



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:21 PM EDT

PDB ID : 1M54 / pdb_00001m54
Title : CYSTATHIONINE-BETA SYNTHASE: REDUCED VICINAL THIOLS
Authors : Taoka, S.; Lepore, B.W.; Kabil, O.; Ojha, S.; Ringe, D.; Banerjee, R.
Deposited on : 2002-07-08
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

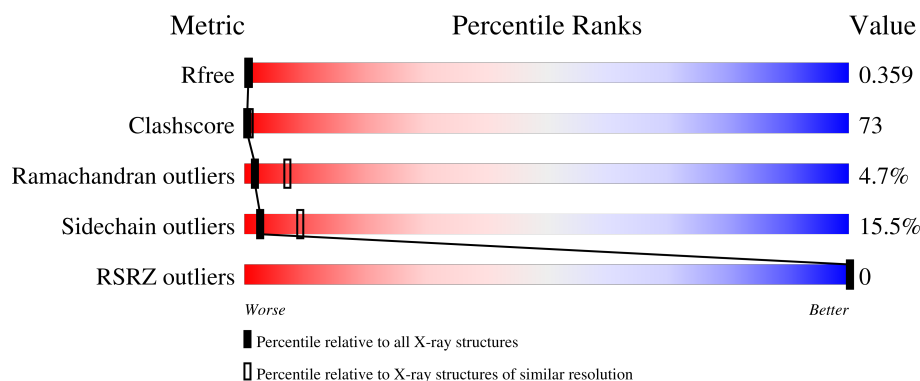
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	24% 51% 16% 6% .
1	B	363	27% 51% 15% . .
1	C	363	21% 58% 12% . 5%
1	D	363	20% 56% 15% . 5%
1	E	363	24% 53% 14% . .

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Mol	Chain	Length	Quality of chain
1	F	363	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	D	1410	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16403 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.

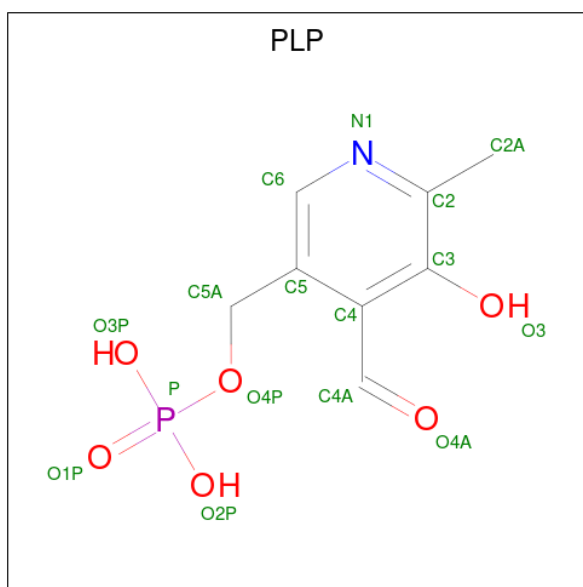
- Molecule 1 is a protein called CYSTATHIONINE BETA-SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2698	1692	471	518	17			
1	B	347	Total	C	N	O	S	0	0	0
			2660	1667	467	509	17			
1	C	346	Total	C	N	O	S	0	0	0
			2651	1664	464	506	17			
1	D	346	Total	C	N	O	S	0	0	0
			2651	1664	464	506	17			
1	E	347	Total	C	N	O	S	0	0	0
			2654	1665	464	508	17			
1	F	344	Total	C	N	O	S	0	0	0
			2637	1655	464	501	17			

There are 6 discrepancies between the modelled and reference sequences:

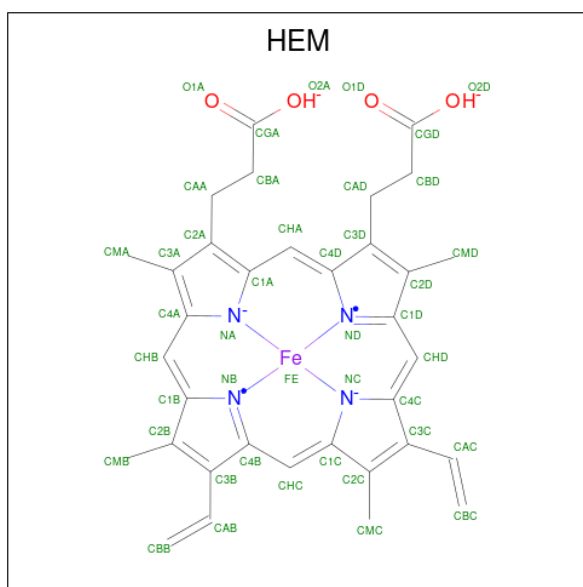
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	ILE	engineered mutation	UNP P35520
B	44	MET	ILE	engineered mutation	UNP P35520
C	44	MET	ILE	engineered mutation	UNP P35520
D	44	MET	ILE	engineered mutation	UNP P35520
E	44	MET	ILE	engineered mutation	UNP P35520
F	44	MET	ILE	engineered mutation	UNP P35520

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

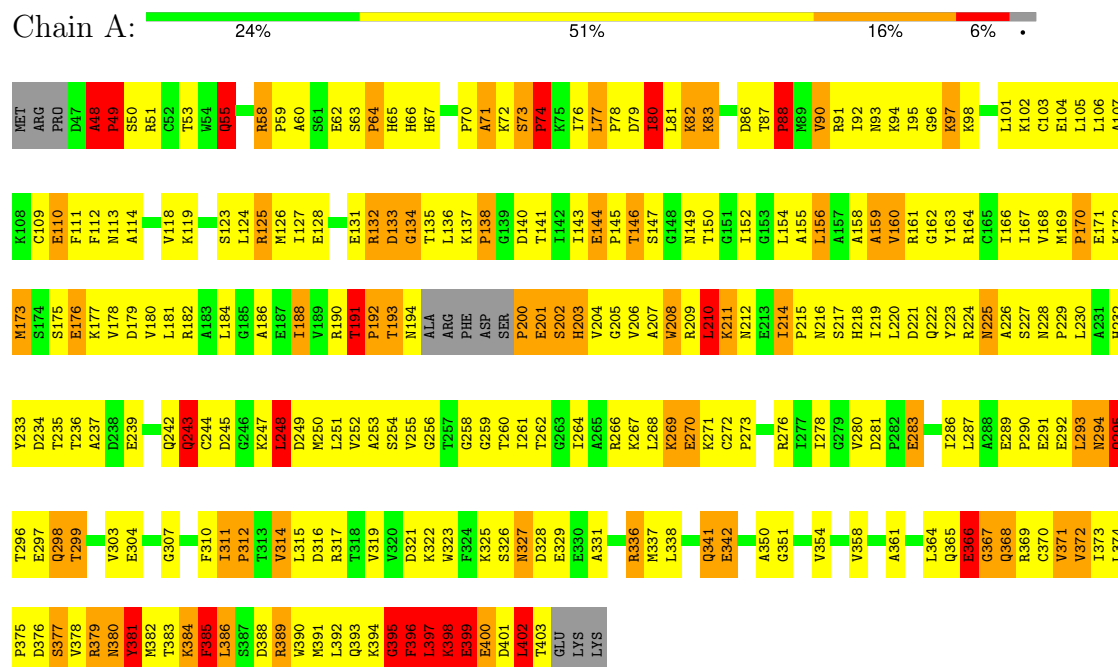
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	12	Total O 12 12	0	0
4	C	14	Total O 14 14	0	0
4	D	26	Total O 26 26	0	0
4	E	24	Total O 24 24	0	0
4	F	16	Total O 16 16	0	0

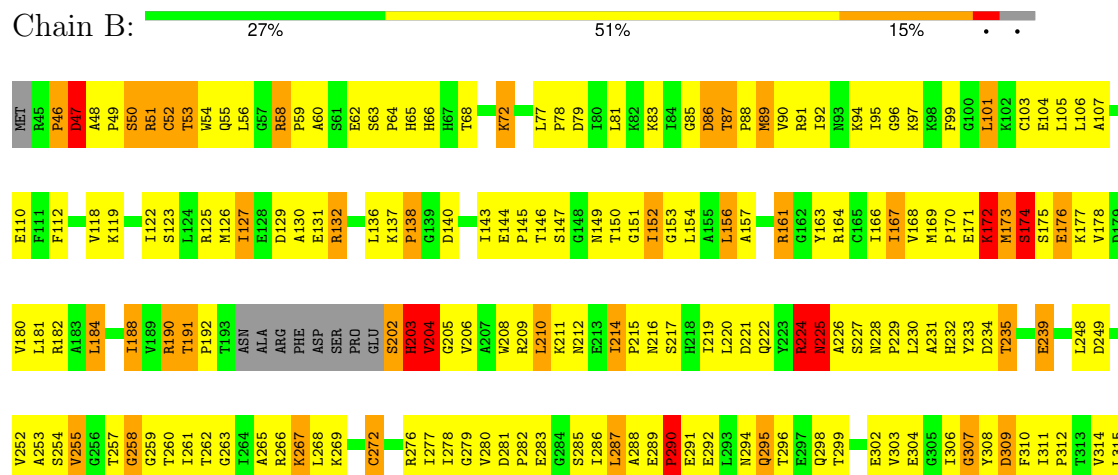
3 Residue-property plots

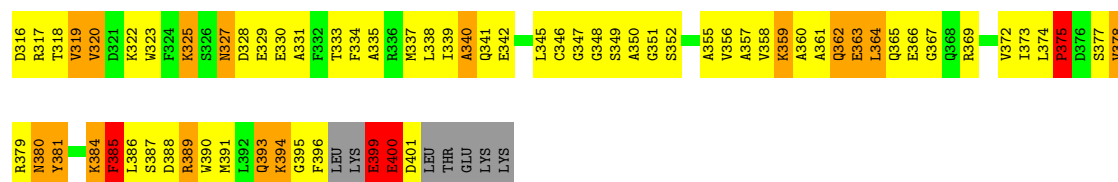
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: CYSTATHIONINE BETA-SYNTASE



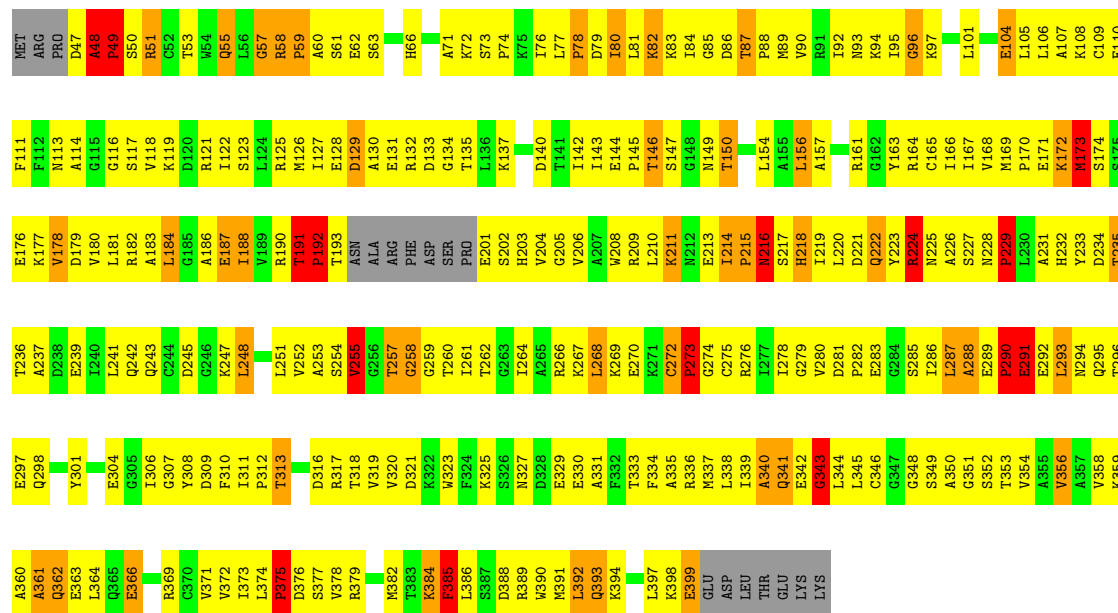
• Molecule 1: CYSTATHIONINE BETA-SYNTASE





