Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 09:50 PM EDT

PDB ID	:	1BE3
Title	:	CYTOCHROME BC1 COMPLEX FROM BOVINE
Authors	:	Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.
Deposited on	:	1998-05-19
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

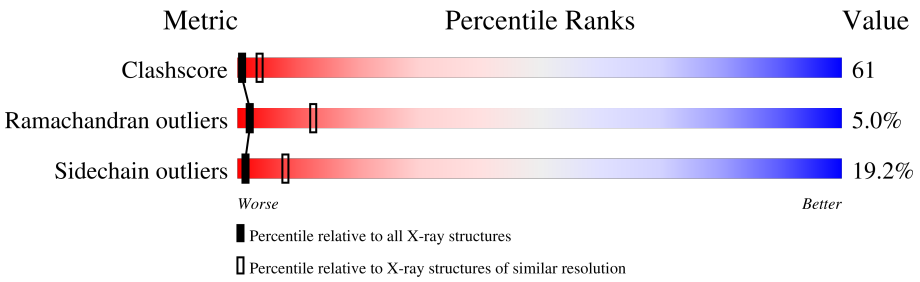
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	446	23% 56% 17% •
2	B	439	23% 55% 15% • 5%
3	C	379	29% 49% 19% •
4	D	241	26% 53% 20% •
5	E	196	25% 51% 22% •
6	F	110	33% 46% 14% • •
7	G	81	21% 58% 16% 5%
8	H	78	24% 41% 17% 18%

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Mol	Chain	Length	Quality of chain
9	I	78	9% 23% 10% 58%
10	J	62	44% 45% 10% •
11	K	56	12% 14% 12% 61%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 16222 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

- Molecule 2 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	419	3141	1972	556	606	7	0	0	0

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3011	2018	472	502	19	0	0	0

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1519	957	263	291	8	0	0	0

- Molecule 6 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	106	916	579	166	169	2	0	0	0

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	81	682	441	128	112	1	0	0	0

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	64	524	316	96	107	5	0	0	0

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	33	248	152	51	44	1	0	0	0

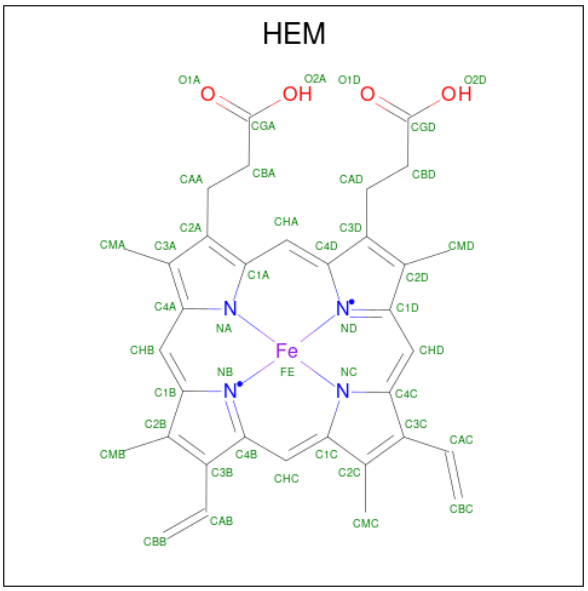
- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	62	512	335	89	88	0	0	0

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

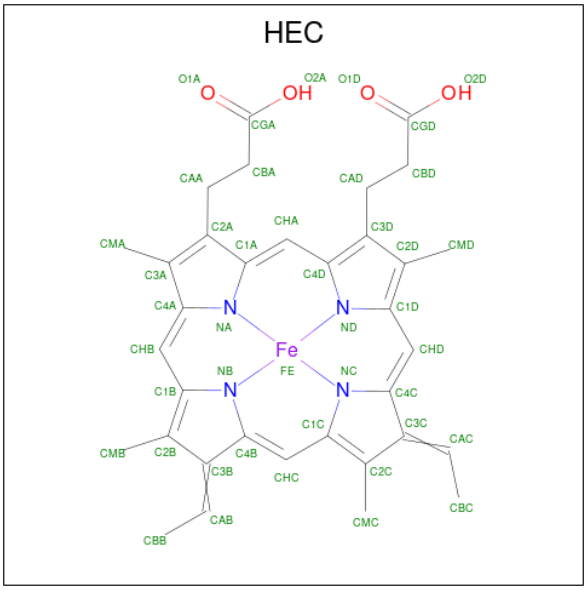
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	K	22	159	103	29	27	0	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



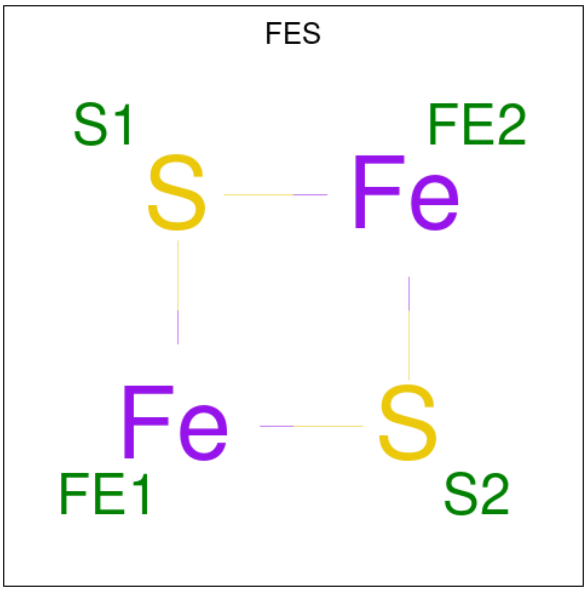
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
14	E	1	4	2	2	0	0

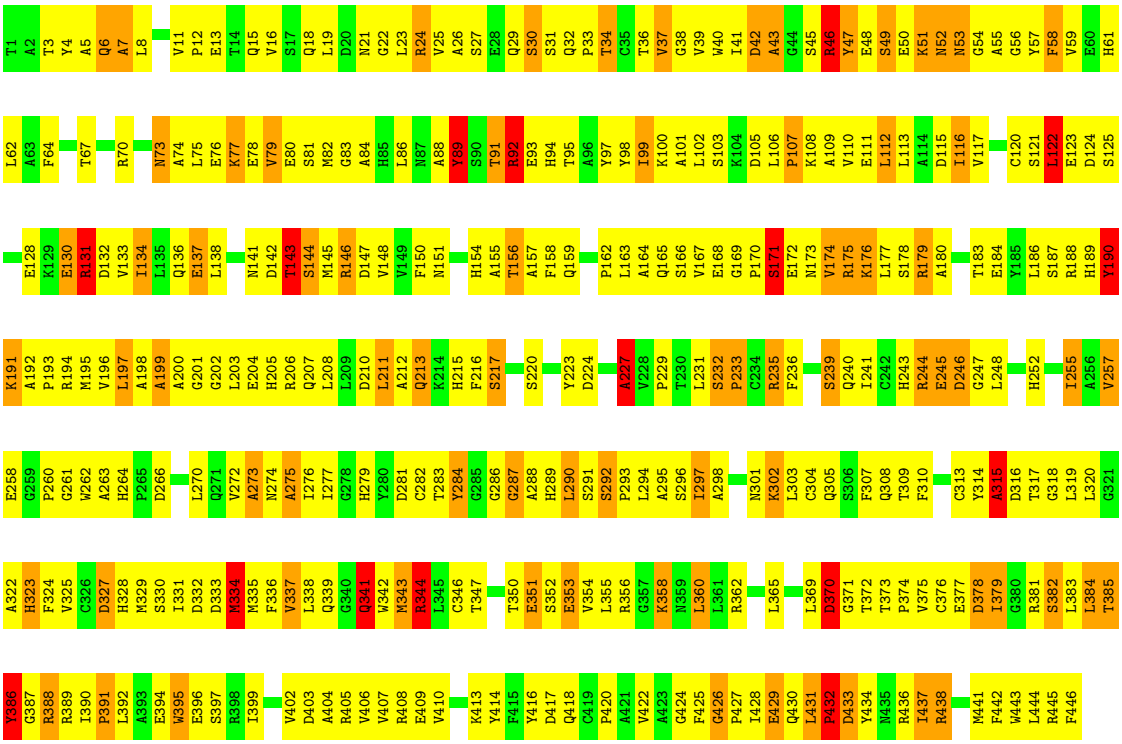
3 Residue-property plots (i)

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.

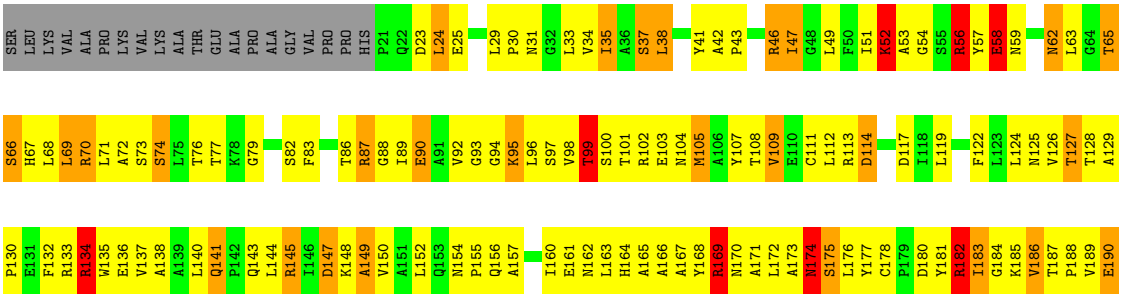
• Molecule 1: CYTOCHROME BC1 COMPLEX

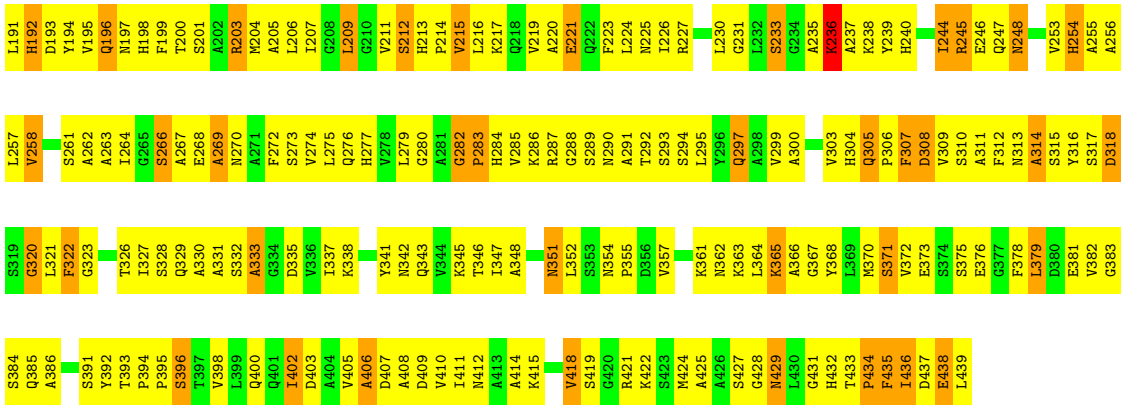
Chain A: 23% 56% 17% •



• Molecule 2: CYTOCHROME BC1 COMPLEX

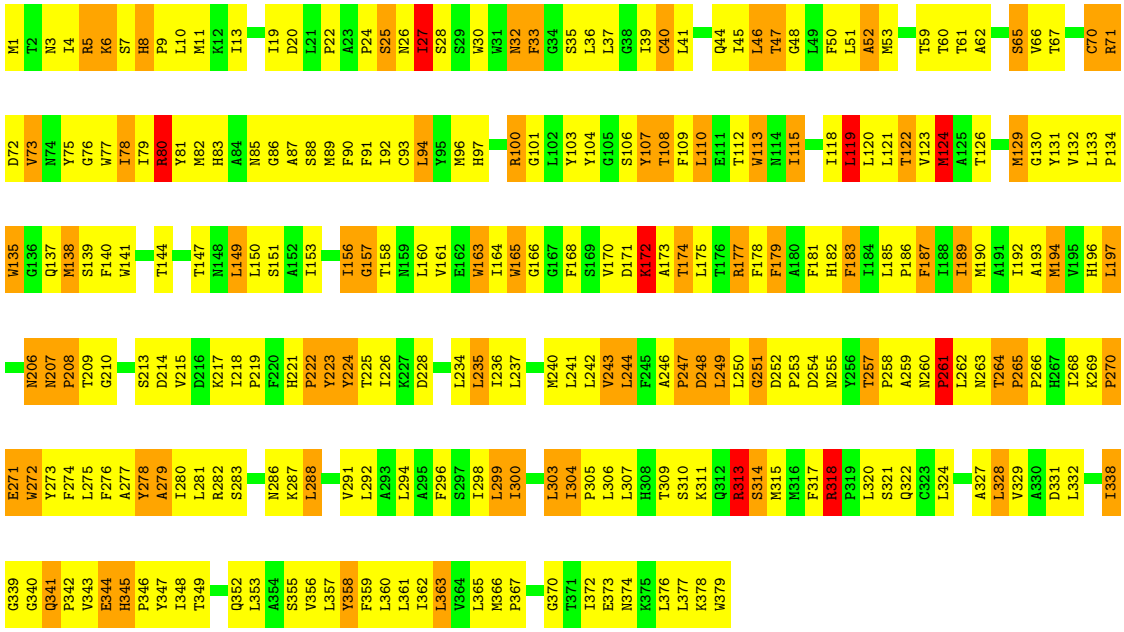
Chain B: 23% 55% 15% • 5%





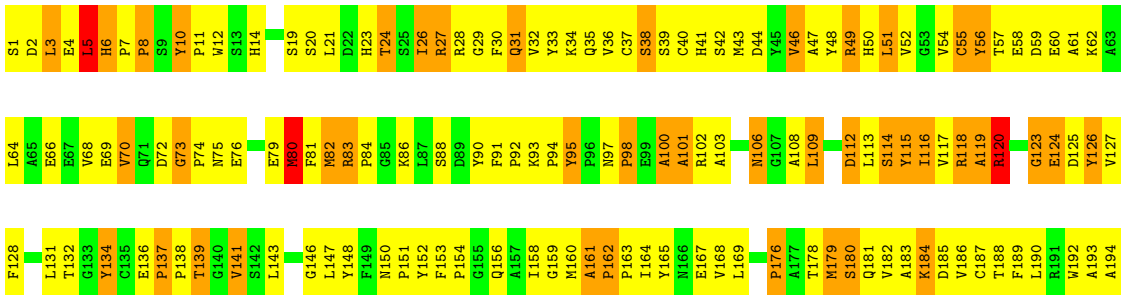
- Molecule 3: CYTOCHROME BC1 COMPLEX

Chain C: 29% 49% 19%



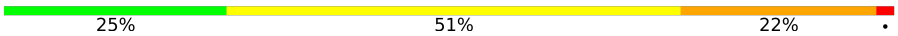
- Molecule 4: CYTOCHROME BC1 COMPLEX

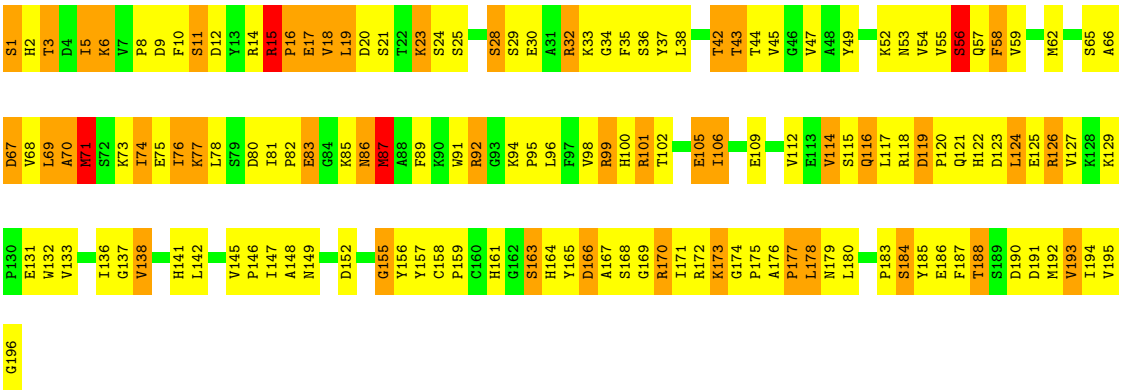
Chain D: 26% 53% 20%



• Molecule 5: CYTOCHROME BC1 COMPLEX

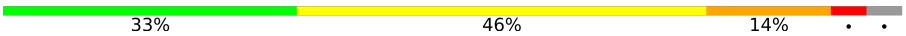
Chain E:

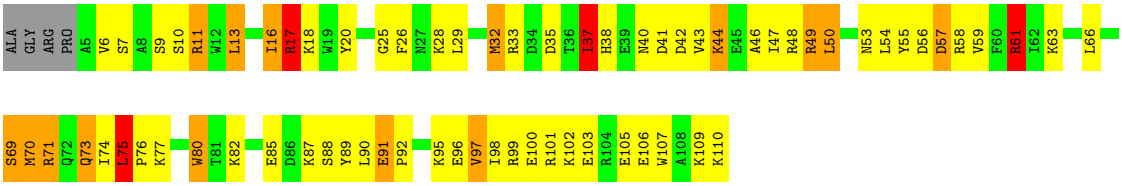




• Molecule 6: CYTOCHROME BC1 COMPLEX

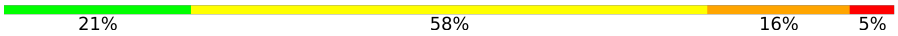
Chain F:

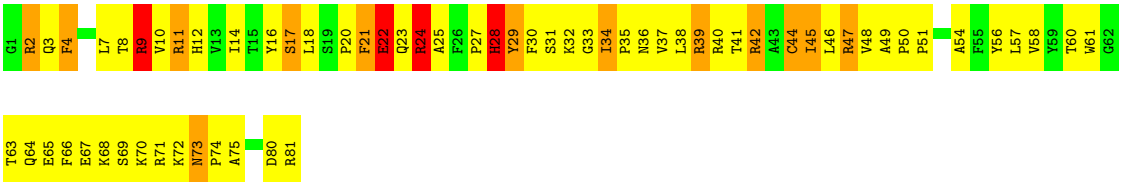




• Molecule 7: CYTOCHROME BC1 COMPLEX

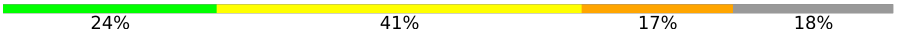
Chain G:

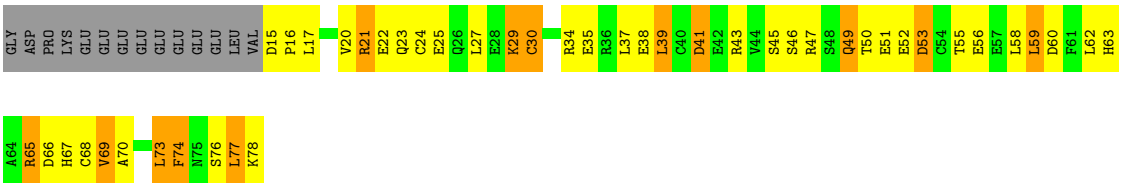




• Molecule 8: CYTOCHROME BC1 COMPLEX

Chain H:





• Molecule 9: CYTOCHROME BC1 COMPLEX

Chain I: 9% 23% 10% 58%

MET LEU SER VAL ALA ALA ARG SER GLY PRO PHE ALA PRO VAL LEU SER ALA THR SER ARG GLY VAL ALA GLY ALA LEU ARG PRO LEU VAL GLN ALA ALA VAL PRO ALA THR SER GLU SER PRO VAL LEU ASP LEU K46 R47 S48 V49 L50 C51 R52 E53 S54 L55 R56 G57 Q58 A59

R62 P63 L64 V65 V68 S69 L70 N71 V72 P73 V76 R77 Y78

- Molecule 10: CYTOCHROME BC1 COMPLEX

Chain J: 44% 45% 10%

V1 A2 P3 T4 L5 T6 A7 R8 L9 Y10 L13 F14 T17 S18 T19 F20 A21 L22 T23 I24 V25 L29 F30 F31 E32 R33 I42 Y43 I46 G49 K50 L51 W52 K53 H54 I55 K56 H57 K58 Y59 E60 N61 K62

- Molecule 11: CYTOCHROME BC1 COMPLEX

Chain K: 12% 14% 12% 61%

MET LEU THR ARG PHE LEU GLY PRO ARG TYR ARG GLN LEU ALA R15 N16 W17 V18 P19 T20 A21 Q22 L23 W24 V30 G31 L32 V33 S34 A35 T36 ASP SER ARG LEU ILE LEU ASP TRP VAL PRO TYR ILE ASN GLY LYS PHE LYS LYS ASP ASP

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	211.20Å 211.20Å 339.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	81.7 (40.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16222	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.62	1/3531 (0.0%)	1.63	35/4792 (0.7%)
2	B	0.59	0/3198	1.52	25/4336 (0.6%)
3	C	0.67	2/3108 (0.1%)	1.56	34/4252 (0.8%)
4	D	0.55	0/1978	1.41	15/2684 (0.6%)
5	E	0.55	1/1553 (0.1%)	1.47	16/2100 (0.8%)
6	F	0.58	1/935 (0.1%)	1.59	12/1253 (1.0%)
7	G	0.56	0/704	1.54	11/951 (1.2%)
8	H	0.51	0/529	1.14	1/708 (0.1%)
9	I	0.64	0/250	1.48	1/335 (0.3%)
10	J	0.54	0/525	1.29	4/707 (0.6%)
11	K	0.55	0/163	1.22	1/225 (0.4%)
All	All	0.60	5/16474 (0.0%)	1.52	155/22343 (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	14
2	B	0	17
3	C	0	8
4	D	0	5
5	E	0	5
6	F	0	5
7	G	0	2
8	H	0	1
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	344	GLU	CD-OE1	7.85	1.34	1.25
6	F	91	GLU	CD-OE1	7.13	1.33	1.25
3	C	261	PRO	N-CD	-6.11	1.39	1.47
1	A	122	LEU	C-O	5.64	1.34	1.23
5	E	56	SER	C-O	5.41	1.33	1.23

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	15	ARG	NE-CZ-NH2	15.63	128.11	120.30
3	C	177	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	235	ARG	NE-CZ-NH2	14.30	127.45	120.30
1	A	235	ARG	NE-CZ-NH1	-13.98	113.31	120.30
3	C	80	ARG	NE-CZ-NH1	-13.54	113.53	120.30
7	G	11	ARG	NE-CZ-NH2	-13.17	113.72	120.30
2	B	134	ARG	NE-CZ-NH1	-12.83	113.89	120.30
4	D	49	ARG	NE-CZ-NH1	-12.60	114.00	120.30
1	A	92	ARG	NE-CZ-NH1	12.13	126.37	120.30
2	B	134	ARG	NE-CZ-NH2	11.66	126.13	120.30
1	A	46	ARG	NE-CZ-NH2	11.48	126.04	120.30
6	F	49	ARG	NE-CZ-NH1	10.54	125.57	120.30
5	E	14	ARG	NE-CZ-NH2	-10.49	115.06	120.30
6	F	49	ARG	CD-NE-CZ	10.42	138.19	123.60
2	B	182	ARG	NE-CZ-NH2	-10.08	115.26	120.30
4	D	10	TYR	CB-CG-CD1	-10.07	114.96	121.00
2	B	56	ARG	NE-CZ-NH1	10.04	125.32	120.30
2	B	56	ARG	CD-NE-CZ	9.95	137.53	123.60
2	B	194	TYR	CG-CD2-CE2	-9.95	113.34	121.30
5	E	14	ARG	CD-NE-CZ	-9.86	109.80	123.60
5	E	32	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	A	89	TYR	CB-CG-CD1	9.39	126.63	121.00
1	A	89	TYR	CB-CG-CD2	-9.35	115.39	121.00
1	A	438	ARG	NE-CZ-NH2	-9.28	115.66	120.30
4	D	27	ARG	NE-CZ-NH2	-9.17	115.72	120.30
3	C	183	PHE	CB-CG-CD2	8.92	127.05	120.80
6	F	49	ARG	NE-CZ-NH2	-8.74	115.93	120.30
3	C	318	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	A	386	TYR	CB-CG-CD1	8.60	126.16	121.00
1	A	344	ARG	NE-CZ-NH1	8.41	124.50	120.30
3	C	196	HIS	CA-CB-CG	8.34	127.78	113.60
5	E	15	ARG	NH1-CZ-NH2	-8.32	110.25	119.40
2	B	308	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	362	ARG	NE-CZ-NH1	-8.15	116.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	122	THR	CA-CB-CG2	-8.15	100.99	112.40
6	F	17	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	131	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	B	245	ARG	CD-NE-CZ	-7.61	112.95	123.60
2	B	70	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	B	169	ARG	NE-CZ-NH2	-7.45	116.58	120.30
7	G	9	ARG	NE-CZ-NH2	7.43	124.02	120.30
3	C	119	LEU	CB-CG-CD1	7.42	123.61	111.00
5	E	99	ARG	NE-CZ-NH1	7.39	123.99	120.30
3	C	71	ARG	NE-CZ-NH1	-7.37	116.61	120.30
3	C	313	ARG	NE-CZ-NH1	7.33	123.97	120.30
10	J	33	ARG	NE-CZ-NH2	7.28	123.94	120.30
5	E	170	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	432	PRO	N-CA-CB	7.21	111.95	103.30
3	C	303	LEU	CA-CB-CG	7.19	131.83	115.30
5	E	14	ARG	NH1-CZ-NH2	7.18	127.30	119.40
3	C	242	LEU	CA-CB-CG	7.18	131.81	115.30
3	C	124	MET	CA-CB-CG	7.10	125.36	113.30
6	F	32	MET	CA-CB-CG	7.05	125.29	113.30
4	D	55	CYS	CA-CB-SG	-6.95	101.48	114.00
2	B	194	TYR	CZ-CE2-CD2	6.81	125.93	119.80
1	A	92	ARG	CD-NE-CZ	6.80	133.12	123.60
7	G	11	ARG	NH1-CZ-NH2	6.74	126.82	119.40
10	J	14	PHE	CB-CG-CD1	6.73	125.51	120.80
4	D	118	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	A	150	PHE	CB-CG-CD2	6.69	125.48	120.80
4	D	120	ARG	CD-NE-CZ	6.58	132.82	123.60
6	F	56	ASP	CB-CG-OD1	-6.56	112.39	118.30
2	B	58	GLU	OE1-CD-OE2	-6.55	115.44	123.30
6	F	61	ARG	CA-CB-CG	6.52	127.73	113.40
3	C	183	PHE	CB-CG-CD1	-6.51	116.24	120.80
1	A	370	ASP	CB-CG-OD1	-6.51	112.44	118.30
7	G	9	ARG	NE-CZ-NH1	-6.48	117.06	120.30
5	E	99	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	146	ARG	NE-CZ-NH2	-6.40	117.10	120.30
4	D	112	ASP	CB-CG-OD2	6.36	124.02	118.30
6	F	57	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	A	199	ALA	N-CA-CB	6.28	118.89	110.10
1	A	190	TYR	CB-CG-CD2	6.27	124.76	121.00
5	E	126	ARG	NE-CZ-NH2	6.26	123.43	120.30
3	C	71	ARG	NE-CZ-NH2	6.26	123.43	120.30
9	I	47	ARG	NE-CZ-NH1	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	177	ARG	NH1-CZ-NH2	6.22	126.24	119.40
2	B	87	ARG	NE-CZ-NH1	-6.20	117.20	120.30
4	D	115	TYR	CB-CG-CD1	6.14	124.68	121.00
8	H	65	ARG	NE-CZ-NH1	-6.13	117.23	120.30
4	D	56	TYR	CB-CG-CD2	-6.13	117.32	121.00
7	G	24	ARG	NE-CZ-NH1	-6.04	117.28	120.30
4	D	10	TYR	CA-CB-CG	-5.99	102.03	113.40
3	C	265	PRO	CB-CA-C	5.95	126.87	112.00
2	B	314	ALA	N-CA-CB	-5.91	101.82	110.10
7	G	21	PHE	CG-CD2-CE2	-5.90	114.31	120.80
1	A	343	MET	N-CA-CB	5.89	121.20	110.60
3	C	248	ASP	CB-CG-OD2	5.86	123.57	118.30
3	C	358	TYR	CB-CG-CD1	5.85	124.51	121.00
6	F	71	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	227	ALA	N-CA-CB	5.83	118.26	110.10
3	C	179	PHE	CB-CG-CD2	-5.79	116.74	120.80
4	D	134	TYR	CB-CG-CD2	-5.78	117.53	121.00
3	C	358	TYR	CB-CG-CD2	-5.78	117.53	121.00
4	D	56	TYR	CB-CG-CD1	5.77	124.46	121.00
7	G	28	HIS	N-CA-CB	5.74	120.93	110.60
1	A	89	TYR	CA-CB-CG	5.74	124.30	113.40
1	A	413	LYS	O-C-N	5.73	131.87	122.70
3	C	100	ARG	NE-CZ-NH1	-5.72	117.44	120.30
3	C	206	ASN	OD1-CG-ND2	5.68	134.97	121.90
2	B	167	ALA	O-C-N	-5.67	113.64	122.70
3	C	318	ARG	CA-CB-CG	5.66	125.86	113.40
2	B	181	TYR	CZ-CE2-CD2	5.66	124.89	119.80
3	C	179	PHE	CB-CG-CD1	5.62	124.74	120.80
7	G	21	PHE	CZ-CE2-CD2	5.62	126.84	120.10
2	B	435	PHE	CB-CG-CD2	-5.62	116.87	120.80
7	G	2	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	B	114	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	378	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	244	ARG	NE-CZ-NH2	5.53	123.06	120.30
3	C	282	ARG	CD-NE-CZ	-5.51	115.88	123.60
1	A	434	TYR	CB-CG-CD2	-5.51	117.69	121.00
2	B	254	HIS	CA-CB-CG	5.50	122.95	113.60
1	A	315	ALA	CA-C-O	5.48	131.61	120.10
5	E	92	ARG	NE-CZ-NH1	-5.47	117.56	120.30
3	C	129	MET	CA-CB-CG	-5.47	104.00	113.30
3	C	206	ASN	CB-CG-OD1	-5.43	110.75	121.60
7	G	22	GLU	CB-CA-C	-5.43	99.55	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	ALA	N-CA-CB	5.42	117.68	110.10
3	C	168	PHE	CB-CG-CD2	-5.40	117.02	120.80
4	D	10	TYR	CB-CG-CD2	5.39	124.23	121.00
10	J	42	ILE	CA-C-O	5.37	131.38	120.10
2	B	65	THR	CA-CB-CG2	-5.33	104.93	112.40
3	C	33	PHE	CB-CG-CD2	-5.33	117.07	120.80
5	E	14	ARG	NE-CZ-NH1	-5.32	117.64	120.30
11	K	17	TRP	CA-CB-CG	-5.31	103.61	113.70
5	E	92	ARG	NE-CZ-NH2	-5.31	117.65	120.30
5	E	58	PHE	CB-CG-CD1	5.30	124.51	120.80
3	C	187	PHE	CB-CG-CD1	-5.29	117.09	120.80
5	E	56	SER	O-C-N	-5.28	114.26	122.70
1	A	92	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
2	B	327	ILE	CB-CA-C	-5.26	101.08	111.60
6	F	61	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	257	VAL	CB-CA-C	-5.25	101.42	111.40
1	A	263	ALA	N-CA-CB	-5.23	102.78	110.10
3	C	194	MET	CA-CB-CG	5.21	122.16	113.30
10	J	14	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	327	ASP	CB-CG-OD2	5.19	122.97	118.30
3	C	113	TRP	CD1-NE1-CE2	-5.17	104.34	109.00
1	A	46	ARG	NE-CZ-NH1	-5.16	117.72	120.30
3	C	62	ALA	N-CA-CB	5.16	117.32	110.10
2	B	134	ARG	CA-CB-CG	5.15	124.74	113.40
2	B	138	ALA	N-CA-CB	5.13	117.29	110.10
7	G	47	ARG	CD-NE-CZ	5.13	130.78	123.60
6	F	58	ARG	CD-NE-CZ	-5.10	116.46	123.60
3	C	235	LEU	CB-CG-CD2	5.10	119.66	111.00
4	D	46	VAL	CA-CB-CG1	-5.08	103.28	110.90
1	A	150	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	A	275	ALA	N-CA-CB	-5.06	103.01	110.10
4	D	49	ARG	NH1-CZ-NH2	5.06	124.96	119.40
5	E	56	SER	CB-CA-C	5.05	119.70	110.10
2	B	169	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	47	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	B	182	ARG	CA-CB-CG	5.03	124.46	113.40
6	F	57	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	THR	Mainchain
1	A	190	TYR	Mainchain
1	A	197	LEU	Mainchain
1	A	210	ASP	Mainchain
1	A	273	ALA	Mainchain
1	A	284	TYR	Mainchain
1	A	297	ILE	Mainchain
1	A	304	CYS	Mainchain
1	A	323	HIS	Mainchain
1	A	334	MET	Mainchain
1	A	341	GLN	Mainchain
1	A	433	ASP	Mainchain
1	A	437	ILE	Mainchain
1	A	47	TYR	Mainchain
2	B	105	MET	Mainchain
2	B	147	ASP	Mainchain
2	B	149	ALA	Mainchain
2	B	172	LEU	Mainchain
2	B	174	ASN	Mainchain
2	B	186	VAL	Mainchain
2	B	244	ILE	Mainchain
2	B	246	GLU	Mainchain
2	B	248	ASN	Mainchain
2	B	282	GLY	Mainchain
2	B	320	GLY	Mainchain
2	B	379	LEU	Mainchain
2	B	391	SER	Mainchain
2	B	406	ALA	Mainchain
2	B	69	LEU	Mainchain
2	B	90	GLU	Mainchain
2	B	99	THR	Mainchain
3	C	108	THR	Mainchain
3	C	149	LEU	Mainchain
3	C	163	TRP	Mainchain
3	C	165	TRP	Mainchain
3	C	213	SER	Mainchain
3	C	264	THR	Mainchain
3	C	40	CYS	Mainchain
3	C	75	TYR	Mainchain
4	D	24	THR	Mainchain
4	D	31	GLN	Mainchain
4	D	41	HIS	Mainchain
4	D	5	LEU	Mainchain

