92	0.42
1:F:99:TYR:CE1	1:F:103:PHE:HD1	2.37	0.42
1:F:101:GLN:HG3	1:F:165:PHE:O	2.19	0.42
1:F:146:PHE:C	1:F:148:PHE:N	2.77	0.42
1:F:338:MET:HA	2:G:184:TYR:CD1	2.52	0.42
1:F:442:LYS:HB2	1:F:541:TRP:CZ3	2.53	0.42
1:F:473:ALA:C	1:F:475:GLY:N	2.77	0.42
2:G:40:GLN:C	2:G:42:SER:H	2.27	0.42
2:G:140:PHE:CE1	2:G:153:ILE:HD13	2.53	0.42
2:G:203:TYR:O	2:G:221:LYS:CA	2.63	0.42
3:H:94:ASN:HB2	3:H:97:GLN:HB3	2.01	0.42
1:A:75:ASP:C	1:A:79:MET:HE2	2.45	0.42
1:A:252:LEU:HD22	1:A:263:PHE:CE2	2.54	0.42
1:A:299:SER:HB3	1:A:310:LEU:HD22	2.00	0.42
1:A:305:PHE:CD1	1:A:305:PHE:N	2.87	0.42
1:A:316:LEU:HD22	1:A:362:LYS:HA	2.01	0.42
1:A:361:VAL:HG22	2:B:93:TRP:CH2	2.55	0.42
1:F:106:HIS:CG	1:F:107:GLY:N	2.84	0.42
1:F:246:LEU:O	1:F:247:THR:C	2.62	0.42
1:F:292:LEU:O	1:F:295:PHE:HB2	2.19	0.42
1:F:363:ILE:O	1:F:364:PHE:C	2.62	0.42
1:A:228:PHE:O	1:A:228:PHE:CG	2.73	0.42
1:A:273:MET:HE1	4:D:105:UNK:N	2.35	0.42
1:A:364:PHE:HB3	2:B:92:VAL:HG21	2.02	0.42
2:B:50:LEU:O	2:B:53:ILE:CG2	2.67	0.42
2:B:140:PHE:CE1	2:B:153:ILE:HD13	2.54	0.42
1:F:318:TRP:O	1:F:319:ALA:C	2.62	0.42
1:F:357:ILE:N	1:F:358:PRO:CD	2.82	0.42
1:F:480:THR:HB	1:F:483:LEU:CG	2.48	0.42
1:F:502:ALA:O	1:F:505:ILE:N	2.52	0.42
1:F:516:MET:O	1:F:519:SER:N	2.45	0.42
1:F:547:PRO:O	1:F:548:PRO:C	2.60	0.42
2:G:262:GLN:O	2:G:264:GLU:N	2.52	0.42
3:H:195:PHE:C	3:H:197:VAL:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PRO:O	1:A:130:GLN:N	2.53	0.42
1:A:331:TRP:CD2	1:A:348:PHE:HE2	2.38	0.42
1:A:341:GLY:O	1:A:342:ALA:C	2.62	0.42
1:A:346:ALA:HA	1:A:350:ILE:HG13	2.00	0.42
1:A:549:PHE:CD1	1:A:549:PHE:N	2.87	0.42
2:B:238:ALA:O	2:B:239:LYS:C	2.62	0.42
1:F:201:THR:O	1:F:201:THR:HG22	2.18	0.42
1:F:233:LEU:O	1:F:236:ASN:N	2.52	0.42
1:F:337:THR:HG23	2:G:183:ILE:HA	2.02	0.42
2:G:53:ILE:C	2:G:55:VAL:N	2.77	0.42
2:G:138:TRP:HE1	2:G:218:MET:HE2	1.85	0.42
2:G:167:SER:HB3	2:G:187:ALA:CA	2.49	0.42
3:H:72:GLU:O	3:H:76:LEU:HD23	2.19	0.42
1:A:68:MET:SD	1:A:113:PHE:HB3	2.60	0.42
1:A:119:VAL:HG13	1:A:120:ILE:N	2.34	0.42
1:A:233:LEU:O	1:A:236:ASN:N	2.52	0.42
1:A:354:ILE:O	1:A:356:ALA:N	2.53	0.42
1:F:216:ARG:NH2	1:F:220:MET:O	2.51	0.42
1:F:243:PHE:HA	1:F:282:TRP:NE1	2.34	0.42
1:F:264:PHE:CD1	1:F:275:TYR:HB2	2.54	0.42
1:F:299:SER:HB3	1:F:310:LEU:HD22	2.00	0.42
1:F:320:THR:OG1	1:F:362:LYS:NZ	2.52	0.42
1:F:354:ILE:O	1:F:356:ALA:N	2.53	0.42
1:F:373:GLY:CA	2:G:71:ALA:O	2.67	0.42
1:F:516:MET:O	1:F:517:TYR:C	2.62	0.42
1:A:72:GLY:O	1:A:73:PHE:C	2.61	0.42
1:A:195:GLN:NE2	1:A:247:THR:CG2	2.71	0.42
1:A:292:LEU:O	1:A:295:PHE:HB2	2.20	0.42
1:A:460:TRP:CZ3	1:A:509:ILE:CD1	3.02	0.42
2:B:89:GLU:HB3	2:B:93:TRP:CD2	2.55	0.42
2:B:239:LYS:HE2	2:B:239:LYS:HA	2.01	0.42
1:F:156:VAL:HG12	1:F:160:LEU:CD1	2.48	0.42
1:F:329:ILE:O	1:F:351:THR:HG21	2.19	0.42
1:F:437:THR:HG23	1:F:448:LEU:HD12	2.01	0.42
1:F:442:LYS:NZ	1:F:543:THR:O	2.53	0.42
1:F:476:PHE:C	1:F:478:GLY:N	2.77	0.42
7:F:1002:HEO:O11	7:F:1002:HEO:HHC	2.19	0.42
1:A:99:TYR:CE1	1:A:103:PHE:HD1	2.37	0.42
1:A:148:PHE:HD2	1:A:148:PHE:HA	1.70	0.42
1:A:404:PRO:HG2	2:B:111:THR:CG2	2.50	0.42
1:A:476:PHE:C	1:A:478:GLY:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PHE:N	1:A:476:PHE:CD1	2.88	0.42
2:B:45:LEU:HD12	2:B:110:THR:CG2	2.46	0.42
2:B:140:PHE:CZ	2:B:153:ILE:HD13	2.54	0.42
2:B:156:PRO:HG3	2:B:231:PHE:CD2	2.55	0.42
3:C:89:ALA:O	3:C:91:TYR:O	2.38	0.42
1:F:248:VAL:HG22	3:H:39:LEU:CD1	2.49	0.42
1:F:335:PHE:O	1:F:336:PHE:C	2.63	0.42
2:G:166:THR:HG23	2:G:167:SER:N	2.34	0.42
1:A:138:PHE:HB3	1:A:141:LEU:HD12	2.02	0.42
1:A:306:SER:HA	1:A:375:ILE:CA	2.41	0.42
1:A:483:LEU:HD22	2:B:216:SER:HA	2.02	0.42
2:B:217:GLY:HA3	2:B:260:TYR:CE1	2.55	0.42
1:F:335:PHE:O	1:F:337:THR:N	2.53	0.42
2:G:97:ILE:O	2:G:101:ILE:HD12	2.19	0.42
2:G:130:GLU:OE1	2:G:141:ILE:CG2	2.68	0.42
2:G:140:PHE:CZ	2:G:153:ILE:HD13	2.54	0.42
3:H:26:ILE:C	3:H:28:GLY:H	2.28	0.42
3:H:77:LEU:HD22	3:H:105:THR:HG23	2.02	0.42
1:A:195:GLN:HG2	1:A:250:VAL:HG11	2.00	0.42
1:A:243:PHE:HA	1:A:282:TRP:NE1	2.34	0.42
1:A:395:GLY:O	1:A:399:VAL:HG23	2.20	0.42
1:A:491:PHE:C	1:A:493:THR:H	2.27	0.42
2:B:72:SER:OG	2:B:73:ASN:N	2.53	0.42
2:B:241:SER:O	2:B:267:SER:OG	2.34	0.42
2:B:254:LEU:HD13	2:B:254:LEU:C	2.44	0.42
1:F:102:ILE:O	1:F:103:PHE:C	2.61	0.42
1:F:191:ILE:HG22	1:F:250:VAL:HG13	2.02	0.42
1:F:227:VAL:HG11	1:F:299:SER:HB2	2.01	0.42
1:F:400:LEU:HD13	2:G:50:LEU:CD2	2.50	0.42
1:F:511:CYS:SG	1:F:512:LEU:N	2.93	0.42
2:G:127:ILE:HG21	2:G:142:TYR:HE2	1.84	0.42
2:G:222:ALA:O	2:G:223:ILE:C	2.63	0.42
1:A:107:GLY:O	1:A:111:ILE:HG13	2.20	0.41
1:A:255:LEU:HB3	1:A:261:THR:CG2	2.50	0.41
1:A:316:LEU:HD21	1:A:365:ASN:CG	2.45	0.41
1:A:375:ILE:CG2	1:A:381:MET:HE2	2.49	0.41
2:B:39:GLU:HG3	2:B:43:LEU:HD12	2.01	0.41
2:B:40:GLN:HB2	2:B:41:ARG:HH11	1.85	0.41