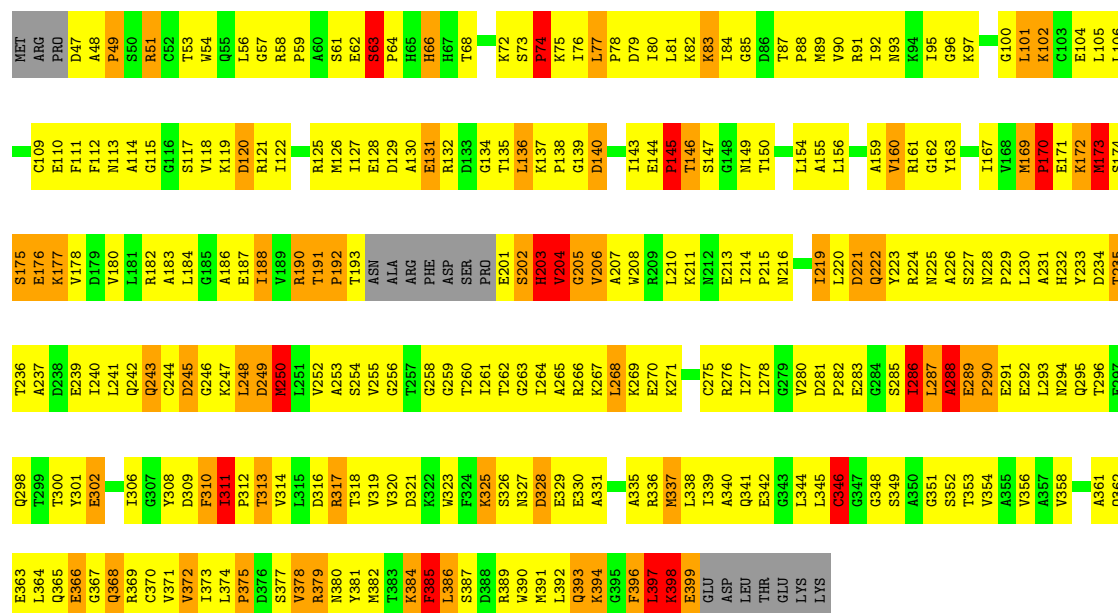
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain C: 21% 58% 12% 5%

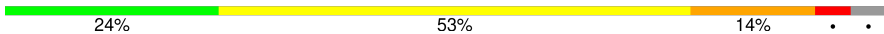


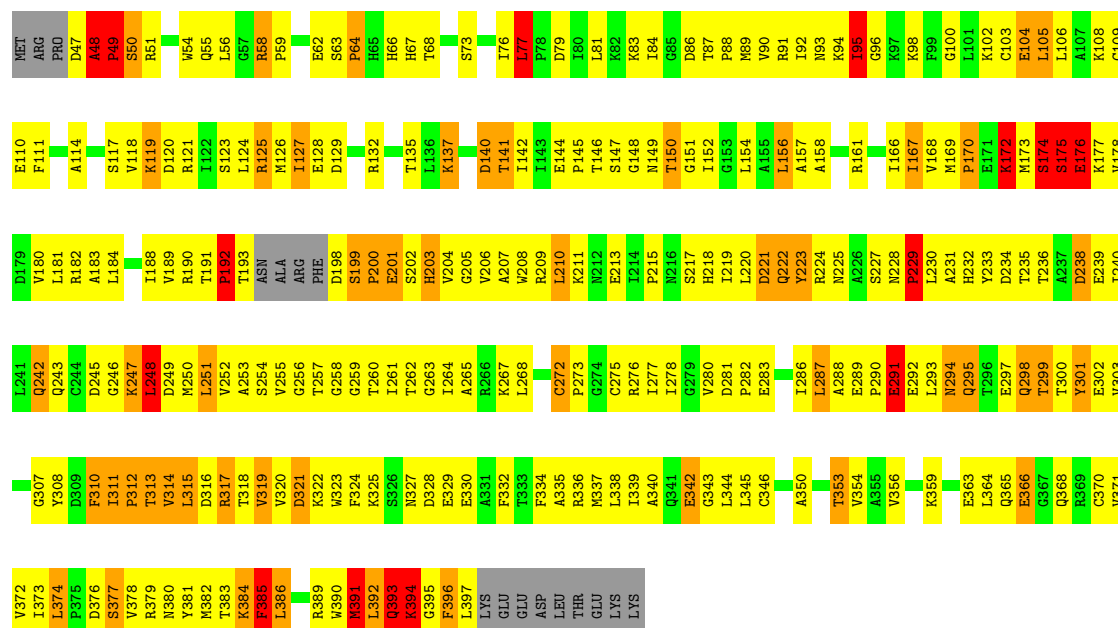
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain D: 20% 56% 15% 5%

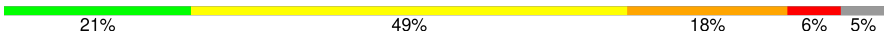


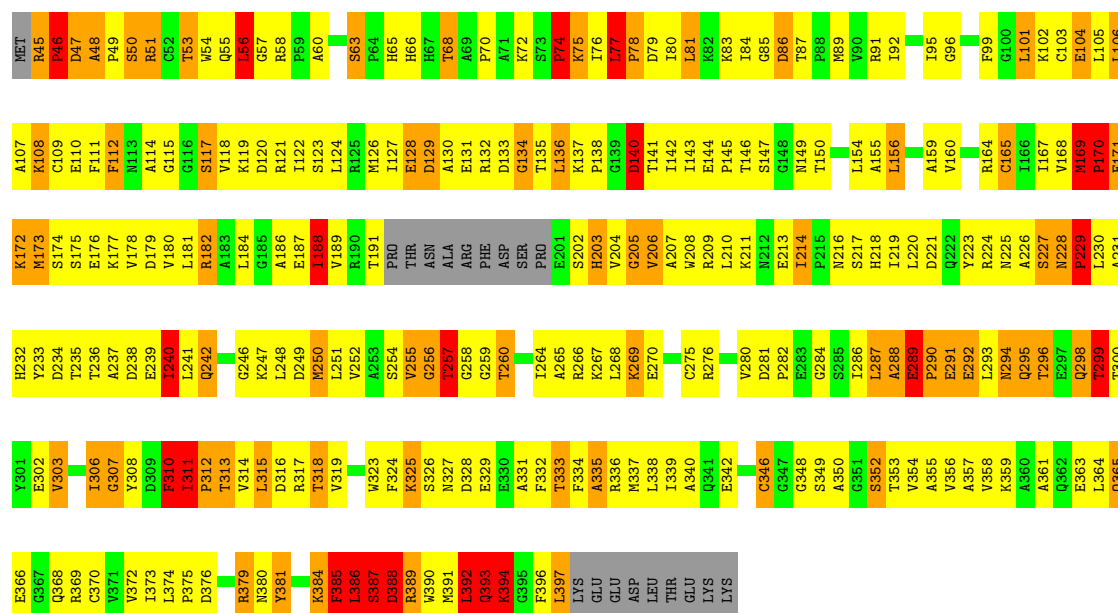
• Molecule 1: CYSTATHIONINE BETA-SYNTASE

Chain E:  24% 53% 14%



• Molecule 1: CYSTATHIONINE BETA-SYNTASE

Chain F:  21% 49% 18% 6% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.74Å 85.63Å 97.08Å 102.01° 101.53° 112.60°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.3 (50.00-2.90) 89.8 (50.00-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.365 0.274 , 0.359	Depositor DCC
R_{free} test set	8143 reflections (8.95%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16403	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4977e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.11	19/2744 (0.7%)	1.71	85/3709 (2.3%)
1	B	2.26	6/2705 (0.2%)	2.11	60/3655 (1.6%)
1	C	0.99	4/2696 (0.1%)	2.17	73/3643 (2.0%)
1	D	0.87	6/2696 (0.2%)	1.68	85/3643 (2.3%)
1	E	0.99	8/2700 (0.3%)	1.67	70/3651 (1.9%)
1	F	0.90	7/2682 (0.3%)	2.09	84/3624 (2.3%)
All	All	1.28	50/16223 (0.3%)	1.92	457/21925 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	225	ASN	N-CA	83.19	2.53	1.46
1	B	401	ASP	C-O	72.69	2.69	1.23
1	C	173	MET	N-CA	28.98	1.83	1.46
1	A	367	GLY	N-CA	23.52	1.79	1.45
1	E	176	GLU	N-CA	21.01	1.73	1.46
1	F	129	ASP	N-CA	15.25	1.64	1.46
1	E	329	GLU	N-CA	12.32	1.61	1.46
1	A	159	ALA	C-N	-11.71	1.19	1.33
1	E	394	LYS	N-CA	11.20	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	ARG	N-CA	11.06	1.61	1.45
1	A	380	ASN	N-CA	10.83	1.60	1.46
1	A	399	GLU	C-N	10.56	1.48	1.33
1	A	160	VAL	N-CA	-8.82	1.34	1.46
1	D	367	GLY	N-CA	8.13	1.56	1.45
1	A	399	GLU	N-CA	7.76	1.56	1.46
1	C	229	PRO	CA-C	-7.54	1.42	1.52
1	F	128	GLU	N-CA	7.51	1.55	1.46
1	A	74	PRO	N-CA	7.47	1.55	1.47
1	C	216	ASN	CA-C	7.42	1.62	1.52
1	E	221	ASP	C-N	7.27	1.43	1.33
1	A	399	GLU	CA-C	7.27	1.62	1.52
1	C	192	PRO	N-CA	7.18	1.56	1.47
1	E	221	ASP	N-CA	6.99	1.55	1.46
1	D	287	LEU	C-N	-6.51	1.24	1.33
1	A	342	GLU	N-CA	6.46	1.54	1.46
1	A	273	PRO	N-CA	6.21	1.55	1.47
1	A	73	SER	CA-C	6.18	1.60	1.53
1	F	229	PRO	CA-C	-6.17	1.43	1.52
1	A	371	VAL	N-CA	6.12	1.53	1.46
1	A	73	SER	N-CA	6.10	1.54	1.46
1	A	74	PRO	CA-C	-6.08	1.46	1.52
1	F	386	LEU	N-CA	-6.08	1.38	1.46
1	D	74	PRO	N-CA	6.03	1.54	1.47
1	E	220	LEU	C-N	6.01	1.42	1.33
1	B	235	THR	CA-C	6.01	1.57	1.52
1	A	398	LYS	C-N	5.97	1.42	1.33
1	B	47	ASP	C-N	-5.93	1.25	1.33
1	A	272	CYS	CA-C	5.90	1.58	1.52
1	D	289	GLU	N-CA	-5.56	1.38	1.46
1	D	289	GLU	CA-C	-5.42	1.46	1.52
1	A	73	SER	C-N	5.38	1.40	1.33
1	F	310	PHE	C-N	-5.36	1.28	1.33
1	F	311	ILE	N-CA	-5.31	1.42	1.46
1	F	50	SER	N-CA	5.29	1.53	1.46
1	D	289	GLU	C-N	-5.25	1.26	1.33
1	B	203	HIS	CB-CG	5.17	1.57	1.50
1	A	71	ALA	CA-CB	5.16	1.64	1.54
1	E	95	ILE	C-N	-5.13	1.26	1.33
1	B	290	PRO	CA-CB	-5.04	1.46	1.53
1	E	199	SER	C-N	5.03	1.40	1.33