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Mol	Chain	Res	Type	Group
4	D	6	HIS	Mainchain
5	E	155	GLY	Mainchain
5	E	184	SER	Mainchain
5	E	43	THR	Mainchain
5	E	56	SER	Mainchain
5	E	71	MET	Mainchain
6	F	17	ARG	Mainchain
6	F	37	ILE	Mainchain
6	F	73	GLN	Mainchain
6	F	75	LEU	Mainchain
6	F	80	TRP	Mainchain
7	G	22	GLU	Mainchain
7	G	73	ASN	Mainchain
8	H	59	LEU	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	3458	0	3356	492	0
2	B	3141	0	3123	408	1
3	C	3011	0	3077	382	2
4	D	1919	0	1868	295	0
5	E	1519	0	1503	184	2
6	F	916	0	909	83	0
7	G	682	0	679	104	0
8	H	524	0	504	58	0
9	I	248	0	265	76	0
10	J	512	0	518	60	0
11	K	159	0	159	23	0
12	C	86	0	60	19	0
13	D	43	0	30	2	0
14	E	4	0	0	1	0
All	All	16222	0	16051	1980	3

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 61.

All (1980) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:CE1	1:A:317:THR:HG21	1.71	1.26
1:A:21:ASN:CB	1:A:217:SER:HB2	1.70	1.20
1:A:392:LEU:HA	1:A:395:TRP:CD1	1.79	1.17
2:B:29:LEU:HD12	2:B:33:LEU:HD21	1.19	1.15
1:A:158:PHE:HE1	1:A:317:THR:HG21	0.97	1.12
4:D:233:ARG:HG2	7:G:17:SER:HB2	1.29	1.12
3:C:26:ASN:HD21	3:C:207:ASN:HB2	1.11	1.11
3:C:174:THR:HG23	3:C:178:PHE:HE1	1.13	1.10
1:A:34:THR:HG21	2:B:370:MET:HG2	1.31	1.09
2:B:304:HIS:CD2	2:B:306:PRO:HD2	1.85	1.09
4:D:83:ARG:HB3	4:D:84:PRO:CD	1.82	1.09
2:B:24:LEU:H	2:B:24:LEU:HD12	1.18	1.08
4:D:83:ARG:CB	4:D:84:PRO:HD2	1.85	1.07
1:A:42:ASP:HB3	1:A:384:LEU:HD22	1.13	1.06
1:A:18:GLN:HE21	1:A:22:GLY:HA2	1.10	1.06
7:G:72:LYS:HB3	7:G:75:ALA:HB2	1.32	1.06
7:G:8:THR:HG22	7:G:9:ARG:H	1.15	1.05
1:A:64:PHE:HE1	1:A:86:LEU:HG	1.19	1.04
9:I:78:TYR:OXT	9:I:78:TYR:HD1	1.38	1.04
3:C:206:ASN:HB2	3:C:313:ARG:NH2	1.72	1.04
3:C:129:MET:HG2	3:C:178:PHE:HD2	1.20	1.03
3:C:108:THR:HB	3:C:313:ARG:HH11	1.21	1.03
1:A:21:ASN:HB3	1:A:217:SER:CB	1.89	1.02
1:A:213:GLN:HB3	1:A:215:HIS:NE2	1.73	1.01
3:C:265:PRO:HB2	3:C:268:ILE:HG12	1.02	1.01
3:C:310:SER:HA	3:C:374:ASN:HD21	1.25	1.01
4:D:70:VAL:HG23	4:D:84:PRO:HD3	1.41	1.01
4:D:57:THR:HG22	4:D:59:ASP:H	1.26	1.01
2:B:305:GLN:HB2	2:B:306:PRO:HD3	1.39	1.00
3:C:26:ASN:HD21	3:C:207:ASN:CB	1.75	1.00
1:A:64:PHE:CE1	1:A:86:LEU:HG	1.96	1.00
1:A:67:THR:HG22	1:A:70:ARG:HB2	1.43	1.00
3:C:265:PRO:HB2	3:C:268:ILE:CG1	1.93	0.99
1:A:383:LEU:HA	1:A:387:GLY:O	1.63	0.98
1:A:378:ASP:O	1:A:382:SER:HB2	1.63	0.97
3:C:174:THR:HG23	3:C:178:PHE:CE1	1.98	0.97
2:B:279:LEU:HD22	2:B:295:LEU:HD13	1.43	0.97
12:C:381:HEM:HBC2	12:C:381:HEM:HMC2	1.46	0.97
1:A:248:LEU:HD11	1:A:425:PHE:HE2	1.27	0.97
9:I:78:TYR:OXT	9:I:78:TYR:CD1	2.19	0.95
2:B:385:GLN:HG2	9:I:62:ARG:HH12	1.31	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:74:PRO:HG2	4:D:82:MET:SD	2.06	0.95
2:B:51:ILE:HG21	2:B:199:PHE:HA	1.46	0.95
1:A:248:LEU:HD11	1:A:425:PHE:CE2	2.02	0.94
3:C:3:ASN:N	3:C:8:HIS:NE2	2.14	0.94
2:B:248:ASN:HB2	2:B:428:GLY:HA2	1.47	0.94
3:C:348:ILE:O	3:C:352:GLN:HG3	1.67	0.94
3:C:106:SER:HB3	12:C:381:HEM:HBD2	1.49	0.94
1:A:36:THR:OG1	1:A:372:THR:HG22	1.69	0.93
1:A:21:ASN:HB3	1:A:217:SER:HB2	0.93	0.92
4:D:233:ARG:CG	7:G:17:SER:HB2	1.98	0.92
3:C:270:PRO:HB2	3:C:274:PHE:HB2	1.51	0.92
1:A:27:SER:HA	1:A:199:ALA:O	1.69	0.92
2:B:283:PRO:HG3	9:I:55:LEU:HD22	1.49	0.92
4:D:219:VAL:HA	4:D:222:MET:HG3	1.50	0.92
3:C:10:LEU:HD12	3:C:13:ILE:HD12	1.51	0.92
1:A:408:ARG:HH12	11:K:15:ARG:HG2	1.34	0.92
2:B:169:ARG:HH11	2:B:238:LYS:NZ	1.68	0.92
3:C:26:ASN:ND2	3:C:207:ASN:HB2	1.84	0.92
1:A:45:SER:HB3	1:A:92:ARG:HA	1.50	0.92
2:B:297:GLN:OE1	2:B:297:GLN:HA	1.67	0.92
2:B:341:TYR:CE2	2:B:345:LYS:HE3	2.05	0.91
4:D:224:ARG:HB2	7:G:25:ALA:HB1	1.53	0.91
12:C:380:HEM:HBB2	12:C:380:HEM:HHC	1.50	0.91
2:B:341:TYR:HE2	2:B:345:LYS:HE3	1.32	0.91
9:I:62:ARG:HB3	9:I:63:PRO:HD3	1.51	0.91
1:A:91:THR:HG22	1:A:93:GLU:H	1.36	0.91
2:B:304:HIS:HD2	2:B:306:PRO:HD2	1.25	0.91
7:G:36:ASN:HA	7:G:39:ARG:HD3	1.52	0.91
4:D:83:ARG:HB3	4:D:84:PRO:HD2	0.94	0.90
2:B:182:ARG:NH1	2:B:185:LYS:HE2	1.86	0.90
3:C:1:MET:SD	3:C:7:SER:HB2	2.12	0.90
10:J:29:LEU:HD13	11:K:34:SER:HB2	1.54	0.90
7:G:29:TYR:HD2	7:G:30:PHE:CD2	1.90	0.90
3:C:210:GLY:HA3	3:C:314:SER:HB2	1.54	0.90
5:E:19:LEU:HD12	5:E:19:LEU:O	1.71	0.90
2:B:237:ALA:HB2	2:B:318:ASP:OD2	1.70	0.89
1:A:236:PHE:CE2	1:A:317:THR:HG23	2.07	0.89
3:C:138:MET:HE3	3:C:269:LYS:H	1.37	0.89
4:D:178:THR:HB	4:D:181:GLN:HG3	1.53	0.89
8:H:70:ALA:HA	8:H:73:LEU:HD22	1.53	0.89
2:B:305:GLN:HB2	2:B:306:PRO:CD	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:345:HIS:HB3	3:C:346:PRO:CD	2.02	0.88
1:A:236:PHE:CE2	1:A:258:GLU:HB3	2.08	0.88
2:B:47:ILE:HD11	2:B:211:VAL:HG21	1.55	0.88
3:C:170:VAL:HG13	3:C:174:THR:HG21	1.56	0.88
3:C:108:THR:HB	3:C:313:ARG:NH1	1.88	0.88
4:D:165:TYR:O	4:D:168:VAL:HG23	1.74	0.88
7:G:73:ASN:N	7:G:74:PRO:HD2	1.89	0.88
4:D:27:ARG:HH12	10:J:58:LYS:HG3	1.40	0.87
9:I:72:VAL:HB	9:I:73:PRO:HD3	1.55	0.87
2:B:132:PHE:CD2	2:B:191:LEU:HD13	2.10	0.87
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.07	0.87
1:A:75:LEU:HD21	1:A:116:ILE:HD11	1.55	0.87
4:D:181:GLN:HA	8:H:77:LEU:HD13	1.56	0.87
6:F:37:ILE:HD11	6:F:90:LEU:CD2	2.05	0.87
1:A:18:GLN:NE2	1:A:22:GLY:HA2	1.90	0.87
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.23	0.86
1:A:155:ALA:HA	1:A:164:ALA:HB1	1.54	0.86
3:C:185:LEU:HB3	3:C:186:PRO:HD3	1.56	0.86
2:B:331:ALA:HA	2:B:432:HIS:ND1	1.89	0.86
1:A:53:ASN:OD1	1:A:165:GLN:HB2	1.75	0.86
1:A:224:ASP:OD1	1:A:227:ALA:HB3	1.76	0.86
3:C:1:MET:SD	3:C:4:ILE:HB	2.14	0.86
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.58	0.86
3:C:310:SER:HB3	3:C:318:ARG:NH1	1.91	0.85
1:A:61:HIS:CD2	1:A:134:ILE:HD11	2.11	0.85
4:D:26:ILE:HG22	4:D:54:VAL:HG13	1.57	0.85
4:D:74:PRO:HB2	4:D:79:GLU:HB2	1.58	0.85
7:G:8:THR:HG22	7:G:9:ARG:N	1.91	0.85
1:A:30:SER:N	1:A:201:GLY:O	2.09	0.85
9:I:72:VAL:HB	9:I:73:PRO:CD	2.05	0.85
1:A:317:THR:HG22	1:A:318:GLY:N	1.87	0.85
3:C:129:MET:HG2	3:C:178:PHE:CD2	2.10	0.85
1:A:39:VAL:HG23	1:A:113:LEU:HD23	1.59	0.85
2:B:29:LEU:HD12	2:B:33:LEU:CD2	2.06	0.85
4:D:27:ARG:HH11	10:J:58:LYS:HZ1	1.23	0.85
1:A:408:ARG:NH1	11:K:15:ARG:HG2	1.91	0.85
4:D:10:TYR:CD1	4:D:11:PRO:HD2	2.11	0.84
4:D:51:LEU:HA	4:D:56:TYR:O	1.77	0.84
4:D:10:TYR:HB2	4:D:125:ASP:OD1	1.75	0.84
1:A:106:LEU:HD22	1:A:203:LEU:HD22	1.59	0.84
4:D:50:HIS:HB3	4:D:54:VAL:HB	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:LEU:HB2	6:F:55:TYR:HB2	1.60	0.84
8:H:25:GLU:HA	8:H:30:CYS:SG	2.17	0.84
2:B:217:LYS:O	2:B:221:GLU:HG3	1.77	0.84
7:G:9:ARG:NH2	7:G:11:ARG:HD2	1.93	0.83
9:I:70:LEU:HD12	9:I:71:ASN:N	1.92	0.83
2:B:200:THR:HG22	2:B:203:ARG:HD2	1.58	0.83
4:D:27:ARG:HH11	10:J:58:LYS:NZ	1.74	0.83
3:C:265:PRO:CB	3:C:268:ILE:HG12	1.98	0.83
6:F:28:LYS:HD3	6:F:74:ILE:HD11	1.58	0.83
3:C:264:THR:O	3:C:266:PRO:HD3	1.78	0.83
3:C:341:GLN:HB3	3:C:347:TYR:CD2	2.14	0.83
1:A:42:ASP:HB3	1:A:384:LEU:CD2	2.05	0.83
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.61	0.83
3:C:59:THR:HG23	3:C:135:TRP:HE1	1.43	0.82
3:C:215:VAL:HG11	6:F:59:VAL:HG13	1.61	0.82
3:C:345:HIS:HB3	3:C:346:PRO:HD3	1.60	0.82
1:A:134:ILE:HD13	1:A:134:ILE:N	1.93	0.82
2:B:24:LEU:HD12	2:B:24:LEU:N	1.94	0.82
1:A:236:PHE:HD2	1:A:258:GLU:HG2	1.42	0.82
1:A:360:LEU:HD13	2:B:93:GLY:HA2	1.61	0.82
2:B:263:ALA:O	2:B:269:ALA:HB2	1.80	0.81
5:E:2:HIS:O	5:E:5:ILE:HG12	1.80	0.81
1:A:334:MET:HA	1:A:334:MET:CE	2.11	0.81
2:B:165:ALA:HA	2:B:173:ALA:HB1	1.61	0.81
4:D:229:VAL:O	4:D:233:ARG:HG3	1.79	0.81
1:A:144:SER:O	1:A:148:VAL:HG23	1.80	0.81
1:A:428:ILE:HG23	1:A:431:LEU:CB	2.11	0.81
9:I:64:LEU:HD12	9:I:65:VAL:N	1.94	0.81
1:A:134:ILE:HA	1:A:137:GLU:HG3	1.63	0.81
4:D:178:THR:OG1	4:D:181:GLN:NE2	2.11	0.81
1:A:293:PRO:O	1:A:297:ILE:HG13	1.81	0.80
1:A:143:THR:HG21	9:I:48:SER:H	1.43	0.80
2:B:169:ARG:HH11	2:B:238:LYS:HZ2	1.26	0.80
3:C:309:THR:CG2	3:C:370:GLY:HA3	2.11	0.80
3:C:309:THR:HG23	3:C:370:GLY:HA3	1.62	0.80
2:B:209:LEU:HD22	2:B:375:SER:HB2	1.64	0.80
4:D:30:PHE:HD1	4:D:189:PHE:CE2	2.00	0.80
3:C:359:PHE:O	3:C:363:LEU:HB2	1.82	0.79
2:B:99:THR:OG1	9:I:68:VAL:HG22	1.81	0.79
4:D:11:PRO:HG3	8:H:70:ALA:O	1.82	0.79
4:D:57:THR:HG22	4:D:59:ASP:N	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:177:PRO:HB2	5:E:178:LEU:HD23	1.62	0.79
3:C:108:THR:CB	3:C:313:ARG:HH11	1.96	0.79
7:G:9:ARG:HH21	7:G:11:ARG:HD2	1.47	0.79
2:B:111:CYS:HB3	2:B:119:LEU:HD22	1.65	0.79
1:A:236:PHE:CD2	1:A:258:GLU:HG2	2.18	0.79
3:C:137:GLN:OE1	3:C:259:ALA:HA	1.83	0.79
2:B:338:LYS:HG2	2:B:439:LEU:HD21	1.65	0.79
3:C:206:ASN:HB2	3:C:313:ARG:HH21	1.48	0.79
8:H:49:GLN:HB2	8:H:52:GLU:HG2	1.63	0.79
4:D:27:ARG:NH1	10:J:58:LYS:NZ	2.31	0.79
4:D:228:SER:HB2	7:G:23:GLN:NE2	1.98	0.79
2:B:31:ASN:HB3	2:B:201:SER:HB3	1.65	0.79
2:B:308:ASP:OD1	2:B:309:VAL:N	2.16	0.79
10:J:18:SER:OG	11:K:23:LEU:HB2	1.83	0.79
1:A:260:PRO:HG3	1:A:414:TYR:CE1	2.18	0.78
6:F:37:ILE:HD11	6:F:90:LEU:HD21	1.64	0.78
10:J:51:LEU:HB3	10:J:52:TRP:CZ3	2.18	0.78
1:A:106:LEU:HD22	1:A:203:LEU:CD2	2.13	0.78
1:A:392:LEU:HA	1:A:395:TRP:NE1	1.98	0.78
2:B:385:GLN:CG	9:I:62:ARG:HH12	1.96	0.78
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.19	0.78
1:A:52:ASN:HB2	1:A:55:ALA:HB2	1.64	0.78
3:C:278:TYR:O	3:C:279:ALA:C	2.22	0.78
2:B:156:GLN:HE22	9:I:56:ARG:HD3	1.47	0.78
5:E:76:ILE:HG23	5:E:194:ILE:HD13	1.65	0.78
1:A:245:GLU:H	1:A:426:GLY:HA3	1.47	0.78
6:F:75:LEU:O	6:F:80:TRP:NE1	2.17	0.78
1:A:102:LEU:HB2	1:A:105:ASP:OD2	1.84	0.77
5:E:169:GLY:HA2	5:E:180:LEU:HD12	1.66	0.77
5:E:164:HIS:CD2	5:E:173:LYS:HG2	2.19	0.77
1:A:39:VAL:HG12	1:A:41:ILE:HD11	1.66	0.77
2:B:203:ARG:NE	2:B:230:LEU:HD23	1.98	0.77
2:B:274:VAL:HG21	2:B:405:VAL:HG21	1.65	0.77
1:A:244:ARG:HG2	7:G:10:VAL:HG12	1.65	0.77
1:A:436:ARG:HE	3:C:222:PRO:HD3	1.50	0.77
2:B:74:SER:O	2:B:82:SER:HB2	1.85	0.77
2:B:200:THR:O	2:B:204:MET:HG3	1.84	0.77
4:D:74:PRO:CB	4:D:79:GLU:HB2	2.15	0.77
3:C:103:TYR:O	3:C:315:MET:HB2	1.83	0.77
7:G:29:TYR:CD2	7:G:30:PHE:CD2	2.73	0.77
1:A:240:GLN:HG3	1:A:422:VAL:HB	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:SER:HA	3:C:13:ILE:HG12	1.65	0.76
2:B:306:PRO:HB2	2:B:329:GLN:NE2	2.00	0.76
1:A:445:ARG:O	1:A:446:PHE:HB2	1.83	0.76
2:B:54:GLY:H	2:B:57:TYR:HD2	1.31	0.76
2:B:67:HIS:HD2	2:B:144:LEU:HD22	1.49	0.76
4:D:97:ASN:OD1	4:D:98:PRO:HD2	1.86	0.76
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.68	0.76
2:B:304:HIS:HD2	2:B:306:PRO:CD	1.99	0.76
1:A:262:TRP:CD2	1:A:385:THR:HG23	2.21	0.76
2:B:200:THR:CG2	2:B:203:ARG:HD2	2.16	0.76
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.68	0.75
2:B:56:ARG:NH2	2:B:318:ASP:OD1	2.16	0.75
4:D:113:LEU:CD2	4:D:116:ILE:HD12	2.16	0.75
5:E:73:LYS:HG3	5:E:196:GLY:O	1.86	0.75
9:I:70:LEU:HD12	9:I:71:ASN:H	1.49	0.75
1:A:73:ASN:O	1:A:77:LYS:HG3	1.86	0.75
2:B:248:ASN:HB2	2:B:428:GLY:CA	2.17	0.75
2:B:262:ALA:HB2	2:B:272:PHE:HE2	1.52	0.74
2:B:162:ASN:HD22	2:B:244:ILE:CG2	2.00	0.74
3:C:8:HIS:HB3	3:C:9:PRO:HD3	1.69	0.74
3:C:100:ARG:HH21	12:C:381:HEM:HBD1	1.52	0.74
4:D:211:MET:HE2	4:D:211:MET:HA	1.69	0.74
4:D:70:VAL:HG23	4:D:84:PRO:CD	2.16	0.74
2:B:198:HIS:HE1	2:B:233:SER:HB3	1.53	0.74
1:A:158:PHE:HE1	1:A:317:THR:CG2	1.91	0.74
1:A:240:GLN:NE2	1:A:431:LEU:HD21	2.01	0.74
1:A:418:GLN:O	1:A:420:PRO:HD3	1.88	0.74
2:B:42:ALA:HB1	2:B:43:PRO:HD2	1.67	0.74
2:B:129:ALA:N	2:B:130:PRO:HD3	2.02	0.74
2:B:264:ILE:CG2	2:B:317:SER:HA	2.17	0.74
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.69	0.74
4:D:54:VAL:O	4:D:54:VAL:HG12	1.87	0.74
1:A:106:LEU:CD2	1:A:203:LEU:HD13	2.16	0.74
1:A:236:PHE:CZ	1:A:317:THR:HG23	2.23	0.73
1:A:37:VAL:HA	1:A:199:ALA:HB2	1.70	0.73
3:C:10:LEU:HD12	3:C:13:ILE:CD1	2.17	0.73
2:B:435:PHE:HB2	2:B:438:GLU:OE1	1.88	0.73
1:A:428:ILE:HG23	1:A:431:LEU:HB2	1.68	0.73
2:B:169:ARG:HD3	2:B:238:LYS:HZ2	1.52	0.73
10:J:51:LEU:HB3	10:J:52:TRP:CE3	2.23	0.73
2:B:385:GLN:HG2	9:I:62:ARG:NH1	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:ALA:O	4:D:103:ALA:N	2.22	0.73
2:B:300:ALA:HA	2:B:307:PHE:CZ	2.24	0.73
2:B:308:ASP:OD2	9:I:55:LEU:HA	1.89	0.73
7:G:72:LYS:CB	7:G:75:ALA:HB2	2.13	0.73
1:A:198:ALA:HB1	1:A:379:ILE:HG22	1.68	0.73
1:A:73:ASN:ND2	1:A:73:ASN:H	1.85	0.73
3:C:135:TRP:HH2	3:C:170:VAL:HG12	1.54	0.73
1:A:184:GLU:O	1:A:188:ARG:HG3	1.88	0.73
2:B:76:THR:HG21	2:B:133:ARG:NH2	2.04	0.73
2:B:83:PHE:CE1	2:B:87:ARG:HG3	2.23	0.73
3:C:78:ILE:HD11	5:E:57:GLN:NE2	2.03	0.73
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.69	0.73
8:H:21:ARG:HB3	8:H:65:ARG:HH21	1.53	0.73
1:A:213:GLN:HB3	1:A:215:HIS:CD2	2.24	0.72
1:A:386:TYR:HD1	1:A:386:TYR:H	1.36	0.72
3:C:138:MET:CE	3:C:269:LYS:H	2.02	0.72
5:E:117:LEU:HD12	5:E:120:PRO:HA	1.71	0.72
1:A:426:GLY:HA2	1:A:428:ILE:N	2.04	0.72
2:B:102:ARG:NH1	2:B:175:SER:HA	2.04	0.72
1:A:64:PHE:HE2	1:A:88:ALA:HB2	1.53	0.72
4:D:102:ARG:HE	4:D:109:LEU:HD22	1.54	0.72
2:B:77:THR:HG22	2:B:130:PRO:HA	1.72	0.72
2:B:309:VAL:HG22	2:B:326:THR:HA	1.71	0.72
4:D:50:HIS:HB3	4:D:54:VAL:CB	2.20	0.72
1:A:351:GLU:OE2	1:A:404:ALA:HB3	1.89	0.72
2:B:261:SER:HB3	2:B:320:GLY:HA3	1.70	0.72
6:F:6:VAL:HB	6:F:10:SER:HB2	1.70	0.72
1:A:383:LEU:HD22	1:A:388:ARG:HA	1.70	0.72
6:F:33:ARG:NH2	6:F:91:GLU:OE2	2.23	0.72
3:C:296:PHE:CE1	3:C:300:ILE:HG13	2.25	0.72
4:D:214:LEU:O	4:D:218:LEU:HG	1.90	0.72
5:E:77:LYS:HD2	5:E:98:VAL:HG21	1.71	0.72
9:I:76:VAL:HG12	9:I:76:VAL:O	1.89	0.72
1:A:15:GLN:O	1:A:26:ALA:HA	1.90	0.72
3:C:81:TYR:OH	4:D:118:ARG:NH2	2.23	0.72
3:C:315:MET:HA	3:C:318:ARG:HG3	1.71	0.71
1:A:392:LEU:CA	1:A:395:TRP:CD1	2.67	0.71
1:A:39:VAL:HG11	1:A:117:VAL:HG21	1.72	0.71
1:A:162:PRO:O	1:A:165:GLN:HG2	1.89	0.71
2:B:76:THR:HG21	2:B:133:ARG:CZ	2.21	0.71
3:C:36:LEU:HD22	3:C:235:LEU:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:HIS:HB3	3:C:222:PRO:HD3	1.71	0.71
3:C:378:LYS:NZ	6:F:91:GLU:OE1	2.24	0.71
5:E:96:LEU:HD21	5:E:195:VAL:HG21	1.71	0.71
1:A:243:HIS:CD2	1:A:425:PHE:CE1	2.79	0.71
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.72	0.71
3:C:300:ILE:HD13	3:C:362:ILE:HG21	1.72	0.71
1:A:223:TYR:CD2	1:A:224:ASP:N	2.57	0.71
3:C:71:ARG:HH21	4:D:196:PRO:HG3	1.56	0.71
2:B:67:HIS:HD2	2:B:144:LEU:CD2	2.04	0.71
5:E:67:ASP:C	5:E:67:ASP:OD1	2.29	0.71
2:B:348:ALA:HB1	2:B:415:LYS:HA	1.73	0.70
5:E:168:SER:OG	5:E:170:ARG:NE	2.20	0.70
3:C:219:PRO:HG2	3:C:222:PRO:HG2	1.73	0.70
7:G:73:ASN:N	7:G:74:PRO:CD	2.55	0.70
3:C:72:ASP:OD1	4:D:49:ARG:NH1	2.15	0.70
3:C:252:ASP:HB3	3:C:253:PRO:HD3	1.74	0.70
3:C:269:LYS:CD	3:C:340:GLY:HA2	2.21	0.70
1:A:32:GLN:HB3	1:A:33:PRO:HD2	1.73	0.70
1:A:67:THR:CG2	1:A:70:ARG:HB2	2.20	0.70
2:B:366:ALA:O	2:B:370:MET:HG3	1.91	0.70
4:D:48:TYR:OH	4:D:68:VAL:HG11	1.92	0.70
5:E:65:SER:O	5:E:69:LEU:HB2	1.92	0.70
3:C:244:LEU:O	4:D:201:ARG:HD3	1.91	0.70
1:A:75:LEU:HD21	1:A:116:ILE:CD1	2.21	0.70
1:A:111:GLU:HG2	1:A:213:GLN:HE22	1.55	0.70
4:D:113:LEU:HD22	4:D:116:ILE:HD12	1.71	0.70
3:C:92:ILE:O	3:C:96:MET:HG2	1.91	0.70
6:F:73:GLN:HG2	7:G:36:ASN:HD21	1.56	0.70
1:A:286:GLY:O	1:A:287:GLY:C	2.31	0.69
1:A:332:ASP:CG	1:A:430:GLN:HE21	1.95	0.69
3:C:206:ASN:ND2	3:C:207:ASN:H	1.90	0.69
4:D:27:ARG:NH1	10:J:58:LYS:HG3	2.06	0.69
4:D:187:CYS:O	4:D:190:LEU:HB2	1.92	0.69
5:E:95:PRO:HB2	5:E:137:GLY:HA3	1.73	0.69
1:A:248:LEU:CD1	1:A:425:PHE:CE2	2.74	0.69
4:D:30:PHE:CE1	4:D:50:HIS:CE1	2.80	0.69
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.74	0.69
6:F:73:GLN:HA	7:G:39:ARG:HH21	1.56	0.69
10:J:58:LYS:HG2	10:J:59:TYR:H	1.56	0.69
1:A:291:SER:O	1:A:293:PRO:HD3	1.91	0.69
1:A:317:THR:CG2	1:A:318:GLY:N	2.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LEU:HD13	2:B:223:PHE:CG	2.28	0.69
2:B:267:ALA:O	2:B:268:GLU:C	2.30	0.69
5:E:33:LYS:HB3	10:J:10:TYR:CE2	2.27	0.69
2:B:89:ILE:HG22	2:B:94:GLY:O	1.92	0.69
2:B:168:TYR:HD1	2:B:238:LYS:O	1.76	0.69
2:B:198:HIS:CE1	2:B:233:SER:HB3	2.28	0.69
6:F:59:VAL:HG11	7:G:10:VAL:HG22	1.74	0.69
1:A:39:VAL:HG12	1:A:41:ILE:CD1	2.22	0.69
1:A:248:LEU:CD1	1:A:425:PHE:HE2	2.03	0.69
2:B:53:ALA:HB2	2:B:198:HIS:HB3	1.74	0.69
2:B:58:GLU:OE2	2:B:66:SER:HB3	1.92	0.69
3:C:26:ASN:OD1	6:F:66:LEU:HD22	1.93	0.69
9:I:64:LEU:HG	9:I:65:VAL:HG23	1.74	0.69
5:E:102:THR:O	5:E:105:GLU:N	2.26	0.69
1:A:317:THR:HG22	1:A:318:GLY:H	1.58	0.69
2:B:109:VAL:HG22	2:B:119:LEU:CD2	2.22	0.68
3:C:328:LEU:O	3:C:332:LEU:HD12	1.92	0.68
4:D:183:ALA:HA	4:D:186:VAL:HG23	1.75	0.68
1:A:158:PHE:CE1	1:A:317:THR:CG2	2.65	0.68
1:A:42:ASP:CB	1:A:384:LEU:HD22	2.08	0.68
2:B:406:ALA:HB3	2:B:409:ASP:HB2	1.74	0.68
3:C:280:ILE:HD13	3:C:355:SER:OG	1.93	0.68
5:E:15:ARG:NH1	7:G:23:GLN:O	2.27	0.68
4:D:82:MET:SD	4:D:86:LYS:HD2	2.33	0.68
2:B:303:VAL:HG12	2:B:304:HIS:N	2.08	0.68
2:B:29:LEU:CD1	2:B:33:LEU:HD21	2.12	0.68
3:C:206:ASN:CB	3:C:313:ARG:NH2	2.54	0.68
3:C:237:LEU:HD22	4:D:216:LEU:HD11	1.75	0.68
4:D:117:VAL:HG13	4:D:124:GLU:N	2.08	0.68
9:I:72:VAL:CB	9:I:73:PRO:HD3	2.24	0.68
1:A:328:HIS:CD2	1:A:329:MET:HG2	2.29	0.68
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.29	0.68
5:E:117:LEU:HD13	5:E:121:GLN:H	1.59	0.68
3:C:248:ASP:O	3:C:249:LEU:C	2.27	0.68
3:C:277:ALA:HB1	3:C:294:LEU:HD11	1.75	0.68
4:D:62:LYS:O	4:D:66:GLU:HG3	1.94	0.68
4:D:165:TYR:CZ	4:D:168:VAL:HG13	2.28	0.68
1:A:192:ALA:HA	1:A:194:ARG:N	2.09	0.67
2:B:156:GLN:NE2	9:I:56:ARG:HD3	2.08	0.67
2:B:183:ILE:HG22	2:B:184:GLY:N	2.08	0.67
4:D:131:LEU:HD13	4:D:164:ILE:HD12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG21	1:A:437:ILE:HD13	1.75	0.67
3:C:379:TRP:CZ3	6:F:37:ILE:HG23	2.29	0.67
4:D:134:TYR:HE2	4:D:163:PRO:HG2	1.58	0.67
6:F:35:ASP:OD1	6:F:89:TYR:OH	2.10	0.67
2:B:200:THR:HG22	2:B:203:ARG:CD	2.24	0.67
2:B:283:PRO:HG3	9:I:55:LEU:CD2	2.23	0.67
3:C:261:PRO:O	3:C:262:LEU:HD23	1.92	0.67
4:D:50:HIS:HB3	4:D:54:VAL:CG2	2.24	0.67
3:C:296:PHE:HD1	3:C:359:PHE:HE1	1.41	0.67
4:D:64:LEU:O	4:D:68:VAL:HG23	1.94	0.67
4:D:26:ILE:CG2	4:D:54:VAL:HG13	2.25	0.67
4:D:57:THR:HB	4:D:60:GLU:HB2	1.77	0.67
5:E:29:SER:HA	5:E:32:ARG:HD3	1.75	0.67
1:A:287:GLY:O	1:A:290:LEU:HG	1.95	0.67
3:C:47:THR:CG2	3:C:83:HIS:HB2	2.25	0.67
9:I:64:LEU:CD1	9:I:65:VAL:HG23	2.24	0.67
1:A:43:ALA:CB	1:A:189:HIS:HB3	2.25	0.67
1:A:111:GLU:HG2	1:A:213:GLN:NE2	2.10	0.67
3:C:59:THR:HG23	3:C:135:TRP:NE1	2.09	0.67
3:C:67:THR:O	3:C:71:ARG:HG3	1.94	0.67
1:A:120:CYS:O	1:A:122:LEU:HG	1.94	0.67
3:C:22:PRO:HG2	7:G:3:GLN:HB3	1.77	0.67
3:C:263:ASN:CG	3:C:264:THR:H	1.98	0.67
4:D:10:TYR:O	4:D:12:TRP:CD1	2.48	0.67
5:E:80:ASP:OD1	5:E:81:ILE:N	2.28	0.67
6:F:28:LYS:HB3	6:F:74:ILE:HD11	1.77	0.67
7:G:28:HIS:CD2	7:G:31:SER:HB3	2.29	0.67
4:D:117:VAL:CG1	4:D:124:GLU:H	2.08	0.67
1:A:38:GLY:HA3	1:A:40:TRP:HZ3	1.58	0.66
5:E:33:LYS:HB3	10:J:10:TYR:HE2	1.60	0.66
1:A:146:ARG:NH2	1:A:308:GLN:HE22	1.92	0.66
2:B:182:ARG:HH12	2:B:185:LYS:HE2	1.60	0.66
2:B:305:GLN:CB	2:B:306:PRO:HD3	2.19	0.66
3:C:44:GLN:HE22	3:C:86:GLY:HA3	1.60	0.66
3:C:137:GLN:HB2	3:C:257:THR:HG22	1.75	0.66
3:C:311:LYS:HD2	3:C:379:TRP:HB3	1.78	0.66
3:C:207:ASN:HD22	3:C:210:GLY:H	1.43	0.66
4:D:50:HIS:O	4:D:54:VAL:N	2.24	0.66
10:J:51:LEU:H	10:J:54:HIS:HD2	1.42	0.66
1:A:198:ALA:HB1	1:A:379:ILE:CG2	2.26	0.66
8:H:35:GLU:O	8:H:39:LEU:HG	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:HB3	1:A:208:LEU:CD2	2.25	0.66
1:A:106:LEU:HD22	1:A:203:LEU:CD1	2.26	0.66
1:A:166:SER:CB	5:E:3:THR:HG22	2.25	0.66
3:C:345:HIS:CB	3:C:346:PRO:CD	2.71	0.66
3:C:357:LEU:HG	3:C:361:LEU:HD11	1.76	0.66
5:E:123:ASP:OD1	5:E:168:SER:HB3	1.95	0.66
2:B:384:SER:HB3	9:I:62:ARG:HG2	1.77	0.66
3:C:310:SER:HB3	3:C:318:ARG:HH12	1.60	0.66
4:D:6:HIS:C	4:D:8:PRO:HD2	2.16	0.66
10:J:58:LYS:HG2	10:J:59:TYR:N	2.11	0.66
2:B:309:VAL:HG22	2:B:326:THR:HG22	1.78	0.65
4:D:23:HIS:CD2	10:J:51:LEU:HA	2.31	0.65
4:D:102:ARG:HA	4:D:108:ALA:O	1.96	0.65
1:A:64:PHE:CE2	1:A:88:ALA:HB2	2.30	0.65
1:A:236:PHE:HE2	1:A:258:GLU:HB3	1.57	0.65
4:D:102:ARG:HE	4:D:109:LEU:CD2	2.09	0.65
4:D:225:HIS:O	4:D:228:SER:OG	2.14	0.65
4:D:150:ASN:OD1	4:D:151:PRO:HD2	1.96	0.65
4:D:161:ALA:O	4:D:163:PRO:HD3	1.95	0.65
1:A:211:LEU:HD12	1:A:211:LEU:O	1.97	0.65
1:A:236:PHE:HD2	1:A:258:GLU:CG	2.08	0.65
2:B:51:ILE:CG2	2:B:199:PHE:HA	2.24	0.65
3:C:151:SER:HB3	3:C:161:VAL:HG21	1.77	0.65
12:C:380:HEM:HHC	12:C:380:HEM:CBB	2.24	0.65
1:A:67:THR:OG1	1:A:115:ASP:OD1	2.12	0.65
4:D:69:GLU:O	4:D:73:GLY:CA	2.44	0.65
1:A:360:LEU:HD13	2:B:93:GLY:CA	2.26	0.65
2:B:261:SER:HB2	2:B:321:LEU:N	2.12	0.65
3:C:25:SER:HA	3:C:218:ILE:HD12	1.77	0.65
3:C:221:HIS:N	3:C:222:PRO:HD2	2.12	0.65
8:H:52:GLU:OE1	8:H:52:GLU:HA	1.96	0.65
9:I:58:GLN:HG2	9:I:78:TYR:CD2	2.32	0.65
1:A:106:LEU:HD22	1:A:203:LEU:HD13	1.78	0.64
3:C:166:GLY:HA3	3:C:177:ARG:NH2	2.12	0.64
4:D:181:GLN:HA	8:H:77:LEU:CD1	2.25	0.64
6:F:28:LYS:CD	6:F:74:ILE:HD11	2.27	0.64
2:B:237:ALA:HB2	2:B:318:ASP:CG	2.17	0.64
4:D:231:LYS:HD3	6:F:71:ARG:HG2	1.78	0.64
1:A:86:LEU:HD13	1:A:99:ILE:CD1	2.27	0.64
1:A:351:GLU:OE2	1:A:404:ALA:N	2.30	0.64
2:B:198:HIS:HE1	2:B:233:SER:CB	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:LEU:O	3:C:276:PHE:C	2.36	0.64
5:E:18:VAL:HG11	5:E:32:ARG:NH1	2.13	0.64
2:B:169:ARG:NH1	2:B:238:LYS:HZ2	1.95	0.64
3:C:214:ASP:HB3	7:G:7:LEU:HB3	1.78	0.64
7:G:71:ARG:HH21	8:H:60:ASP:CG	2.00	0.64
3:C:272:TRP:CE2	3:C:273:TYR:HD1	2.15	0.64
8:H:21:ARG:HB3	8:H:65:ARG:NH2	2.12	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.97	0.64
1:A:41:ILE:HD12	1:A:41:ILE:H	1.63	0.64
2:B:162:ASN:HD22	2:B:244:ILE:HG22	1.62	0.64
2:B:209:LEU:HG	2:B:209:LEU:O	1.96	0.64
3:C:206:ASN:CB	3:C:313:ARG:HH21	2.08	0.64
1:A:417:ASP:OD1	1:A:438:ARG:NH2	2.30	0.64
2:B:378:PHE:O	2:B:382:VAL:HG23	1.98	0.64
3:C:8:HIS:CB	3:C:9:PRO:CD	2.75	0.64
3:C:78:ILE:HD11	5:E:57:GLN:HE22	1.63	0.64
7:G:34:ILE:CB	7:G:35:PRO:HD3	2.28	0.64
9:I:53:GLU:O	9:I:54:SER:C	2.37	0.64
9:I:64:LEU:HG	9:I:64:LEU:O	1.97	0.64
1:A:255:ILE:HD13	1:A:342:TRP:CH2	2.33	0.64
2:B:262:ALA:HB2	2:B:272:PHE:CE2	2.32	0.64
5:E:136:ILE:HG22	5:E:138:VAL:HG23	1.80	0.64
9:I:53:GLU:O	9:I:55:LEU:HG	1.98	0.64
1:A:173:ASN:O	1:A:174:VAL:C	2.37	0.64
2:B:124:LEU:O	2:B:128:THR:HB	1.98	0.64