3:C:195:PHE:C	3:C:197:VAL:H	2.28	0.41
1:F:113:PHE:CE2	1:F:152:GLY:C	2.98	0.41
1:F:305:PHE:N	1:F:305:PHE:CD1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:SER:CB	1:F:375:ILE:HG13	2.50	0.41
1:F:356:ALA:HA	7:F:1002:HEO:H262	2.01	0.41
1:F:433:PHE:O	1:F:434:ALA:C	2.63	0.41
2:G:38:LEU:O	2:G:39:GLU:C	2.63	0.41
3:H:72:GLU:O	3:H:73:THR:C	2.62	0.41
1:A:168:THR:CB	1:A:172:ALA:HA	2.44	0.41
1:A:308:LYS:HE3	1:A:372:GLN:HB2	1.99	0.41
1:A:318:TRP:O	1:A:319:ALA:C	2.63	0.41
1:A:461:ILE:HG13	1:A:461:ILE:H	1.61	0.41
2:B:158:ASN:O	2:B:159:THR:HG23	2.20	0.41
3:C:166:ARG:NE	3:C:167:ARG:NH2	2.67	0.41
1:F:111:ILE:CD1	1:F:170:TRP:CE3	3.03	0.41
1:F:238:LEU:C	1:F:240:ILE:N	2.78	0.41
1:F:373:GLY:HA2	2:G:71:ALA:C	2.45	0.41
1:F:375:ILE:HD12	2:G:71:ALA:O	2.21	0.41
2:G:40:GLN:HB2	2:G:41:ARG:HH11	1.85	0.41
2:G:91:VAL:HG12	2:G:92:VAL:HG13	2.02	0.41
2:G:183:ILE:HG13	2:G:184:TYR:N	2.35	0.41
2:G:245:MET:O	2:G:269:VAL:HA	2.21	0.41
3:H:85:MET:SD	3:H:178:MET:HG3	2.61	0.41
4:I:66:UNK:C	4:I:68:UNK:N	2.79	0.41
1:A:76:ALA:O	1:A:77:ILE:C	2.61	0.41
1:A:100:ASP:CG	2:B:212:GLY:HA2	2.45	0.41
1:A:156:VAL:O	1:A:160:LEU:CD1	2.68	0.41
1:A:238:LEU:HB3	1:A:289:ILE:HD11	2.02	0.41
2:B:203:TYR:O	2:B:221:LYS:CA	2.65	0.41
3:C:33:LEU:C	3:C:35:SER:H	2.27	0.41
1:F:61:TYR:O	1:F:64:VAL:N	2.53	0.41
2:G:36:ILE:O	2:G:39:GLU:OE2	2.38	0.41
2:G:53:ILE:O	2:G:55:VAL:N	2.53	0.41
2:G:178:ARG:HA	2:G:178:ARG:HD2	1.86	0.41
2:G:183:ILE:HB	2:G:193:LEU:HD12	2.02	0.41
3:H:88:ILE:HG23	3:H:98:VAL:HG13	2.01	0.41
1:A:201:THR:O	1:A:201:THR:HG22	2.19	0.41
1:A:433:PHE:O	1:A:434:ALA:C	2.63	0.41
2:B:40:GLN:C	2:B:42:SER:H	2.28	0.41
3:C:67:PRO:HB2	3:C:195:PHE:CE1	2.55	0.41
1:F:137:ALA:H	1:F:215:MET:CE	2.29	0.41
1:F:190:TRP:CE3	1:F:191:ILE:HG12	2.52	0.41
1:F:383:TRP:O	1:F:384:THR:C	2.63	0.41
2:G:156:PRO:HD3	2:G:231:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:148:LEU:O	3:H:151:THR:N	2.53	0.41
3:H:202:GLY:O	3:H:203:ALA:HB3	2.20	0.41
1:A:101:GLN:HG3	1:A:165:PHE:O	2.20	0.41
1:A:176:LEU:HD13	2:B:170:VAL:HG11	2.03	0.41
1:A:246:LEU:O	1:A:247:THR:C	2.63	0.41
1:A:383:TRP:CD1	1:A:434:ALA:HA	2.56	0.41
1:A:486:GLN:CD	1:A:486:GLN:H	2.29	0.41
1:A:509:ILE:HD13	1:A:509:ILE:HA	1.77	0.41
3:C:154:LEU:HD13	3:C:184:TRP:HH2	1.84	0.41
1:F:306:SER:OG	1:F:375:ILE:HG23	2.21	0.41
1:F:332:LEU:HD22	1:F:335:PHE:HB2	2.02	0.41
2:G:269:VAL:O	2:G:269:VAL:HG23	2.20	0.41
3:H:84:GLY:O	3:H:88:ILE:CG1	2.67	0.41
3:H:180:LEU:C	3:H:182:LEU:N	2.79	0.41
1:A:238:LEU:C	1:A:240:ILE:N	2.78	0.41
1:A:316:LEU:O	1:A:319:ALA:HB3	2.21	0.41
1:F:76:ALA:O	1:F:77:ILE:C	2.62	0.41
1:F:480:THR:OG1	2:G:206:ILE:HB	2.20	0.41
2:G:153:ILE:HD11	2:G:220:PHE:CE2	2.55	0.41
2:G:264:GLU:CG	2:G:265:TYR:N	2.79	0.41
3:H:78:PHE:CZ	4:I:57:UNK:HA	2.54	0.41
3:H:82:THR:CG2	4:I:10:UNK:O	2.68	0.41
4:I:104:UNK:C	4:I:106:UNK:N	2.79	0.41
1:A:79:MET:SD	1:A:102:ILE:CG2	3.09	0.41
1:A:106:HIS:CG	1:A:107:GLY:N	2.85	0.41
1:A:168:THR:O	1:A:172:ALA:HA	2.20	0.41
1:A:245:ILE:HB	1:A:282:TRP:HB2	2.03	0.41
1:A:396:MET:HB3	2:B:53:ILE:CD1	2.50	0.41
2:B:127:ILE:HG21	2:B:142:TYR:HE2	1.85	0.41
2:B:178:ARG:HA	2:B:178:ARG:HD2	1.86	0.41
3:C:49:VAL:C	3:C:51:VAL:N	2.79	0.41
3:C:77:LEU:HD22	3:C:105:THR:HG23	2.01	0.41
3:C:199:TYR:HD1	3:C:199:TYR:H	1.66	0.41
4:D:104:UNK:C	4:D:106:UNK:N	2.79	0.41
1:F:316:LEU:O	1:F:319:ALA:HB3	2.21	0.41
1:F:461:ILE:HG13	1:F:461:ILE:H	1.61	0.41
1:F:543:THR:CG2	1:F:544:SER:H	2.33	0.41
3:H:195:PHE:CD1	3:H:199:TYR:CB	3.04	0.41
1:A:102:ILE:O	1:A:103:PHE:C	2.61	0.41
1:A:106:HIS:O	1:A:108:VAL:N	2.53	0.41
1:A:310:LEU:HD11	1:A:366:TRP:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HD23	1:A:513:VAL:HG23	2.03	0.41
2:B:38:LEU:O	2:B:39:GLU:C	2.64	0.41
3:C:145:THR:O	3:C:147:GLY:N	2.53	0.41
1:F:57:LEU:HA	1:F:60:MET:HB2	2.02	0.41
1:F:228:PHE:CD1	1:F:297:VAL:HG23	2.56	0.41
3:H:78:PHE:CZ	3:H:185:HIS:CE1	3.09	0.41
3:H:81:ILE:HD11	3:H:105:THR:HG21	2.02	0.41
3:H:150:VAL:HG22	3:H:187:LEU:HD11	2.03	0.41
1:A:98:HIS:HB3	1:A:102:ILE:HD11	2.03	0.41
1:A:227:VAL:HG11	1:A:299:SER:HB2	2.01	0.41
1:A:283:GLY:O	1:A:284:HIS:C	2.63	0.41
1:A:335:PHE:O	1:A:337:THR:N	2.54	0.41
1:A:346:ALA:C	1:A:348:PHE:N	2.79	0.41
1:A:397:THR:O	1:A:401:LEU:HG	2.20	0.41
1:A:417:ILE:HD13	6:A:1001:HEM:CBA	2.50	0.41
1:A:420:PHE:C	1:A:422:ASN:N	2.76	0.41
2:B:130:GLU:OE1	2:B:141:ILE:CG2	2.69	0.41
3:C:42:ILE:CG2	3:C:43:LEU:N	2.84	0.41
3:C:94:ASN:HD22	3:C:97:GLN:HE22	1.68	0.41
1:F:76:ALA:C	1:F:78:MET:N	2.78	0.41
1:F:110:MET:C	6:F:1001:HEM:HBC2	2.45	0.41
1:F:159:SER:OG	1:F:189:TYR:HB2	2.18	0.41
1:F:238:LEU:HB3	1:F:289:ILE:HD11	2.03	0.41
1:F:314:THR:O	1:F:315:SER:C	2.63	0.41
1:F:341:GLY:O	1:F:344:VAL:N	2.54	0.41
1:F:408:PHE:O	2:G:182:GLN:NE2	2.45	0.41
1:F:409:VAL:HG21	2:G:43:LEU:CD2	2.51	0.41