All (457) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	45	ARG	CA-C-N	46.77	178.30	119.84
1	F	45	ARG	C-N-CA	46.77	178.30	119.84
1	B	289	GLU	CA-C-N	46.26	177.66	119.84
1	B	289	GLU	C-N-CA	46.26	177.66	119.84
1	C	48	ALA	CA-C-N	43.15	173.78	119.84
1	C	48	ALA	C-N-CA	43.15	173.78	119.84
1	C	289	GLU	CA-C-N	42.25	172.66	119.84
1	C	289	GLU	C-N-CA	42.25	172.66	119.84
1	B	225	ASN	N-CA-CB	30.25	161.61	110.49
1	F	129	ASP	N-CA-C	-26.16	79.24	112.72
1	B	47	ASP	CA-C-N	-23.82	97.50	122.74
1	B	47	ASP	C-N-CA	-23.82	97.50	122.74
1	B	224	ARG	CA-C-N	-23.47	76.71	121.54
1	B	224	ARG	C-N-CA	-23.47	76.71	121.54
1	A	161	ARG	N-CA-C	-21.54	85.71	113.72
1	E	48	ALA	CA-C-N	20.42	145.37	119.84
1	E	48	ALA	C-N-CA	20.42	145.37	119.84
1	E	176	GLU	N-CA-CB	18.91	142.44	110.49
1	B	401	ASP	CA-C-O	-18.74	88.94	120.80
1	D	289	GLU	CA-C-N	-18.42	101.34	119.76
1	D	289	GLU	C-N-CA	-18.42	101.34	119.76
1	B	225	ASN	N-CA-C	-18.25	71.93	110.80
1	D	222	GLN	N-CA-C	-17.91	91.55	113.41
1	F	46	PRO	CA-N-CD	-17.57	87.40	112.00
1	C	290	PRO	CA-N-CD	-17.50	87.50	112.00
1	A	366	GLU	CB-CA-C	16.71	134.90	109.84
1	A	367	GLY	N-CA-C	15.21	149.23	113.18
1	B	401	ASP	CA-CB-CG	-14.72	97.88	112.60
1	C	290	PRO	N-CA-CB	14.70	118.69	103.25
1	F	46	PRO	N-CA-CB	14.70	118.69	103.25
1	F	289	GLU	CA-C-N	-14.13	102.17	119.84
1	F	289	GLU	C-N-CA	-14.13	102.17	119.84
1	B	47	ASP	CB-CA-C	-13.90	90.24	112.06
1	E	329	GLU	N-CA-C	-13.72	93.38	112.45
1	E	394	LYS	N-CA-C	13.32	130.28	110.17
1	F	45	ARG	O-C-N	12.80	143.48	123.00
1	F	128	GLU	N-CA-CB	-12.24	91.76	110.73
1	C	191	THR	CA-C-N	12.09	134.95	119.84
1	C	191	THR	C-N-CA	12.09	134.95	119.84
1	C	290	PRO	N-CD-CG	11.95	121.12	103.20
1	B	289	GLU	C-N-CD	-11.89	76.27	125.00
1	F	229	PRO	CA-N-CD	-11.81	95.47	112.00
1	F	128	GLU	N-CA-C	11.75	128.04	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	173	MET	N-CA-C	-11.74	85.78	110.80
1	E	221	ASP	CA-C-N	11.59	139.21	122.05
1	E	221	ASP	C-N-CA	11.59	139.21	122.05
1	D	367	GLY	N-CA-C	11.54	129.93	114.92
1	F	46	PRO	N-CD-CG	11.54	120.50	103.20
1	C	48	ALA	C-N-CD	-11.50	77.85	125.00
1	F	140	ASP	N-CA-C	11.45	127.25	113.28
1	C	192	PRO	N-CA-C	11.26	135.66	112.47
1	D	365	GLN	OE1-CD-NE2	-11.13	111.47	122.60
1	D	206	VAL	N-CA-C	-11.08	95.93	111.89
1	A	342	GLU	N-CA-C	-10.92	99.69	113.23
1	B	400	GLU	CA-C-N	-10.85	102.17	121.70
1	B	400	GLU	C-N-CA	-10.85	102.17	121.70
1	A	203	HIS	CA-CB-CG	-10.76	103.04	113.80
1	C	341	GLN	CA-C-N	-10.69	106.78	122.07
1	C	341	GLN	C-N-CA	-10.69	106.78	122.07
1	E	394	LYS	N-CA-CB	-10.69	93.31	110.51
1	C	393	GLN	OE1-CD-NE2	-10.57	112.03	122.60
1	D	289	GLU	O-C-N	-10.57	109.16	121.32
1	F	65	HIS	N-CA-C	10.51	125.62	109.96
1	C	222	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	C	172	LYS	CA-C-N	-10.44	101.61	121.54
1	C	172	LYS	C-N-CA	-10.44	101.61	121.54
1	D	203	HIS	CA-CB-CG	-10.35	103.45	113.80
1	E	295	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	A	74	PRO	CA-N-CD	-10.28	97.61	112.00
1	A	341	GLN	OE1-CD-NE2	-10.23	112.37	122.60
1	D	160	VAL	CB-CA-C	-10.22	102.06	111.06
1	F	63	SER	CA-C-N	10.21	129.88	119.56
1	F	63	SER	C-N-CA	10.21	129.88	119.56
1	B	381	TYR	N-CA-C	10.15	124.98	112.59
1	C	341	GLN	OE1-CD-NE2	-10.15	112.45	122.60
1	A	402	LEU	N-CA-C	10.10	122.24	111.03
1	A	243	GLN	OE1-CD-NE2	-10.10	112.50	122.60
1	A	295	GLN	OE1-CD-NE2	-10.08	112.52	122.60
1	F	295	GLN	OE1-CD-NE2	-10.08	112.52	122.60
1	D	243	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	B	393	GLN	OE1-CD-NE2	-9.98	112.62	122.60
1	D	222	GLN	OE1-CD-NE2	-9.96	112.64	122.60
1	A	55	GLN	OE1-CD-NE2	-9.93	112.67	122.60
1	A	379	ARG	CA-C-N	-9.92	102.59	121.54
1	A	379	ARG	C-N-CA	-9.92	102.59	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	55	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	A	298	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	368	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	C	385	PHE	CA-CB-CG	9.74	123.54	113.80
1	A	273	PRO	N-CA-C	9.73	127.38	113.47
1	B	365	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	E	393	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	F	298	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	C	289	GLU	C-N-CD	-9.65	85.42	125.00
1	E	298	GLN	OE1-CD-NE2	-9.64	112.95	122.60
1	B	381	TYR	N-CA-CB	-9.64	95.50	110.92
1	F	311	ILE	N-CA-C	9.63	116.32	107.56
1	D	393	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	B	362	GLN	OE1-CD-NE2	-9.60	113.00	122.60
1	A	204	VAL	N-CA-C	-9.59	89.40	109.34
1	F	393	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	C	362	GLN	OE1-CD-NE2	-9.52	113.08	122.60
1	E	222	GLN	OE1-CD-NE2	-9.47	113.13	122.60
1	E	314	VAL	N-CA-C	-9.45	96.17	107.70
1	D	120	ASP	N-CA-C	-9.37	101.61	113.23
1	C	341	GLN	N-CA-C	-9.36	94.33	108.46
1	B	400	GLU	O-C-N	-9.34	109.98	122.49
1	A	204	VAL	CA-C-N	-9.32	103.14	121.41
1	A	204	VAL	C-N-CA	-9.32	103.14	121.41
1	F	75	LYS	N-CA-C	-9.31	99.38	112.13
1	F	310	PHE	CB-CA-C	-9.31	90.71	109.79
1	A	365	GLN	OE1-CD-NE2	-9.23	113.37	122.60
1	D	295	GLN	OE1-CD-NE2	-9.18	113.42	122.60
1	D	289	GLU	CA-C-O	-9.11	107.68	120.16
1	B	203	HIS	CA-CB-CG	9.03	122.83	113.80
1	E	298	GLN	N-CA-C	9.01	125.01	111.04
1	D	289	GLU	N-CA-C	9.01	129.71	109.81
1	E	313	THR	CA-C-N	8.99	130.96	121.97
1	E	313	THR	C-N-CA	8.99	130.96	121.97
1	D	84	ILE	N-CA-CB	-8.77	99.32	111.25
1	A	401	ASP	CA-C-N	8.77	132.55	120.63
1	A	401	ASP	C-N-CA	8.77	132.55	120.63
1	D	287	LEU	CA-C-N	-8.77	104.80	121.54
1	D	287	LEU	C-N-CA	-8.77	104.80	121.54
1	B	214	ILE	N-CA-C	8.74	116.20	107.55
1	A	370	CYS	CA-C-N	-8.71	108.81	120.91
1	A	370	CYS	C-N-CA	-8.71	108.81	120.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	LEU	N-CA-C	-8.70	92.26	110.80
1	F	169	MET	CA-C-N	8.60	130.59	119.84
1	F	169	MET	C-N-CA	8.60	130.59	119.84
1	C	59	PRO	N-CA-C	8.59	125.27	111.26
1	A	210	LEU	N-CA-C	-8.57	103.95	114.75
1	E	221	ASP	CA-C-O	8.56	130.05	120.80
1	F	310	PHE	CA-CB-CG	8.52	122.31	113.80
1	E	229	PRO	CA-N-CD	-8.49	100.11	112.00
1	E	176	GLU	N-CA-C	-8.48	92.74	110.80
1	E	200	PRO	CA-N-CD	-8.42	100.21	112.00
1	B	87	THR	CA-C-N	8.35	128.28	119.85
1	B	87	THR	C-N-CA	8.35	128.28	119.85
1	A	396	PHE	CA-CB-CG	8.31	122.11	113.80
1	D	74	PRO	CA-N-CD	-8.31	100.37	112.00
1	B	50	SER	N-CA-C	-8.27	102.06	112.90
1	F	45	ARG	C-N-CD	-8.26	91.12	125.00
1	D	385	PHE	CA-CB-CG	8.23	122.03	113.80
1	F	104	GLU	N-CA-C	-8.23	98.30	110.48
1	E	86	ASP	N-CA-C	-8.20	102.58	112.58