2:B:262:ALA:HB3	2:B:269:ALA:HA	1.80	0.64
4:D:138:PRO:HD2	4:D:141:VAL:HG11	1.80	0.64
5:E:118:ARG:HE	5:E:171:ILE:HG13	1.63	0.64
7:G:54:ALA:O	7:G:58:VAL:HG23	1.98	0.64
10:J:9:LEU:HD12	10:J:13:LEU:HD12	1.80	0.64
1:A:80:GLU:O	1:A:83:GLY:N	2.31	0.63
4:D:115:TYR:HD2	4:D:119:ALA:HB2	1.63	0.63
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.78	0.63
6:F:13:LEU:HA	6:F:16:ILE:HD11	1.79	0.63
6:F:44:LYS:HA	6:F:44:LYS:NZ	2.12	0.63
6:F:101:ARG:HG2	6:F:105:GLU:OE2	1.98	0.63
1:A:334:MET:HA	1:A:334:MET:HE2	1.78	0.63
6:F:37:ILE:HD11	6:F:90:LEU:HD23	1.79	0.63
4:D:82:MET:CE	4:D:86:LYS:HD2	2.29	0.63
8:H:62:LEU:HA	8:H:65:ARG:HG2	1.80	0.63
9:I:64:LEU:HD12	9:I:65:VAL:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PHE:HZ	1:A:317:THR:HA	1.63	0.63
3:C:254:ASP:HB3	4:D:119:ALA:O	1.98	0.63
4:D:7:PRO:HB2	8:H:63:HIS:HE1	1.63	0.63
1:A:70:ARG:HB3	1:A:74:ALA:HB3	1.81	0.63
1:A:75:LEU:HD21	1:A:116:ILE:CG1	2.28	0.63
3:C:306:LEU:N	3:C:306:LEU:HD23	2.14	0.63
4:D:23:HIS:NE2	10:J:51:LEU:HA	2.14	0.63
9:I:70:LEU:CD2	9:I:73:PRO:HD2	2.28	0.63
1:A:240:GLN:NE2	1:A:431:LEU:CD2	2.61	0.63
2:B:180:ASP:HA	2:B:183:ILE:HD12	1.79	0.63
2:B:309:VAL:CG2	2:B:326:THR:HG22	2.28	0.63
3:C:47:THR:HG22	3:C:48:GLY:N	2.13	0.63
4:D:211:MET:HA	4:D:211:MET:CE	2.27	0.63
1:A:18:GLN:HE21	1:A:22:GLY:CA	2.00	0.63
2:B:129:ALA:N	2:B:130:PRO:CD	2.61	0.63
3:C:124:MET:HG2	3:C:274:PHE:HE1	1.63	0.63
3:C:298:ILE:HG22	3:C:299:LEU:HD23	1.81	0.63
4:D:3:LEU:HD22	7:G:70:LYS:NZ	2.13	0.63
4:D:34:LYS:O	4:D:34:LYS:HG2	1.99	0.63
3:C:27:ILE:O	3:C:27:ILE:HG22	1.99	0.62
1:A:36:THR:CB	1:A:372:THR:HG22	2.29	0.62
2:B:56:ARG:NE	2:B:103:GLU:OE1	2.16	0.62
3:C:88:SER:HA	3:C:272:TRP:HZ2	1.64	0.62
7:G:29:TYR:CD2	7:G:30:PHE:HD2	2.17	0.62
1:A:392:LEU:HA	1:A:395:TRP:HD1	1.53	0.62
4:D:75:ASN:ND2	4:D:80:MET:O	2.32	0.62
4:D:165:TYR:CD1	4:D:168:VAL:HG22	2.34	0.62
4:D:229:VAL:HG22	7:G:20:PRO:HD3	1.81	0.62
11:K:18:VAL:HB	11:K:19:PRO:HD3	1.81	0.62
1:A:334:MET:HA	1:A:334:MET:HE3	1.81	0.62
1:A:385:THR:CG2	1:A:386:TYR:CD1	2.82	0.62
2:B:264:ILE:HG21	2:B:317:SER:HA	1.81	0.62
2:B:292:THR:HG21	2:B:363:LYS:NZ	2.15	0.62
3:C:320:LEU:HB2	3:C:373:GLU:OE2	1.99	0.62
2:B:102:ARG:HH12	2:B:175:SER:HA	1.63	0.62
3:C:157:GLY:O	3:C:160:LEU:HB3	2.00	0.62
11:K:20:THR:HG23	11:K:24:TRP:CD1	2.35	0.62
1:A:188:ARG:O	1:A:191:LYS:HE2	1.99	0.62
1:A:262:TRP:CG	1:A:385:THR:HG23	2.34	0.62
3:C:327:ALA:O	3:C:331:ASP:N	2.29	0.62
5:E:117:LEU:CD1	5:E:120:PRO:HA	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:122:HIS:O	5:E:125:GLU:HG2	2.00	0.62
7:G:67:GLU:O	7:G:71:ARG:HB3	1.99	0.62
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.33	0.62
2:B:304:HIS:CD2	2:B:305:GLN:N	2.68	0.62
3:C:190:MET:O	3:C:194:MET:HG3	1.99	0.62
5:E:116:GLN:HA	5:E:116:GLN:HE21	1.65	0.62
1:A:159:GLN:HE22	7:G:18:LEU:HD21	1.65	0.61
4:D:126:TYR:OH	13:D:242:HEC:HBA2	2.00	0.61
5:E:29:SER:CB	5:E:32:ARG:HD3	2.30	0.61
1:A:134:ILE:N	1:A:134:ILE:CD1	2.62	0.61
3:C:90:PHE:CE1	3:C:123:VAL:HG11	2.35	0.61
6:F:57:ASP:O	6:F:61:ARG:HG2	2.00	0.61
6:F:91:GLU:O	6:F:95:LYS:HG3	1.98	0.61
1:A:61:HIS:CD2	1:A:134:ILE:CD1	2.81	0.61
1:A:91:THR:CG2	1:A:92:ARG:N	2.63	0.61
1:A:25:VAL:HG12	1:A:205:HIS:CE1	2.35	0.61
1:A:308:GLN:HG3	1:A:308:GLN:O	1.98	0.61
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.31	0.61
5:E:158:CYS:HB3	5:E:163:SER:HB2	1.83	0.61
1:A:385:THR:HB	1:A:386:TYR:CD1	2.35	0.61
2:B:247:GLN:NE2	2:B:429:ASN:HA	2.15	0.61
3:C:8:HIS:HB3	3:C:9:PRO:CD	2.31	0.61
4:D:176:PRO:HB2	4:D:181:GLN:HE22	1.64	0.61
6:F:96:GLU:OE1	6:F:99:ARG:HD2	2.00	0.61
8:H:21:ARG:CB	8:H:65:ARG:HH21	2.13	0.61
1:A:86:LEU:CD1	1:A:99:ILE:HG12	2.30	0.61
2:B:264:ILE:HG22	2:B:317:SER:HA	1.82	0.61
2:B:270:ASN:O	2:B:274:VAL:HG23	2.00	0.61
3:C:132:VAL:HA	3:C:139:SER:HB2	1.82	0.61
7:G:56:TYR:HD1	7:G:57:LEU:HD23	1.65	0.61
3:C:185:LEU:HB3	3:C:186:PRO:CD	2.27	0.61
4:D:11:PRO:HG2	8:H:74:PHE:CD1	2.35	0.61
4:D:48:TYR:OH	4:D:68:VAL:HG21	2.01	0.61
2:B:174:ASN:O	2:B:174:ASN:ND2	2.26	0.61
3:C:214:ASP:HA	3:C:217:LYS:HE2	1.82	0.61
3:C:234:LEU:HD23	4:D:216:LEU:HD21	1.82	0.61
3:C:269:LYS:HD3	3:C:340:GLY:HA2	1.81	0.61
1:A:4:TYR:O	1:A:7:ALA:HB3	2.00	0.61
1:A:317:THR:CG2	1:A:318:GLY:H	2.14	0.61
1:A:408:ARG:NH2	11:K:15:ARG:HE	1.99	0.61
3:C:40:CYS:HB3	3:C:90:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:SER:O	3:C:92:ILE:HG13	2.01	0.61
3:C:240:MET:O	3:C:244:LEU:HB2	2.01	0.61
4:D:72:ASP:O	4:D:73:GLY:O	2.19	0.61
4:D:76:GLU:O	4:D:76:GLU:HG2	2.01	0.61
4:D:178:THR:HB	4:D:181:GLN:CG	2.28	0.61
7:G:8:THR:CG2	7:G:9:ARG:H	2.03	0.61
3:C:41:LEU:O	3:C:45:ILE:HG13	2.01	0.61
4:D:34:LYS:HD3	4:D:35:GLN:NE2	2.15	0.61
5:E:147:ILE:O	5:E:156:TYR:HA	2.00	0.61
1:A:11:VAL:HG13	1:A:12:PRO:HD2	1.82	0.60
1:A:34:THR:HB	2:B:373:GLU:OE1	1.99	0.60
1:A:236:PHE:CD2	1:A:258:GLU:HB3	2.35	0.60
4:D:113:LEU:O	4:D:114:SER:C	2.39	0.60
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.16	0.60
1:A:106:LEU:HD21	1:A:203:LEU:HD13	1.83	0.60
2:B:275:LEU:HB2	2:B:410:VAL:HG13	1.83	0.60
5:E:34:GLY:CA	10:J:10:TYR:HD2	2.14	0.60
1:A:332:ASP:OD1	1:A:430:GLN:NE2	2.34	0.60
2:B:62:ASN:HD22	2:B:62:ASN:C	2.01	0.60
5:E:9:ASP:OD1	5:E:11:SER:OG	2.20	0.60
3:C:135:TRP:CE3	3:C:175:LEU:HD22	2.36	0.60
5:E:6:LYS:H	5:E:6:LYS:HD2	1.65	0.60
5:E:136:ILE:HD11	5:E:183:PRO:HG3	1.84	0.60
8:H:49:GLN:NE2	8:H:52:GLU:OE2	2.34	0.60
1:A:241:ILE:HD12	7:G:16:TYR:HE1	1.65	0.60
2:B:101:THR:HG23	2:B:103:GLU:H	1.67	0.60
2:B:328:SER:OG	2:B:333:ALA:HA	2.02	0.60
5:E:42:THR:O	5:E:45:VAL:N	2.34	0.60
5:E:141:HIS:CE1	5:E:142:LEU:HG	2.36	0.60
2:B:68:LEU:HD22	2:B:186:VAL:HB	1.84	0.60
2:B:304:HIS:CD2	2:B:305:GLN:H	2.19	0.60
5:E:172:ARG:NE	5:E:172:ARG:HA	2.15	0.60
1:A:51:LYS:HE2	1:A:177:LEU:HD12	1.83	0.60
1:A:163:LEU:HD21	1:A:314:TYR:CD2	2.37	0.60
3:C:296:PHE:CD1	3:C:359:PHE:HE1	2.20	0.60
4:D:27:ARG:NH2	4:D:60:GLU:OE2	2.35	0.60
4:D:51:LEU:HD22	4:D:58:GLU:HA	1.84	0.60
7:G:28:HIS:O	7:G:29:TYR:C	2.39	0.60
2:B:384:SER:CB	9:I:62:ARG:HG2	2.32	0.60
4:D:27:ARG:NH1	10:J:58:LYS:CE	2.64	0.60
5:E:29:SER:CA	5:E:32:ARG:HD3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:ILE:CD1	5:E:183:PRO:HG3	2.31	0.60
1:A:106:LEU:N	1:A:107:PRO:HD2	2.17	0.60
1:A:385:THR:HG22	1:A:386:TYR:N	2.16	0.60
2:B:174:ASN:C	2:B:174:ASN:HD22	1.96	0.60
3:C:329:VAL:O	3:C:332:LEU:HB2	2.01	0.60
5:E:77:LYS:CE	5:E:98:VAL:HG21	2.32	0.60
1:A:91:THR:HG23	1:A:92:ARG:H	1.66	0.60
1:A:198:ALA:CB	1:A:379:ILE:HG22	2.32	0.60
1:A:390:ILE:N	1:A:391:PRO:HD3	2.17	0.60
2:B:262:ALA:HB3	2:B:269:ALA:N	2.17	0.60
4:D:72:ASP:OD1	4:D:76:GLU:OE1	2.20	0.60
5:E:123:ASP:HB2	5:E:170:ARG:NH2	2.16	0.60
4:D:161:ALA:HB1	4:D:162:PRO:HD2	1.84	0.59
5:E:77:LYS:CD	5:E:98:VAL:HG21	2.32	0.59
1:A:143:THR:HG23	1:A:143:THR:O	2.02	0.59
2:B:169:ARG:NH1	2:B:238:LYS:NZ	2.47	0.59
3:C:44:GLN:OE1	3:C:44:GLN:HA	2.01	0.59
4:D:178:THR:CB	4:D:181:GLN:HE21	2.15	0.59
1:A:142:ASP:OD2	5:E:1:SER:HB2	2.02	0.59
1:A:151:ASN:HD22	5:E:2:HIS:CD2	2.20	0.59
2:B:299:VAL:O	2:B:303:VAL:HG23	2.03	0.59
4:D:50:HIS:O	4:D:51:LEU:C	2.40	0.59
4:D:117:VAL:HG13	4:D:124:GLU:H	1.64	0.59
6:F:88:SER:HB3	6:F:91:GLU:CD	2.22	0.59
1:A:6:GLN:O	1:A:7:ALA:C	2.40	0.59
1:A:106:LEU:O	1:A:107:PRO:C	2.40	0.59
1:A:442:PHE:O	1:A:443:TRP:CD1	2.56	0.59
1:A:379:ILE:HD12	1:A:390:ILE:CD1	2.32	0.59
2:B:109:VAL:HG22	2:B:119:LEU:HD21	1.84	0.59
2:B:279:LEU:HD23	2:B:294:SER:HB3	1.84	0.59
3:C:177:ARG:O	3:C:181:PHE:HD2	1.85	0.59
5:E:122:HIS:O	5:E:123:ASP:C	2.40	0.59
5:E:161:HIS:HB2	14:E:197:FES:S1	2.42	0.59
1:A:328:HIS:NE2	1:A:329:MET:HG2	2.17	0.59
1:A:373:THR:N	1:A:374:PRO:HD2	2.17	0.59
3:C:44:GLN:OE1	3:C:83:HIS:ND1	2.35	0.59
4:D:27:ARG:NH1	10:J:58:LYS:HZ1	1.92	0.59
5:E:77:LYS:HG3	5:E:193:VAL:HG13	1.83	0.59
8:H:22:GLU:O	8:H:25:GLU:HG2	2.02	0.59
3:C:41:LEU:CD1	12:C:380:HEM:HBB1	2.33	0.59
5:E:33:LYS:HA	7:G:21:PHE:CE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:SER:N	1:A:52:ASN:OD1	2.34	0.59
1:A:171:SER:O	1:A:174:VAL:HB	2.02	0.59
2:B:266:SER:O	2:B:269:ALA:HB3	2.03	0.59
2:B:322:PHE:CD1	2:B:322:PHE:C	2.76	0.59
3:C:170:VAL:HG12	3:C:170:VAL:O	2.01	0.59
5:E:119:ASP:OD1	5:E:178:LEU:HA	2.02	0.59
2:B:182:ARG:HH11	2:B:185:LYS:HE2	1.64	0.59
7:G:33:GLY:O	7:G:34:ILE:C	2.41	0.59
1:A:166:SER:HB3	5:E:3:THR:HG22	1.84	0.59
1:A:428:ILE:CG2	1:A:431:LEU:HB3	2.33	0.59
2:B:207:ILE:HD11	2:B:383:GLY:HA2	1.85	0.59
3:C:292:LEU:N	3:C:292:LEU:HD23	2.17	0.59
4:D:28:ARG:NH1	8:H:78:LYS:OXT	2.35	0.59
5:E:147:ILE:H	5:E:157:TYR:H	1.48	0.59
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.84	0.58
1:A:255:ILE:HD13	1:A:342:TRP:CZ3	2.38	0.58
1:A:136:GLN:HE21	9:I:50:LEU:HB3	1.68	0.58
1:A:252:HIS:CD2	1:A:325:VAL:HG22	2.38	0.58
1:A:444:LEU:O	1:A:445:ARG:HG3	2.03	0.58
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.85	0.58
2:B:303:VAL:CG1	2:B:304:HIS:N	2.66	0.58
4:D:5:LEU:CD1	8:H:59:LEU:HB3	2.33	0.58
5:E:67:ASP:OD1	5:E:68:VAL:N	2.36	0.58
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.39	0.58
2:B:95:LYS:NZ	9:I:70:LEU:HD22	2.17	0.58
1:A:373:THR:N	1:A:374:PRO:CD	2.66	0.58
12:C:381:HEM:O2A	12:C:381:HEM:HHA	2.02	0.58
6:F:55:TYR:C	6:F:55:TYR:CD1	2.77	0.58
9:I:58:GLN:HG2	9:I:78:TYR:HD2	1.66	0.58
2:B:175:SER:OG	2:B:176:LEU:N	2.35	0.58
3:C:246:ALA:N	3:C:247:PRO:CD	2.67	0.58
3:C:361:LEU:HD23	3:C:365:LEU:HD12	1.84	0.58
4:D:119:ALA:O	4:D:120:ARG:C	2.40	0.58
8:H:65:ARG:HG3	8:H:66:ASP:N	2.17	0.58
1:A:11:VAL:CG1	1:A:12:PRO:HD2	2.32	0.58
1:A:73:ASN:ND2	1:A:73:ASN:N	2.52	0.58
1:A:385:THR:HB	1:A:386:TYR:HD1	1.68	0.58
2:B:97:SER:OG	9:I:70:LEU:HB2	2.02	0.58
2:B:132:PHE:HB3	2:B:137:VAL:HG21	1.85	0.58
2:B:147:ASP:O	2:B:150:VAL:HG22	2.04	0.58
2:B:203:ARG:HE	2:B:230:LEU:HD23	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:HIS:CG	2:B:305:GLN:H	2.21	0.58
3:C:27:ILE:O	3:C:27:ILE:CG2	2.51	0.58
10:J:49:GLY:HA2	10:J:54:HIS:CB	2.33	0.58
1:A:389:ARG:C	1:A:391:PRO:HD3	2.23	0.58
2:B:24:LEU:HG	2:B:38:LEU:HD11	1.86	0.58
2:B:304:HIS:CG	2:B:305:GLN:N	2.71	0.58
2:B:395:PRO:O	2:B:398:VAL:HB	2.04	0.58
4:D:187:CYS:O	4:D:190:LEU:N	2.36	0.58
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.04	0.58
9:I:58:GLN:HA	9:I:78:TYR:CD2	2.38	0.58
2:B:182:ARG:NH1	2:B:185:LYS:HG2	2.18	0.58
2:B:203:ARG:HH21	2:B:230:LEU:HA	1.69	0.58
2:B:212:SER:OG	2:B:215:VAL:HB	2.03	0.58
2:B:247:GLN:HE22	2:B:429:ASN:ND2	2.00	0.58
4:D:72:ASP:OD2	4:D:92:PRO:HB2	2.03	0.58
4:D:76:GLU:O	4:D:76:GLU:CG	2.52	0.58
2:B:206:LEU:O	2:B:207:ILE:HD13	2.04	0.58
2:B:300:ALA:HB2	2:B:307:PHE:HZ	1.69	0.58
8:H:37:LEU:HD21	8:H:58:LEU:HA	1.84	0.58
1:A:3:THR:HG23	2:B:114:ASP:OD1	2.03	0.57
1:A:333:ASP:O	1:A:337:VAL:HG23	2.04	0.57
8:H:15:ASP:HB2	8:H:16:PRO:CD	2.33	0.57
2:B:99:THR:CG2	2:B:100:SER:N	2.67	0.57
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.39	0.57
5:E:185:TYR:HB3	5:E:195:VAL:HA	1.86	0.57
1:A:46:ARG:HG2	1:A:46:ARG:O	2.02	0.57
2:B:58:GLU:OE1	2:B:63:LEU:HA	2.04	0.57
3:C:85:ASN:OD1	3:C:243:VAL:HG23	2.04	0.57
3:C:103:TYR:OH	3:C:322:GLN:HG3	2.04	0.57
3:C:153:ILE:CG2	3:C:156:ILE:HG12	2.34	0.57
3:C:272:TRP:NE1	3:C:273:TYR:HD1	2.02	0.57
1:A:335:MET:HE3	1:A:338:LEU:HD23	1.86	0.57
2:B:35:ILE:HB	2:B:206:LEU:HB3	1.84	0.57
2:B:279:LEU:HD22	2:B:295:LEU:CD1	2.26	0.57
3:C:181:PHE:O	3:C:185:LEU:HB2	2.04	0.57
4:D:6:HIS:N	4:D:7:PRO:HD2	2.19	0.57
1:A:428:ILE:CG2	1:A:431:LEU:CB	2.80	0.57
3:C:264:THR:O	3:C:266:PRO:CD	2.50	0.57
3:C:313:ARG:HB3	6:F:38:HIS:CD2	2.40	0.57
4:D:3:LEU:HD11	7:G:71:ARG:HB2	1.85	0.57
5:E:23:LYS:HG3	5:E:24:SER:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:59:VAL:O	5:E:59:VAL:HG12	2.04	0.57
7:G:3:GLN:HA	7:G:3:GLN:OE1	2.04	0.57
7:G:64:GLN:O	7:G:65:GLU:C	2.41	0.57
9:I:64:LEU:CG	9:I:65:VAL:HG23	2.35	0.57
11:K:23:LEU:HD23	11:K:23:LEU:N	2.19	0.57
2:B:318:ASP:OD1	2:B:318:ASP:N	2.38	0.57
2:B:412:ASN:O	2:B:415:LYS:HB2	2.05	0.57
1:A:76:GLU:HA	1:A:79:VAL:HG23	1.86	0.57
2:B:62:ASN:O	2:B:62:ASN:ND2	2.36	0.57
5:E:175:PRO:O	5:E:176:ALA:C	2.42	0.57
2:B:166:ALA:HB2	2:B:244:ILE:HD12	1.86	0.57
2:B:239:TYR:OH	2:B:421:ARG:O	2.17	0.57
4:D:23:HIS:CD2	10:J:52:TRP:N	2.73	0.57
4:D:222:MET:HE2	5:E:43:THR:HG21	1.87	0.57
1:A:224:ASP:OD1	1:A:227:ALA:CB	2.52	0.57
1:A:274:ASN:HD21	1:A:320:LEU:HD11	1.69	0.57
1:A:308:GLN:O	1:A:308:GLN:CG	2.52	0.57
3:C:170:VAL:HG13	3:C:174:THR:CG2	2.32	0.57
4:D:6:HIS:CG	4:D:7:PRO:HD3	2.39	0.57
4:D:23:HIS:CD2	10:J:52:TRP:H	2.23	0.57
2:B:262:ALA:HB3	2:B:269:ALA:CA	2.35	0.57
3:C:19:ILE:HG22	3:C:20:ASP:OD1	2.05	0.57
5:E:114:VAL:HA	5:E:117:LEU:HD11	1.86	0.57
1:A:53:ASN:CG	1:A:165:GLN:HB2	2.25	0.56
1:A:431:LEU:O	1:A:432:PRO:O	2.22	0.56
1:A:442:PHE:O	1:A:443:TRP:HD1	1.88	0.56
12:C:380:HEM:O2D	12:C:380:HEM:HBA2	2.04	0.56
4:D:182:VAL:O	4:D:186:VAL:HG23	2.04	0.56
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.35	0.56
2:B:257:LEU:HD13	2:B:424:MET:HE2	1.87	0.56
3:C:218:ILE:HG23	3:C:223:TYR:CD2	2.40	0.56
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.40	0.56
8:H:34:ARG:O	8:H:38:GLU:HG2	2.04	0.56
2:B:49:LEU:HD11	2:B:204:MET:HB3	1.87	0.56
2:B:362:ASN:HA	2:B:365:LYS:HD2	1.87	0.56
3:C:104:TYR:CE1	3:C:208:PRO:HA	2.40	0.56
3:C:215:VAL:HG11	6:F:59:VAL:CG1	2.34	0.56
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.87	0.56
4:D:43:MET:HE3	4:D:91:PHE:CD2	2.40	0.56
4:D:131:LEU:HD13	4:D:164:ILE:CD1	2.36	0.56
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:55:ILE:CG2	10:J:58:LYS:HE2	2.34	0.56
1:A:236:PHE:CZ	1:A:317:THR:HA	2.40	0.56
2:B:71:LEU:HD13	2:B:143:GLN:HG3	1.87	0.56
3:C:51:LEU:O	3:C:53:MET:N	2.38	0.56
1:A:46:ARG:O	1:A:46:ARG:CG	2.53	0.56
1:A:351:GLU:OE2	1:A:404:ALA:CB	2.52	0.56
4:D:49:ARG:HG3	4:D:49:ARG:O	2.06	0.56
5:E:127:VAL:HG12	5:E:133:VAL:HA	1.87	0.56
7:G:68:LYS:HD3	7:G:72:LYS:NZ	2.19	0.56
1:A:262:TRP:CE3	1:A:385:THR:CG2	2.87	0.56
3:C:51:LEU:HD13	12:C:380:HEM:O1D	2.05	0.56
5:E:29:SER:OG	5:E:32:ARG:HD3	2.05	0.56
1:A:166:SER:O	1:A:167:VAL:C	2.43	0.56
1:A:343:MET:HE1	1:A:441:MET:O	2.06	0.56
1:A:351:GLU:OE2	1:A:403:ASP:OD1	2.23	0.56
1:A:18:GLN:HG2	1:A:19:LEU:O	2.06	0.56
1:A:39:VAL:CG1	1:A:41:ILE:HD11	2.36	0.56
1:A:77:LYS:HG2	2:B:291:ALA:CB	2.36	0.56
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.40	0.56
2:B:213:HIS:N	2:B:214:PRO:CD	2.69	0.56
2:B:375:SER:OG	2:B:376:GLU:N	2.38	0.56
3:C:25:SER:CA	3:C:218:ILE:HD12	2.35	0.56
3:C:130:GLY:HA3	3:C:182:HIS:CE1	2.41	0.56
3:C:307:LEU:HD13	3:C:362:ILE:O	2.06	0.56
3:C:343:VAL:O	3:C:348:ILE:HD11	2.05	0.56
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.41	0.56
6:F:55:TYR:O	6:F:59:VAL:HG23	2.06	0.56
1:A:4:TYR:CE2	1:A:396:GLU:HG3	2.39	0.56
3:C:124:MET:CE	3:C:298:ILE:HD13	2.35	0.56
3:C:78:ILE:O	3:C:79:ILE:C	2.43	0.56
3:C:135:TRP:CH2	3:C:170:VAL:HG12	2.40	0.56
4:D:5:LEU:HD23	4:D:152:TYR:CE1	2.41	0.56
4:D:228:SER:HB2	7:G:23:GLN:HE22	1.70	0.56
5:E:91:TRP:HZ3	5:E:136:ILE:HD11	1.69	0.56
10:J:17:THR:HA	10:J:20:PHE:HB3	1.87	0.56
2:B:25:GLU:HB3	2:B:213:HIS:ND1	2.20	0.55
5:E:117:LEU:HB2	5:E:120:PRO:HA	1.88	0.55
9:I:70:LEU:HD21	9:I:73:PRO:HD2	1.88	0.55
1:A:39:VAL:HG23	1:A:113:LEU:CD2	2.33	0.55
1:A:54:GLY:HA3	1:A:169:GLY:HA3	1.86	0.55
1:A:322:ALA:HB3	1:A:338:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:7:SER:HA	6:F:11:ARG:HE	1.71	0.55
10:J:21:ALA:O	10:J:22:LEU:C	2.43	0.55
2:B:33:LEU:HD23	2:B:33:LEU:H	1.70	0.55
1:A:279:HIS:ND1	1:A:284:TYR:OH	2.38	0.55
3:C:25:SER:HA	3:C:218:ILE:CD1	2.37	0.55
3:C:259:ALA:O	3:C:261:PRO:HD3	2.06	0.55
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.89	0.55
5:E:168:SER:HB3	5:E:170:ARG:HH21	1.72	0.55
2:B:148:LYS:HG3	2:B:177:TYR:HB3	1.89	0.55
2:B:332:SER:O	2:B:333:ALA:C	2.45	0.55
3:C:270:PRO:CB	3:C:274:PHE:HB2	2.32	0.55
1:A:243:HIS:CD2	1:A:425:PHE:HE1	2.24	0.55
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.88	0.55
3:C:313:ARG:HG3	3:C:313:ARG:O	2.05	0.55
4:D:206:LEU:C	4:D:206:LEU:HD22	2.27	0.55
5:E:69:LEU:O	5:E:70:ALA:C	2.45	0.55
1:A:131:ARG:NH2	1:A:177:LEU:O	2.39	0.55
1:A:262:TRP:CE3	1:A:385:THR:HG23	2.42	0.55
2:B:140:LEU:O	2:B:141:GLN:C	2.44	0.55
4:D:165:TYR:CG	4:D:168:VAL:HG22	2.41	0.55
5:E:95:PRO:HD2	5:E:138:VAL:HG22	1.88	0.55
6:F:88:SER:HB3	6:F:91:GLU:CG	2.36	0.55
10:J:32:GLU:HG2	10:J:33:ARG:N	2.20	0.55
1:A:170:PRO:O	1:A:171:SER:C	2.45	0.55
1:A:224:ASP:O	1:A:227:ALA:N	2.40	0.55
1:A:429:GLU:HG3	1:A:429:GLU:O	2.06	0.55
2:B:162:ASN:HD22	2:B:244:ILE:HG21	1.70	0.55
2:B:345:LYS:HD3	2:B:418:VAL:CG1	2.37	0.55
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.42	0.55
1:A:213:GLN:CB	1:A:215:HIS:CD2	2.90	0.55
2:B:304:HIS:CD2	2:B:306:PRO:CD	2.73	0.55
2:B:348:ALA:CB	2:B:415:LYS:HA	2.36	0.55
5:E:53:ASN:N	5:E:53:ASN:OD1	2.40	0.55
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.88	0.55
1:A:276:ILE:HD11	1:A:354:VAL:HA	1.88	0.55
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.07	0.55
7:G:73:ASN:H	7:G:74:PRO:HD2	1.69	0.55
2:B:342:ASN:O	2:B:345:LYS:HB2	2.07	0.54
3:C:338:ILE:HD13	3:C:338:ILE:N	2.22	0.54
4:D:138:PRO:O	4:D:139:THR:C	2.45	0.54
1:A:163:LEU:HD21	1:A:314:TYR:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:VAL:CG1	2:B:303:VAL:HG21	2.37	0.54
4:D:153:PHE:CD2	4:D:158:ILE:HD12	2.43	0.54
1:A:240:GLN:HE21	1:A:431:LEU:HD21	1.70	0.54
1:A:243:HIS:CD2	1:A:425:PHE:CD1	2.94	0.54
2:B:203:ARG:CZ	2:B:230:LEU:HD23	2.37	0.54
4:D:69:GLU:O	4:D:73:GLY:HA3	2.08	0.54
4:D:211:MET:SD	5:E:49:TYR:HD2	2.29	0.54
7:G:68:LYS:O	7:G:72:LYS:N	2.31	0.54
1:A:74:ALA:O	1:A:75:LEU:C	2.45	0.54
3:C:26:ASN:HB2	6:F:69:SER:OG	2.08	0.54
3:C:33:PHE:CE1	3:C:96:MET:HG3	2.42	0.54
4:D:3:LEU:HD22	7:G:70:LYS:HZ3	1.72	0.54
2:B:204:MET:HE3	2:B:224:LEU:HD13	1.89	0.54
2:B:357:VAL:O	2:B:361:LYS:HG3	2.07	0.54
3:C:24:PRO:O	3:C:224:TYR:OH	2.13	0.54
3:C:107:TYR:HB3	3:C:113:TRP:CE3	2.43	0.54
4:D:2:ASP:HB3	4:D:156:GLN:NE2	2.22	0.54
1:A:46:ARG:HH12	1:A:315:ALA:HB3	1.73	0.54
1:A:291:SER:HA	2:B:87:ARG:NH1	2.22	0.54
2:B:169:ARG:HH11	2:B:238:LYS:HZ1	1.49	0.54
3:C:263:ASN:OD1	3:C:264:THR:N	2.33	0.54
4:D:56:TYR:HD1	4:D:60:GLU:CD	2.10	0.54
4:D:178:THR:HG21	8:H:16:PRO:HG2	1.90	0.54
1:A:128:GLU:OE2	1:A:131:ARG:NH1	2.40	0.54
1:A:223:TYR:CE2	1:A:224:ASP:HB3	2.42	0.54
1:A:281:ASP:OD1	1:A:282:CYS:N	2.40	0.54
1:A:386:TYR:CD1	1:A:386:TYR:N	2.75	0.54
1:A:406:VAL:O	1:A:410:VAL:HG23	2.08	0.54
2:B:299:VAL:HG13	2:B:303:VAL:HG21	1.89	0.54
3:C:269:LYS:NZ	3:C:340:GLY:CA	2.70	0.54
3:C:328:LEU:HB2	3:C:361:LEU:HD13	1.89	0.54
4:D:123:GLY:O	4:D:125:ASP:N	2.41	0.54
5:E:33:LYS:HA	7:G:21:PHE:CD2	2.43	0.54
1:A:162:PRO:O	1:A:165:GLN:NE2	2.41	0.54
1:A:414:TYR:O	1:A:418:GLN:HG3	2.08	0.54
2:B:168:TYR:CD1	2:B:238:LYS:O	2.60	0.54
2:B:338:LYS:CG	2:B:439:LEU:HD21	2.36	0.54
3:C:91:PHE:HB2	3:C:272:TRP:CZ2	2.43	0.54
4:D:5:LEU:C	4:D:7:PRO:HD2	2.28	0.54
4:D:82:MET:SD	4:D:86:LYS:HE3	2.47	0.54
5:E:155:GLY:HA3	5:E:165:TYR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:28:HIS:HD2	7:G:31:SER:H	1.55	0.54
7:G:33:GLY:O	7:G:36:ASN:N	2.40	0.54
4:D:6:HIS:N	4:D:7:PRO:CD	2.71	0.54
4:D:143:LEU:HD22	4:D:147:LEU:O	2.07	0.54
1:A:86:LEU:HD13	1:A:99:ILE:HD13	1.90	0.54
1:A:261:GLY:HA2	1:A:314:TYR:O	2.08	0.54
2:B:183:ILE:O	2:B:186:VAL:HG23	2.08	0.54
3:C:108:THR:O	3:C:110:LEU:N	2.40	0.54
3:C:122:THR:CG2	3:C:185:LEU:HD11	2.38	0.54
3:C:210:GLY:HA3	3:C:314:SER:CB	2.32	0.54
5:E:23:LYS:HG3	5:E:24:SER:N	2.22	0.54
8:H:16:PRO:O	8:H:20:VAL:HG23	2.08	0.54
1:A:5:ALA:O	1:A:8:LEU:HB2	2.08	0.53
1:A:106:LEU:CD2	1:A:203:LEU:HD22	2.35	0.53
1:A:347:THR:HA	11:K:16:ASN:HD22	1.73	0.53
6:F:73:GLN:NE2	7:G:32:LYS:NZ	2.55	0.53
6:F:87:LYS:HE2	6:F:89:TYR:HB3	1.90	0.53
2:B:95:LYS:HG2	2:B:96:LEU:N	2.21	0.53
3:C:355:SER:O	3:C:356:VAL:C	2.43	0.53
4:D:102:ARG:HG2	4:D:108:ALA:O	2.07	0.53
5:E:112:VAL:CG1	5:E:117:LEU:HD21	2.39	0.53
7:G:34:ILE:HB	7:G:35:PRO:CD	2.36	0.53
2:B:393:THR:HG22	2:B:394:PRO:O	2.09	0.53
3:C:107:TYR:C	3:C:107:TYR:CD1	2.81	0.53
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.73	0.53
4:D:128:PHE:HB2	4:D:187:CYS:SG	2.48	0.53
5:E:34:GLY:HA2	10:J:10:TYR:HD2	1.71	0.53
5:E:45:VAL:HG23	10:J:24:ILE:HG23	1.90	0.53
5:E:121:GLN:HG2	5:E:125:GLU:OE2	2.08	0.53
6:F:106:GLU:OE1	6:F:109:LYS:HE2	2.09	0.53
1:A:27:SER:HB3	1:A:208:LEU:HD22	1.90	0.53
1:A:51:LYS:O	1:A:53:ASN:N	2.42	0.53
2:B:213:HIS:O	2:B:213:HIS:HD2	1.90	0.53
4:D:118:ARG:HG3	4:D:194:ALA:HB1	1.91	0.53
5:E:137:GLY:O	5:E:145:VAL:HG22	2.08	0.53
7:G:68:LYS:O	7:G:69:SER:C	2.46	0.53
1:A:29:GLN:HG3	1:A:203:LEU:O	2.09	0.53
1:A:429:GLU:OE2	7:G:4:PHE:O	2.26	0.53
2:B:38:LEU:CD1	2:B:378:PHE:CE2	2.92	0.53
3:C:177:ARG:O	3:C:181:PHE:CD2	2.61	0.53
3:C:309:THR:HG21	3:C:370:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:TYR:O	5:E:159:PRO:HD3	2.08	0.53
9:I:72:VAL:CB	9:I:73:PRO:CD	2.78	0.53
3:C:300:ILE:HD13	3:C:362:ILE:CG2	2.39	0.53
5:E:15:ARG:CB	5:E:16:PRO:HD2	2.38	0.53
5:E:191:ASP:N	5:E:191:ASP:OD1	2.41	0.53
7:G:56:TYR:CD1	7:G:57:LEU:HD23	2.43	0.53
1:A:48:GLU:OE1	1:A:52:ASN:O	2.27	0.53
2:B:59:ASN:O	2:B:63:LEU:HG	2.09	0.53
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.91	0.53
3:C:91:PHE:CB	3:C:272:TRP:CH2	2.92	0.53
5:E:91:TRP:NE1	5:E:92:ARG:HG3	2.23	0.53
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.44	0.53
1:A:156:THR:HG23	1:A:239:SER:OG	2.08	0.53
1:A:227:ALA:O	1:A:229:PRO:HD3	2.09	0.53
12:C:380:HEM:CMC	12:C:380:HEM:HBC2	2.39	0.53
4:D:233:ARG:HG2	7:G:17:SER:CB	2.20	0.53
1:A:78:GLU:HG2	1:A:112:LEU:HD21	1.91	0.53
2:B:177:TYR:O	2:B:178:CYS:C	2.47	0.53
2:B:248:ASN:CB	2:B:428:GLY:HA2	2.31	0.53
6:F:73:GLN:HA	7:G:39:ARG:NH2	2.21	0.53
7:G:29:TYR:HD2	7:G:30:PHE:HD2	1.46	0.53
8:H:55:THR:O	8:H:56:GLU:C	2.46	0.53
1:A:159:GLN:HE22	7:G:18:LEU:CD2	2.22	0.52
2:B:135:TRP:NE1	2:B:136:GLU:HG3	2.24	0.52
2:B:379:LEU:HG	2:B:379:LEU:O	2.09	0.52
4:D:176:PRO:HB2	4:D:181:GLN:NE2	2.24	0.52
5:E:6:LYS:HD2	5:E:6:LYS:N	2.24	0.52
3:C:65:SER:OG	3:C:66:VAL:N	2.42	0.52
4:D:98:PRO:O	4:D:101:ALA:HB3	2.10	0.52
10:J:49:GLY:HA2	10:J:54:HIS:HB3	1.90	0.52
1:A:174:VAL:HG12	1:A:175:ARG:N	2.19	0.52