1:F:452:TRP:O	1:F:455:ARG:HB2	2.20	0.41
1:F:476:PHE:N	1:F:476:PHE:CD1	2.89	0.41
1:F:508:GLY:C	1:F:510:LEU:N	2.78	0.41
2:G:106:LEU:O	2:G:107:THR:C	2.63	0.41
2:G:107:THR:O	2:G:108:TRP:C	2.64	0.41
2:G:147:ILE:HG21	2:G:238:ALA:HB3	2.01	0.41
2:G:225:THR:HB	2:G:226:PRO:CD	2.51	0.41
2:G:271:PRO:O	2:G:272:ASP:OD1	2.39	0.41
3:H:102:LEU:HD23	3:H:161:MET:HG3	2.03	0.41
1:A:252:LEU:HD13	1:A:263:PHE:CD2	2.55	0.41
1:A:335:PHE:O	1:A:336:PHE:C	2.64	0.41
1:A:355:ILE:HG22	1:A:355:ILE:O	2.21	0.41
1:A:387:PHE:C	1:A:389:VAL:H	2.29	0.41
1:A:481:ARG:O	1:A:483:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:MET:HA	2:B:251:PHE:HB3	2.02	0.41
3:C:102:LEU:HD23	3:C:161:MET:HG3	2.03	0.41
3:C:164:ILE:O	3:C:168:GLY:CA	2.64	0.41
1:F:53:ASP:O	1:F:54:HIS:C	2.64	0.41
1:F:120:ILE:CD1	1:F:201:THR:OG1	2.69	0.41
1:F:170:TRP:NE1	1:F:171:LEU:HG	2.35	0.41
1:F:195:GLN:NE2	1:F:247:THR:CG2	2.71	0.41
1:F:397:THR:O	1:F:401:LEU:HG	2.20	0.41
1:F:411:HIS:C	1:F:413:SER:N	2.78	0.41
1:F:480:THR:HB	1:F:483:LEU:CD1	2.50	0.41
3:H:112:PHE:HZ	3:H:191:TRP:CZ3	2.39	0.41
1:A:341:GLY:O	1:A:344:VAL:N	2.54	0.40
1:A:502:ALA:O	1:A:505:ILE:N	2.54	0.40
2:B:60:LEU:C	2:B:62:ALA:N	2.72	0.40
2:B:89:GLU:HB3	2:B:93:TRP:CE3	2.56	0.40
2:B:91:VAL:HG12	2:B:92:VAL:HG13	2.03	0.40
2:B:129:ILE:C	2:B:130:GLU:HG3	2.46	0.40
2:B:251:PHE:CE2	2:B:273:LEU:HD21	2.56	0.40
3:C:138:ALA:O	3:C:139:PHE:C	2.62	0.40
1:F:170:TRP:CE2	1:F:171:LEU:CD2	3.04	0.40
1:F:251:ALA:O	1:F:254:THR:CB	2.68	0.40
2:G:134:MET:CE	2:G:255:ALA:HB2	2.50	0.40
2:G:277:VAL:O	2:G:278:ILE:C	2.63	0.40
3:H:138:ALA:O	3:H:139:PHE:C	2.63	0.40
1:A:155:LEU:HA	1:A:155:LEU:HD23	1.89	0.40
1:A:251:ALA:HA	1:A:254:THR:OG1	2.21	0.40
1:A:452:TRP:CD1	1:A:452:TRP:H	2.39	0.40
1:A:547:PRO:O	1:A:548:PRO:C	2.63	0.40
2:B:126:PRO:HG3	2:B:160:PRO:HG2	2.03	0.40
2:B:167:SER:HB3	2:B:187:ALA:CA	2.51	0.40
3:C:141:ALA:O	3:C:142:LEU:C	2.62	0.40
3:C:180:LEU:C	3:C:182:LEU:N	2.79	0.40
1:F:228:PHE:O	1:F:228:PHE:CG	2.75	0.40
1:F:252:LEU:HD22	1:F:263:PHE:CE2	2.56	0.40
1:F:409:VAL:HG21	2:G:43:LEU:HD21	2.03	0.40
1:F:481:ARG:HG2	1:F:482:ARG:H	1.85	0.40
1:F:509:ILE:HD13	1:F:509:ILE:HA	1.75	0.40
2:G:50:LEU:O	2:G:53:ILE:CG2	2.69	0.40
2:G:140:PHE:HD2	2:G:149:THR:HG1	1.69	0.40
3:H:110:ALA:O	3:H:114:GLY:N	2.54	0.40
4:I:108:UNK:O	4:I:109:UNK:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:MET:SD	1:A:103:PHE:N	2.94	0.40
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.83	0.40
1:A:255:LEU:HD22	1:A:259:LEU:HD12	2.03	0.40
1:A:328:PHE:O	1:A:331:TRP:HZ3	2.05	0.40
1:A:356:ALA:O	1:A:357:ILE:C	2.64	0.40
1:A:463:GLY:HA3	1:A:505:ILE:HG13	2.03	0.40
7:A:1002:HEO:O11	7:A:1002:HEO:HHC	2.21	0.40
2:B:155:PHE:CZ	2:B:222:ALA:HB1	2.56	0.40
2:B:222:ALA:O	2:B:223:ILE:C	2.64	0.40
3:C:177:ILE:HD12	3:C:178:MET:N	2.36	0.40
1:F:315:SER:HB3	1:F:365:ASN:HD21	1.86	0.40
2:G:45:LEU:HD12	2:G:110:THR:CG2	2.48	0.40
2:G:53:ILE:CG2	2:G:54:VAL:N	2.84	0.40
3:H:26:ILE:HG22	3:H:27:PHE:N	2.35	0.40
3:H:85:MET:C	3:H:88:ILE:HB	2.46	0.40
3:H:122:HIS:O	3:H:122:HIS:ND1	2.54	0.40
1:A:363:ILE:O	1:A:364:PHE:C	2.64	0.40
1:A:440:TRP:O	1:A:444:PHE:HB2	2.22	0.40
1:A:481:ARG:CG	1:A:482:ARG:N	2.80	0.40
2:B:99:ILE:O	2:B:103:LEU:HB2	2.21	0.40
3:C:146:HIS:NE2	3:C:187:LEU:HD23	2.36	0.40
1:F:63:ILE:O	1:F:64:VAL:C	2.64	0.40
1:F:200:GLY:O	1:F:202:THR:N	2.54	0.40
1:F:257:ARG:CB	1:F:257:ARG:NH1	2.74	0.40
1:F:311:PHE:HZ	2:G:88:VAL:HG21	1.85	0.40
1:F:498:ALA:C	1:F:500:SER:N	2.79	0.40
2:G:184:TYR:OH	2:G:189:MET:CE	2.70	0.40
2:G:278:ILE:HG22	2:G:282:MET:HG3	2.03	0.40
3:H:33:LEU:O	3:H:37:CYS:N	2.55	0.40
3:H:87:ALA:HB1	3:H:97:GLN:CD	2.47	0.40
1:A:122:LEU:CD1	1:A:297:VAL:HG21	2.51	0.40
1:A:228:PHE:CD1	1:A:297:VAL:HG23	2.56	0.40
1:A:242:SER:OG	1:A:282:TRP:HD1	2.05	0.40
1:A:305:PHE:N	1:A:305:PHE:HD1	2.19	0.40
1:A:369:THR:O	1:A:369:THR:CG2	2.69	0.40
1:A:411:HIS:ND1	7:A:1002:HEO:O2A	2.52	0.40
2:B:43:LEU:O	2:B:46:THR:OG1	2.36	0.40
3:C:51:VAL:HG12	3:C:135:PHE:CZ	2.57	0.40
3:C:116:GLU:OE1	3:C:143:VAL:HG11	2.21	0.40
1:F:383:TRP:CD1	1:F:434:ALA:HA	2.57	0.40
2:G:74:LYS:H	2:G:74:LYS:HG3	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:134:MET:HE2	2:G:255:ALA:HB2	2.03	0.40
2:G:139:PHE:HA	2:G:149:THR:O	2.21	0.40
3:H:94:ASN:HD22	3:H:97:GLN:HE22	1.69	0.40
3:H:167:ARG:HG3	3:H:167:ARG:NH1	2.36	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	499/663 (75%)	331 (66%)	110 (22%)	58 (12%)	0 4
1	F	499/663 (75%)	333 (67%)	108 (22%)	58 (12%)	0 4
2	B	255/315 (81%)	162 (64%)	66 (26%)	27 (11%)	0 5
2	G	255/315 (81%)	167 (66%)	58 (23%)	30 (12%)	0 4
3	C	183/204 (90%)	112 (61%)	52 (28%)	19 (10%)	0 5
3	H	183/204 (90%)	107 (58%)	56 (31%)	20 (11%)	0 5
All	All	1874/2364 (79%)	1212 (65%)	450 (24%)	212 (11%)	0 5