1	F	134	GLY	N-CA-C	-8.16	103.92	115.43
1	B	399	GLU	CB-CA-C	-8.12	94.66	110.10
1	B	112	PHE	N-CA-C	8.11	123.01	113.20
1	A	255	VAL	N-CA-C	7.99	119.35	108.17
1	A	74	PRO	CB-CA-C	-7.93	99.01	110.75
1	F	388	ASP	CA-C-N	-7.93	109.77	120.79
1	F	388	ASP	C-N-CA	-7.93	109.77	120.79
1	F	295	GLN	CA-C-N	7.91	132.10	120.87
1	F	295	GLN	C-N-CA	7.91	132.10	120.87
1	D	250	MET	N-CA-C	7.87	127.56	110.80
1	E	49	PRO	N-CA-C	7.87	128.68	112.47
1	E	200	PRO	N-CA-C	-7.78	103.14	113.65
1	C	104	GLU	N-CA-C	-7.77	100.06	110.55
1	F	214	ILE	CA-C-N	7.70	127.71	119.78
1	F	214	ILE	C-N-CA	7.70	127.71	119.78
1	A	399	GLU	N-CA-C	7.69	127.17	110.80
1	A	73	SER	CA-C-N	7.58	128.02	120.52
1	A	73	SER	C-N-CA	7.58	128.02	120.52
1	F	128	GLU	CA-C-N	-7.55	108.88	122.46
1	F	128	GLU	C-N-CA	-7.55	108.88	122.46
1	B	172	LYS	CA-C-N	7.53	135.92	121.54
1	B	172	LYS	C-N-CA	7.53	135.92	121.54
1	E	209	ARG	N-CA-C	-7.51	104.57	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	229	PRO	O-C-N	7.51	131.24	122.23
1	A	386	LEU	N-CA-C	-7.46	103.00	112.93
1	F	388	ASP	CA-CB-CG	7.39	119.99	112.60
1	E	175	SER	CA-C-N	-7.38	107.44	121.54
1	E	175	SER	C-N-CA	-7.38	107.44	121.54
1	B	295	GLN	N-CA-C	7.35	122.10	107.62
1	D	146	THR	N-CA-C	7.35	120.98	109.96
1	F	86	ASP	N-CA-C	-7.32	103.64	112.58
1	E	222	GLN	CG-CD-NE2	7.32	127.37	116.40
1	A	88	PRO	CA-N-CD	-7.31	101.77	112.00
1	E	295	GLN	CG-CD-NE2	7.30	127.34	116.40
1	B	393	GLN	CG-CD-NE2	7.29	127.34	116.40
1	E	314	VAL	CA-C-O	-7.29	115.78	120.66
1	E	221	ASP	N-CA-C	7.28	121.22	110.30
1	E	393	GLN	CG-CD-NE2	7.27	127.31	116.40
1	C	229	PRO	CA-N-CD	-7.27	101.83	112.00
1	C	362	GLN	CG-CD-NE2	7.24	127.26	116.40
1	C	375	PRO	N-CA-C	7.23	127.36	112.47
1	C	393	GLN	CG-CD-NE2	7.22	127.23	116.40
1	F	295	GLN	CG-CD-NE2	7.22	127.23	116.40
1	E	221	ASP	O-C-N	7.20	132.94	123.07
1	F	303	VAL	CA-C-N	7.17	132.66	121.26
1	F	303	VAL	C-N-CA	7.17	132.66	121.26
1	D	310	PHE	N-CA-C	7.13	123.51	114.31
1	B	365	GLN	CG-CD-NE2	7.12	127.08	116.40
1	F	313	THR	N-CA-C	-7.11	104.07	112.89
1	D	295	GLN	CG-CD-NE2	7.11	127.07	116.40
1	A	295	GLN	CG-CD-NE2	7.10	127.05	116.40
1	C	192	PRO	CA-N-CD	-7.08	102.08	112.00
1	D	243	GLN	CG-CD-NE2	7.07	127.00	116.40
1	A	88	PRO	CA-C-N	-7.04	113.07	122.99
1	A	88	PRO	C-N-CA	-7.04	113.07	122.99
1	B	290	PRO	CA-N-CD	-7.02	102.17	112.00
1	C	173	MET	N-CA-CB	6.99	122.31	110.49
1	A	341	GLN	CG-CD-NE2	6.99	126.88	116.40
1	A	398	LYS	N-CA-C	6.96	119.18	109.15
1	A	401	ASP	N-CA-C	6.96	119.45	108.67
1	D	73	SER	CA-C-N	6.92	126.88	120.03
1	D	73	SER	C-N-CA	6.92	126.88	120.03
1	D	204	VAL	N-CA-C	-6.92	94.94	109.34
1	C	222	GLN	CG-CD-NE2	6.89	126.74	116.40
1	D	310	PHE	CB-CA-C	-6.87	97.48	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	ALA	N-CA-C	6.87	118.77	111.28
1	D	290	PRO	N-CA-C	-6.86	100.42	111.19
1	E	96	GLY	N-CA-C	-6.85	96.94	113.18
1	F	46	PRO	CB-CA-C	6.84	122.86	111.56
1	E	105	LEU	CB-CA-C	-6.83	99.74	112.30
1	A	192	PRO	N-CA-C	-6.81	103.94	113.81
1	B	290	PRO	N-CA-C	-6.80	98.46	112.47
1	C	49	PRO	CA-N-CD	-6.79	102.50	112.00
1	E	222	GLN	O-C-N	6.77	131.18	122.71
1	A	193	THR	CA-C-N	-6.75	109.54	121.70
1	A	193	THR	C-N-CA	-6.75	109.54	121.70
1	E	192	PRO	CA-N-CD	-6.75	102.55	112.00
1	D	288	ALA	CA-C-N	-6.73	105.38	121.80
1	D	288	ALA	C-N-CA	-6.73	105.38	121.80
1	D	366	GLU	CA-C-N	-6.73	111.95	122.51
1	D	366	GLU	C-N-CA	-6.73	111.95	122.51
1	E	51	ARG	N-CA-C	-6.70	104.42	112.59
1	E	298	GLN	CG-CD-NE2	6.70	126.45	116.40
1	D	205	GLY	CA-C-N	-6.70	109.67	120.86
1	D	205	GLY	C-N-CA	-6.70	109.67	120.86
1	A	73	SER	N-CA-C	6.67	119.08	109.48
1	F	290	PRO	CB-CA-C	6.67	122.57	111.56
1	D	222	GLN	CG-CD-NE2	6.66	126.39	116.40
1	D	384	LYS	N-CA-C	6.66	118.66	109.54
1	A	159	ALA	O-C-N	6.65	129.17	122.12
1	E	272	CYS	CA-C-N	6.64	128.15	119.84
1	E	272	CYS	C-N-CA	6.64	128.15	119.84
1	F	393	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	397	LEU	N-CA-C	6.61	124.88	110.80
1	D	365	GLN	CG-CD-NE2	6.60	126.30	116.40
1	F	55	GLN	CG-CD-NE2	6.60	126.30	116.40
1	A	381	TYR	N-CA-C	6.58	121.02	112.92
1	C	129	ASP	N-CA-C	-6.56	105.38	113.19
1	A	74	PRO	CA-C-N	-6.56	111.99	120.65
1	A	74	PRO	C-N-CA	-6.56	111.99	120.65
1	B	312	PRO	CB-CA-C	6.55	119.96	111.64
1	D	131	GLU	N-CA-C	-6.53	104.00	112.23
1	F	240	ILE	CB-CA-C	6.53	121.99	111.29
1	A	365	GLN	CG-CD-NE2	6.52	126.18	116.40
1	D	140	ASP	CA-CB-CG	-6.50	106.09	112.60
1	F	312	PRO	N-CA-C	6.50	121.45	111.11
1	F	290	PRO	N-CA-C	-6.49	99.10	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	GLY	N-CA-C	-6.49	107.36	115.08
1	F	77	LEU	CA-C-N	6.45	126.21	119.05
1	F	77	LEU	C-N-CA	6.45	126.21	119.05
1	D	393	GLN	CG-CD-NE2	6.44	126.06	116.40
1	F	298	GLN	CG-CD-NE2	6.43	126.05	116.40
1	B	364	LEU	N-CA-C	6.42	118.59	110.24
1	F	117	SER	N-CA-C	6.42	117.05	108.38
1	A	243	GLN	CG-CD-NE2	6.41	126.02	116.40
1	D	145	PRO	CA-N-CD	-6.41	103.03	112.00
1	D	63	SER	CA-C-N	6.41	125.83	118.85
1	D	63	SER	C-N-CA	6.41	125.83	118.85
1	D	255	VAL	N-CA-C	6.40	116.89	106.72
1	B	375	PRO	N-CA-C	6.39	124.13	113.78
1	C	235	THR	CB-CA-C	-6.39	98.29	109.02
1	D	192	PRO	CB-CA-C	6.39	122.10	111.56
1	B	283	GLU	N-CA-C	-6.38	101.50	110.50
1	A	82	LYS	N-CA-C	-6.38	105.60	113.19
1	E	117	SER	N-CA-C	6.36	117.51	108.74
1	D	235	THR	N-CA-C	6.35	120.92	111.96
1	C	224	ARG	CB-CA-C	-6.35	100.84	109.28
1	B	362	GLN	CG-CD-NE2	6.33	125.89	116.40
1	E	105	LEU	N-CA-C	6.32	118.92	111.02
1	A	298	GLN	CG-CD-NE2	6.31	125.87	116.40
1	F	60	ALA	N-CA-C	-6.28	103.71	111.75
1	D	147	SER	N-CA-C	-6.26	106.18	113.88
1	C	341	GLN	CG-CD-NE2	6.26	125.79	116.40
1	D	170	PRO	CB-CA-C	6.26	121.89	111.56
1	A	55	GLN	CG-CD-NE2	6.26	125.79	116.40
1	F	296	THR	N-CA-C	-6.26	101.02	110.28
1	B	171	GLU	CA-C-N	6.24	133.46	121.54
1	B	171	GLU	C-N-CA	6.24	133.46	121.54
1	C	293	LEU	N-CA-C	6.20	124.01	110.80
1	F	392	LEU	CA-C-N	-6.20	109.70	121.54
1	F	392	LEU	C-N-CA	-6.20	109.70	121.54
1	C	273	PRO	CB-CA-C	6.18	121.76	111.56
1	A	133	ASP	CA-CB-CG	6.17	118.77	112.60
1	F	284	GLY	N-CA-C	-6.16	106.65	115.64
1	C	340	ALA	N-CA-C	6.14	117.81	110.44
1	C	191	THR	O-C-N	6.14	128.38	121.32
1	C	255	VAL	N-CA-C	6.11	116.92	108.12
1	D	385	PHE	N-CA-CB	6.11	120.81	110.49
1	B	239	GLU	N-CA-C	-6.10	104.55	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	384	LYS	N-CA-C	-6.10	100.26	108.86
1	B	375	PRO	CA-N-CD	-6.07	103.50	112.00
1	A	366	GLU	N-CA-C	-6.06	101.33	110.24
1	C	361	ALA	CA-C-N	-6.06	109.97	121.54
1	C	361	ALA	C-N-CA	-6.06	109.97	121.54