1:A:240:GLN:HE22	1:A:431:LEU:CD2	2.21	0.52
1:A:371:GLY:O	1:A:375:VAL:HG22	2.09	0.52
1:A:391:PRO:HB2	1:A:395:TRP:CZ2	2.44	0.52
3:C:37:LEU:HD23	3:C:93:CYS:HB3	1.91	0.52
5:E:191:ASP:OD1	5:E:192:MET:HG2	2.10	0.52
10:J:32:GLU:HG2	10:J:33:ARG:H	1.74	0.52
1:A:157:ALA:HB1	1:A:319:LEU:HD21	1.92	0.52
2:B:187:THR:O	2:B:190:GLU:HB2	2.08	0.52
2:B:303:VAL:CG1	2:B:307:PHE:CD2	2.92	0.52
8:H:66:ASP:O	8:H:67:HIS:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:OG	1:A:172:GLU:N	2.41	0.52
2:B:67:HIS:CD2	2:B:144:LEU:HD22	2.37	0.52
2:B:300:ALA:CB	2:B:307:PHE:HZ	2.22	0.52
3:C:47:THR:HG23	3:C:83:HIS:HB2	1.92	0.52
3:C:121:LEU:HD23	3:C:124:MET:CE	2.39	0.52
12:C:380:HEM:HBC2	12:C:380:HEM:HMC1	1.92	0.52
1:A:158:PHE:CZ	1:A:317:THR:HG21	2.38	0.52
1:A:180:ALA:O	1:A:183:THR:HB	2.10	0.52
1:A:350:THR:HB	1:A:353:GLU:CG	2.39	0.52
2:B:352:LEU:HD21	2:B:357:VAL:HG23	1.90	0.52
3:C:207:ASN:ND2	3:C:210:GLY:H	2.07	0.52
4:D:46:VAL:HG12	4:D:47:ALA:O	2.10	0.52
2:B:174:ASN:ND2	2:B:174:ASN:C	2.63	0.52
2:B:408:ALA:HA	2:B:411:ILE:HG13	1.92	0.52
3:C:223:TYR:HB3	4:D:227:TRP:CE2	2.45	0.52
4:D:6:HIS:O	4:D:8:PRO:HD2	2.10	0.52
4:D:137:PRO:HG3	4:D:143:LEU:HD11	1.92	0.52
10:J:32:GLU:CG	10:J:33:ARG:N	2.73	0.52
1:A:21:ASN:CB	1:A:217:SER:CB	2.64	0.52
2:B:169:ARG:HD3	2:B:238:LYS:NZ	2.22	0.52
4:D:10:TYR:CB	4:D:125:ASP:OD1	2.54	0.52
1:A:50:GLU:O	1:A:173:ASN:ND2	2.42	0.52
2:B:56:ARG:HH21	2:B:103:GLU:CD	2.14	0.52
2:B:196:GLN:HG2	2:B:197:ASN:OD1	2.09	0.52
2:B:262:ALA:HB2	2:B:268:GLU:HB3	1.92	0.52
4:D:239:PRO:HB2	4:D:241:LYS:HB3	1.92	0.52
1:A:75:LEU:CD2	1:A:116:ILE:HD11	2.35	0.52
1:A:91:THR:CG2	1:A:92:ARG:H	2.23	0.52
1:A:270:LEU:O	1:A:273:ALA:N	2.43	0.52
2:B:68:LEU:HB2	2:B:144:LEU:HD21	1.91	0.52
4:D:23:HIS:CD2	10:J:50:LYS:O	2.63	0.52
4:D:228:SER:HB2	7:G:23:GLN:HE21	1.74	0.52
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.92	0.52
3:C:269:LYS:NZ	3:C:340:GLY:HA3	2.24	0.51
7:G:18:LEU:HB2	7:G:23:GLN:OE1	2.09	0.51
8:H:27:LEU:O	8:H:30:CYS:N	2.36	0.51
2:B:24:LEU:H	2:B:24:LEU:CD1	1.98	0.51
2:B:192:HIS:O	2:B:193:ASP:C	2.49	0.51
3:C:243:VAL:HG12	3:C:244:LEU:N	2.25	0.51
3:C:310:SER:HB3	3:C:318:ARG:HH11	1.72	0.51
3:C:338:ILE:HA	3:C:341:GLN:HG2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:5:LEU:HD13	8:H:59:LEU:HB3	1.92	0.51
4:D:220:TYR:O	4:D:224:ARG:HG2	2.09	0.51
1:A:381:ARG:HA	1:A:384:LEU:HD12	1.92	0.51
1:A:428:ILE:O	1:A:431:LEU:N	2.39	0.51
2:B:197:ASN:HB2	2:B:198:HIS:CD2	2.45	0.51
2:B:354:ASN:N	2:B:355:PRO:HD2	2.25	0.51
4:D:76:GLU:OE2	4:D:93:LYS:O	2.28	0.51
6:F:7:SER:O	6:F:11:ARG:HB2	2.11	0.51
6:F:32:MET:O	6:F:33:ARG:C	2.49	0.51
7:G:39:ARG:HA	7:G:42:ARG:HD2	1.92	0.51
10:J:43:TYR:O	10:J:46:ILE:HG13	2.10	0.51
1:A:239:SER:HB2	7:G:18:LEU:HD23	1.92	0.51
2:B:46:ARG:HH12	2:B:376:GLU:HG3	1.75	0.51
4:D:11:PRO:CD	8:H:70:ALA:HB1	2.39	0.51
9:I:76:VAL:O	9:I:76:VAL:CG1	2.58	0.51
10:J:9:LEU:HD12	10:J:13:LEU:CD1	2.40	0.51
1:A:48:GLU:OE1	1:A:53:ASN:O	2.28	0.51
4:D:120:ARG:HH11	4:D:120:ARG:CG	2.24	0.51
4:D:127:VAL:HG12	4:D:187:CYS:SG	2.50	0.51
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.26	0.51
5:E:94:LYS:HB3	5:E:95:PRO:CD	2.41	0.51
1:A:51:LYS:HE2	1:A:177:LEU:CD1	2.41	0.51
3:C:91:PHE:HB3	3:C:272:TRP:CH2	2.46	0.51
3:C:172:LYS:O	3:C:173:ALA:C	2.47	0.51
4:D:79:GLU:O	4:D:80:MET:C	2.48	0.51
4:D:138:PRO:O	4:D:141:VAL:HB	2.11	0.51
4:D:161:ALA:O	4:D:163:PRO:CD	2.59	0.51
1:A:124:ASP:O	1:A:128:GLU:HG2	2.11	0.51
1:A:192:ALA:HB2	1:A:195:MET:HB2	1.92	0.51
1:A:408:ARG:HH22	11:K:15:ARG:HE	1.59	0.51
2:B:58:GLU:HB3	2:B:62:ASN:HB3	1.92	0.51
2:B:257:LEU:HD13	2:B:424:MET:CE	2.41	0.51
3:C:153:ILE:HG21	3:C:156:ILE:HD11	1.91	0.51
3:C:186:PRO:HA	3:C:189:ILE:HG13	1.93	0.51
4:D:106:ASN:HD22	4:D:106:ASN:C	2.14	0.51
6:F:87:LYS:HG3	6:F:89:TYR:HB3	1.91	0.51
1:A:327:ASP:OD1	1:A:328:HIS:N	2.43	0.51
1:A:390:ILE:N	1:A:391:PRO:CD	2.74	0.51
3:C:341:GLN:HA	3:C:341:GLN:NE2	2.25	0.51
4:D:4:GLU:HG3	4:D:6:HIS:ND1	2.26	0.51
4:D:46:VAL:HG11	4:D:91:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:PRO:HA	1:A:316:ASP:HB3	1.92	0.51
2:B:47:ILE:HB	2:B:109:VAL:HG12	1.93	0.51
3:C:119:LEU:HG	12:C:381:HEM:CAB	2.40	0.51
3:C:250:LEU:O	3:C:252:ASP:N	2.44	0.51
3:C:328:LEU:HG	3:C:332:LEU:HD12	1.93	0.51
4:D:27:ARG:NH1	10:J:58:LYS:HE3	2.25	0.51
5:E:147:ILE:N	5:E:157:TYR:H	2.09	0.51
1:A:99:ILE:HG13	1:A:113:LEU:HD13	1.93	0.51
1:A:260:PRO:HG3	1:A:414:TYR:CZ	2.46	0.51
2:B:237:ALA:CB	2:B:318:ASP:HB2	2.40	0.51
2:B:383:GLY:O	2:B:386:ALA:HB3	2.11	0.51
3:C:353:LEU:HD23	3:C:353:LEU:N	2.25	0.51
5:E:129:LYS:HG3	5:E:187:PHE:CE1	2.46	0.51
7:G:60:THR:O	7:G:61:TRP:C	2.50	0.51
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.40	0.50
1:A:179:ARG:HG3	1:A:180:ALA:N	2.25	0.50
1:A:204:GLU:HG2	1:A:206:ARG:HB3	1.93	0.50
2:B:98:VAL:HG13	2:B:107:TYR:CE2	2.47	0.50
3:C:206:ASN:ND2	3:C:207:ASN:N	2.59	0.50
3:C:207:ASN:O	3:C:208:PRO:C	2.48	0.50
1:A:136:GLN:HE21	9:I:50:LEU:HG	1.76	0.50
1:A:236:PHE:CD2	1:A:258:GLU:CB	2.93	0.50
2:B:255:ALA:HA	2:B:425:ALA:O	2.11	0.50
4:D:212:MET:HG3	4:D:216:LEU:HD12	1.93	0.50
5:E:82:PRO:O	5:E:83:GLU:C	2.48	0.50
5:E:123:ASP:O	5:E:125:GLU:N	2.44	0.50
1:A:236:PHE:CD2	1:A:258:GLU:CG	2.89	0.50
2:B:300:ALA:HA	2:B:307:PHE:HZ	1.75	0.50
4:D:33:TYR:HA	4:D:37:CYS:HB2	1.93	0.50
4:D:44:ASP:OD1	4:D:93:LYS:NZ	2.40	0.50
4:D:211:MET:SD	5:E:49:TYR:CD2	3.05	0.50
5:E:123:ASP:OD1	5:E:168:SER:CB	2.59	0.50
6:F:44:LYS:HA	6:F:44:LYS:HZ3	1.73	0.50
1:A:383:LEU:HD22	1:A:388:ARG:CA	2.40	0.50
2:B:122:PHE:O	2:B:126:VAL:HG23	2.11	0.50
4:D:6:HIS:O	4:D:8:PRO:CD	2.60	0.50
1:A:166:SER:O	1:A:169:GLY:N	2.41	0.50
3:C:303:LEU:O	3:C:304:ILE:C	2.50	0.50
5:E:188:THR:OG1	5:E:192:MET:HB2	2.11	0.50
10:J:55:ILE:O	10:J:58:LYS:HD3	2.12	0.50
1:A:136:GLN:NE2	9:I:50:LEU:HG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:LEU:HD21	2:B:204:MET:SD	2.50	0.50
2:B:62:ASN:ND2	2:B:65:THR:OG1	2.45	0.50
2:B:262:ALA:CB	2:B:272:PHE:CE2	2.95	0.50
3:C:309:THR:HG21	3:C:367:PRO:O	2.11	0.50
4:D:7:PRO:N	4:D:8:PRO:HD2	2.27	0.50
4:D:29:GLY:HA3	4:D:185:ASP:O	2.11	0.50
6:F:71:ARG:HH11	6:F:71:ARG:HB3	1.76	0.50
11:K:20:THR:HG23	11:K:24:TRP:HD1	1.76	0.50
1:A:26:ALA:O	1:A:27:SER:HB3	2.12	0.50
1:A:42:ASP:HB2	1:A:94:HIS:ND1	2.26	0.50
2:B:71:LEU:HD21	2:B:147:ASP:OD2	2.11	0.50
2:B:198:HIS:O	2:B:203:ARG:HD3	2.12	0.50
2:B:406:ALA:O	2:B:407:ASP:C	2.49	0.50
4:D:35:GLN:OE1	4:D:35:GLN:HA	2.11	0.50
1:A:252:HIS:O	1:A:424:GLY:HA2	2.11	0.50
5:E:96:LEU:HD21	5:E:195:VAL:HG11	1.94	0.50
9:I:64:LEU:HD11	9:I:65:VAL:HG23	1.93	0.50
1:A:111:GLU:O	1:A:115:ASP:HB2	2.12	0.50
2:B:56:ARG:HA	2:B:174:ASN:HD21	1.77	0.50
2:B:268:GLU:O	2:B:269:ALA:C	2.51	0.50
3:C:19:ILE:HG23	3:C:221:HIS:HB2	1.94	0.50
3:C:310:SER:OG	3:C:311:LYS:N	2.43	0.50
5:E:76:ILE:HA	5:E:193:VAL:O	2.12	0.50
11:K:32:LEU:HD12	11:K:36:THR:OG1	2.11	0.50
1:A:262:TRP:CE3	1:A:385:THR:HG21	2.47	0.49
1:A:329:MET:HA	1:A:430:GLN:OE1	2.12	0.49
3:C:164:ILE:O	3:C:177:ARG:NH1	2.44	0.49
3:C:186:PRO:HG2	12:C:380:HEM:HMC3	1.94	0.49
3:C:376:LEU:HD12	6:F:20:TYR:CD2	2.47	0.49
6:F:13:LEU:HB3	6:F:16:ILE:HD11	1.93	0.49
6:F:76:PRO:O	6:F:80:TRP:CD1	2.64	0.49
1:A:30:SER:OG	1:A:32:GLN:HG2	2.12	0.49
1:A:192:ALA:HB1	1:A:193:PRO:HA	1.94	0.49
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.42	0.49
7:G:45:ILE:O	7:G:49:ALA:HB3	2.13	0.49
10:J:23:THR:HG22	10:J:24:ILE:N	2.25	0.49
2:B:217:LYS:HE3	2:B:221:GLU:OE2	2.11	0.49
3:C:40:CYS:HB3	3:C:90:PHE:HD2	1.77	0.49
3:C:140:PHE:C	3:C:140:PHE:CD1	2.85	0.49
3:C:271:GLU:O	3:C:272:TRP:C	2.50	0.49
5:E:116:GLN:HA	5:E:116:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:VAL:HG12	5:E:146:PRO:O	2.12	0.49
5:E:166:ASP:C	5:E:166:ASP:OD1	2.50	0.49
2:B:306:PRO:HB2	2:B:329:GLN:HE22	1.74	0.49
3:C:26:ASN:HA	6:F:70:MET:HA	1.94	0.49
3:C:129:MET:O	3:C:132:VAL:HB	2.12	0.49
4:D:178:THR:O	4:D:179:MET:C	2.50	0.49
1:A:53:ASN:HB3	1:A:170:PRO:HD2	1.95	0.49
1:A:322:ALA:HB2	1:A:338:LEU:HD11	1.95	0.49
1:A:433:ASP:O	1:A:437:ILE:HG13	2.13	0.49
2:B:286:LYS:HD3	2:B:287:ARG:NH1	2.28	0.49
2:B:367:GLY:O	2:B:371:SER:OG	2.28	0.49
3:C:345:HIS:HB3	3:C:346:PRO:HD2	1.89	0.49
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.42	0.49
10:J:3:PRO:HG2	10:J:8:ARG:HG2	1.94	0.49
1:A:379:ILE:HD12	1:A:390:ILE:HD12	1.94	0.49
1:A:433:ASP:OD2	3:C:223:TYR:OH	2.24	0.49
2:B:408:ALA:O	2:B:411:ILE:N	2.45	0.49
3:C:153:ILE:HG21	3:C:156:ILE:CG1	2.42	0.49
3:C:276:PHE:O	3:C:277:ALA:C	2.51	0.49
5:E:37:TYR:CZ	7:G:21:PHE:HZ	2.31	0.49
2:B:100:SER:HB2	2:B:105:MET:HG3	1.94	0.49
2:B:182:ARG:HH12	2:B:185:LYS:HG2	1.78	0.49
2:B:219:VAL:HG12	2:B:220:ALA:N	2.27	0.49
3:C:78:ILE:O	3:C:82:MET:HB2	2.13	0.49
3:C:163:TRP:O	3:C:177:ARG:NH1	2.38	0.49
3:C:344:GLU:OE1	7:G:66:PHE:CE1	2.65	0.49
1:A:51:LYS:O	1:A:173:ASN:ND2	2.46	0.49
1:A:144:SER:OG	1:A:147:ASP:HB2	2.13	0.49
1:A:297:ILE:HD12	1:A:337:VAL:CG1	2.43	0.49
1:A:301:ASN:O	1:A:302:LYS:C	2.50	0.49
2:B:283:PRO:HG3	9:I:55:LEU:CG	2.43	0.49
9:I:54:SER:O	9:I:55:LEU:HD23	2.13	0.49
2:B:188:PRO:O	2:B:189:VAL:C	2.49	0.49
4:D:165:TYR:CE1	4:D:168:VAL:HG22	2.47	0.49
5:E:129:LYS:HD2	5:E:187:PHE:CE2	2.48	0.49
6:F:95:LYS:O	6:F:96:GLU:C	2.49	0.49
7:G:36:ASN:HA	7:G:39:ARG:CD	2.33	0.49
1:A:4:TYR:HE2	1:A:396:GLU:HG3	1.78	0.49
1:A:309:THR:HA	1:A:322:ALA:HA	1.94	0.49
1:A:379:ILE:HD12	1:A:390:ILE:HD11	1.95	0.49
2:B:276:GLN:HG2	2:B:277:HIS:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:THR:HG22	2:B:398:VAL:HG23	1.94	0.49
5:E:81:ILE:HG22	5:E:100:HIS:CB	2.42	0.49
1:A:369:LEU:HD21	1:A:378:ASP:OD2	2.13	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.13	0.48
2:B:434:PRO:HB3	2:B:438:GLU:HB3	1.95	0.48
3:C:71:ARG:NH2	4:D:193:ALA:O	2.46	0.48
3:C:88:SER:HA	3:C:272:TRP:CZ2	2.45	0.48
3:C:257:THR:HG22	3:C:257:THR:O	2.13	0.48
3:C:379:TRP:CH2	6:F:37:ILE:HG23	2.48	0.48
4:D:30:PHE:CD1	4:D:189:PHE:CE2	2.92	0.48
8:H:15:ASP:CB	8:H:16:PRO:CD	2.91	0.48
1:A:67:THR:HG22	1:A:70:ARG:CB	2.30	0.48
2:B:262:ALA:CB	2:B:269:ALA:N	2.76	0.48
2:B:384:SER:HB3	9:I:62:ARG:HD2	1.94	0.48
3:C:153:ILE:HG21	3:C:156:ILE:HG12	1.95	0.48
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.46	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.48	0.48
1:A:36:THR:HA	1:A:99:ILE:O	2.13	0.48
2:B:99:THR:HG22	2:B:100:SER:N	2.27	0.48
3:C:243:VAL:CG1	3:C:244:LEU:N	2.75	0.48
9:I:58:GLN:HB3	9:I:78:TYR:HB2	1.95	0.48
2:B:303:VAL:HG11	2:B:307:PHE:CD2	2.48	0.48
3:C:77:TRP:O	3:C:81:TYR:HD2	1.97	0.48
3:C:296:PHE:O	3:C:300:ILE:HB	2.14	0.48
3:C:304:ILE:HB	3:C:305:PRO:HD3	1.94	0.48
5:E:32:ARG:HH12	7:G:22:GLU:CD	2.16	0.48
1:A:255:ILE:HD12	1:A:335:MET:HE1	1.96	0.48
2:B:135:TRP:CD1	2:B:136:GLU:HG3	2.48	0.48
4:D:48:TYR:OH	4:D:68:VAL:CB	2.61	0.48
1:A:19:LEU:HG	1:A:23:LEU:HB3	1.96	0.48
1:A:34:THR:HG22	1:A:101:ALA:O	2.14	0.48
1:A:245:GLU:O	1:A:247:GLY:N	2.47	0.48
1:A:279:HIS:CE1	1:A:284:TYR:HH	2.29	0.48
1:A:365:LEU:O	1:A:369:LEU:HD12	2.13	0.48
2:B:69:LEU:O	2:B:72:ALA:N	2.44	0.48
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.13	0.48
2:B:289:SER:OG	2:B:290:ASN:N	2.46	0.48
3:C:36:LEU:HD22	3:C:235:LEU:CB	2.42	0.48
3:C:47:THR:HG21	3:C:83:HIS:CB	2.43	0.48
8:H:21:ARG:O	8:H:24:CYS:HB2	2.14	0.48
8:H:68:CYS:O	8:H:69:VAL:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLY:HA2	1:A:427:PRO:C	2.33	0.48
2:B:155:PRO:O	2:B:156:GLN:C	2.52	0.48
2:B:258:VAL:CG1	2:B:321:LEU:HB3	2.43	0.48
3:C:3:ASN:CA	3:C:8:HIS:NE2	2.77	0.48
3:C:73:VAL:HG12	3:C:76:GLY:HA3	1.93	0.48
3:C:304:ILE:O	3:C:305:PRO:C	2.50	0.48
4:D:43:MET:HA	4:D:112:ASP:OD1	2.14	0.48
4:D:102:ARG:HH21	4:D:109:LEU:HD23	1.78	0.48
5:E:12:ASP:O	7:G:24:ARG:NH2	2.39	0.48
9:I:64:LEU:HD12	9:I:64:LEU:C	2.31	0.48
1:A:394:GLU:O	1:A:395:TRP:C	2.49	0.48
1:A:408:ARG:HH22	11:K:15:ARG:NE	2.11	0.48
1:A:417:ASP:OD1	1:A:438:ARG:NH1	2.46	0.48
2:B:140:LEU:O	2:B:143:GLN:N	2.46	0.48
3:C:4:ILE:O	3:C:5:ARG:C	2.52	0.48
4:D:35:GLN:HB2	4:D:169:LEU:CD1	2.43	0.48
4:D:136:GLU:O	4:D:137:PRO:C	2.50	0.48
4:D:138:PRO:HD2	4:D:141:VAL:CG1	2.43	0.48
6:F:28:LYS:HB3	6:F:74:ILE:CD1	2.43	0.48
1:A:240:GLN:HG3	1:A:422:VAL:CB	2.38	0.48
1:A:343:MET:CE	1:A:416:TYR:CD2	2.97	0.48
1:A:381:ARG:HA	1:A:384:LEU:CD1	2.44	0.48
2:B:46:ARG:CZ	2:B:376:GLU:HB2	2.43	0.48
2:B:46:ARG:NH1	2:B:376:GLU:HB2	2.29	0.48
2:B:46:ARG:NH2	2:B:376:GLU:HB2	2.28	0.48
2:B:203:ARG:HG2	2:B:230:LEU:HD21	1.95	0.48
2:B:322:PHE:CD1	2:B:323:GLY:N	2.82	0.48
2:B:333:ALA:O	2:B:337:ILE:HD12	2.14	0.48
3:C:218:ILE:CG2	3:C:223:TYR:CD2	2.96	0.48
3:C:366:MET:HB2	3:C:367:PRO:HD3	1.95	0.48
5:E:101:ARG:HG3	5:E:131:GLU:O	2.12	0.48
1:A:36:THR:HG21	1:A:373:THR:HA	1.96	0.48
1:A:45:SER:HA	1:A:48:GLU:HG3	1.95	0.48
2:B:156:GLN:OE1	9:I:58:GLN:NE2	2.33	0.48
2:B:306:PRO:HB2	2:B:329:GLN:HE21	1.77	0.48
2:B:348:ALA:HB3	2:B:418:VAL:HG21	1.95	0.48
3:C:3:ASN:HA	3:C:8:HIS:CD2	2.49	0.48
3:C:124:MET:HE3	3:C:298:ILE:HD13	1.96	0.48
3:C:182:HIS:O	3:C:186:PRO:HD2	2.14	0.48
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.80	0.48
4:D:72:ASP:O	4:D:72:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:79:GLU:OE1	4:D:82:MET:HG3	2.13	0.48
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.96	0.48
1:A:61:HIS:CB	1:A:130:GLU:HG3	2.44	0.47
1:A:223:TYR:CE2	1:A:224:ASP:CB	2.97	0.47
1:A:307:PHE:CD1	1:A:307:PHE:C	2.86	0.47
1:A:383:LEU:HD22	1:A:388:ARG:C	2.34	0.47
1:A:399:ILE:O	1:A:402:VAL:HG23	2.14	0.47
2:B:258:VAL:CG1	2:B:321:LEU:HD22	2.44	0.47
5:E:171:ILE:O	5:E:172:ARG:HD2	2.14	0.47
1:A:34:THR:CG2	2:B:370:MET:HG2	2.23	0.47
1:A:395:TRP:O	1:A:396:GLU:C	2.51	0.47
1:A:431:LEU:O	1:A:432:PRO:C	2.53	0.47
2:B:308:ASP:HB2	9:I:54:SER:HB2	1.96	0.47
3:C:47:THR:HG21	3:C:83:HIS:HB2	1.96	0.47
3:C:149:LEU:HD21	3:C:281:LEU:CD2	2.44	0.47
4:D:26:ILE:HG22	4:D:27:ARG:N	2.29	0.47
5:E:77:LYS:HZ1	5:E:193:VAL:HG21	1.80	0.47
5:E:168:SER:CB	5:E:170:ARG:HH21	2.26	0.47
8:H:53:ASP:C	8:H:53:ASP:OD1	2.53	0.47
1:A:136:GLN:CD	9:I:51:CYS:HB3	2.35	0.47
2:B:341:TYR:CD2	2:B:345:LYS:HE3	2.48	0.47
3:C:44:GLN:HE22	3:C:86:GLY:CA	2.24	0.47
3:C:90:PHE:O	3:C:94:LEU:HB2	2.15	0.47
3:C:317:PHE:CD1	6:F:26:PHE:HB3	2.49	0.47
6:F:50:LEU:N	6:F:50:LEU:HD23	2.30	0.47
6:F:91:GLU:N	6:F:92:PRO:CD	2.77	0.47
2:B:261:SER:HB2	2:B:321:LEU:C	2.35	0.47
2:B:283:PRO:CG	9:I:55:LEU:HD13	2.44	0.47
2:B:303:VAL:HG11	2:B:307:PHE:CG	2.50	0.47
3:C:313:ARG:CB	6:F:38:HIS:CD2	2.98	0.47
4:D:165:TYR:O	4:D:168:VAL:CG2	2.55	0.47
9:I:58:GLN:O	9:I:59:ALA:HB2	2.14	0.47
1:A:52:ASN:HB2	1:A:55:ALA:CB	2.38	0.47
2:B:213:HIS:O	2:B:213:HIS:CD2	2.67	0.47
3:C:70:CYS:SG	3:C:80:ARG:HD2	2.55	0.47
3:C:299:LEU:O	3:C:300:ILE:C	2.52	0.47
3:C:342:PRO:HG2	7:G:66:PHE:CZ	2.50	0.47
4:D:69:GLU:O	4:D:73:GLY:HA2	2.15	0.47
5:E:81:ILE:CD1	5:E:87:MET:HB2	2.44	0.47
9:I:57:GLY:O	9:I:78:TYR:CE2	2.68	0.47
9:I:72:VAL:HB	9:I:73:PRO:HD2	1.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:VAL:O	1:A:275:ALA:HB3	2.14	0.47
1:A:355:LEU:HD22	1:A:358:LYS:HZ3	1.79	0.47
2:B:37:SER:HB3	2:B:213:HIS:HB2	1.95	0.47
3:C:131:TYR:O	3:C:134:PRO:HD2	2.13	0.47
3:C:178:PHE:O	3:C:179:PHE:C	2.52	0.47
4:D:48:TYR:OH	4:D:68:VAL:CG1	2.61	0.47
4:D:165:TYR:CE1	4:D:168:VAL:HA	2.49	0.47
8:H:70:ALA:HA	8:H:73:LEU:CD2	2.37	0.47
1:A:257:VAL:O	1:A:257:VAL:HG23	2.15	0.47
3:C:107:TYR:C	3:C:107:TYR:HD1	2.17	0.47
3:C:137:GLN:NE2	3:C:263:ASN:HB3	2.29	0.47
3:C:156:ILE:HG12	3:C:157:GLY:H	1.79	0.47
3:C:221:HIS:HB3	3:C:222:PRO:CD	2.41	0.47
4:D:3:LEU:N	4:D:3:LEU:HD23	2.30	0.47
4:D:10:TYR:H	4:D:125:ASP:CG	2.18	0.47
4:D:183:ALA:O	4:D:184:LYS:C	2.53	0.47
5:E:16:PRO:HB2	5:E:17:GLU:HG2	1.96	0.47
5:E:20:ASP:O	5:E:21:SER:C	2.53	0.47
6:F:91:GLU:HB2	6:F:92:PRO:HD3	1.96	0.47
7:G:50:PRO:CB	7:G:51:PRO:HD3	2.44	0.47
1:A:46:ARG:HB3	1:A:92:ARG:O	2.14	0.47
1:A:334:MET:O	1:A:336:PHE:N	2.47	0.47
2:B:231:GLY:C	2:B:233:SER:N	2.67	0.47
3:C:4:ILE:O	3:C:4:ILE:HG22	2.15	0.47
3:C:32:ASN:HD21	3:C:228:ASP:HA	1.79	0.47
3:C:120:LEU:HB2	12:C:381:HEM:CMC	2.45	0.47
4:D:23:HIS:HA	4:D:26:ILE:HB	1.97	0.47
5:E:33:LYS:CB	10:J:10:TYR:CE2	2.97	0.47
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.96	0.47
1:A:95:THR:HG21	1:A:190:TYR:OH	2.15	0.47
1:A:422:VAL:HG21	1:A:437:ILE:CD1	2.44	0.47
3:C:7:SER:O	3:C:8:HIS:O	2.32	0.47
3:C:186:PRO:HB3	12:C:380:HEM:CBB	2.45	0.47
6:F:33:ARG:O	6:F:35:ASP:N	2.48	0.47
8:H:66:ASP:HA	8:H:69:VAL:HG23	1.96	0.47
3:C:183:PHE:CE1	3:C:187:PHE:HE2	2.33	0.47
3:C:272:TRP:NE1	3:C:273:TYR:CD1	2.82	0.47
3:C:291:VAL:O	3:C:294:LEU:HB3	2.15	0.47
4:D:70:VAL:CG2	4:D:84:PRO:HD3	2.29	0.47
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.30	0.47
4:D:165:TYR:H	4:D:168:VAL:CG2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:32:LEU:O	11:K:33:VAL:C	2.53	0.47
1:A:241:ILE:HD12	7:G:16:TYR:CE1	2.48	0.46
1:A:343:MET:HE3	1:A:416:TYR:CD2	2.51	0.46
3:C:153:ILE:HG22	3:C:156:ILE:HG12	1.97	0.46
5:E:74:ILE:HG23	5:E:74:ILE:O	2.15	0.46
5:E:163:SER:HA	5:E:173:LYS:O	2.15	0.46
8:H:21:ARG:NH1	8:H:66:ASP:OD1	2.47	0.46
8:H:59:LEU:O	8:H:60:ASP:C	2.52	0.46
1:A:243:HIS:NE2	1:A:425:PHE:HE1	2.14	0.46
1:A:426:GLY:HA2	1:A:428:ILE:H	1.79	0.46
2:B:285:VAL:CG1	2:B:288:GLY:HA3	2.45	0.46
3:C:81:TYR:OH	4:D:118:ARG:CZ	2.63	0.46
4:D:31:GLN:OE1	4:D:31:GLN:HA	2.15	0.46
7:G:45:ILE:HD12	7:G:45:ILE:HA	1.74	0.46
1:A:53:ASN:OD1	1:A:170:PRO:CD	2.64	0.46
1:A:64:PHE:HA	1:A:75:LEU:CD2	2.46	0.46
1:A:106:LEU:HB3	1:A:107:PRO:CD	2.45	0.46
1:A:123:GLU:O	1:A:124:ASP:C	2.52	0.46
1:A:176:LYS:O	1:A:177:LEU:C	2.52	0.46
1:A:426:GLY:HA2	1:A:428:ILE:HG13	1.97	0.46
2:B:300:ALA:CA	2:B:307:PHE:HZ	2.28	0.46
4:D:206:LEU:HD12	10:J:43:TYR:HB2	1.97	0.46
10:J:18:SER:HB3	11:K:23:LEU:HD12	1.97	0.46
11:K:18:VAL:HB	11:K:19:PRO:CD	2.45	0.46
1:A:18:GLN:HA	1:A:23:LEU:O	2.14	0.46
1:A:143:THR:O	1:A:143:THR:CG2	2.64	0.46
1:A:379:ILE:N	1:A:379:ILE:HD13	2.31	0.46
2:B:101:THR:CG2	2:B:104:ASN:H	2.28	0.46
2:B:283:PRO:HG3	9:I:55:LEU:HB3	1.98	0.46
2:B:385:GLN:O	2:B:386:ALA:C	2.53	0.46
3:C:166:GLY:HA3	3:C:177:ARG:CZ	2.45	0.46
3:C:304:ILE:HB	3:C:305:PRO:CD	2.45	0.46
7:G:67:GLU:O	7:G:71:ARG:CB	2.61	0.46
1:A:61:HIS:CD2	2:B:287:ARG:HD3	2.51	0.46
2:B:155:PRO:HB2	2:B:254:HIS:CE1	2.50	0.46
2:B:314:ALA:CB	9:I:64:LEU:HD22	2.46	0.46
2:B:408:ALA:O	2:B:411:ILE:HB	2.16	0.46
2:B:433:THR:O	2:B:434:PRO:C	2.53	0.46
3:C:280:ILE:O	3:C:283:SER:OG	2.32	0.46
3:C:328:LEU:HG	3:C:332:LEU:CD1	2.46	0.46
5:E:89:PHE:N	5:E:89:PHE:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:ARG:HG2	8:H:43:ARG:O	2.14	0.46
9:I:62:ARG:HB3	9:I:63:PRO:CD	2.35	0.46
1:A:157:ALA:CB	1:A:319:LEU:HD21	2.46	0.46
1:A:158:PHE:O	1:A:159:GLN:C	2.53	0.46
1:A:172:GLU:O	1:A:173:ASN:C	2.53	0.46
2:B:33:LEU:HB3	2:B:201:SER:O	2.16	0.46
4:D:137:PRO:HG3	4:D:143:LEU:CD1	2.46	0.46
5:E:59:VAL:O	5:E:59:VAL:CG1	2.64	0.46
7:G:33:GLY:O	7:G:37:VAL:N	2.35	0.46
9:I:78:TYR:CD1	9:I:78:TYR:C	2.88	0.46
1:A:279:HIS:CE1	1:A:284:TYR:OH	2.69	0.46
3:C:166:GLY:CA	3:C:177:ARG:NH2	2.79	0.46
3:C:272:TRP:CE2	3:C:273:TYR:CD1	3.00	0.46
4:D:165:TYR:OH	4:D:168:VAL:HG13	2.15	0.46
4:D:218:LEU:O	4:D:221:ALA:HB3	2.16	0.46
10:J:56:LYS:HG2	10:J:60:GLU:OE1	2.15	0.46
1:A:19:LEU:HB2	1:A:23:LEU:HB3	1.98	0.46
1:A:130:GLU:OE2	9:I:52:ARG:NH2	2.49	0.46
1:A:385:THR:HG22	1:A:386:TYR:CD1	2.50	0.46
3:C:276:PHE:CG	3:C:277:ALA:N	2.83	0.46
4:D:21:LEU:CD1	4:D:192:TRP:HB2	2.46	0.46
4:D:39:SER:O	4:D:94:PRO:HB3	2.15	0.46
4:D:200:HIS:CD2	4:D:204:MET:HG3	2.51	0.46
4:D:208:MET:CE	4:D:208:MET:C	2.84	0.46
5:E:173:LYS:HG3	5:E:174:GLY:N	2.30	0.46
6:F:106:GLU:O	6:F:109:LYS:HG2	2.16	0.46
7:G:3:GLN:O	7:G:7:LEU:HG	2.15	0.46
10:J:31:PHE:O	10:J:32:GLU:C	2.51	0.46
1:A:146:ARG:HH21	1:A:308:GLN:HE22	1.62	0.46
1:A:207:GLN:O	1:A:208:LEU:C	2.55	0.46
1:A:276:ILE:O	1:A:292:SER:HB2	2.16	0.46
3:C:51:LEU:O	3:C:52:ALA:C	2.54	0.46
3:C:279:ALA:O	3:C:280:ILE:C	2.54	0.46
4:D:183:ALA:CA	4:D:186:VAL:HG23	2.45	0.46
8:H:65:ARG:O	8:H:69:VAL:HG23	2.16	0.46
10:J:4:THR:HG22	10:J:6:THR:N	2.31	0.46
1:A:39:VAL:HG11	1:A:117:VAL:CG2	2.43	0.46
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.51	0.46
3:C:263:ASN:O	3:C:265:PRO:HD3	2.16	0.46
3:C:296:PHE:HE1	3:C:300:ILE:HG13	1.74	0.46
3:C:318:ARG:HB3	3:C:373:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:HIS:ND1	4:D:7:PRO:HD3	2.30	0.46
6:F:10:SER:HA	6:F:13:LEU:HG	1.97	0.46
1:A:70:ARG:HB3	1:A:74:ALA:CB	2.45	0.45
2:B:67:HIS:CD2	2:B:144:LEU:CD2	2.93	0.45
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.52	0.45
2:B:162:ASN:ND2	2:B:244:ILE:HG21	2.31	0.45
2:B:292:THR:CG2	2:B:363:LYS:NZ	2.80	0.45
3:C:47:THR:CG2	3:C:83:HIS:CB	2.94	0.45
1:A:64:PHE:HA	1:A:75:LEU:HD22	1.98	0.45
1:A:289:HIS:O	1:A:290:LEU:C	2.54	0.45
1:A:310:PHE:O	1:A:310:PHE:CD1	2.69	0.45
2:B:79:GLY:HA3	2:B:125:ASN:HD21	1.81	0.45
2:B:292:THR:HG21	2:B:363:LYS:HZ1	1.81	0.45
2:B:431:GLY:O	2:B:432:HIS:HD2	1.98	0.45
3:C:221:HIS:CB	3:C:222:PRO:CD	2.94	0.45
3:C:237:LEU:O	3:C:241:LEU:HB2	2.16	0.45
6:F:25:GLY:O	6:F:26:PHE:C	2.54	0.45
6:F:73:GLN:HG2	7:G:36:ASN:ND2	2.29	0.45
1:A:243:HIS:O	1:A:425:PHE:HA	2.17	0.45
2:B:316:TYR:OH	9:I:64:LEU:HD23	2.15	0.45
3:C:257:THR:O	3:C:258:PRO:C	2.52	0.45
4:D:181:GLN:CA	8:H:77:LEU:HD13	2.39	0.45
1:A:51:LYS:CG	1:A:52:ASN:N	2.78	0.45
1:A:58:PHE:O	1:A:59:VAL:C	2.54	0.45
1:A:136:GLN:HE21	9:I:50:LEU:CB	2.28	0.45
2:B:161:GLU:OE1	2:B:175:SER:HB2	2.16	0.45
3:C:378:LYS:HD3	6:F:33:ARG:HH12	1.80	0.45
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.81	0.45
4:D:50:HIS:HB3	4:D:54:VAL:HG21	1.96	0.45
4:D:69:GLU:HA	4:D:73:GLY:HA2	1.99	0.45
5:E:77:LYS:HG3	5:E:193:VAL:CG1	2.46	0.45
1:A:428:ILE:HG22	1:A:431:LEU:HB3	1.98	0.45
2:B:352:LEU:O	2:B:352:LEU:HG	2.16	0.45
3:C:39:ILE:O	3:C:40:CYS:C	2.53	0.45
3:C:260:ASN:O	3:C:262:LEU:N	2.49	0.45
3:C:341:GLN:NE2	3:C:341:GLN:CA	2.79	0.45
4:D:160:MET:HE2	4:D:163:PRO:HG3	1.97	0.45
5:E:71:MET:HA	5:E:74:ILE:HG22	1.98	0.45
5:E:127:VAL:CG1	5:E:133:VAL:HG23	2.47	0.45
6:F:75:LEU:HD12	6:F:75:LEU:HA	1.78	0.45
1:A:248:LEU:HD12	1:A:425:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PHE:CZ	3:C:6:LYS:HE3	2.51	0.45