All (212) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	102	ILE
1	A	106	HIS
1	A	135	ASP
1	A	175	PRO
1	A	330	VAL
1	A	336	PHE
1	A	379	SER

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Mol	Chain	Res	Type
1	A	451	THR
1	A	482	ARG
1	A	549	PHE
2	B	85	SER
2	B	101	ILE
2	B	116	PRO
2	B	118	LYS
2	B	119	PRO
3	C	97	GLN
3	C	197	VAL
1	F	96	PRO
1	F	102	ILE
1	F	106	HIS
1	F	135	ASP
1	F	175	PRO
1	F	330	VAL
1	F	336	PHE
1	F	379	SER
1	F	451	THR
1	F	482	ARG
1	F	549	PHE
1	F	551	ASN
2	G	85	SER
2	G	116	PRO
2	G	118	LYS
2	G	119	PRO
3	H	97	GLN
3	H	197	VAL
1	A	62	ILE
1	A	95	PRO
1	A	97	HIS
1	A	103	PHE
1	A	110	MET
1	A	129	LEU
1	A	139	PRO
1	A	147	TRP
1	A	166	ALA
1	A	184	GLY
1	A	304	THR
1	A	355	ILE
1	A	363	ILE
1	A	442	LYS

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Mol	Chain	Res	Type
1	A	481	ARG
1	A	525	GLN
1	A	551	ASN
2	B	67	TRP
2	B	113	ALA
2	B	125	LYS
2	B	178	ARG
2	B	200	PRO
2	B	223	ILE
2	B	263	VAL
3	C	20	ASP
3	C	50	LEU
3	C	89	ALA
3	C	165	ALA
3	C	168	GLY
3	C	194	VAL
3	C	199	TYR
3	C	202	GLY
1	F	95	PRO
1	F	97	HIS
1	F	103	PHE
1	F	110	MET
1	F	129	LEU
1	F	139	PRO
1	F	147	TRP
1	F	166	ALA
1	F	184	GLY
1	F	234	CYS
1	F	355	ILE
1	F	363	ILE
1	F	442	LYS
1	F	481	ARG
1	F	525	GLN
2	G	67	TRP
2	G	113	ALA
2	G	125	LYS
2	G	178	ARG
2	G	223	ILE
2	G	263	VAL
3	H	20	ASP
3	H	50	LEU
3	H	52	ASN