1	B	255	VAL	N-CA-C	6.05	116.58	108.11
1	D	386	LEU	N-CA-C	-6.04	105.40	112.89
1	D	75	LYS	N-CA-C	-6.04	104.33	111.03
1	D	290	PRO	CA-N-CD	-6.02	103.57	112.00
1	A	368	GLN	CG-CD-NE2	6.02	125.43	116.40
1	D	129	ASP	N-CA-C	-6.01	106.10	113.50
1	C	49	PRO	N-CA-C	6.01	124.86	112.47
1	A	248	LEU	N-CA-C	-6.00	99.57	108.99
1	F	81	LEU	CB-CA-C	6.00	122.36	110.42
1	A	272	CYS	CA-C-N	5.99	125.20	118.97
1	A	272	CYS	C-N-CA	5.99	125.20	118.97
1	A	385	PHE	CA-CB-CG	5.98	119.78	113.80
1	D	397	LEU	N-CA-C	5.97	123.53	110.80
1	E	203	HIS	N-CA-C	-5.97	104.83	114.09
1	E	64	PRO	N-CA-C	-5.95	106.30	114.98
1	A	48	ALA	N-CA-C	5.94	122.94	109.81
1	E	172	LYS	N-CA-C	5.94	120.60	113.23
1	C	178	VAL	N-CA-C	-5.93	104.73	110.72
1	F	346	CYS	CA-C-N	-5.93	117.15	122.43
1	F	346	CYS	C-N-CA	-5.93	117.15	122.43
1	A	365	GLN	CA-C-N	5.92	129.51	121.05
1	A	365	GLN	C-N-CA	5.92	129.51	121.05
1	D	385	PHE	N-CA-C	-5.87	98.29	110.80
1	C	221	ASP	N-CA-C	5.87	117.96	108.34
1	C	289	GLU	O-C-N	5.87	128.07	121.32
1	D	368	GLN	N-CA-C	-5.86	101.06	110.14
1	F	333	THR	N-CA-C	-5.84	104.61	110.97
1	D	397	LEU	CA-C-N	-5.82	110.42	121.54
1	D	397	LEU	C-N-CA	-5.82	110.42	121.54
1	D	249	ASP	N-CA-C	-5.82	99.68	107.88
1	E	48	ALA	C-N-CD	-5.82	101.14	125.00
1	D	221	ASP	CA-C-O	5.81	127.08	120.80
1	B	47	ASP	CA-C-O	-5.80	115.54	122.27
1	E	312	PRO	CB-CA-C	5.80	119.00	111.64
1	C	356	VAL	N-CA-C	-5.79	107.21	111.90
1	A	200	PRO	CB-CA-C	5.76	121.05	110.10
1	A	90	VAL	N-CA-C	5.75	116.27	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ILE	N-CA-C	5.73	113.73	107.60
1	C	290	PRO	CB-CA-C	5.73	121.01	111.56
1	C	59	PRO	O-C-N	-5.71	115.88	122.85
1	A	144	GLU	CA-C-N	5.71	125.41	119.64
1	A	144	GLU	C-N-CA	5.71	125.41	119.64
1	B	58	ARG	CA-C-N	5.70	125.72	119.90
1	B	58	ARG	C-N-CA	5.70	125.72	119.90
1	C	295	GLN	N-CA-C	5.70	118.92	107.41
1	A	161	ARG	N-CA-CB	5.69	119.02	110.65
1	F	188	ILE	N-CA-C	5.69	117.19	108.71
1	C	385	PHE	N-CA-C	5.68	122.91	110.80
1	A	380	ASN	N-CA-C	5.66	122.85	110.80
1	D	321	ASP	N-CA-C	5.65	120.17	113.28
1	E	95	ILE	CB-CA-C	-5.64	102.05	111.29
1	C	258	GLY	N-CA-C	-5.62	108.00	114.69
1	D	221	ASP	N-CA-CB	5.61	118.48	109.28
1	F	260	THR	N-CA-C	5.61	117.20	111.14
1	D	337	MET	N-CA-C	-5.61	104.38	111.11
1	F	46	PRO	N-CA-C	-5.61	100.92	112.47
1	E	140	ASP	N-CA-C	5.60	118.24	111.40
1	E	374	LEU	CA-C-N	5.59	126.83	119.84
1	E	374	LEU	C-N-CA	5.59	126.83	119.84
1	A	184	LEU	N-CA-C	-5.59	106.35	114.12
1	B	224	ARG	O-C-N	-5.58	117.09	123.40
1	D	378	VAL	N-CA-C	5.58	116.31	110.62
1	B	89	MET	N-CA-C	-5.57	100.11	109.07
1	C	289	GLU	CA-C-O	5.55	127.77	120.16
1	E	229	PRO	N-CA-C	-5.55	105.82	113.53
1	C	272	CYS	CA-C-N	-5.54	112.91	119.84
1	C	272	CYS	C-N-CA	-5.54	112.91	119.84
1	C	392	LEU	CB-CA-C	-5.54	99.63	110.11
1	F	56	LEU	CA-C-N	5.54	132.26	121.41
1	F	56	LEU	C-N-CA	5.54	132.26	121.41
1	C	63	SER	N-CA-C	5.53	117.04	110.07
1	F	299	THR	N-CA-C	5.52	119.52	112.12
1	A	389	ARG	N-CA-C	-5.50	105.28	111.28
1	C	218	HIS	CA-CB-CG	-5.48	108.32	113.80
1	D	203	HIS	CB-CA-C	-5.46	99.56	110.42
1	F	335	ALA	N-CA-C	-5.45	104.74	111.33
1	F	289	GLU	N-CA-C	5.45	121.85	109.81
1	E	291	GLU	N-CA-C	-5.43	106.61	113.18
1	A	86	ASP	N-CA-C	-5.42	105.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	396	PHE	CA-C-N	-5.40	111.23	121.54
1	D	396	PHE	C-N-CA	-5.40	111.23	121.54
1	F	56	LEU	O-C-N	5.40	129.53	123.06
1	C	343	GLY	N-CA-C	5.39	125.96	113.18
1	D	286	ILE	CA-C-N	5.39	131.84	121.54
1	D	286	ILE	C-N-CA	5.39	131.84	121.54
1	A	64	PRO	N-CA-C	-5.39	101.38	112.47
1	E	77	LEU	N-CA-C	-5.39	102.86	109.65
1	E	314	VAL	O-C-N	-5.38	117.30	122.94
1	D	160	VAL	N-CA-C	5.36	118.32	112.96
1	F	229	PRO	N-CA-CB	5.36	109.22	103.33
1	A	211	LYS	N-CA-C	-5.35	105.14	110.97
1	B	172	LYS	N-CA-C	5.34	122.18	110.80
1	F	269	LYS	N-CA-C	-5.34	105.57	111.71
1	F	203	HIS	N-CA-C	5.33	117.52	111.02
1	C	270	GLU	N-CA-C	-5.32	105.05	112.45
1	E	314	VAL	CB-CA-C	5.32	116.74	111.74
1	F	102	LYS	N-CA-C	-5.31	107.34	113.88
1	F	291	GLU	N-CA-C	-5.31	106.04	113.37
1	E	384	LYS	N-CA-C	-5.29	101.39	109.65
1	C	234	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	53	THR	CB-CA-C	-5.29	104.43	111.88
1	B	86	ASP	N-CA-C	-5.28	105.64	113.40
1	B	389	ARG	N-CA-C	-5.27	105.23	110.97
1	B	49	PRO	CB-CA-C	5.26	118.24	111.56
1	C	257	THR	N-CA-C	-5.26	105.96	112.38
1	F	112	PHE	N-CA-C	-5.26	107.39	112.97
1	A	365	GLN	N-CA-C	5.26	117.67	109.52
1	F	165	CYS	N-CA-C	5.26	118.05	109.59
1	D	102	LYS	N-CA-C	-5.25	106.72	113.23
1	A	293	LEU	CB-CA-C	-5.24	99.99	110.42
1	D	84	ILE	N-CA-C	5.24	115.51	108.17
1	E	176	GLU	CB-CG-CD	5.23	121.49	112.60
1	C	87	THR	CA-C-N	5.23	125.43	120.31
1	C	87	THR	C-N-CA	5.23	125.43	120.31
1	A	204	VAL	CA-C-O	-5.21	114.27	120.78
1	F	299	THR	CB-CA-C	-5.21	102.61	111.26
1	C	192	PRO	CA-C-N	-5.19	112.35	121.70
1	C	192	PRO	C-N-CA	-5.19	112.35	121.70
1	E	191	THR	CA-C-N	5.19	126.33	119.84
1	E	191	THR	C-N-CA	5.19	126.33	119.84
1	A	377	SER	N-CA-C	5.18	118.08	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	172	LYS	CA-C-N	-5.18	111.64	121.54
1	E	172	LYS	C-N-CA	-5.18	111.64	121.54
1	C	146	THR	N-CA-C	5.18	117.08	108.02
1	B	400	GLU	N-CA-CB	-5.17	102.92	110.53
1	A	191	THR	O-C-N	5.17	125.85	121.20
1	C	186	ALA	N-CA-C	5.17	118.13	110.48
1	A	170	PRO	CB-CA-C	5.16	118.00	111.39
1	E	311	ILE	N-CA-C	5.16	112.26	107.56
1	D	249	ASP	CA-C-N	-5.14	111.72	121.54
1	D	249	ASP	C-N-CA	-5.14	111.72	121.54
1	C	288	ALA	N-CA-C	5.13	117.48	109.52
1	C	214	ILE	CB-CA-C	-5.13	104.88	110.78
1	B	46	PRO	CA-N-CD	-5.13	104.82	112.00
1	E	137	LYS	N-CA-C	5.12	116.52	110.07
1	E	104	GLU	CA-C-N	5.11	130.55	122.78
1	E	104	GLU	C-N-CA	5.11	130.55	122.78
1	A	291	GLU	N-CA-C	-5.11	105.90	111.82
1	D	302	GLU	N-CA-C	5.11	118.66	112.23
1	C	384	LYS	N-CA-C	-5.10	101.69	109.65
1	F	325	LYS	N-CA-C	-5.10	103.79	110.53
1	B	252	VAL	N-CA-C	-5.10	101.06	109.12
1	D	271	LYS	CA-C-N	5.10	127.51	122.00
1	D	271	LYS	C-N-CA	5.10	127.51	122.00
1	A	188	ILE	N-CA-C	5.09	115.30	108.17
1	D	310	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	395	GLY	O-C-N	5.09	129.32	122.70
1	D	221	ASP	O-C-N	5.09	130.05	123.07
1	E	73	SER	CA-C-N	5.09	126.20	119.84
1	E	73	SER	C-N-CA	5.09	126.20	119.84
1	E	49	PRO	CA-N-CD	-5.09	104.88	112.00
1	F	56	LEU	CA-C-O	5.08	126.50	120.96
1	E	255	VAL	N-CA-C	5.07	115.28	107.77
1	B	210	LEU	N-CA-C	-5.06	107.17	113.55
1	B	151	GLY	N-CA-C	-5.01	109.10	115.31
1	D	177	LYS	CA-C-N	5.01	127.59	120.53
1	D	177	LYS	C-N-CA	5.01	127.59	120.53