2:B:157:ALA:O	2:B:161:GLU:CG	2.65	0.45
2:B:170:ASN:OD1	2:B:171:ALA:N	2.47	0.45
3:C:26:ASN:ND2	3:C:26:ASN:C	2.70	0.45
3:C:124:MET:HE1	3:C:298:ILE:HD13	1.97	0.45
3:C:310:SER:CB	3:C:318:ARG:HH11	2.30	0.45
4:D:14:HIS:HA	4:D:19:SER:HB3	1.99	0.45
4:D:27:ARG:CZ	10:J:58:LYS:HE3	2.47	0.45
6:F:49:ARG:NH1	6:F:97:VAL:CG2	2.80	0.45
1:A:79:VAL:HG12	1:A:84:ALA:HB3	1.99	0.45
1:A:343:MET:CE	1:A:416:TYR:CE2	3.00	0.45
2:B:124:LEU:HD13	2:B:223:PHE:CB	2.47	0.45
2:B:133:ARG:O	2:B:134:ARG:C	2.54	0.45
3:C:46:LEU:O	3:C:47:THR:C	2.55	0.45
5:E:43:THR:O	5:E:47:VAL:HG23	2.17	0.45
5:E:77:LYS:CE	5:E:98:VAL:CG2	2.94	0.45
10:J:25:VAL:HG12	11:K:30:VAL:HG12	1.99	0.45
2:B:303:VAL:CG1	2:B:304:HIS:H	2.30	0.45
2:B:433:THR:HA	2:B:434:PRO:HD2	1.71	0.45
3:C:133:LEU:HD23	3:C:133:LEU:HA	1.79	0.45
3:C:138:MET:HG2	3:C:253:PRO:HB3	1.97	0.45
3:C:269:LYS:HZ2	3:C:340:GLY:HA3	1.80	0.45
3:C:373:GLU:O	3:C:377:LEU:HD12	2.17	0.45
4:D:160:MET:HE3	13:D:242:HEC:C1C	2.46	0.45
6:F:44:LYS:HA	6:F:44:LYS:CE	2.47	0.45
3:C:122:THR:HG23	3:C:185:LEU:HD11	1.97	0.45
3:C:221:HIS:N	3:C:222:PRO:CD	2.78	0.45
3:C:275:LEU:HB3	3:C:339:GLY:HA3	1.99	0.45
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.85	0.45
4:D:200:HIS:HD2	4:D:204:MET:HG3	1.81	0.45
5:E:137:GLY:O	5:E:146:PRO:HD2	2.17	0.45
1:A:31:SER:N	1:A:202:GLY:HA2	2.31	0.45
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.45
4:D:44:ASP:O	4:D:90:TYR:CD2	2.70	0.45
4:D:146:GLY:O	4:D:159:GLY:HA2	2.17	0.45
4:D:187:CYS:O	4:D:188:THR:C	2.55	0.45
4:D:189:PHE:O	4:D:189:PHE:CG	2.69	0.45
6:F:71:ARG:O	6:F:73:GLN:HG3	2.17	0.45
6:F:91:GLU:N	6:F:92:PRO:HD2	2.32	0.45
7:G:34:ILE:CB	7:G:35:PRO:CD	2.93	0.45
1:A:16:VAL:HG11	1:A:388:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HG21	1:A:414:TYR:O	2.17	0.44
1:A:436:ARG:HE	3:C:222:PRO:CD	2.26	0.44
3:C:82:MET:HA	3:C:243:VAL:HG21	1.98	0.44
3:C:101:GLY:HA2	3:C:106:SER:HB2	1.97	0.44
4:D:34:LYS:O	4:D:38:SER:OG	2.26	0.44
4:D:54:VAL:O	4:D:54:VAL:CG1	2.59	0.44
7:G:71:ARG:O	7:G:73:ASN:N	2.50	0.44
7:G:72:LYS:HB3	7:G:75:ALA:CB	2.24	0.44
8:H:49:GLN:O	8:H:51:GLU:N	2.50	0.44
1:A:61:HIS:NE2	1:A:134:ILE:HD12	2.32	0.44
1:A:394:GLU:O	1:A:397:SER:N	2.50	0.44
2:B:47:ILE:CD1	2:B:211:VAL:HG21	2.36	0.44
2:B:381:GLU:O	2:B:381:GLU:HG3	2.16	0.44
2:B:392:TYR:O	2:B:392:TYR:CG	2.66	0.44
3:C:97:HIS:HD2	12:C:381:HEM:C1C	2.35	0.44
5:E:71:MET:HA	5:E:74:ILE:CG2	2.48	0.44
9:I:54:SER:O	9:I:55:LEU:HG	2.17	0.44
1:A:145:MET:SD	1:A:248:LEU:HD13	2.57	0.44
2:B:51:ILE:HD13	2:B:199:PHE:CG	2.52	0.44
2:B:101:THR:HG23	2:B:104:ASN:H	1.82	0.44
2:B:261:SER:HB2	2:B:321:LEU:CA	2.47	0.44
4:D:43:MET:CE	4:D:91:PHE:CE2	3.01	0.44
4:D:82:MET:SD	4:D:86:LYS:CD	3.05	0.44
6:F:29:LEU:HD23	6:F:29:LEU:HA	1.72	0.44
1:A:38:GLY:HA3	1:A:40:TRP:CZ3	2.46	0.44
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.75	0.44
1:A:200:ALA:CB	1:A:375:VAL:HG23	2.48	0.44
1:A:232:SER:O	1:A:233:PRO:C	2.54	0.44
2:B:211:VAL:HG12	2:B:212:SER:N	2.33	0.44
2:B:314:ALA:CB	9:I:64:LEU:CD2	2.95	0.44
3:C:288:LEU:HD12	3:C:288:LEU:O	2.17	0.44
4:D:117:VAL:O	4:D:123:GLY:HA2	2.17	0.44
5:E:81:ILE:HD13	5:E:98:VAL:O	2.17	0.44
1:A:31:SER:H	1:A:202:GLY:HA2	1.82	0.44
1:A:32:GLN:HB3	1:A:33:PRO:CD	2.44	0.44
1:A:116:ILE:HG22	1:A:117:VAL:N	2.32	0.44
1:A:162:PRO:O	1:A:165:GLN:CG	2.63	0.44
1:A:370:ASP:O	1:A:374:PRO:HG2	2.17	0.44
3:C:5:ARG:O	3:C:9:PRO:HD2	2.17	0.44
3:C:71:ARG:HH21	4:D:196:PRO:CG	2.29	0.44
3:C:207:ASN:ND2	3:C:209:THR:OG1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:O	1:A:292:SER:OG	2.33	0.44
1:A:350:THR:HB	1:A:353:GLU:HG3	1.99	0.44
1:A:355:LEU:HD22	1:A:358:LYS:NZ	2.32	0.44
2:B:53:ALA:O	2:B:105:MET:HB2	2.17	0.44
2:B:95:LYS:HZ3	9:I:70:LEU:HD22	1.80	0.44
2:B:283:PRO:CG	9:I:55:LEU:HB3	2.48	0.44
2:B:345:LYS:HD3	2:B:418:VAL:HG11	1.99	0.44
4:D:24:THR:O	4:D:27:ARG:HB3	2.17	0.44
5:E:25:SER:HA	5:E:28:SER:OG	2.17	0.44
5:E:109:GLU:HG3	5:E:167:ALA:HB3	2.00	0.44
5:E:148:ALA:O	5:E:149:ASN:C	2.56	0.44
5:E:165:TYR:HD1	5:E:169:GLY:O	2.01	0.44
6:F:13:LEU:HA	6:F:16:ILE:CD1	2.47	0.44
1:A:45:SER:HB3	1:A:92:ARG:HG3	2.00	0.44
1:A:53:ASN:ND2	1:A:165:GLN:HG3	2.32	0.44
1:A:416:TYR:O	1:A:418:GLN:HG2	2.18	0.44
2:B:69:LEU:O	2:B:72:ALA:HB3	2.18	0.44
2:B:343:GLN:O	2:B:343:GLN:HG3	2.17	0.44
3:C:345:HIS:O	3:C:346:PRO:C	2.55	0.44
5:E:53:ASN:O	5:E:54:VAL:C	2.54	0.44
5:E:55:VAL:O	5:E:59:VAL:HG23	2.18	0.44
5:E:118:ARG:HE	5:E:171:ILE:CG1	2.28	0.44
11:K:34:SER:O	11:K:35:ALA:C	2.55	0.44
1:A:62:LEU:HB3	1:A:122:LEU:HD22	1.99	0.44
1:A:248:LEU:CD1	1:A:425:PHE:CD2	3.01	0.44
1:A:347:THR:O	11:K:16:ASN:HB2	2.18	0.44
3:C:91:PHE:HB2	3:C:272:TRP:CH2	2.52	0.44
3:C:341:GLN:CA	3:C:341:GLN:HE21	2.29	0.44
8:H:49:GLN:H	8:H:49:GLN:HG3	1.61	0.44
1:A:61:HIS:HB3	1:A:130:GLU:HG3	1.99	0.44
1:A:166:SER:CB	5:E:3:THR:CG2	2.95	0.44
1:A:172:GLU:O	1:A:175:ARG:N	2.51	0.44
2:B:200:THR:HG22	2:B:203:ARG:CG	2.48	0.44
2:B:209:LEU:CD2	2:B:375:SER:HB2	2.42	0.44
2:B:264:ILE:HB	2:B:316:TYR:O	2.18	0.44
2:B:436:ILE:H	2:B:436:ILE:HG13	1.16	0.44
4:D:210:LEU:O	4:D:211:MET:C	2.57	0.44
5:E:35:PHE:O	5:E:38:LEU:HB3	2.17	0.44
5:E:43:THR:HG22	5:E:44:THR:N	2.31	0.44
8:H:73:LEU:HD21	8:H:74:PHE:HD1	1.83	0.44
1:A:45:SER:HB2	1:A:167:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:OD1	1:A:170:PRO:HD3	2.18	0.43
2:B:42:ALA:HB1	2:B:43:PRO:CD	2.44	0.43
2:B:294:SER:OG	2:B:343:GLN:NE2	2.46	0.43
2:B:308:ASP:CB	9:I:54:SER:HB2	2.48	0.43
2:B:312:PHE:CD1	9:I:58:GLN:O	2.71	0.43
3:C:72:ASP:HB3	5:E:67:ASP:H	1.83	0.43
3:C:345:HIS:CB	3:C:346:PRO:HD3	2.37	0.43
12:C:381:HEM:HMC2	12:C:381:HEM:CBC	2.32	0.43
4:D:115:TYR:O	4:D:118:ARG:N	2.51	0.43
5:E:19:LEU:O	5:E:19:LEU:CD1	2.54	0.43
10:J:62:LYS:HD3	10:J:62:LYS:HA	1.49	0.43
1:A:86:LEU:HD12	1:A:98:TYR:O	2.18	0.43
2:B:219:VAL:O	2:B:220:ALA:C	2.56	0.43
2:B:372:VAL:O	2:B:372:VAL:HG12	2.18	0.43
3:C:268:ILE:H	3:C:268:ILE:HG13	1.59	0.43
3:C:342:PRO:HD2	3:C:347:TYR:CE2	2.53	0.43
5:E:127:VAL:HG13	5:E:133:VAL:HG23	2.00	0.43
8:H:49:GLN:O	8:H:52:GLU:N	2.32	0.43
1:A:19:LEU:HD11	1:A:212:ALA:HB3	2.00	0.43
1:A:112:LEU:HD13	1:A:112:LEU:HA	1.72	0.43
1:A:405:ARG:O	1:A:409:GLU:HG3	2.17	0.43
1:A:428:ILE:O	1:A:428:ILE:HG22	2.18	0.43
2:B:269:ALA:O	2:B:272:PHE:HB2	2.18	0.43
2:B:308:ASP:OD2	9:I:54:SER:O	2.36	0.43
3:C:8:HIS:O	3:C:9:PRO:C	2.56	0.43
3:C:252:ASP:CB	3:C:253:PRO:HD3	2.46	0.43
3:C:315:MET:HG2	3:C:321:SER:HB2	1.99	0.43
4:D:83:ARG:CB	4:D:84:PRO:CD	2.62	0.43
10:J:60:GLU:HG3	10:J:60:GLU:O	2.17	0.43
1:A:61:HIS:NE2	1:A:134:ILE:CD1	2.81	0.43
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.66	0.43
2:B:97:SER:OG	9:I:70:LEU:HD22	2.18	0.43
2:B:187:THR:HB	2:B:188:PRO:HD2	2.01	0.43
3:C:33:PHE:O	3:C:37:LEU:N	2.48	0.43
3:C:163:TRP:O	3:C:164:ILE:C	2.57	0.43
5:E:18:VAL:HG12	5:E:25:SER:HB3	2.01	0.43
5:E:68:VAL:O	5:E:69:LEU:C	2.57	0.43
5:E:69:LEU:HA	5:E:69:LEU:HD12	1.66	0.43
8:H:52:GLU:O	8:H:53:ASP:C	2.57	0.43
11:K:34:SER:OG	11:K:35:ALA:N	2.50	0.43
1:A:46:ARG:HB2	1:A:163:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:HIS:ND1	7:G:14:ILE:HG13	2.33	0.43
1:A:324:PHE:CD2	1:A:334:MET:HG2	2.53	0.43
2:B:227:ARG:N	2:B:227:ARG:HD2	2.33	0.43
3:C:153:ILE:HG21	3:C:156:ILE:CD1	2.48	0.43
3:C:304:ILE:O	3:C:307:LEU:N	2.40	0.43
4:D:136:GLU:O	4:D:137:PRO:O	2.37	0.43
5:E:23:LYS:CG	5:E:24:SER:H	2.29	0.43
6:F:40:ASN:CG	6:F:41:ASP:H	2.21	0.43
8:H:22:GLU:O	8:H:23:GLN:C	2.54	0.43
1:A:106:LEU:HD12	1:A:110:VAL:HG23	1.99	0.43
2:B:119:LEU:HD12	2:B:119:LEU:HA	1.80	0.43
2:B:206:LEU:HD12	2:B:206:LEU:HA	1.72	0.43
2:B:280:GLY:HA2	2:B:311:ALA:HB3	2.01	0.43
3:C:121:LEU:HD23	3:C:124:MET:HE1	2.01	0.43
3:C:121:LEU:HD21	3:C:298:ILE:HG21	2.00	0.43
3:C:192:ILE:O	3:C:193:ALA:C	2.54	0.43
3:C:269:LYS:NZ	3:C:340:GLY:HA2	2.32	0.43
4:D:79:GLU:HB3	4:D:82:MET:HB2	2.01	0.43
4:D:199:ASP:O	4:D:200:HIS:C	2.55	0.43
5:E:116:GLN:HE21	5:E:116:GLN:CA	2.29	0.43
7:G:35:PRO:O	7:G:39:ARG:HB3	2.18	0.43
7:G:44:CYS:O	7:G:47:ARG:N	2.48	0.43
1:A:40:TRP:O	1:A:384:LEU:HD21	2.19	0.43
1:A:57:TYR:CE2	1:A:61:HIS:HE1	2.37	0.43
1:A:145:MET:SD	1:A:248:LEU:CD1	3.06	0.43
2:B:235:ALA:O	2:B:236:LYS:CB	2.66	0.43
2:B:332:SER:O	2:B:335:ASP:N	2.52	0.43
3:C:8:HIS:CB	3:C:9:PRO:HD3	2.38	0.43
3:C:37:LEU:CD2	3:C:93:CYS:HB3	2.48	0.43
3:C:151:SER:OG	3:C:287:LYS:NZ	2.51	0.43
3:C:278:TYR:O	3:C:281:LEU:N	2.50	0.43
3:C:358:TYR:CD1	3:C:358:TYR:C	2.92	0.43
4:D:32:VAL:HG11	4:D:186:VAL:CG2	2.48	0.43
4:D:100:ALA:O	4:D:101:ALA:C	2.56	0.43
4:D:160:MET:O	4:D:161:ALA:O	2.37	0.43
4:D:206:LEU:HD22	4:D:206:LEU:O	2.18	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.82	0.43
10:J:18:SER:CB	11:K:23:LEU:HB2	2.48	0.43
1:A:141:ASN:HD22	1:A:168:GLU:CD	2.22	0.43
2:B:166:ALA:HB2	2:B:244:ILE:CD1	2.48	0.43
2:B:381:GLU:O	2:B:385:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:ASN:CA	3:C:8:HIS:CD2	3.02	0.43
3:C:134:PRO:O	3:C:135:TRP:CB	2.65	0.43
3:C:171:ASP:O	3:C:172:LYS:C	2.56	0.43
3:C:246:ALA:N	3:C:247:PRO:HD3	2.34	0.43
3:C:304:ILE:H	3:C:304:ILE:HG12	1.66	0.43
3:C:361:LEU:O	3:C:366:MET:HG3	2.18	0.43
1:A:341:GLN:O	1:A:342:TRP:C	2.56	0.43
1:A:377:GLU:O	1:A:378:ASP:C	2.57	0.43
2:B:31:ASN:ND2	2:B:225:ASN:OD1	2.52	0.43
2:B:46:ARG:NE	2:B:375:SER:OG	2.52	0.43
2:B:304:HIS:NE2	2:B:306:PRO:HD2	2.27	0.43
2:B:347:ILE:O	2:B:411:ILE:HG23	2.19	0.43
2:B:378:PHE:CE2	2:B:382:VAL:HG21	2.53	0.43
4:D:28:ARG:CD	4:D:185:ASP:OD2	2.66	0.43
4:D:36:VAL:HG23	4:D:169:LEU:HD11	2.01	0.43
4:D:180:SER:HB3	8:H:17:LEU:HB2	2.00	0.43
5:E:77:LYS:NZ	5:E:98:VAL:CG2	2.82	0.43
10:J:56:LYS:NZ	10:J:60:GLU:OE1	2.49	0.43
1:A:83:GLY:O	2:B:370:MET:HE1	2.18	0.43
1:A:194:ARG:O	1:A:384:LEU:HD23	2.18	0.43
2:B:137:VAL:O	2:B:137:VAL:HG12	2.19	0.43
2:B:163:LEU:O	2:B:164:HIS:C	2.54	0.43
3:C:135:TRP:CD2	3:C:175:LEU:HD22	2.53	0.43
3:C:357:LEU:HG	3:C:361:LEU:CD1	2.45	0.43
4:D:195:GLU:HG3	4:D:198:HIS:HB2	2.01	0.43
4:D:206:LEU:C	4:D:206:LEU:CD2	2.87	0.43
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.49	0.42
1:A:277:ILE:H	1:A:277:ILE:HG12	1.64	0.42
2:B:207:ILE:CD1	2:B:383:GLY:HA2	2.47	0.42
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.42
4:D:162:PRO:O	4:D:163:PRO:C	2.57	0.42
5:E:15:ARG:H	5:E:15:ARG:HG2	1.50	0.42
5:E:34:GLY:N	10:J:10:TYR:CD2	2.87	0.42
5:E:73:LYS:O	5:E:73:LYS:HG2	2.19	0.42
1:A:106:LEU:O	1:A:107:PRO:O	2.37	0.42
2:B:62:ASN:O	2:B:63:LEU:C	2.57	0.42
2:B:79:GLY:H	2:B:125:ASN:ND2	2.17	0.42
3:C:37:LEU:HD12	3:C:97:HIS:CD2	2.54	0.42
4:D:3:LEU:CD2	7:G:70:LYS:HZ3	2.32	0.42
4:D:167:GLU:HG2	4:D:167:GLU:O	2.19	0.42
4:D:224:ARG:O	4:D:225:HIS:C	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:GLU:HA	7:G:65:GLU:OE1	2.19	0.42
7:G:80:ASP:O	7:G:81:ARG:HB2	2.20	0.42
11:K:20:THR:O	11:K:24:TRP:CD1	2.72	0.42
1:A:24:ARG:HB2	1:A:196:VAL:HG22	2.01	0.42
1:A:169:GLY:HA2	1:A:170:PRO:HD2	1.77	0.42
1:A:186:LEU:O	1:A:187:SER:C	2.58	0.42
1:A:244:ARG:CZ	1:A:429:GLU:HB2	2.49	0.42
2:B:90:GLU:O	2:B:92:VAL:N	2.52	0.42
2:B:109:VAL:HG13	2:B:109:VAL:O	2.19	0.42
2:B:126:VAL:O	2:B:130:PRO:HG3	2.19	0.42
3:C:37:LEU:HD23	3:C:37:LEU:HA	1.81	0.42
3:C:130:GLY:O	3:C:131:TYR:C	2.56	0.42
12:C:381:HEM:HBC2	12:C:381:HEM:CMC	2.26	0.42
4:D:203:ARG:HA	10:J:43:TYR:CE1	2.55	0.42
10:J:52:TRP:CG	10:J:53:LYS:N	2.86	0.42
1:A:53:ASN:O	1:A:53:ASN:ND2	2.51	0.42
1:A:167:VAL:O	1:A:168:GLU:C	2.55	0.42
1:A:287:GLY:O	1:A:289:HIS:N	2.53	0.42
2:B:346:THR:HG23	2:B:351:ASN:HB3	2.01	0.42
3:C:25:SER:HB3	3:C:218:ILE:HD11	2.01	0.42
3:C:122:THR:O	3:C:122:THR:HG22	2.18	0.42
3:C:248:ASP:O	3:C:251:GLY:N	2.52	0.42
1:A:385:THR:CB	1:A:386:TYR:CD1	3.02	0.42
2:B:201:SER:OG	2:B:226:ILE:N	2.51	0.42
2:B:312:PHE:HD1	9:I:58:GLN:O	2.02	0.42
3:C:221:HIS:HA	3:C:225:THR:HG23	2.00	0.42
4:D:43:MET:HE3	4:D:91:PHE:HD2	1.83	0.42
4:D:48:TYR:OH	4:D:68:VAL:CG2	2.67	0.42
4:D:117:VAL:CG2	4:D:190:LEU:HB3	2.50	0.42
4:D:208:MET:C	4:D:208:MET:HE2	2.39	0.42
4:D:227:TRP:CE3	4:D:230:LEU:HD12	2.53	0.42
6:F:16:ILE:H	6:F:16:ILE:HG13	1.34	0.42
2:B:348:ALA:CB	2:B:418:VAL:HG21	2.49	0.42
2:B:396:SER:O	2:B:400:GLN:HG3	2.20	0.42
5:E:75:GLU:O	5:E:194:ILE:HA	2.20	0.42
5:E:112:VAL:HG12	5:E:117:LEU:HD21	2.01	0.42
6:F:46:ALA:O	6:F:50:LEU:HD23	2.20	0.42
8:H:27:LEU:O	8:H:29:LYS:N	2.52	0.42
1:A:56:GLY:O	1:A:59:VAL:N	2.52	0.42
1:A:235:ARG:O	1:A:235:ARG:HG2	2.20	0.42
2:B:63:LEU:HD22	2:B:174:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:ASN:CG	2:B:171:ALA:N	2.73	0.42
3:C:25:SER:HB3	3:C:218:ILE:CD1	2.50	0.42
3:C:121:LEU:HD23	3:C:124:MET:HE2	2.01	0.42
3:C:156:ILE:O	3:C:157:GLY:C	2.57	0.42
4:D:5:LEU:HD23	4:D:152:TYR:HE1	1.82	0.42
4:D:153:PHE:CE2	4:D:158:ILE:HD12	2.55	0.42
5:E:86:ASN:HB2	5:E:99:ARG:HD2	2.01	0.42
1:A:131:ARG:O	1:A:132:ASP:C	2.58	0.42
1:A:235:ARG:HB3	5:E:21:SER:O	2.20	0.42
1:A:264:HIS:CE1	1:A:266:ASP:OD1	2.72	0.42
1:A:322:ALA:HB3	1:A:338:LEU:CD2	2.50	0.42
1:A:429:GLU:CG	7:G:4:PHE:O	2.67	0.42
2:B:180:ASP:HA	2:B:183:ILE:CD1	2.46	0.42
3:C:50:PHE:CD2	3:C:53:MET:HE3	2.55	0.42
3:C:115:ILE:H	3:C:115:ILE:HG12	1.47	0.42
3:C:138:MET:HE3	3:C:269:LYS:N	2.18	0.42
3:C:160:LEU:O	3:C:161:VAL:C	2.58	0.42
3:C:310:SER:CB	3:C:318:ARG:NH1	2.73	0.42
4:D:31:GLN:O	4:D:32:VAL:C	2.58	0.42
4:D:216:LEU:N	4:D:217:PRO:CD	2.83	0.42
5:E:18:VAL:HG11	5:E:32:ARG:HH12	1.85	0.42
5:E:171:ILE:HD13	5:E:176:ALA:HB3	2.02	0.42
6:F:75:LEU:HB3	6:F:80:TRP:HE1	1.84	0.42
1:A:33:PRO:O	1:A:103:SER:N	2.47	0.42
1:A:134:ILE:HD13	1:A:134:ILE:H	1.79	0.42
1:A:243:HIS:NE2	1:A:425:PHE:CE1	2.87	0.42
2:B:283:PRO:HG3	9:I:55:LEU:HD13	2.02	0.42
2:B:368:TYR:HA	2:B:371:SER:OG	2.20	0.42
3:C:156:ILE:CG1	3:C:157:GLY:H	2.32	0.42
12:C:380:HEM:CBB	12:C:380:HEM:CHC	2.92	0.42
4:D:57:THR:N	4:D:60:GLU:HB3	2.35	0.42
4:D:74:PRO:HB3	4:D:79:GLU:HB2	1.95	0.42
4:D:220:TYR:CE2	4:D:224:ARG:HD3	2.55	0.42
6:F:7:SER:O	6:F:11:ARG:HD2	2.20	0.42
7:G:61:TRP:O	7:G:64:GLN:HB2	2.20	0.42
10:J:55:ILE:O	10:J:55:ILE:HG22	2.20	0.42
1:A:37:VAL:HA	1:A:199:ALA:CB	2.44	0.42
1:A:198:ALA:O	1:A:199:ALA:HB2	2.20	0.42
2:B:25:GLU:O	2:B:213:HIS:CE1	2.73	0.42
2:B:57:TYR:HB3	2:B:198:HIS:CE1	2.55	0.42
2:B:100:SER:CB	2:B:105:MET:HG3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:O	2:B:109:VAL:CG1	2.67	0.42
3:C:46:LEU:HB3	3:C:47:THR:H	1.54	0.42
3:C:217:LYS:HG3	7:G:7:LEU:CD1	2.45	0.42
4:D:51:LEU:HD23	4:D:61:ALA:HB3	2.02	0.42
6:F:96:GLU:O	6:F:97:VAL:C	2.58	0.42
8:H:77:LEU:N	8:H:77:LEU:HD23	2.35	0.42
1:A:5:ALA:O	1:A:6:GLN:O	2.38	0.41
1:A:154:HIS:O	1:A:155:ALA:C	2.57	0.41
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.79	0.41
2:B:381:GLU:OE2	9:I:62:ARG:NH2	2.53	0.41
2:B:414:ALA:O	2:B:418:VAL:HG23	2.19	0.41
3:C:131:TYR:OH	3:C:253:PRO:HG2	2.20	0.41
6:F:13:LEU:CA	6:F:16:ILE:HD11	2.47	0.41
6:F:96:GLU:OE1	6:F:96:GLU:HA	2.20	0.41
8:H:73:LEU:HD23	8:H:74:PHE:N	2.34	0.41
1:A:80:GLU:HG2	2:B:284:HIS:HD2	1.85	0.41
1:A:223:TYR:CD2	1:A:224:ASP:HB3	2.55	0.41
2:B:148:LYS:HE2	2:B:152:LEU:HD11	2.03	0.41
3:C:218:ILE:HG23	3:C:219:PRO:HD2	2.02	0.41
4:D:56:TYR:CD1	4:D:60:GLU:OE2	2.73	0.41
4:D:118:ARG:CG	4:D:194:ALA:HB1	2.50	0.41
4:D:189:PHE:CD1	4:D:189:PHE:C	2.92	0.41
5:E:185:TYR:CB	5:E:195:VAL:HA	2.50	0.41
7:G:48:VAL:O	7:G:51:PRO:HD2	2.20	0.41
8:H:73:LEU:CD2	8:H:74:PHE:HD1	2.33	0.41
10:J:20:PHE:O	10:J:23:THR:HB	2.20	0.41
1:A:381:ARG:O	1:A:384:LEU:HD12	2.19	0.41
4:D:30:PHE:CE1	4:D:50:HIS:HE1	2.34	0.41
4:D:150:ASN:OD1	4:D:151:PRO:CD	2.68	0.41
5:E:29:SER:O	5:E:30:GLU:C	2.58	0.41
5:E:77:LYS:HZ3	5:E:98:VAL:HG22	1.85	0.41
5:E:158:CYS:HA	5:E:159:PRO:HD2	1.93	0.41
1:A:45:SER:HB3	1:A:92:ARG:CA	2.36	0.41
1:A:55:ALA:O	1:A:56:GLY:C	2.57	0.41
1:A:335:MET:CE	1:A:339:GLN:HG3	2.50	0.41
2:B:79:GLY:CA	2:B:125:ASN:HD21	2.33	0.41
2:B:154:ASN:O	2:B:155:PRO:C	2.59	0.41
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.35	0.41
2:B:303:VAL:HG12	2:B:307:PHE:CD2	2.55	0.41
2:B:308:ASP:OD1	2:B:308:ASP:C	2.56	0.41
3:C:51:LEU:HD12	3:C:83:HIS:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:TYR:CZ	4:D:118:ARG:NH2	2.85	0.41
3:C:140:PHE:HD1	3:C:141:TRP:CD1	2.38	0.41
5:E:129:LYS:HD2	5:E:187:PHE:CD2	2.55	0.41
6:F:88:SER:HB3	6:F:91:GLU:HG3	2.01	0.41
7:G:71:ARG:NH2	8:H:60:ASP:OD1	2.37	0.41
9:I:64:LEU:CD1	9:I:64:LEU:C	2.85	0.41
1:A:106:LEU:CD1	1:A:110:VAL:HG23	2.51	0.41
1:A:282:CYS:SG	1:A:305:GLN:OE1	2.79	0.41
1:A:341:GLN:OE1	1:A:344:ARG:NH1	2.53	0.41
1:A:376:CYS:O	1:A:379:ILE:HB	2.21	0.41
2:B:35:ILE:HG13	2:B:216:LEU:HD23	2.02	0.41
2:B:195:VAL:HG13	2:B:199:PHE:CD2	2.54	0.41
2:B:308:ASP:O	2:B:309:VAL:HG23	2.20	0.41
2:B:331:ALA:CA	2:B:432:HIS:ND1	2.73	0.41
3:C:87:ALA:O	3:C:91:PHE:HD2	2.03	0.41
4:D:79:GLU:O	4:D:80:MET:O	2.39	0.41
5:E:102:THR:OG1	5:E:105:GLU:HB2	2.20	0.41
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.03	0.41
8:H:45:SER:OG	8:H:46:SER:N	2.43	0.41
1:A:37:VAL:HG13	1:A:199:ALA:CB	2.51	0.41
1:A:240:GLN:CG	1:A:422:VAL:HB	2.45	0.41
1:A:292:SER:O	1:A:295:ALA:N	2.53	0.41
1:A:336:PHE:HE2	1:A:446:PHE:HD2	1.68	0.41
2:B:41:TYR:CG	2:B:42:ALA:N	2.88	0.41
3:C:80:ARG:HD2	3:C:80:ARG:HH11	1.43	0.41
3:C:173:ALA:O	3:C:174:THR:C	2.58	0.41
3:C:299:LEU:HD23	3:C:299:LEU:N	2.35	0.41
3:C:304:ILE:N	3:C:305:PRO:HD2	2.36	0.41
4:D:3:LEU:HD22	7:G:70:LYS:HZ1	1.84	0.41
4:D:52:VAL:HG13	10:J:52:TRP:CD1	2.56	0.41
4:D:147:LEU:O	4:D:148:TYR:C	2.58	0.41
5:E:38:LEU:O	5:E:42:THR:OG1	2.38	0.41
5:E:81:ILE:HD11	5:E:87:MET:HB2	2.03	0.41
7:G:11:ARG:O	7:G:12:HIS:HB2	2.19	0.41
7:G:49:ALA:N	7:G:50:PRO:HD2	2.36	0.41
7:G:71:ARG:O	7:G:73:ASN:ND2	2.54	0.41
11:K:17:TRP:O	11:K:21:ALA:N	2.36	0.41
1:A:223:TYR:CD2	1:A:224:ASP:CB	3.03	0.41
1:A:310:PHE:CD1	1:A:310:PHE:C	2.94	0.41
2:B:65:THR:O	2:B:66:SER:C	2.59	0.41
2:B:191:LEU:O	2:B:192:HIS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:TYR:HB3	3:C:113:TRP:CZ3	2.55	0.41
3:C:147:THR:HG21	3:C:165:TRP:NE1	2.36	0.41
3:C:172:LYS:H	3:C:172:LYS:HG2	1.35	0.41
3:C:338:ILE:HA	3:C:338:ILE:HD12	1.87	0.41
4:D:74:PRO:HG2	4:D:82:MET:CE	2.49	0.41
4:D:81:PHE:O	4:D:81:PHE:CD2	2.74	0.41
10:J:51:LEU:HB3	10:J:52:TRP:HZ3	1.82	0.41
1:A:52:ASN:O	1:A:53:ASN:C	2.59	0.41
1:A:136:GLN:HE21	9:I:50:LEU:CG	2.34	0.41
2:B:47:ILE:HB	2:B:109:VAL:CG1	2.51	0.41
3:C:30:TRP:HA	3:C:33:PHE:HE2	1.86	0.41
3:C:341:GLN:HA	3:C:341:GLN:HE21	1.86	0.41
4:D:23:HIS:O	4:D:24:THR:C	2.55	0.41
4:D:36:VAL:O	4:D:36:VAL:HG12	2.20	0.41
10:J:52:TRP:CE3	10:J:52:TRP:N	2.89	0.41
1:A:5:ALA:O	1:A:6:GLN:C	2.59	0.41
1:A:46:ARG:HB2	1:A:163:LEU:CD1	2.51	0.41
1:A:286:GLY:O	1:A:287:GLY:O	2.38	0.41
1:A:313:CYS:O	1:A:314:TYR:CD1	2.74	0.41
1:A:313:CYS:O	1:A:314:TYR:HD1	2.03	0.41
2:B:51:ILE:CD1	2:B:199:PHE:CG	3.04	0.41
2:B:122:PHE:HD1	2:B:122:PHE:HA	1.73	0.41
2:B:145:ARG:O	2:B:149:ALA:HB2	2.21	0.41
2:B:245:ARG:HH21	2:B:433:THR:HB	1.86	0.41
2:B:352:LEU:HD21	2:B:357:VAL:CG2	2.51	0.41
3:C:262:LEU:HD23	3:C:262:LEU:HA	1.86	0.41
3:C:272:TRP:CG	3:C:273:TYR:N	2.88	0.41
3:C:360:LEU:HG	3:C:365:LEU:HD21	2.02	0.41
3:C:376:LEU:O	6:F:17:ARG:HG2	2.20	0.41
4:D:26:ILE:HG21	4:D:54:VAL:HG22	2.03	0.41
4:D:165:TYR:CD2	4:D:168:VAL:HG22	2.56	0.41
5:E:10:PHE:O	5:E:11:SER:C	2.58	0.41
6:F:37:ILE:HD13	6:F:37:ILE:HG21	1.87	0.41
8:H:15:ASP:N	8:H:16:PRO:HD2	2.35	0.41
1:A:93:GLU:O	1:A:94:HIS:ND1	2.54	0.41
1:A:106:LEU:HD22	1:A:203:LEU:CG	2.50	0.41
1:A:133:VAL:HG12	1:A:134:ILE:HD13	2.03	0.41
1:A:284:TYR:CD1	9:I:72:VAL:O	2.74	0.41
2:B:148:LYS:O	2:B:152:LEU:HG	2.21	0.41
2:B:211:VAL:HG11	2:B:216:LEU:HD13	2.03	0.41
2:B:211:VAL:CG1	2:B:212:SER:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:ASP:OD2	4:D:92:PRO:CB	2.68	0.41
4:D:208:MET:HE2	4:D:208:MET:HB3	1.61	0.41
5:E:94:LYS:HB3	5:E:95:PRO:HD2	2.02	0.41
8:H:15:ASP:HB2	8:H:16:PRO:HD2	2.00	0.41
10:J:56:LYS:CE	10:J:60:GLU:OE1	2.69	0.41
1:A:89:TYR:CD1	1:A:89:TYR:C	2.95	0.40
1:A:329:MET:CE	7:G:2:ARG:HD2	2.52	0.40
1:A:428:ILE:O	1:A:430:GLN:N	2.55	0.40
2:B:97:SER:HG	9:I:70:LEU:HB2	1.84	0.40
3:C:149:LEU:HD21	3:C:281:LEU:HD22	2.02	0.40
4:D:208:MET:CE	4:D:209:LEU:HG	2.51	0.40
5:E:23:LYS:CG	5:E:24:SER:N	2.83	0.40
5:E:65:SER:O	5:E:66:ALA:C	2.58	0.40
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.51	0.40
6:F:49:ARG:NH1	6:F:97:VAL:HG22	2.36	0.40
1:A:159:GLN:NE2	7:G:18:LEU:HD21	2.33	0.40
1:A:240:GLN:HE22	1:A:431:LEU:HD21	1.80	0.40
2:B:68:LEU:CD2	2:B:186:VAL:HB	2.50	0.40
3:C:138:MET:HE1	3:C:268:ILE:HA	2.03	0.40
3:C:150:LEU:HD12	3:C:150:LEU:HA	1.87	0.40
3:C:338:ILE:O	3:C:341:GLN:HB2	2.20	0.40
3:C:341:GLN:HE21	3:C:341:GLN:N	2.19	0.40
6:F:43:VAL:O	6:F:47:ILE:HG13	2.22	0.40
8:H:66:ASP:O	8:H:67:HIS:O	2.39	0.40
1:A:22:GLY:O	1:A:24:ARG:HG2	2.21	0.40
1:A:24:ARG:HH11	1:A:24:ARG:HD2	1.72	0.40
1:A:168:GLU:H	1:A:168:GLU:HG3	1.60	0.40
2:B:163:LEU:HD22	2:B:256:ALA:CB	2.51	0.40
2:B:198:HIS:HE1	2:B:233:SER:OG	2.03	0.40
3:C:130:GLY:O	3:C:133:LEU:HB2	2.21	0.40
3:C:286:ASN:C	3:C:286:ASN:OD1	2.60	0.40
3:C:372:ILE:O	3:C:376:LEU:HG	2.21	0.40
4:D:102:ARG:CG	4:D:109:LEU:HB2	2.50	0.40
5:E:15:ARG:HB2	5:E:16:PRO:CD	2.51	0.40
6:F:102:LYS:O	6:F:103:GLU:C	2.58	0.40
1:A:200:ALA:HB3	1:A:375:VAL:HG23	2.02	0.40
1:A:385:THR:HG21	1:A:386:TYR:CE1	2.56	0.40
2:B:34:VAL:O	2:B:205:ALA:HA	2.20	0.40
2:B:38:LEU:CD1	2:B:378:PHE:HE2	2.34	0.40
2:B:394:PRO:O	2:B:398:VAL:HG23	2.21	0.40
3:C:44:GLN:NE2	3:C:86:GLY:C	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:MET:HE3	4:D:209:LEU:HA	2.04	0.40
5:E:15:ARG:HD3	7:G:23:GLN:C	2.42	0.40
7:G:37:VAL:O	7:G:41:THR:HG23	2.21	0.40
1:A:61:HIS:HB3	1:A:130:GLU:CG	2.52	0.40
2:B:24:LEU:N	2:B:24:LEU:CD1	2.68	0.40
2:B:109:VAL:CG2	2:B:119:LEU:HG	2.51	0.40
2:B:309:VAL:CG1	2:B:310:SER:N	2.83	0.40
4:D:131:LEU:HD22	4:D:163:PRO:HB3	2.03	0.40
4:D:139:THR:OG1	8:H:41:ASP:OD1	2.34	0.40
5:E:15:ARG:CB	5:E:16:PRO:CD	2.98	0.40
5:E:33:LYS:HB2	5:E:33:LYS:HE3	1.91	0.40
5:E:100:HIS:HD2	5:E:101:ARG:N	2.19	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:THR:OG1	5:E:141:HIS:O[10_665]	1.93	0.27
2:B:169:ARG:NH2	2:B:438:GLU:OE2[10_665]	1.99	0.21
3:C:177:ARG:NH2	5:E:62:MET:O[10_665]	2.12	0.08