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Mol	Chain	Res	Type
3	H	89	ALA
3	H	109	GLY
3	H	165	ALA
3	H	168	GLY
3	H	194	VAL
3	H	199	TYR
3	H	202	GLY
1	A	82	GLN
1	A	101	GLN
1	A	128	PRO
1	A	137	ALA
1	A	200	GLY
1	A	201	THR
1	A	234	CYS
1	A	273	MET
1	A	326	LEU
1	A	338	MET
1	A	474	LEU
2	B	112	HIS
2	B	117	SER
2	B	121	ALA
2	B	209	SER
2	B	213	PRO
2	B	260	TYR
3	C	48	ALA
3	C	52	ASN
3	C	54	THR
3	C	92	LYS
3	C	93	ASN
3	C	140	PHE
1	F	62	ILE
1	F	82	GLN
1	F	101	GLN
1	F	128	PRO
1	F	137	ALA
1	F	200	GLY
1	F	201	THR
1	F	273	MET
1	F	304	THR
1	F	338	MET
1	F	436	MET
2	G	77	LYS

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Mol	Chain	Res	Type
2	G	112	HIS
2	G	117	SER
2	G	121	ALA
2	G	200	PRO
2	G	209	SER
2	G	213	PRO
2	G	260	TYR
3	H	48	ALA
3	H	54	THR
3	H	92	LYS
3	H	140	PHE
1	A	60	MET
1	A	153	VAL
1	A	170	TRP
1	A	361	VAL
1	A	436	MET
1	A	539	LEU
2	B	32	PRO
2	B	54	VAL
2	B	77	LYS
1	F	153	VAL
1	F	170	TRP
1	F	326	LEU
1	F	474	LEU
1	F	539	LEU
2	G	32	PRO
3	H	93	ASN
1	A	172	ALA
1	A	207	ASN
1	A	313	TYR
1	A	317	VAL
1	A	371	TYR
1	A	462	ILE
2	B	56	ILE
2	B	177	PRO
1	F	60	MET
1	F	172	ALA
1	F	207	ASN
1	F	317	VAL
1	F	361	VAL
1	F	371	TYR
1	F	492	HIS

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Mol	Chain	Res	Type
2	G	54	VAL
2	G	65	PHE
2	G	66	ALA
2	G	108	TRP
2	G	133	SER
2	G	177	PRO
3	H	181	SER
1	A	404	PRO
1	A	408	PHE
2	B	41	ARG
2	B	108	TRP
3	C	124	ILE
3	C	181	SER
1	F	174	PRO
1	F	313	TYR
1	F	462	ILE
1	F	503	VAL
2	G	41	ARG
2	G	56	ILE
2	G	158	ASN
3	H	124	ILE
1	A	503	VAL
2	B	257	PRO
1	F	404	PRO
1	F	441	PRO
2	G	126	PRO
2	G	257	PRO
3	C	150	VAL
3	H	150	VAL
1	A	107	GLY
1	A	441	PRO
2	B	126	PRO
1	A	245	ILE
1	A	329	ILE
1	F	329	ILE
1	F	138	PHE

5.3.2 Protein sidechains (i)

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	413/547 (76%)	370 (90%)	43 (10%)	7	27
1	F	413/547 (76%)	368 (89%)	45 (11%)	6	26
2	B	215/262 (82%)	188 (87%)	27 (13%)	4	21
2	G	215/262 (82%)	186 (86%)	29 (14%)	4	20
3	C	152/166 (92%)	132 (87%)	20 (13%)	4	20
3	H	152/166 (92%)	132 (87%)	20 (13%)	4	20
All	All	1560/1950 (80%)	1376 (88%)	184 (12%)	5	23

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	80	ARG
1	A	95	PRO
1	A	101	GLN
1	A	103	PHE
1	A	116	MET
1	A	145	SER
1	A	148	PHE
1	A	155	LEU
1	A	159	SER
1	A	162	VAL
1	A	168	THR
1	A	188	ASP
1	A	192	TRP
1	A	223	PHE
1	A	229	THR
1	A	236	ASN
1	A	247	THR
1	A	249	THR
1	A	256	ASP
1	A	263	PHE
1	A	267	ASP
1	A	268	MET
1	A	274	MET
1	A	279	ILE
1	A	280	TRP
1	A	287	VAL

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Mol	Chain	Res	Type
1	A	294	VAL
1	A	300	GLU
1	A	314	THR
1	A	326	LEU
1	A	330	VAL
1	A	359	THR
1	A	377	PHE
1	A	388	ILE
1	A	397	THR
1	A	409	VAL
1	A	416	LEU
1	A	461	ILE
1	A	509	ILE
1	A	512	LEU
1	A	514	ILE
1	A	545	SER
2	B	36	ILE
2	B	39	GLU
2	B	41	ARG
2	B	61	MET
2	B	67	TRP
2	B	74	LYS
2	B	77	LYS
2	B	93	TRP
2	B	94	THR
2	B	112	HIS
2	B	115	GLU
2	B	118	LYS
2	B	119	PRO
2	B	120	LEU
2	B	134	MET
2	B	144	GLU
2	B	153	ILE
2	B	155	PHE
2	B	159	THR
2	B	161	VAL
2	B	172	ASN
2	B	181	SER
2	B	189	MET
2	B	192	ARG
2	B	227	ASP
2	B	276	ASP

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Mol	Chain	Res	Type
2	B	277	VAL
3	C	29	PHE
3	C	31	ILE
3	C	43	LEU
3	C	44	PHE
3	C	46	THR
3	C	50	LEU
3	C	72	GLU
3	C	78	PHE
3	C	85	MET
3	C	99	ILE
3	C	122	HIS
3	C	135	PHE
3	C	143	VAL
3	C	155	ILE
3	C	156	TRP
3	C	167	ARG
3	C	172	THR
3	C	179	CYS
3	C	182	LEU
3	C	187	LEU
1	F	53	ASP
1	F	80	ARG
1	F	95	PRO
1	F	101	GLN
1	F	103	PHE
1	F	116	MET
1	F	145	SER
1	F	148	PHE
1	F	155	LEU
1	F	159	SER
1	F	162	VAL
1	F	168	THR
1	F	188	ASP
1	F	192	TRP
1	F	223	PHE
1	F	229	THR
1	F	236	ASN
1	F	247	THR
1	F	249	THR
1	F	256	ASP
1	F	263	PHE