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	400	GLU	Mainchain
1	C	224	ARG	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2698	0	2721	383	0
1	B	2660	0	2678	345	0
1	C	2651	0	2678	427	0
1	D	2651	0	2679	460	1
1	E	2654	0	2676	468	1
1	F	2637	0	2668	414	0
2	A	15	0	7	2	0
2	B	15	0	7	2	0
2	C	15	0	7	4	0
2	D	15	0	7	6	0
2	E	15	0	7	2	0
2	F	15	0	7	2	0
3	A	43	0	30	6	0
3	B	43	0	30	6	0
3	C	43	0	30	9	0
3	D	43	0	30	8	0
3	E	43	0	30	6	0
3	F	43	0	30	10	0
4	A	12	0	0	1	0
4	B	12	0	0	0	0
4	C	14	0	0	2	0
4	D	26	0	0	1	0
4	E	24	0	0	0	0
4	F	16	0	0	4	0
All	All	16403	0	16322	2395	1

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 73.

All (2395) 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:D:203:HIS:CE1	1:D:204:VAL:CG1	1.87	1.56
1:E:176:GLU:N	1:E:176:GLU:CA	1.73	1.49
1:D:203:HIS:CE1	1:D:204:VAL:HG12	1.47	1.46
1:A:367:GLY:N	1:A:367:GLY:CA	1.79	1.44
1:D:173:MET:CE	1:D:173:MET:HA	1.49	1.42
1:D:339:ILE:HG23	1:D:345:LEU:CD2	1.48	1.41
1:C:173:MET:N	1:C:173:MET:CA	1.83	1.39
1:D:310:PHE:O	1:D:311:ILE:CG1	1.71	1.39
1:B:399:GLU:CG	1:B:399:GLU:O	1.67	1.31
1:C:384:LYS:HE3	4:C:1322:HOH:O	1.31	1.30
1:D:173:MET:HE3	1:D:173:MET:CA	1.61	1.30
1:D:398:LYS:HZ2	1:D:398:LYS:CB	0.87	1.29
1:D:396:PHE:O	1:D:397:LEU:CB	1.74	1.27
1:C:190:ARG:O	1:C:192:PRO:CD	1.82	1.27
1:D:249:ASP:OD2	1:D:368:GLN:CB	1.81	1.27
1:E:299:THR:CG2	1:E:300:THR:HG23	1.64	1.27
1:D:310:PHE:O	1:D:311:ILE:HG13	1.16	1.26
1:E:384:LYS:O	1:E:386:LEU:N	1.67	1.26
1:A:190:ARG:O	1:A:192:PRO:HD3	1.37	1.23
1:D:339:ILE:CG2	1:D:345:LEU:CD2	2.19	1.21
1:C:59:PRO:HB2	1:C:62:GLU:CG	1.70	1.21
1:A:304:GLU:OE1	1:A:384:LYS:NZ	1.73	1.20
1:D:310:PHE:C	1:D:311:ILE:HG13	1.47	1.19
1:E:95:ILE:CG1	1:E:337:MET:HE3	1.72	1.19
1:E:94:LYS:O	1:E:95:ILE:HG22	1.44	1.18
1:C:190:ARG:O	1:C:192:PRO:HD3	1.02	1.18
1:D:345:LEU:O	1:D:378:VAL:CG1	1.91	1.18
1:D:339:ILE:HG23	1:D:345:LEU:HD21	1.25	1.17
1:D:345:LEU:O	1:D:378:VAL:HG13	1.03	1.17
1:E:222:GLN:O	1:E:223:TYR:CD2	1.96	1.17
1:E:299:THR:HG22	1:E:300:THR:CG2	1.75	1.16
1:B:224:ARG:O	1:B:225:ASN:CA	1.94	1.16
1:D:248:LEU:HD22	1:D:249:ASP:O	1.44	1.16
1:D:397:LEU:O	1:D:398:LYS:CB	1.89	1.16
1:D:398:LYS:HB2	1:D:398:LYS:NZ	0.98	1.16
1:B:399:GLU:O	1:B:399:GLU:CD	1.87	1.15
1:C:397:LEU:O	1:C:398:LYS:HD3	1.47	1.15
1:E:48:ALA:N	1:E:49:PRO:HD3	1.54	1.15
1:F:289:GLU:O	1:F:291:GLU:N	1.78	1.15
1:A:191:THR:HG21	1:A:203:HIS:CG	1.83	1.14
1:D:248:LEU:CD2	1:D:249:ASP:H	1.60	1.14
1:D:397:LEU:O	1:D:398:LYS:HB2	1.39	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ASP:O	1:F:216:ASN:O	1.67	1.12
1:B:287:LEU:HD22	1:B:310:PHE:O	1.49	1.12
1:D:398:LYS:HZ2	1:D:398:LYS:HB3	1.07	1.12
1:E:127:ILE:HD13	1:E:142:ILE:HD13	1.31	1.12
1:B:287:LEU:CD2	1:B:310:PHE:O	1.96	1.12
1:C:191:THR:HG23	1:C:201:GLU:O	1.50	1.12
1:E:317:ARG:HB2	1:E:317:ARG:HH11	0.95	1.11
1:C:255:VAL:HB	1:C:287:LEU:HD11	1.22	1.11
1:A:201:GLU:O	1:A:201:GLU:HG3	1.36	1.10
1:D:171:GLU:C	1:D:172:LYS:HD2	1.76	1.10
1:D:203:HIS:CG	1:D:203:HIS:O	2.02	1.10
1:B:101:LEU:HD11	1:B:361:ALA:HB3	1.11	1.10
1:D:249:ASP:OD2	1:D:368:GLN:HB3	0.94	1.10
1:D:339:ILE:CG2	1:D:345:LEU:HD21	1.76	1.09
1:A:192:PRO:O	1:A:193:THR:HG22	1.52	1.09
1:B:170:PRO:HG3	1:B:191:THR:HG21	1.31	1.09
1:D:205:GLY:HA2	1:D:208:TRP:HB2	1.29	1.09
1:E:298:GLN:O	1:E:299:THR:HB	1.39	1.09
1:A:91:ARG:HH12	1:B:78:PRO:HA	1.04	1.09
1:E:106:LEU:HD11	1:F:76:ILE:HD13	1.33	1.09
1:E:394:LYS:HE3	1:E:394:LYS:H	1.11	1.09
1:D:248:LEU:HD22	1:D:249:ASP:H	1.13	1.08
1:F:289:GLU:O	1:F:290:PRO:C	1.88	1.08
1:E:201:GLU:OE1	1:E:201:GLU:O	1.70	1.08
1:A:283:GLU:HB3	1:A:298:GLN:OE1	1.51	1.08
1:E:144:GLU:HB2	1:E:154:LEU:HD12	1.33	1.08
1:F:299:THR:HG22	1:F:300:THR:N	1.69	1.07
1:E:48:ALA:H	1:E:313:THR:HG21	1.17	1.07
1:E:105:LEU:O	1:E:105:LEU:CG	1.96	1.07
1:E:47:ASP:N	1:E:313:THR:HG23	1.69	1.07
1:E:299:THR:HG22	1:E:300:THR:HG23	1.15	1.07
1:C:290:PRO:O	1:C:292:GLU:N	1.87	1.07
1:D:339:ILE:HG23	1:D:345:LEU:HD23	1.17	1.07
1:E:170:PRO:HD3	1:E:203:HIS:NE2	1.71	1.06
1:A:125:ARG:HG2	1:A:125:ARG:HH11	1.19	1.06
1:D:384:LYS:O	1:D:385:PHE:HB3	1.50	1.06
1:F:379:ARG:NH1	1:F:379:ARG:HB3	1.70	1.06
1:C:290:PRO:O	1:C:291:GLU:C	1.98	1.05
1:E:170:PRO:CD	1:E:203:HIS:NE2	2.19	1.05
1:F:379:ARG:HB3	1:F:379:ARG:HH11	0.90	1.05
1:E:48:ALA:CB	1:E:224:ARG:HH22	1.68	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:O	1:A:192:PRO:CD	2.04	1.05
1:B:384:LYS:O	1:B:385:PHE:HB3	1.55	1.04
1:B:399:GLU:O	1:B:399:GLU:HG3	1.28	1.04
1:C:101:LEU:CA	1:C:362:GLN:HE21	1.62	1.04
1:C:110:GLU:HG2	1:C:118:VAL:HG23	1.34	1.04
1:C:190:ARG:C	1:C:192:PRO:HD3	1.83	1.04
1:E:299:THR:HG22	1:E:300:THR:N	1.65	1.04
1:C:288:ALA:HB3	1:C:294:ASN:HD21	1.19	1.04
1:E:314:VAL:O	1:E:315:LEU:HB3	1.54	1.04
1:A:193:THR:HG23	1:A:193:THR:O	1.58	1.04
1:C:59:PRO:CB	1:C:62:GLU:HG3	1.88	1.04
1:C:215:PRO:O	1:C:217:SER:N	1.89	1.04
1:F:228:ASN:OD1	1:F:229:PRO:HD3	1.58	1.04
1:C:255:VAL:CB	1:C:287:LEU:HD11	1.87	1.03
1:D:393:GLN:O	1:D:394:LYS:HG2	1.59	1.03
1:F:127:ILE:HD11	1:F:154:LEU:HD22	1.36	1.03
1:C:101:LEU:HA	1:C:362:GLN:HE21	1.18	1.02
1:E:317:ARG:HH11	1:E:317:ARG:CB	1.72	1.02
1:A:168:VAL:HG12	1:A:203:HIS:HD2	1.20	1.02
1:D:72:LYS:HB2	1:F:66:HIS:CE1	1.94	1.02
1:F:392:LEU:O	1:F:393:GLN:CB	1.98	1.02
1:F:373:ILE:HG22	1:F:375:PRO:HD3	1.40	1.02
1:D:221:ASP:OD2	1:D:223:TYR:N	1.91	1.01
1:F:290:PRO:HB2	1:F:293:LEU:HG	1.35	1.01
1:E:95:ILE:HG13	1:E:337:MET:HE3	1.04	1.01
1:E:317:ARG:HB2	1:E:317:ARG:NH1	1.76	1.00
1:E:207:ALA:O	1:E:210:LEU:HB2	1.61	1.00
1:E:105:LEU:O	1:E:105:LEU:HG	1.24	1.00
1:C:59:PRO:HB2	1:C:62:GLU:HG3	1.00	1.00
1:F:56:LEU:HD12	1:F:57:GLY:H	1.27	1.00
1:C:201:GLU:HB2	1:C:209:ARG:HH22	1.26	0.99
1:E:298:GLN:O	1:E:299:THR:CB	2.07	0.99
1:C:48:ALA:HB1	1:C:49:PRO:HD3	1.42	0.99
1:E:289:GLU:OE2	1:E:317:ARG:NH1	1.95	0.99
1:F:156:LEU:HD23	1:F:184:LEU:HD22	1.40	0.99
1:D:311:ILE:HG23	1:D:317:ARG:HH12	1.27	0.98
1:C:385:PHE:HA	1:C:391:MET:HG2	1.42	0.98
1:D:203:HIS:CE1	1:D:204:VAL:HG11	1.99	0.98
1:F:392:LEU:O	1:F:393:GLN:HB2	1.61	0.98
1:D:311:ILE:HG23	1:D:317:ARG:NH1	1.79	0.97
1:D:201:GLU:O	1:D:201:GLU:CD	2.07	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:HIS:CE1	1:D:204:VAL:HG13	1.96	0.97
1:F:379:ARG:HH11	1:F:379:ARG:CB	1.77	0.97
1:A:95:ILE:HG23	1:A:337:MET:HE3	1.44	0.97
1:C:59:PRO:CD	1:C:62:GLU:OE2	2.13	0.97
1:D:203:HIS:HE1	1:D:204:VAL:CG1	1.70	0.96
1:A:191:THR:CG2	1:A:203:HIS:CG	2.49	0.96
1:A:132:ARG:O	1:C:74:PRO:HB3	1.63	0.96
1:D:111:PHE:HB2	1:D:377:SER:HB3	1.45	0.96
1:D:250:MET:HB2	1:D:364:LEU:HD21	1.46	0.96
1:C:340:ALA:HB2	1:D:183:ALA:O	1.64	0.96
1:B:101:LEU:HD11	1:B:361:ALA:CB	1.95	0.96
1:E:336:ARG:HA	1:E:339:ILE:HD12	1.46	0.95
1:E:394:LYS:H	1:E:394:LYS:CE	1.79	0.95
1:E:48:ALA:N	1:E:49:PRO:CD	2.26	0.95
1:B:224:ARG:HH11	1:B:224:ARG:HG3	1.29	0.95
1:C:255:VAL:CG1	1:C:287:LEU:CD1	2.45	0.95
1:E:201:GLU:HB2	1:E:205:GLY:HA3	1.48	0.95
1:B:327:ASN:HD22	1:B:327:ASN:H	1.05	0.95
1:B:373:ILE:HG22	1:B:375:PRO:HD3	1.45	0.95
1:E:169:MET:O	1:E:190:ARG:HA	1.66	0.95
1:B:285:SER:O	1:B:294:ASN:OD1	1.85	0.94
1:B:288:ALA:HB3	1:B:294:ASN:HD21	1.30	0.94
1:A:170:PRO:HD3	1:A:203:HIS:NE2	1.82	0.94