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	444/446 (100%)	359 (81%)	65 (15%)	20 (4%)	2 14
2	B	417/439 (95%)	360 (86%)	43 (10%)	14 (3%)	3 20
3	C	377/379 (100%)	300 (80%)	55 (15%)	22 (6%)	1 10
4	D	239/241 (99%)	188 (79%)	32 (13%)	19 (8%)	1 4
5	E	194/196 (99%)	144 (74%)	40 (21%)	10 (5%)	2 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	104/110 (94%)	89 (86%)	14 (14%)	1 (1%)	15	53
7	G	79/81 (98%)	57 (72%)	18 (23%)	4 (5%)	2	12
8	H	62/78 (80%)	46 (74%)	11 (18%)	5 (8%)	1	4
9	I	31/78 (40%)	17 (55%)	9 (29%)	5 (16%)	0	1
10	J	60/62 (97%)	47 (78%)	13 (22%)	0	100	100
11	K	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0	2
All	All	2027/2166 (94%)	1622 (80%)	303 (15%)	102 (5%)	2	12

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
1	A	432	PRO
2	B	183	ILE
3	C	8	HIS
3	C	27	ILE
3	C	46	LEU
3	C	157	GLY
3	C	223	TYR
3	C	224	TYR
3	C	272	TRP
4	D	73	GLY
4	D	124	GLU
5	E	16	PRO
5	E	70	ALA
5	E	177	PRO
7	G	27	PRO
9	I	72	VAL
1	A	52	ASN
1	A	171	SER
1	A	246	ASP
1	A	287	GLY
1	A	288	ALA
1	A	315	ALA
1	A	385	THR
1	A	429	GLU
2	B	333	ALA
2	B	351	ASN
3	C	28	SER
3	C	52	ALA