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Mol	Chain	Res	Type
1	F	267	ASP
1	F	268	MET
1	F	274	MET
1	F	279	ILE
1	F	280	TRP
1	F	287	VAL
1	F	294	VAL
1	F	300	GLU
1	F	314	THR
1	F	326	LEU
1	F	330	VAL
1	F	359	THR
1	F	377	PHE
1	F	388	ILE
1	F	397	THR
1	F	409	VAL
1	F	416	LEU
1	F	461	ILE
1	F	509	ILE
1	F	512	LEU
1	F	514	ILE
1	F	545	SER
1	F	548	PRO
1	F	552	PHE
2	G	36	ILE
2	G	39	GLU
2	G	41	ARG
2	G	61	MET
2	G	67	TRP
2	G	74	LYS
2	G	77	LYS
2	G	93	TRP
2	G	94	THR
2	G	95	VAL
2	G	99	ILE
2	G	112	HIS
2	G	115	GLU
2	G	118	LYS
2	G	119	PRO
2	G	120	LEU
2	G	134	MET
2	G	144	GLU

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Mol	Chain	Res	Type
2	G	153	ILE
2	G	155	PHE
2	G	159	THR
2	G	161	VAL
2	G	172	ASN
2	G	181	SER
2	G	189	MET
2	G	192	ARG
2	G	227	ASP
2	G	276	ASP
2	G	277	VAL
3	H	29	PHE
3	H	39	LEU
3	H	43	LEU
3	H	44	PHE
3	H	46	THR
3	H	50	LEU
3	H	72	GLU
3	H	78	PHE
3	H	85	MET
3	H	99	ILE
3	H	122	HIS
3	H	135	PHE
3	H	143	VAL
3	H	155	ILE
3	H	156	TRP
3	H	167	ARG
3	H	172	THR
3	H	179	CYS
3	H	182	LEU
3	H	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	124	ASN
1	A	130	GLN
1	A	142	ASN
1	A	157	ASN
1	A	195	GLN
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	365	ASN
1	A	378	HIS
1	A	486	GLN
1	A	492	HIS
2	B	145	GLN
2	B	151	ASN
2	B	168	ASN
2	B	190	GLN
2	B	198	ASN
2	B	233	GLN
2	B	261	ASN
2	B	268	ASN
3	C	94	ASN
3	C	97	GLN
3	C	173	ASN
1	F	124	ASN
1	F	142	ASN
1	F	157	ASN
1	F	195	GLN
1	F	266	ASN
1	F	345	ASN
1	F	365	ASN
1	F	486	GLN
1	F	492	HIS
2	G	145	GLN
2	G	151	ASN
2	G	168	ASN
2	G	190	GLN
2	G	198	ASN
2	G	233	GLN
2	G	261	ASN
2	G	268	ASN
3	H	94	ASN
3	H	97	GLN
3	H	173	ASN

5.3.3 RNA

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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEM	A	1001	1	50,50,50	1.13	2 (4%)	67,82,82	1.02	2 (2%)
7	HEO	F	1002	1	66,66,66	0.97	2 (3%)	84,102,102	1.15	7 (8%)
7	HEO	A	1002	1	66,66,66	0.95	1 (1%)	84,102,102	1.15	5 (5%)
6	HEM	F	1001	1	50,50,50	1.14	2 (4%)	67,82,82	1.03	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	A	1001	1	-	8/14/54/54	-
7	HEO	F	1002	1	2/2/7/15	9/34/74/74	-
7	HEO	A	1002	1	2/2/7/15	9/34/74/74	-
6	HEM	F	1001	1	-	8/14/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1001	HEM	CBB-CAB	4.81	1.53	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1001	HEM	CBB-CAB	4.71	1.53	1.30
7	A	1002	HEO	CAC-C3C	-2.94	1.39	1.47
7	F	1002	HEO	CAC-C3C	-2.90	1.39	1.47
6	F	1001	HEM	CAC-C3C	-2.84	1.39	1.47
6	A	1001	HEM	CAC-C3C	-2.80	1.39	1.47
7	F	1002	HEO	C18-C19	2.24	1.38	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1001	HEM	CBB-CAB-C3B	-3.56	109.76	127.53
6	F	1001	HEM	CBB-CAB-C3B	-3.52	109.95	127.53
7	A	1002	HEO	C3C-C4C-NC	3.17	112.47	109.80
7	F	1002	HEO	C3C-C4C-NC	3.06	112.37	109.80
7	A	1002	HEO	C1D-ND-C4D	-2.68	102.03	105.21
7	F	1002	HEO	C1D-ND-C4D	-2.61	102.12	105.21
6	F	1001	HEM	C3B-C4B-NB	2.47	111.24	109.47
7	A	1002	HEO	C3D-C4D-ND	2.35	112.62	110.35
7	A	1002	HEO	C13-C14-C15	-2.31	122.33	127.62
7	F	1002	HEO	C3D-C4D-ND	2.27	112.55	110.35
7	F	1002	HEO	C13-C14-C15	-2.24	122.50	127.62
7	F	1002	HEO	C17-C18-C19	-2.23	122.53	127.62
7	A	1002	HEO	C17-C18-C19	-2.22	122.54	127.62
6	A	1001	HEM	C3B-C4B-NB	2.18	111.03	109.47
7	F	1002	HEO	C2D-C1D-ND	2.07	112.21	109.84
7	F	1002	HEO	C2B-C1B-NB	2.01	112.22	109.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	1002	HEO	NB
7	A	1002	HEO	ND
7	F	1002	HEO	NB
7	F	1002	HEO	ND

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	HEM	C2B-C3B-CAB-CBB
6	A	1001	HEM	C2C-C3C-CAC-CBC
6	F	1001	HEM	C2B-C3B-CAB-CBB
6	F	1001	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	A	1002	HEO	C15-C16-C17-C18
7	F	1002	HEO	C15-C16-C17-C18
7	A	1002	HEO	C4C-C3C-CAC-CBC
7	F	1002	HEO	C4C-C3C-CAC-CBC
7	A	1002	HEO	C2C-C3C-CAC-CBC
7	F	1002	HEO	C2C-C3C-CAC-CBC
6	A	1001	HEM	C4B-C3B-CAB-CBB
6	A	1001	HEM	C4C-C3C-CAC-CBC
6	F	1001	HEM	C4B-C3B-CAB-CBB
6	F	1001	HEM	C4C-C3C-CAC-CBC
7	A	1002	HEO	C2A-CAA-CBA-CGA
7	F	1002	HEO	C2A-CAA-CBA-CGA
7	F	1002	HEO	CAD-CBD-CGD-O1D
7	A	1002	HEO	CAD-CBD-CGD-O1D
7	A	1002	HEO	CAD-CBD-CGD-O2D
7	F	1002	HEO	CAD-CBD-CGD-O2D
6	A	1001	HEM	CAD-CBD-CGD-O2D
6	F	1001	HEM	CAA-CBA-CGA-O2A
6	F	1001	HEM	CAD-CBD-CGD-O2D
6	A	1001	HEM	CAA-CBA-CGA-O2A
6	F	1001	HEM	CAA-CBA-CGA-O1A
6	A	1001	HEM	CAA-CBA-CGA-O1A
6	F	1001	HEM	CAD-CBD-CGD-O1D
7	F	1002	HEO	CAA-CBA-CGA-O2A
7	A	1002	HEO	CAA-CBA-CGA-O2A
6	A	1001	HEM	CAD-CBD-CGD-O1D
7	A	1002	HEO	CAA-CBA-CGA-O1A
7	F	1002	HEO	CAA-CBA-CGA-O1A
7	F	1002	HEO	C26-C15-C16-C17
7	A	1002	HEO	C26-C15-C16-C17

There are no ring outliers.