1:B:224:ARG:O	1:B:225:ASN:HA	1.66	0.94
1:B:214:ILE:O	1:B:217:SER:HB2	1.66	0.94
1:D:397:LEU:HD22	1:D:398:LYS:HE3	1.48	0.94
1:A:91:ARG:HD2	1:A:93:ASN:OD1	1.68	0.94
1:D:398:LYS:HB2	1:D:398:LYS:HZ1	1.20	0.94
1:C:269:LYS:O	1:C:273:PRO:HG3	1.68	0.94
1:A:201:GLU:O	1:A:201:GLU:CG	2.15	0.93
1:F:56:LEU:HD12	1:F:57:GLY:N	1.82	0.93
1:D:171:GLU:C	1:D:172:LYS:CD	2.41	0.93
1:E:55:GLN:HB2	1:E:58:ARG:HG3	1.49	0.93
1:E:299:THR:CG2	1:E:300:THR:CG2	2.40	0.93
1:C:59:PRO:HD2	1:C:62:GLU:OE2	1.69	0.93
1:D:172:LYS:CD	1:D:172:LYS:N	2.30	0.93
1:D:286:ILE:HA	1:D:294:ASN:ND2	1.84	0.92
1:E:49:PRO:HG3	1:E:313:THR:HG22	1.51	0.92
1:E:207:ALA:HB1	1:E:219:ILE:HD11	1.50	0.92
1:E:221:ASP:O	1:E:225:ASN:N	2.01	0.92
1:F:176:GLU:O	1:F:180:VAL:HG23	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ARG:O	1:D:192:PRO:CD	2.18	0.92
1:F:294:ASN:N	1:F:294:ASN:HD22	1.67	0.92
1:A:110:GLU:HG3	1:A:113:ASN:HD21	1.35	0.92
1:E:127:ILE:HD13	1:E:142:ILE:CD1	1.99	0.91
1:D:250:MET:HG2	1:D:370:CYS:SG	2.10	0.91
1:B:161:ARG:HH11	1:B:161:ARG:HG2	1.35	0.91
1:B:164:ARG:NH2	1:B:166:ILE:HD11	1.85	0.91
1:F:77:LEU:HD23	1:F:77:LEU:H	1.35	0.91
1:B:358:VAL:HG23	1:B:359:LYS:HD3	1.52	0.91
1:A:191:THR:CG2	1:A:203:HIS:HB3	2.00	0.91
1:B:46:PRO:HD3	1:B:310:PHE:CG	2.06	0.91
1:A:194:ASN:O	1:A:200:PRO:HD3	1.71	0.91
1:B:170:PRO:HG3	1:B:191:THR:CG2	2.01	0.91
1:E:198:ASP:HB3	1:E:310:PHE:CZ	2.06	0.90
1:A:168:VAL:HG12	1:A:203:HIS:CD2	2.05	0.90
1:C:397:LEU:O	1:C:398:LYS:CD	2.19	0.90
1:D:203:HIS:ND1	1:D:204:VAL:CG1	2.33	0.90
1:C:363:GLU:OE2	1:C:364:LEU:CD2	2.19	0.90
1:C:255:VAL:HB	1:C:287:LEU:CD1	2.02	0.90
1:F:385:PHE:O	1:F:386:LEU:HB3	1.71	0.90
1:D:397:LEU:O	1:D:398:LYS:CG	2.20	0.90
1:E:350:ALA:HB1	1:E:374:LEU:HD22	1.54	0.90
1:E:92:ILE:CG2	1:E:95:ILE:CG2	2.50	0.90
1:C:173:MET:N	1:C:173:MET:C	2.30	0.89
1:D:205:GLY:CA	1:D:208:TRP:H	1.84	0.89
1:D:72:LYS:HB2	1:F:66:HIS:HE1	1.37	0.89
1:D:310:PHE:C	1:D:311:ILE:CG1	2.33	0.89
1:C:59:PRO:CG	1:C:62:GLU:OE2	2.20	0.89
1:C:101:LEU:HA	1:C:362:GLN:NE2	1.87	0.89
1:C:101:LEU:CA	1:C:362:GLN:NE2	2.35	0.89
1:B:355:ALA:O	1:B:359:LYS:HE2	1.71	0.89
1:D:190:ARG:O	1:D:192:PRO:HD3	1.72	0.89
1:E:174:SER:O	1:E:175:SER:HB2	1.73	0.89
1:E:172:LYS:O	1:E:173:MET:C	2.14	0.89
1:A:170:PRO:HA	1:A:191:THR:OG1	1.73	0.89
1:E:48:ALA:HB2	1:E:224:ARG:HH22	1.38	0.88
1:E:238:ASP:O	1:E:242:GLN:HB2	1.73	0.88
1:C:268:LEU:O	1:C:272:CYS:N	2.06	0.88
1:F:168:VAL:HG22	1:F:189:VAL:HB	1.54	0.88
1:A:210:LEU:HD22	1:A:214:ILE:HD11	1.54	0.88
1:D:76:ILE:HB	1:F:134:GLY:HA3	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LYS:HE3	1:F:380:ASN:HB3	1.55	0.88
1:E:299:THR:HG21	1:E:300:THR:HG23	1.53	0.88
1:A:91:ARG:HH12	1:B:78:PRO:CA	1.87	0.88
1:D:205:GLY:HA2	1:D:208:TRP:CB	2.02	0.88
1:D:249:ASP:O	1:D:250:MET:O	1.92	0.88
1:D:338:LEU:HD22	1:D:344:LEU:HD12	1.56	0.88
1:E:176:GLU:HA	1:E:396:PHE:CE1	2.09	0.87
1:B:146:THR:HG21	1:B:222:GLN:NE2	1.89	0.87
1:D:339:ILE:CG2	1:D:345:LEU:HD23	1.93	0.87
1:D:397:LEU:O	1:D:398:LYS:NZ	2.07	0.87
1:D:91:ARG:CD	1:D:93:ASN:HD21	1.87	0.87
1:C:126:MET:SD	1:C:220:LEU:HB3	2.14	0.87
1:E:223:TYR:CE1	1:E:257:THR:HG22	2.09	0.87
1:F:396:PHE:O	1:F:397:LEU:HB2	1.71	0.87
1:A:91:ARG:HB3	1:A:91:ARG:HH11	1.39	0.86
1:C:382:MET:HE2	1:D:176:GLU:HG3	1.56	0.86
1:F:363:GLU:HG3	1:F:364:LEU:HD22	1.56	0.86
1:F:127:ILE:HD11	1:F:154:LEU:CD2	2.05	0.86
1:E:317:ARG:CB	1:E:317:ARG:NH1	2.36	0.86
1:A:91:ARG:NH1	1:B:78:PRO:HA	1.88	0.86
1:A:399:GLU:O	1:A:400:GLU:HB2	1.73	0.86
1:D:281:ASP:OD1	1:D:287:LEU:O	1.94	0.86
1:F:393:GLN:O	1:F:394:LYS:HB2	1.73	0.86
1:C:350:ALA:HB1	1:C:374:LEU:HD22	1.58	0.86
1:E:170:PRO:HD2	1:E:203:HIS:NE2	1.88	0.86
1:E:336:ARG:HD3	1:E:385:PHE:O	1.76	0.86
1:E:48:ALA:H	1:E:49:PRO:CD	1.89	0.85
1:E:199:SER:H	1:E:202:SER:HB2	1.39	0.85
1:F:176:GLU:HG2	1:F:380:ASN:O	1.76	0.85
1:C:172:LYS:C	1:C:173:MET:CA	2.49	0.85
1:D:397:LEU:O	1:D:398:LYS:CE	2.24	0.85
1:F:135:THR:O	1:F:136:LEU:C	2.15	0.85
1:E:48:ALA:H	1:E:49:PRO:HD3	1.41	0.85
1:E:48:ALA:N	1:E:313:THR:HG21	1.92	0.85
1:C:106:LEU:HD11	1:C:369:ARG:HD2	1.54	0.85
1:C:331:ALA:O	1:C:351:GLY:HA3	1.76	0.85
1:C:77:LEU:HB2	1:D:90:VAL:HG22	1.59	0.85
1:C:336:ARG:NH1	1:C:385:PHE:O	2.08	0.85
1:D:345:LEU:O	1:D:346:CYS:O	1.94	0.85
1:C:48:ALA:CB	1:C:49:PRO:HD3	2.03	0.85
1:D:310:PHE:O	1:D:311:ILE:CD1	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:SER:C	1:E:176:GLU:CA	2.50	0.84
1:F:299:THR:HG22	1:F:300:THR:OG1	1.76	0.84
1:E:55:GLN:O	1:E:58:ARG:HB2	1.77	0.84
1:E:59:PRO:HB2	1:E:62:GLU:HG3	1.57	0.84
1:B:46:PRO:O	1:B:48:ALA:HB2	1.77	0.84
1:E:299:THR:CG2	1:E:300:THR:N	2.39	0.84
1:A:194:ASN:N	1:A:200:PRO:HD2	1.93	0.84
1:A:80:ILE:CD1	1:A:83:LYS:HB2	2.08	0.84
1:D:266:ARG:O	1:D:270:GLU:HG3	1.76	0.84
1:C:106:LEU:HD12	1:C:371:VAL:HG22	1.60	0.84
1:E:335:ALA:HB1	1:E:385:PHE:HE1	1.43	0.84
1:F:242:GLN:HA	1:F:242:GLN:HE21	1.42	0.84
1:D:253:ALA:HB2	1:D:373:ILE:HD12	1.59	0.83
1:F:384:LYS:O	1:F:385:PHE:C	2.18	0.83
1:B:164:ARG:HH21	1:B:166:ILE:HD11	1.40	0.83
1:D:248:LEU:CD2	1:D:249:ASP:O	2.24	0.83
1:E:92:ILE:HG22	1:E:95:ILE:CG2	2.08	0.83
1:A:80:ILE:HD12	1:A:83:LYS:HB2	1.59	0.83
1:A:202:SER:OG	1:A:203:HIS:N	2.06	0.83
1:D:202:SER:O	1:D:204:VAL:HG13	1.78	0.83
1:F:167:ILE:HD12	1:F:181:LEU:HD13	1.60	0.83
1:F:336:ARG:HH12	1:F:388:ASP:CA	1.92	0.83
1:F:264:ILE:HG22	1:F:268:LEU:HD12	1.60	0.83
1:C:47:ASP:CG	1:C:48:ALA:H	1.86	0.83
1:E:262:THR:OG1	1:E:315:LEU:HA	1.77	0.83
1:F:135:THR:O	1:F:136:LEU:O	1.95	0.83
1:D:66:HIS:CD2	1:D:132:ARG:HD3	2.14	0.83
1:E:176:GLU:N	1:E:176:GLU:C	2.36	0.83
1:C:192:PRO:O	1:C:193:THR:OG1	1.95	0.82
1:E:94:LYS:O	1:E:95:ILE:CG2	2.27	0.82
1:B:72:LYS:HZ3	1:B:72:LYS:HA	1.44	0.82
1:E:176:GLU:HA	1:E:396:PHE:CZ	2.13	0.82
1:B:224:ARG:HG3	1:B:224:ARG:NH1	1.90	0.82
1:D:248:LEU:CD2	1:D:249:ASP:N	2.42	0.82
1:B:95:ILE:HG23	1:B:337:MET:HE3	1.62	0.82
1:E:140:ASP:O	1:E:141:THR:OG1	1.96	0.82
1:E:397:LEU:CD1	1:F:390:TRP:HB2	2.09	0.82
1:A:242:GLN:HE21	1:C:61:SER:HB2	1.43	0.82
1:F:392:LEU:O	1:F:393:GLN:CG	2.27	0.82
1:C:224:ARG:HD2	1:C:225:ASN:N	1.94	0.82
1:D:170:PRO:HA	1:D:191:THR:HB	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:CD1	1:F:76:ILE:HD13	2.09	0.82
1:E:211:LYS:HE3	1:E:218:HIS:HA	1.60	0.82
1:F:384:LYS:O	1:F:385:PHE:O	1.98	0.82
1:E:102:LYS:HD3	1:E:365:GLN:HG2	1.62	0.82
1:E:222:GLN:O	1:E:223:TYR:CG	2.31	0.81
1:E:335:ALA:HB1	1:E:385:PHE:CE1	2.14	0.81
1:F:68:THR:O	1:F:234:ASP:HB3	1.80	0.81
1:B:327:ASN:HD22	1:B:327:ASN:N	1.73	0.81
1:E:392:LEU:O	1:E:393:GLN:HB2	1.77	0.81
1:A:102:LYS:HG2	1:A:366:GLU:OE2	1.79	0.81
1:B:47:ASP:OD1	1:B:48:ALA:CA	2.22	0.81
1:F:144:GLU:CG	1:F:146:THR:HG22	2.11	0.81
1:E:201:GLU:HB2	1:E:205:GLY:CA	2.10	0.81
1:E:84:ILE:HD13	1:E:120:ASP:HB3	1.62	0.81
1:F:254:SER:HA	1:F:280:VAL:HB	1.62	0.81
1:D:203:HIS:O	1:D:203:HIS:CD2	2.33	0.81
1:A:66:HIS:NE2	1:C:71:ALA:HA	1.96	0.81
1:F:287:LEU:H	1:F:287:LEU:HD12	1.45	0.81
1:A:205:GLY:H	1:A:208:TRP:H	1.30	0.80
1:E:199:SER:OG	1:E:202:SER:HA	1.81	0.80
1:C:146:THR:HG21	1:C:222:GLN:HE22	1.46	0.80
1:D:172:LYS:HD2	1:D:172:LYS:N	1.90	0.80
1:E:145:PRO:HB3	1:E:204:VAL:HG12	1.63	0.80
1:A:191:THR:CG2	1:A:203:HIS:CB	2.59	0.80