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Mol	Chain	Res	Type
3	C	109	PHE
3	C	255	ASN
4	D	38	SER
4	D	51	LEU
4	D	101	ALA
5	E	71	MET
5	E	87	MET
5	E	124	LEU
7	G	29	TYR
11	K	33	VAL
1	A	233	PRO
1	A	290	LEU
1	A	391	PRO
2	B	236	LYS
2	B	269	ALA
2	B	283	PRO
2	B	305	GLN
3	C	172	LYS
3	C	278	TYR
3	C	279	ALA
4	D	98	PRO
4	D	119	ALA
4	D	123	GLY
5	E	69	LEU
6	F	97	VAL
7	G	45	ILE
8	H	49	GLN
8	H	50	THR
9	I	54	SER
9	I	59	ALA
1	A	109	ALA
1	A	395	TRP
2	B	52	LYS
2	B	88	GLY
3	C	345	HIS
4	D	139	THR
4	D	162	PRO
11	K	32	LEU
1	A	6	GLN
1	A	7	ALA
1	A	227	ALA
2	B	330	ALA

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Mol	Chain	Res	Type
3	C	110	LEU
3	C	208	PRO
3	C	222	PRO
3	C	247	PRO
3	C	261	PRO
3	C	270	PRO
4	D	8	PRO
4	D	80	MET
4	D	100	ALA
4	D	120	ARG
4	D	137	PRO
4	D	161	ALA
5	E	8	PRO
5	E	152	ASP
7	G	34	ILE
8	H	39	LEU
8	H	53	ASP
2	B	192	HIS
2	B	307	PHE
3	C	251	GLY
5	E	106	ILE
1	A	174	VAL
4	D	83	ARG
4	D	154	PRO
8	H	69	VAL
1	A	426	GLY
9	I	65	VAL
2	B	434	PRO
4	D	176	PRO
9	I	73	PRO
2	B	141	GLN