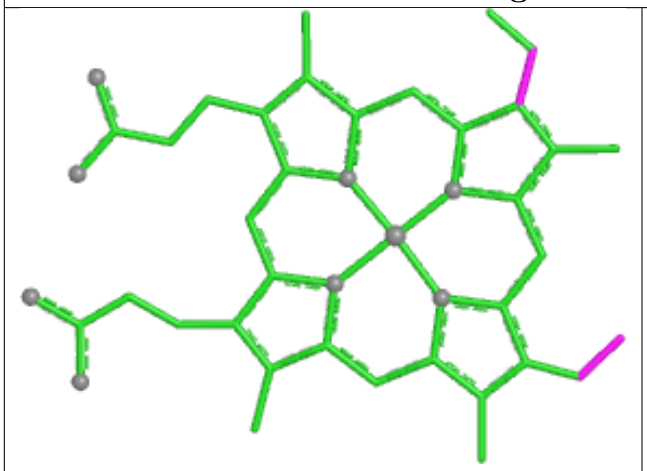
4 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	HEM	18	0
7	F	1002	HEO	12	0
7	A	1002	HEO	14	0
6	F	1001	HEM	18	0

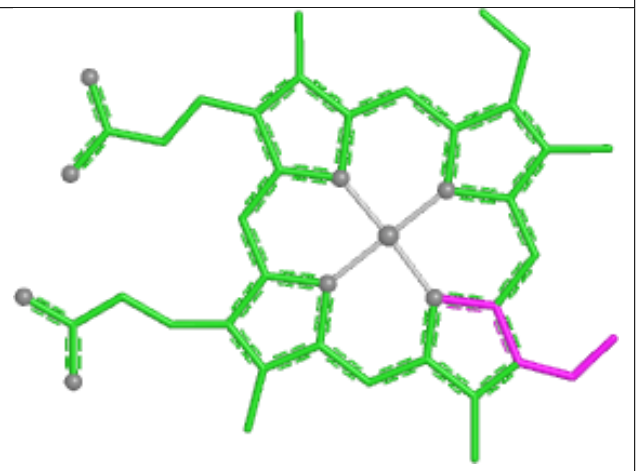
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