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	291 (79%)	79 (21%)	1 5
2	B	328/343 (96%)	265 (81%)	63 (19%)	1 8
3	C	327/327 (100%)	273 (84%)	54 (16%)	2 11
4	D	206/206 (100%)	177 (86%)	29 (14%)	3 16
5	E	168/168 (100%)	124 (74%)	44 (26%)	0 2
6	F	96/98 (98%)	73 (76%)	23 (24%)	0 3
7	G	71/71 (100%)	59 (83%)	12 (17%)	2 11
8	H	61/74 (82%)	52 (85%)	9 (15%)	3 14
9	I	27/60 (45%)	21 (78%)	6 (22%)	1 4
10	J	52/52 (100%)	45 (86%)	7 (14%)	4 17
11	K	15/46 (33%)	11 (73%)	4 (27%)	0 2
All	All	1721/1815 (95%)	1391 (81%)	330 (19%)	1 8

All (330) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	24	ARG
1	A	30	SER
1	A	34	THR
1	A	37	VAL
1	A	42	ASP
1	A	46	ARG
1	A	49	SER
1	A	51	LYS
1	A	53	ASN
1	A	58	PHE
1	A	73	ASN
1	A	77	LYS
1	A	79	VAL
1	A	81	SER
1	A	82	MET
1	A	89	TYR
1	A	91	THR
1	A	92	ARG
1	A	97	TYR

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Mol	Chain	Res	Type
1	A	99	ILE
1	A	100	LYS
1	A	108	LYS
1	A	112	LEU
1	A	116	ILE
1	A	121	SER
1	A	122	LEU
1	A	125	SER
1	A	130	GLU
1	A	131	ARG
1	A	134	ILE
1	A	137	GLU
1	A	138	LEU
1	A	143	THR
1	A	144	SER
1	A	156	THR
1	A	171	SER
1	A	175	ARG
1	A	176	LYS
1	A	178	SER
1	A	179	ARG
1	A	191	LYS
1	A	197	LEU
1	A	211	LEU
1	A	213	GLN
1	A	216	PHE
1	A	217	SER
1	A	220	SER
1	A	231	LEU
1	A	232	SER
1	A	239	SER
1	A	245	GLU
1	A	246	ASP
1	A	255	ILE
1	A	283	THR
1	A	292	SER
1	A	296	SER
1	A	302	LYS
1	A	330	SER
1	A	331	ILE
1	A	334	MET
1	A	337	VAL

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Mol	Chain	Res	Type
1	A	341	GLN
1	A	344	ARG
1	A	346	CYS
1	A	351	GLU
1	A	352	SER
1	A	353	GLU
1	A	356	ARG
1	A	358	LYS
1	A	360	LEU
1	A	370	ASP
1	A	379	ILE
1	A	382	SER
1	A	384	LEU
1	A	386	TYR
1	A	388	ARG
1	A	407	VAL
1	A	431	LEU
2	B	23	ASP
2	B	24	LEU
2	B	35	ILE
2	B	37	SER
2	B	38	LEU
2	B	46	ARG
2	B	47	ILE
2	B	52	LYS
2	B	56	ARG
2	B	58	GLU
2	B	62	ASN
2	B	66	SER
2	B	70	ARG
2	B	73	SER
2	B	74	SER
2	B	86	THR
2	B	95	LYS
2	B	99	THR
2	B	108	THR
2	B	109	VAL
2	B	112	LEU
2	B	113	ARG
2	B	117	ASP
2	B	127	THR
2	B	134	ARG

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Mol	Chain	Res	Type
2	B	145	ARG
2	B	160	ILE
2	B	169	ARG
2	B	174	ASN
2	B	175	SER
2	B	182	ARG
2	B	190	GLU
2	B	196	GLN
2	B	203	ARG
2	B	209	LEU
2	B	212	SER
2	B	215	VAL
2	B	221	GLU
2	B	233	SER
2	B	236	LYS
2	B	240	HIS
2	B	253	VAL
2	B	258	VAL
2	B	266	SER
2	B	273	SER
2	B	293	SER
2	B	297	GLN
2	B	315	SER
2	B	318	ASP
2	B	322	PHE
2	B	365	LYS
2	B	371	SER
2	B	396	SER
2	B	402	ILE
2	B	403	ASP
2	B	418	VAL
2	B	419	SER
2	B	422	LYS
2	B	427	SER
2	B	429	ASN
2	B	436	ILE
2	B	437	ASP
2	B	438	GLU
3	C	5	ARG
3	C	6	LYS
3	C	11	MET
3	C	25	SER

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Mol	Chain	Res	Type
3	C	27	ILE
3	C	32	ASN
3	C	35	SER
3	C	47	THR
3	C	60	THR
3	C	61	THR
3	C	65	SER
3	C	70	CYS
3	C	73	VAL
3	C	78	ILE
3	C	80	ARG
3	C	89	MET
3	C	94	LEU
3	C	107	TYR
3	C	112	THR
3	C	115	ILE
3	C	118	ILE
3	C	119	LEU
3	C	124	MET
3	C	126	THR
3	C	135	TRP
3	C	138	MET
3	C	144	THR
3	C	156	ILE
3	C	158	THR
3	C	172	LYS
3	C	174	THR
3	C	189	ILE
3	C	197	LEU
3	C	207	ASN
3	C	226	ILE
3	C	236	ILE
3	C	243	VAL
3	C	244	LEU
3	C	249	LEU
3	C	257	THR
3	C	271	GLU
3	C	288	LEU
3	C	299	LEU
3	C	300	ILE
3	C	304	ILE
3	C	313	ARG

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Mol	Chain	Res	Type
3	C	314	SER
3	C	318	ARG
3	C	324	LEU
3	C	328	LEU
3	C	338	ILE
3	C	341	GLN
3	C	349	THR
3	C	363	LEU
4	D	1	SER
4	D	3	LEU
4	D	5	LEU
4	D	20	SER
4	D	26	ILE
4	D	40	CYS
4	D	42	SER
4	D	55	CYS
4	D	70	VAL
4	D	80	MET
4	D	82	MET
4	D	88	SER
4	D	95	TYR
4	D	106	ASN
4	D	109	LEU
4	D	114	SER
4	D	116	ILE
4	D	120	ARG
4	D	126	TYR
4	D	132	THR
4	D	141	VAL
4	D	179	MET
4	D	180	SER
4	D	184	LYS
4	D	206	LEU
4	D	208	MET
4	D	211	MET
4	D	222	MET
4	D	224	ARG
5	E	1	SER
5	E	3	THR
5	E	5	ILE
5	E	6	LYS
5	E	11	SER

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Mol	Chain	Res	Type
5	E	15	ARG
5	E	17	GLU
5	E	18	VAL
5	E	19	LEU
5	E	23	LYS
5	E	28	SER
5	E	36	SER
5	E	42	THR
5	E	52	LYS
5	E	56	SER
5	E	58	PHE
5	E	67	ASP
5	E	71	MET
5	E	74	ILE
5	E	76	ILE
5	E	77	LYS
5	E	78	LEU
5	E	83	GLU
5	E	85	LYS
5	E	86	ASN
5	E	87	MET
5	E	101	ARG
5	E	105	GLU
5	E	114	VAL
5	E	115	SER
5	E	116	GLN
5	E	119	ASP
5	E	124	LEU
5	E	126	ARG
5	E	138	VAL
5	E	163	SER
5	E	166	ASP
5	E	173	LYS
5	E	178	LEU
5	E	184	SER
5	E	186	GLU
5	E	188	THR
5	E	190	ASP
5	E	193	VAL
6	F	9	SER
6	F	11	ARG
6	F	13	LEU

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Mol	Chain	Res	Type
6	F	16	ILE
6	F	18	LYS
6	F	37	ILE
6	F	44	LYS
6	F	48	ARG
6	F	50	LEU
6	F	53	ASN
6	F	54	LEU
6	F	61	ARG
6	F	63	LYS
6	F	69	SER
6	F	70	MET
6	F	75	LEU
6	F	77	LYS
6	F	82	LYS
6	F	85	GLU
6	F	98	ILE
6	F	100	GLU
6	F	107	TRP
6	F	110	LYS
7	G	4	PHE
7	G	9	ARG
7	G	17	SER
7	G	24	ARG
7	G	28	HIS
7	G	38	LEU
7	G	39	ARG
7	G	40	ARG
7	G	42	ARG
7	G	44	CYS
7	G	46	LEU
7	G	63	THR
8	H	21	ARG
8	H	29	LYS
8	H	30	CYS
8	H	41	ASP
8	H	47	ARG
8	H	73	LEU
8	H	74	PHE
8	H	76	SER
8	H	77	LEU
9	I	46	LYS

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Mol	Chain	Res	Type
9	I	49	VAL
9	I	62	ARG
9	I	70	LEU
9	I	77	ARG
9	I	78	TYR
10	J	4	THR
10	J	18	SER
10	J	33	ARG
10	J	46	ILE
10	J	52	TRP
10	J	58	LYS
10	J	62	LYS
11	K	20	THR
11	K	23	LEU
11	K	34	SER
11	K	36	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	85	HIS
1	A	136	GLN
1	A	151	ASN
1	A	154	HIS
1	A	159	GLN
1	A	189	HIS
1	A	213	GLN
1	A	240	GLN
1	A	243	HIS
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	323	HIS
2	B	62	ASN
2	B	67	HIS
2	B	125	ASN
2	B	158	HIS
2	B	162	ASN
2	B	174	ASN
2	B	198	HIS
2	B	304	HIS

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Mol	Chain	Res	Type
2	B	329	GLN
2	B	343	GLN
2	B	429	ASN
3	C	15	ASN
3	C	26	ASN
3	C	32	ASN
3	C	206	ASN
3	C	267	HIS
3	C	312	GLN
3	C	341	GLN
3	C	374	ASN
4	D	50	HIS
4	D	75	ASN
4	D	106	ASN
4	D	181	GLN
4	D	200	HIS
5	E	86	ASN
5	E	108	GLN
5	E	116	GLN
6	F	38	HIS
6	F	73	GLN
7	G	12	HIS
7	G	28	HIS
7	G	36	ASN
8	H	49	GLN
8	H	63	HIS
10	J	54	HIS
11	K	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	HEC	D	242	4	32,50,50	2.26	5 (15%)	24,82,82	2.26	11 (45%)
12	HEM	C	380	3	41,50,50	1.56	4 (9%)	45,82,82	1.53	9 (20%)
12	HEM	C	381	3	41,50,50	1.41	4 (9%)	45,82,82	1.72	12 (26%)
14	FES	E	197	5	0,4,4	-	-	-		

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
13	HEC	D	242	4	-	7/10/54/54	-
12	HEM	C	380	3	-	5/12/54/54	-
12	HEM	C	381	3	-	5/12/54/54	-
14	FES	E	197	5	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	C2B-C3B	-7.23	1.33	1.40
13	D	242	HEC	C3C-C2C	-6.61	1.33	1.40
12	C	380	HEM	C3C-C2C	-5.23	1.33	1.40
12	C	381	HEM	C3C-C2C	-4.84	1.33	1.40
13	D	242	HEC	CBB-CAB	-4.01	1.34	1.49
13	D	242	HEC	CBC-CAC	-3.66	1.35	1.49
12	C	380	HEM	C3C-CAC	3.28	1.54	1.47
12	C	380	HEM	CAB-C3B	2.87	1.55	1.47
12	C	381	HEM	C3B-C2B	-2.43	1.32	1.37
12	C	381	HEM	CAB-C3B	2.42	1.54	1.47
12	C	381	HEM	C3C-CAC	2.37	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	CAD-C3D	2.24	1.55	1.52
12	C	380	HEM	C3B-C2B	-2.13	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	380	HEM	CMA-C3A-C4A	-4.97	120.83	128.46
12	C	381	HEM	C2C-C3C-C4C	4.23	109.85	106.90
12	C	380	HEM	CMA-C3A-C2A	4.02	132.53	124.94
12	C	380	HEM	CBD-CAD-C3D	3.92	123.52	112.63
13	D	242	HEC	CMD-C2D-C1D	-3.60	122.94	128.46
13	D	242	HEC	O2A-CGA-O1A	3.58	132.23	123.30
13	D	242	HEC	CBD-CAD-C3D	3.55	118.68	112.62
13	D	242	HEC	CBA-CAA-C2A	3.52	118.53	112.60
12	C	381	HEM	C4D-C3D-C2D	3.47	111.95	106.90
13	D	242	HEC	CMB-C2B-C1B	-3.43	123.19	128.46
12	C	381	HEM	C3D-C4D-ND	-3.43	106.35	110.17
13	D	242	HEC	CMC-C2C-C1C	-3.24	123.48	128.46
12	C	381	HEM	O1D-CGD-CBD	-3.14	113.01	123.08
12	C	381	HEM	O2D-CGD-O1D	3.02	130.83	123.30
12	C	381	HEM	CMA-C3A-C4A	-2.93	123.95	128.46
13	D	242	HEC	CMC-C2C-C3C	2.90	129.23	125.82
13	D	242	HEC	CMB-C2B-C3B	2.83	129.15	125.82
12	C	380	HEM	O2A-CGA-O1A	2.45	129.41	123.30
12	C	381	HEM	C3B-C2B-C1B	2.42	108.28	106.49
12	C	381	HEM	CHA-C4D-C3D	2.36	129.75	125.33
12	C	381	HEM	CBD-CAD-C3D	2.34	119.14	112.63
12	C	380	HEM	C4C-CHD-C1D	2.34	125.65	122.56
13	D	242	HEC	CMD-C2D-C3D	2.28	129.25	124.94
12	C	381	HEM	CAD-C3D-C4D	-2.27	120.69	124.66
13	D	242	HEC	O1A-CGA-CBA	-2.16	116.14	123.08
12	C	381	HEM	C1D-C2D-C3D	-2.14	104.71	106.96
12	C	380	HEM	CBA-CAA-C2A	2.11	116.23	112.62
12	C	380	HEM	O1A-CGA-CBA	-2.04	116.51	123.08
12	C	381	HEM	CMA-C3A-C2A	2.04	128.79	124.94
13	D	242	HEC	C4C-C3C-C2C	2.03	108.54	106.35
12	C	380	HEM	O1D-CGD-CBD	-2.03	116.57	123.08
12	C	380	HEM	CHA-C4D-ND	-2.01	121.90	124.38

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	242	HEC	C2A-CAA-CBA-CGA
12	C	380	HEM	C2A-CAA-CBA-CGA
13	D	242	HEC	C1A-C2A-CAA-CBA
13	D	242	HEC	C3A-C2A-CAA-CBA
12	C	381	HEM	C2D-C3D-CAD-CBD
12	C	380	HEM	CAD-CBD-CGD-O2D
12	C	380	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	CAA-CBA-CGA-O1A
12	C	381	HEM	CAD-CBD-CGD-O2D
13	D	242	HEC	CAA-CBA-CGA-O2A
12	C	380	HEM	CAA-CBA-CGA-O2A
12	C	381	HEM	CAA-CBA-CGA-O2A
13	D	242	HEC	CAA-CBA-CGA-O1A
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	380	HEM	CAA-CBA-CGA-O1A
13	D	242	HEC	CAD-CBD-CGD-O2D
13	D	242	HEC	CAD-CBD-CGD-O1D

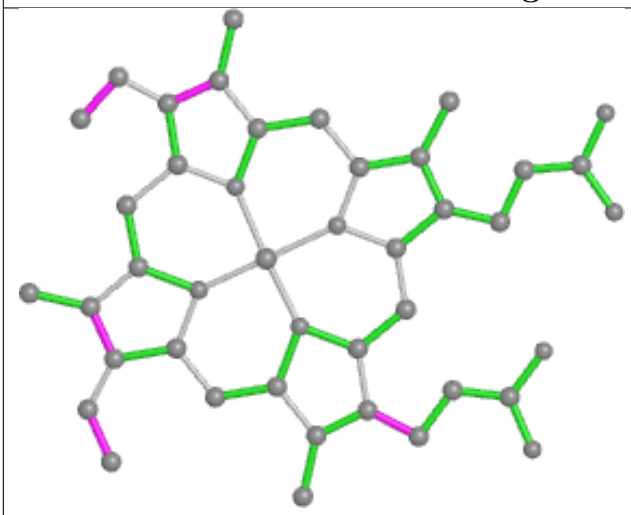
There are no ring outliers.

4 monomers are involved in 22 short contacts:

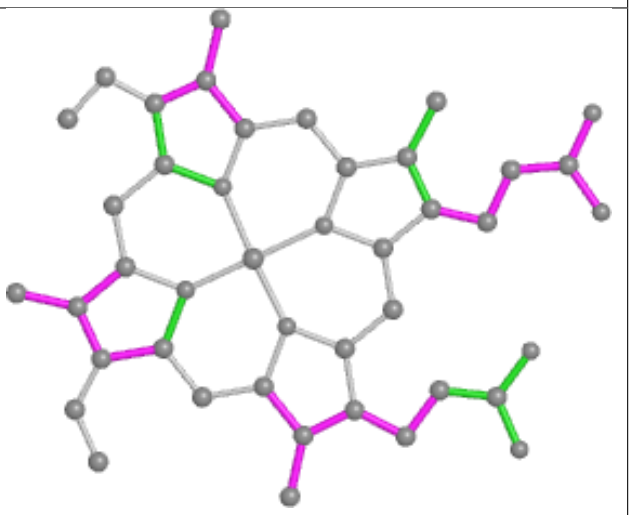
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	242	HEC	2	0
12	C	380	HEM	10	0
12	C	381	HEM	9	0
14	E	197	FES	1	0

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.

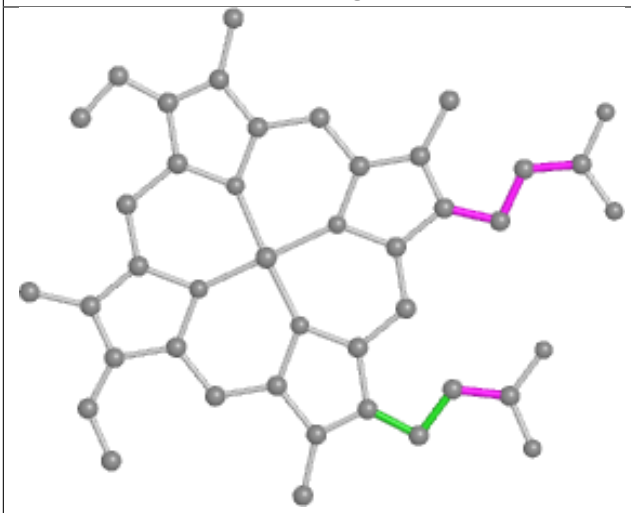
Ligand HEC D 242



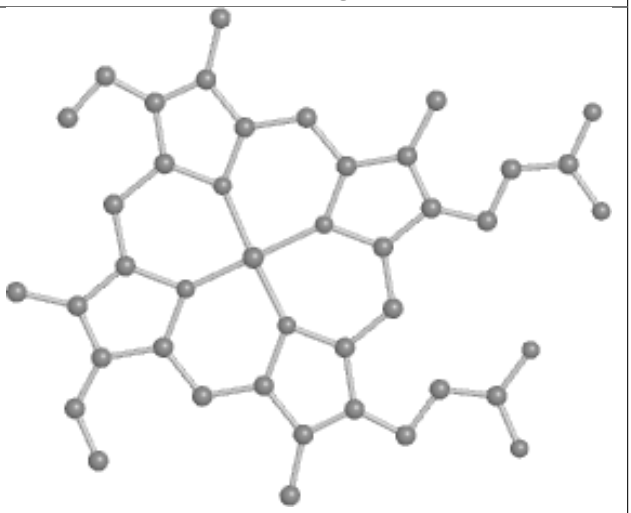
Bond lengths



Bond angles

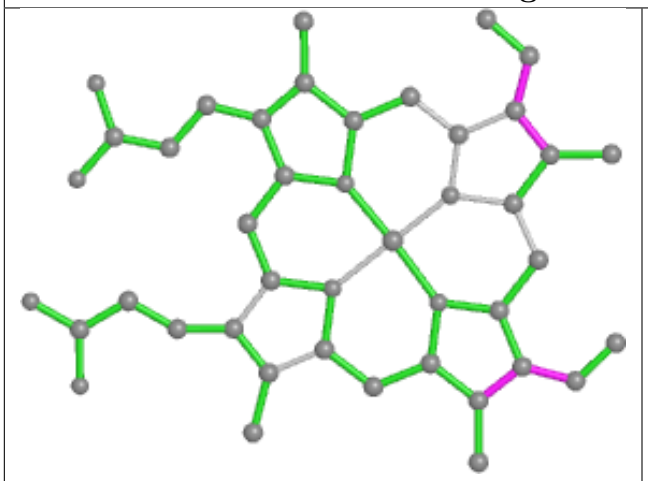


Torsions

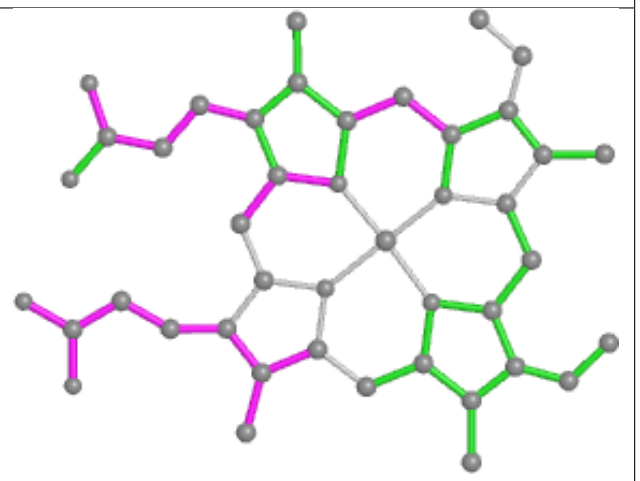


Rings

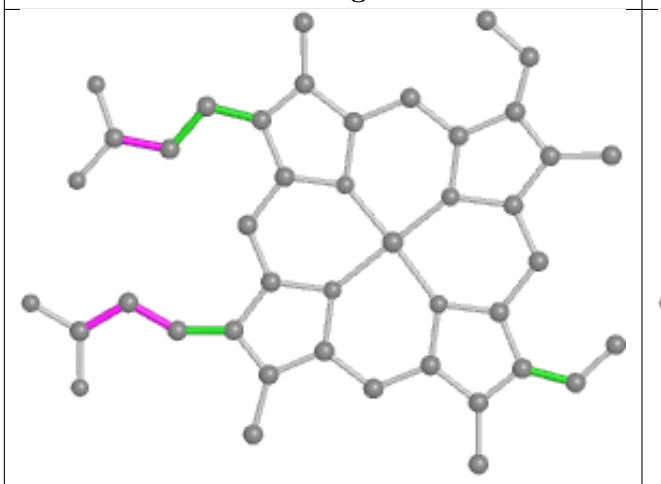
Ligand HEM C 380



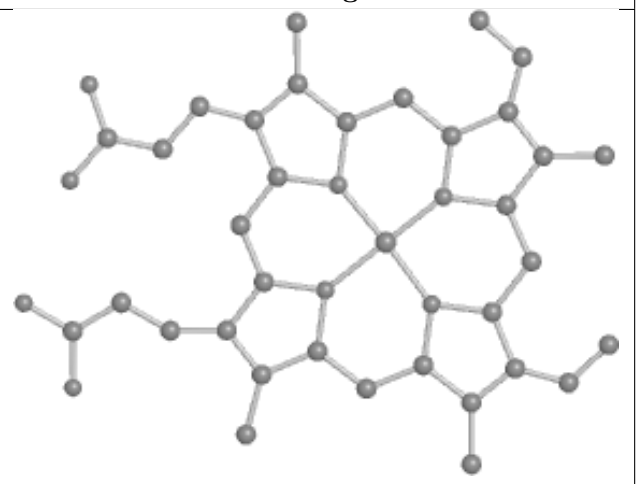
Bond lengths



Bond angles

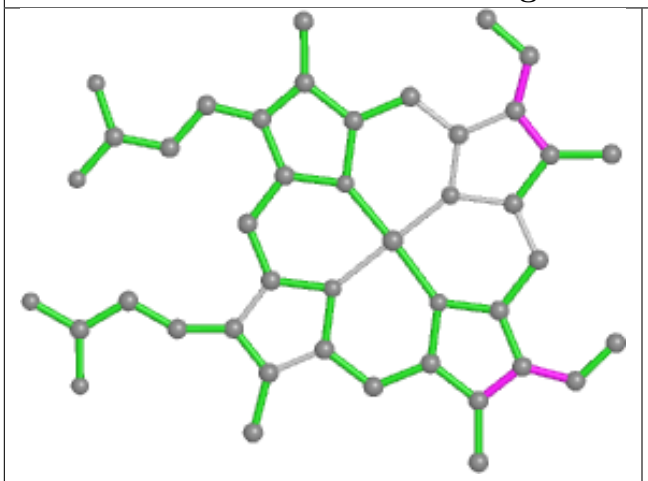


Torsions

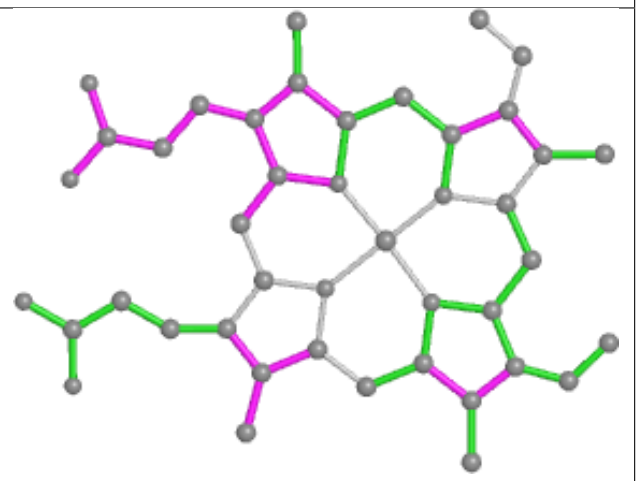


Rings

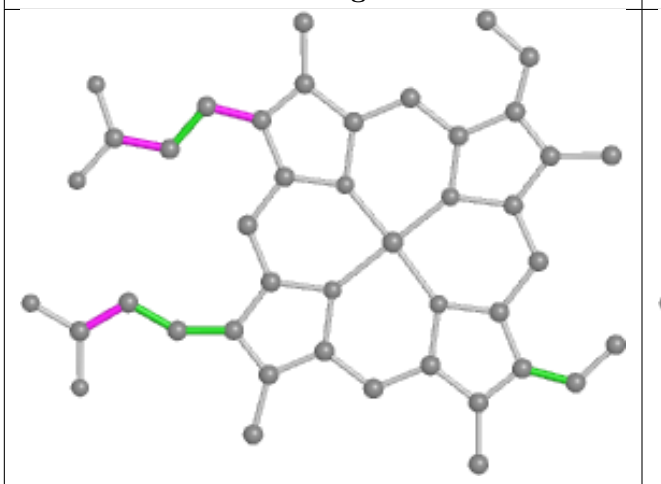
Ligand HEM C 381



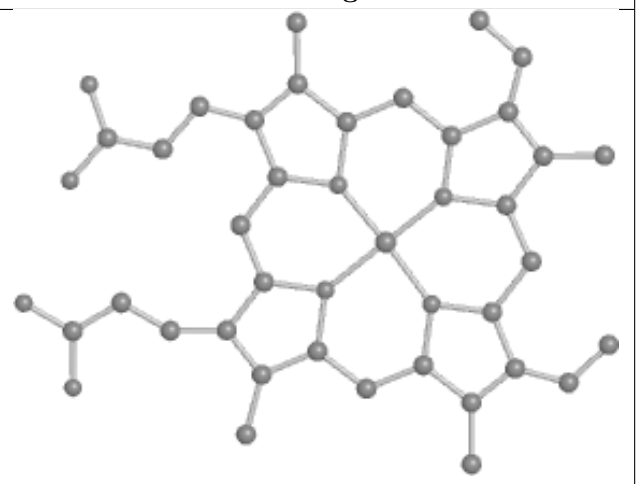
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.