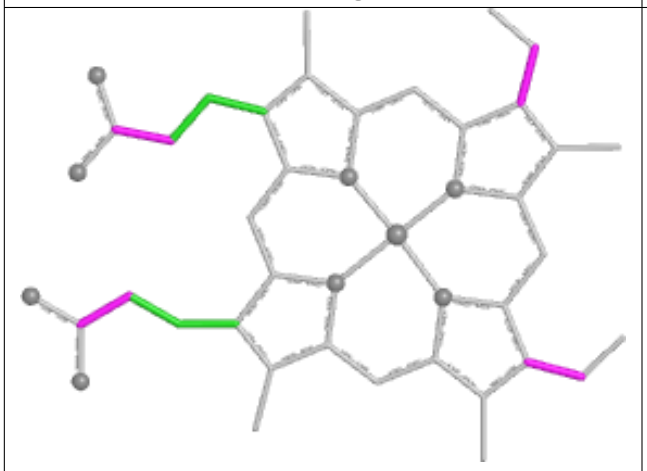
Ligand HEM A 1001



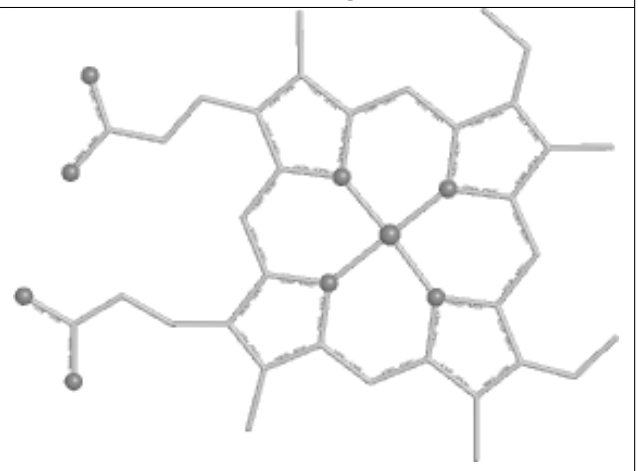
Bond lengths



Bond angles

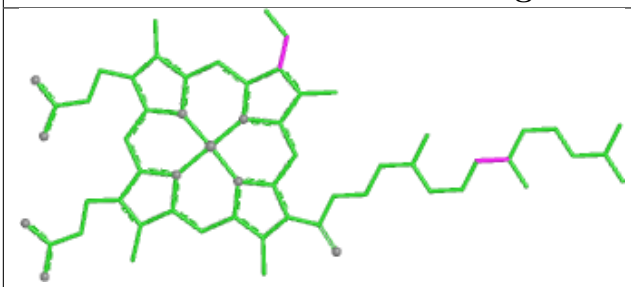


Torsions

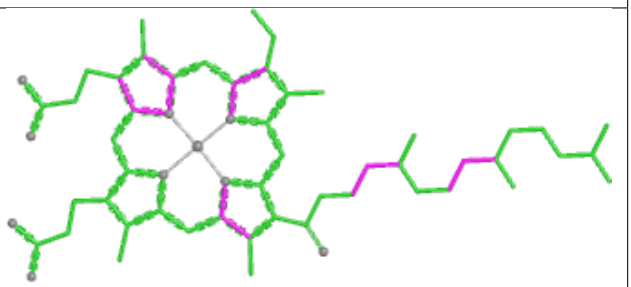


Rings

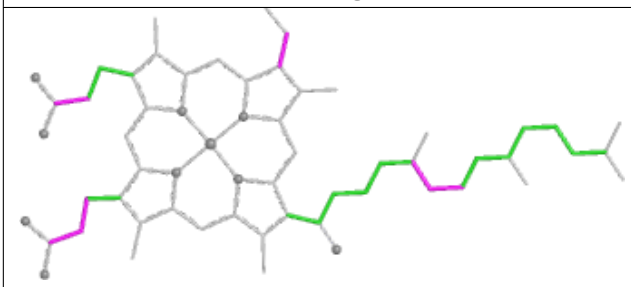
Ligand HEO F 1002



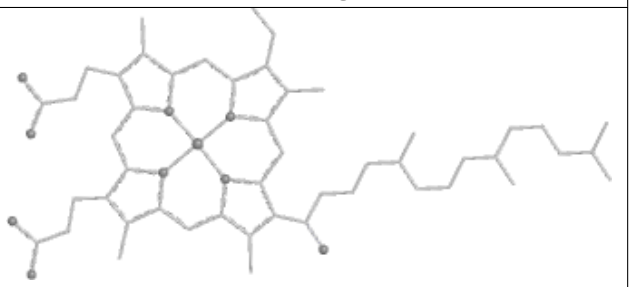
Bond lengths



Bond angles

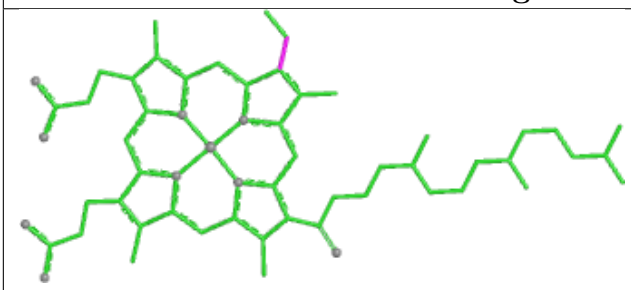


Torsions

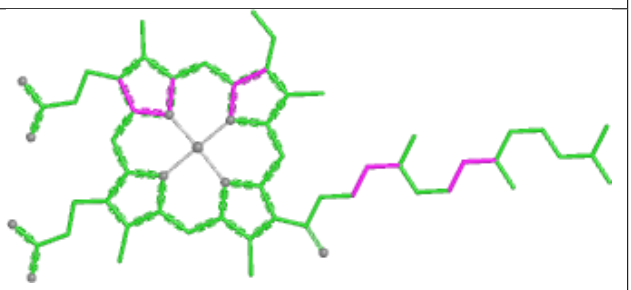


Rings

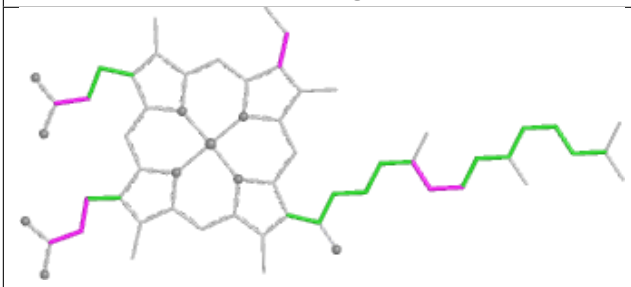
Ligand HEO A 1002



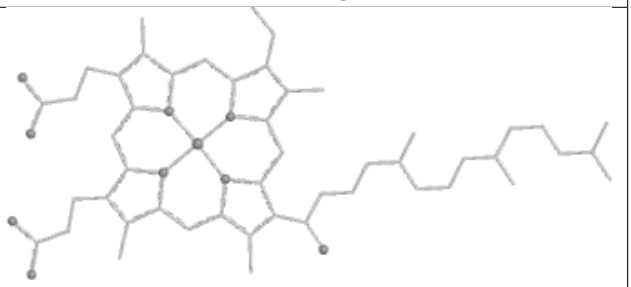
Bond lengths



Bond angles

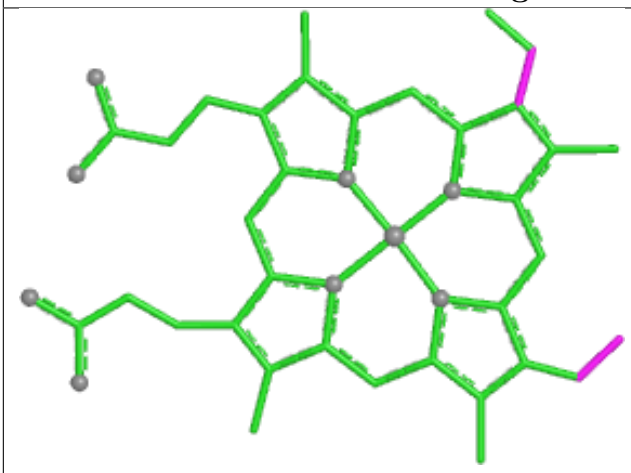


Torsions

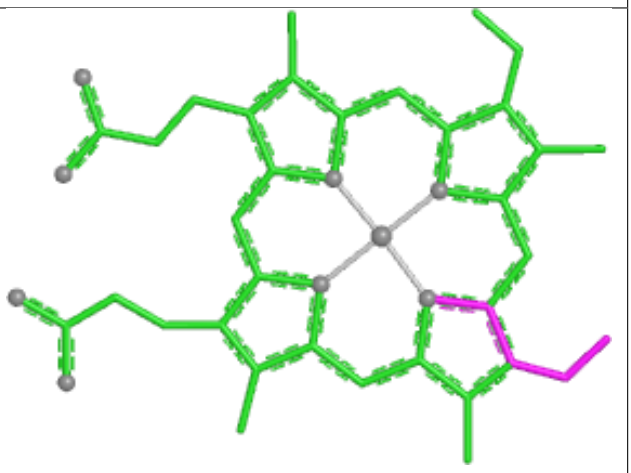


Rings

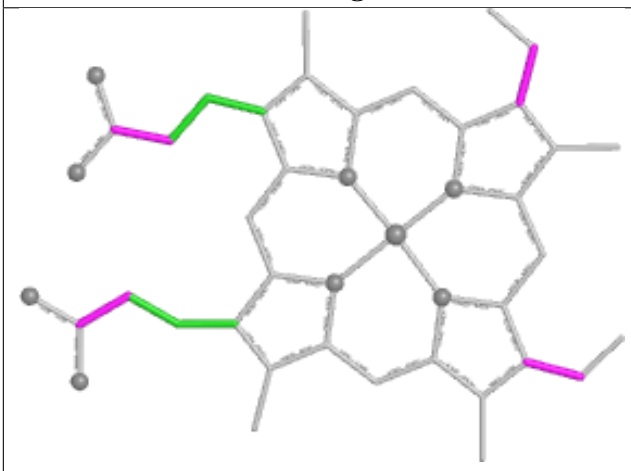
Ligand HEM F 1001



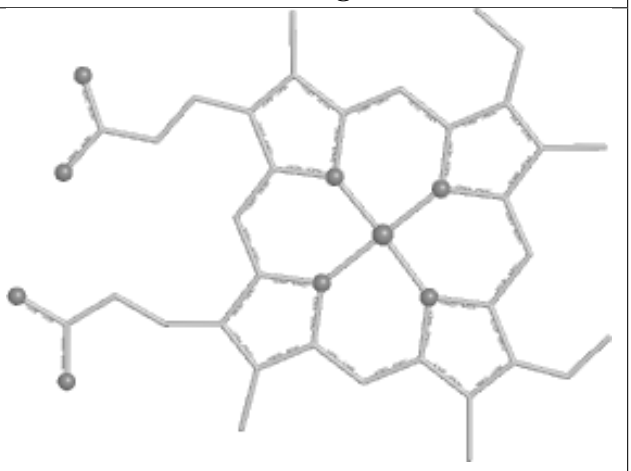
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	174:PRO	C	175:PRO	N	1.16

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.