1:B:384:LYS:HB3	1:B:390:TRP:CE2	2.16	0.80
1:A:191:THR:HG21	1:A:203:HIS:ND1	1.97	0.80
1:A:192:PRO:O	1:A:193:THR:CG2	2.28	0.80
1:F:250:MET:CE	1:F:364:LEU:HD21	2.11	0.80
1:A:391:MET:HB3	1:A:397:LEU:HD21	1.64	0.80
1:E:394:LYS:HE3	1:E:394:LYS:N	1.95	0.80
1:F:267:LYS:O	1:F:270:GLU:HB2	1.81	0.80
1:C:95:ILE:HG12	1:C:337:MET:HE2	1.64	0.80
1:F:336:ARG:HH12	1:F:388:ASP:CB	1.95	0.80
1:F:311:ILE:O	1:F:311:ILE:HG22	1.80	0.79
1:D:203:HIS:ND1	1:D:204:VAL:HG13	1.95	0.79
1:F:254:SER:HB2	1:F:306:ILE:HG21	1.64	0.79
1:D:203:HIS:ND1	1:D:204:VAL:HG12	1.97	0.79
1:D:310:PHE:O	1:D:311:ILE:CB	2.25	0.79
1:E:176:GLU:OE2	1:E:380:ASN:O	2.00	0.79
1:C:280:VAL:HG21	1:C:353:THR:HA	1.61	0.79
1:D:398:LYS:CB	1:D:398:LYS:NZ	1.73	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASP:O	1:A:135:THR:N	2.14	0.79
1:C:247:LYS:N	1:C:247:LYS:HD2	1.98	0.79
1:C:339:ILE:HG23	1:C:345:LEU:HD23	1.65	0.79
1:D:203:HIS:NE2	1:D:204:VAL:HG12	1.97	0.79
1:D:243:GLN:O	1:D:245:ASP:N	2.16	0.79
1:F:172:LYS:O	1:F:173:MET:O	2.01	0.79
1:F:394:LYS:HZ3	1:F:394:LYS:HA	1.48	0.78
1:E:199:SER:OG	1:E:201:GLU:C	2.26	0.78
1:F:81:LEU:HD23	1:F:84:ILE:HD11	1.65	0.78
1:D:78:PRO:HD2	1:D:82:LYS:HG3	1.65	0.78
1:E:198:ASP:HA	1:E:202:SER:HB2	1.65	0.78
1:A:83:LYS:NZ	1:A:83:LYS:HA	1.99	0.78
1:A:322:LYS:HG2	1:A:323:TRP:N	1.98	0.78
1:B:94:LYS:HD2	1:B:341:GLN:HB3	1.65	0.78
1:F:364:LEU:HD22	1:F:364:LEU:H	1.49	0.78
1:B:101:LEU:CD1	1:B:361:ALA:HB3	2.05	0.78
1:D:311:ILE:CG2	1:D:317:ARG:NH1	2.45	0.78
1:B:224:ARG:HH11	1:B:224:ARG:CG	1.95	0.78
1:C:93:ASN:N	1:C:342:GLU:OE2	2.17	0.78
1:D:48:ALA:O	1:D:313:THR:HB	1.83	0.78
1:C:145:PRO:HA	1:C:168:VAL:HB	1.65	0.78
1:F:250:MET:HE3	1:F:364:LEU:HD21	1.65	0.78
1:A:101:LEU:HD11	1:A:358:VAL:HA	1.65	0.77
1:A:110:GLU:HG3	1:A:113:ASN:ND2	1.99	0.77
1:C:111:PHE:HZ	1:C:344:LEU:HD22	1.49	0.77
1:A:170:PRO:HD3	1:A:203:HIS:CE1	2.18	0.77
1:E:392:LEU:O	1:E:393:GLN:CB	2.31	0.77
1:B:258:GLY:HA3	1:B:315:LEU:HB2	1.64	0.77
1:B:203:HIS:C	1:B:204:VAL:HG23	2.10	0.77
1:E:199:SER:OG	1:E:202:SER:N	2.17	0.77
1:E:320:VAL:HG11	1:E:323:TRP:NE1	1.99	0.77
1:C:79:ASP:OD1	1:C:81:LEU:HB2	1.84	0.77
1:C:128:GLU:HA	1:C:131:GLU:HG3	1.65	0.77
1:C:398:LYS:O	1:C:399:GLU:HB3	1.82	0.77
1:E:150:THR:OG1	1:E:222:GLN:OE1	2.00	0.77
1:E:199:SER:N	1:E:202:SER:HB2	1.99	0.77
1:B:357:ALA:O	1:B:361:ALA:HB3	1.83	0.77
1:C:172:LYS:O	1:C:173:MET:HB2	1.84	0.77
1:E:47:ASP:N	1:E:313:THR:CG2	2.48	0.77
1:D:178:VAL:O	1:D:182:ARG:HG3	1.84	0.76
1:D:219:ILE:HG22	1:D:220:LEU:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:ARG:HD2	3:C:1320:HEM:HBC2	1.66	0.76
1:D:396:PHE:O	1:D:397:LEU:HB2	0.81	0.76
1:F:130:ALA:HA	1:F:133:ASP:OD2	1.84	0.76
1:F:228:ASN:OD1	1:F:229:PRO:CD	2.33	0.76
1:B:225:ASN:N	1:B:314:VAL:HG12	1.99	0.76
1:C:224:ARG:HD2	1:C:225:ASN:CA	2.14	0.76
1:E:316:ASP:OD2	1:E:318:THR:HB	1.85	0.76
1:F:257:THR:HG22	2:F:1610:PLP:O3P	1.86	0.76
1:C:248:LEU:HD21	1:C:371:VAL:HG23	1.65	0.76
1:C:336:ARG:HH22	1:C:397:LEU:HD11	1.48	0.76
1:A:175:SER:HA	1:A:178:VAL:HB	1.67	0.76
1:A:223:TYR:O	1:A:314:VAL:HG22	1.86	0.76
1:C:339:ILE:HG23	1:C:345:LEU:CD2	2.15	0.76
1:D:205:GLY:C	1:D:207:ALA:N	2.35	0.76
1:D:171:GLU:OE1	1:D:190:ARG:HD3	1.85	0.76
1:B:224:ARG:C	1:B:225:ASN:CA	2.58	0.76
1:B:391:MET:SD	1:B:396:PHE:CD1	2.79	0.76
1:D:235:THR:O	1:D:239:GLU:HG3	1.86	0.76
1:D:286:ILE:HD12	1:D:286:ILE:H	1.49	0.76
1:F:87:THR:HB	1:F:109:CYS:O	1.86	0.76
1:A:194:ASN:H	1:A:200:PRO:HD2	1.51	0.75
1:F:95:ILE:HD11	1:F:337:MET:O	1.86	0.75
1:F:56:LEU:CD2	1:F:269:LYS:HB3	2.16	0.75
1:B:46:PRO:HG3	1:B:310:PHE:CD2	2.21	0.75
1:D:203:HIS:HE1	1:D:204:VAL:HG11	1.40	0.75
1:E:48:ALA:HB3	1:E:224:ARG:HH22	1.51	0.75
1:A:95:ILE:HG23	1:A:337:MET:CE	2.16	0.75
1:B:292:GLU:HA	1:B:295:GLN:HE21	1.50	0.75
1:C:59:PRO:HG2	1:C:62:GLU:OE2	1.86	0.75
1:C:235:THR:O	1:C:239:GLU:HG3	1.87	0.75
1:F:147:SER:HB3	1:F:169:MET:HB3	1.68	0.75
1:F:396:PHE:O	1:F:396:PHE:CD2	2.39	0.75
1:A:298:GLN:O	1:A:298:GLN:HG2	1.85	0.75
1:C:121:ARG:HH12	1:C:235:THR:HG22	1.52	0.75
1:E:397:LEU:HD11	1:F:390:TRP:HB2	1.69	0.75
1:F:169:MET:HB2	1:F:173:MET:SD	2.26	0.75
1:F:289:GLU:OE2	1:F:317:ARG:HD3	1.86	0.75
1:E:125:ARG:HG2	1:E:125:ARG:HH11	1.49	0.75
1:F:124:LEU:O	1:F:128:GLU:HB2	1.87	0.75
1:A:95:ILE:HD12	1:A:338:LEU:HD23	1.69	0.75
1:C:90:VAL:HG22	1:D:77:LEU:CD1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:THR:O	1:C:235:THR:HG22	1.86	0.75
1:D:283:GLU:HA	1:D:325:LYS:HZ1	1.52	0.74
1:A:62:GLU:O	3:A:1120:HEM:HMB1	1.86	0.74
1:A:126:MET:HG2	1:A:220:LEU:HB3	1.69	0.74
1:A:132:ARG:HB2	1:A:132:ARG:HH11	1.51	0.74
1:B:169:MET:HG3	1:B:190:ARG:NH2	2.02	0.74
1:C:77:LEU:HD21	1:C:83:LYS:HB2	1.69	0.74
1:C:335:ALA:HB1	1:C:385:PHE:CZ	2.22	0.74
1:D:248:LEU:HD22	1:D:249:ASP:N	1.97	0.74
1:B:366:GLU:HB3	1:C:216:ASN:HD22	1.52	0.74
1:C:335:ALA:HB3	1:C:385:PHE:CE1	2.23	0.74
1:D:119:LYS:HD3	1:D:150:THR:OG1	1.86	0.74
1:F:394:LYS:HA	1:F:394:LYS:NZ	2.03	0.74
1:B:387:SER:HB3	1:B:389:ARG:HH21	1.53	0.74
1:C:201:GLU:CB	1:C:209:ARG:HH22	1.99	0.74
1:E:283:GLU:HG2	1:E:325:LYS:HB3	1.69	0.74
1:C:164:ARG:HE	1:C:187:GLU:CD	1.96	0.74
1:E:199:SER:OG	1:E:202:SER:CA	2.35	0.74
1:A:322:LYS:HG2	1:A:323:TRP:H	1.52	0.74
1:C:50:SER:O	1:C:51:ARG:HB2	1.86	0.74
1:E:281:ASP:O	1:E:325:LYS:HA	1.88	0.74
1:A:205:GLY:O	1:A:206:VAL:C	2.21	0.74
1:A:290:PRO:HD2	1:A:293:LEU:HG	1.68	0.74
1:B:367:GLY:H	1:C:216:ASN:HD21	1.33	0.74
1:C:101:LEU:HD11	1:C:358:VAL:HA	1.69	0.74
1:E:144:GLU:HB2	1:E:154:LEU:CD1	2.13	0.74
1:E:303:VAL:HG23	1:E:328:ASP:OD2	1.87	0.74
1:D:393:GLN:O	1:D:393:GLN:HG3	1.86	0.74
1:A:244:CYS:O	1:A:245:ASP:HB2	1.87	0.73
1:D:48:ALA:HB1	1:D:49:PRO:HD2	1.70	0.73
1:C:172:LYS:O	1:C:173:MET:CB	2.36	0.73
1:C:255:VAL:CG1	1:C:287:LEU:HD11	2.14	0.73
1:F:303:VAL:CG2	1:F:328:ASP:OD2	2.36	0.73
1:F:336:ARG:HH22	1:F:388:ASP:HB3	1.54	0.73
1:C:110:GLU:HG2	1:C:118:VAL:CG2	2.16	0.73
1:C:137:LYS:HB2	1:C:140:ASP:OD1	1.87	0.73
1:E:176:GLU:N	1:E:177:LYS:N	2.37	0.73
1:C:388:ASP:C	1:C:392:LEU:HD12	2.14	0.73
1:E:286:ILE:HG13	1:E:286:ILE:O	1.86	0.73
1:B:169:MET:HG3	1:B:190:ARG:HH21	1.54	0.73
1:D:237:ALA:HB2	1:D:264:ILE:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:VAL:HG22	1:F:356:VAL:HG21	1.70	0.73
1:F:303:VAL:HG23	1:F:328:ASP:OD2	1.88	0.73
1:E:346:CYS:O	1:E:378:VAL:HG12	1.89	0.73
1:B:379:ARG:HB3	1:B:379:ARG:NH1	2.04	0.72
1:A:131:GLU:HG3	1:A:136:LEU:HD23	1.71	0.72
1:C:288:ALA:HB3	1:C:294:ASN:ND2	2.00	0.72
1:D:137:LYS:HD3	1:E:104:GLU:CD	2.14	0.72
1:D:232:HIS:CD2	1:D:260:THR:HA	2.23	0.72
1:A:134:GLY:HA3	1:C:76:ILE:HB	1.69	0.72
1:B:173:MET:HE1	1:B:304:GLU:OE2	1.89	0.72
1:C:272:CYS:O	1:C:273:PRO:C	2.31	0.72
1:E:170:PRO:HD3	1:E:203:HIS:CD2	2.25	0.72
1:B:329:GLU:O	1:B:333:THR:HG23	1.88	0.72
1:C:366:GLU:CD	1:C:366:GLU:H	1.98	0.72
1:D:74:PRO:HB2	1:D:76:ILE:O	1.90	0.72
1:E:192:PRO:O	1:E:202:SER:O	2.07	0.72
1:B:287:LEU:HD11	1:B:308:TYR:CB	2.20	0.72
1:E:92:ILE:HG22	1:E:95:ILE:HG22	1.72	0.72
1:E:343:GLY:HA2	1:F:156:LEU:HD21	1.70	0.72
1:D:391:MET:O	1:D:394:LYS:HB2	1.90	0.72
1:E:391:MET:HE3	1:E:391:MET:O	1.89	0.72
1:B:357:ALA:O	1:B:361:ALA:CB	2.38	0.72
1:D:190:ARG:O	1:D:192:PRO:HD2	1.88	0.72
1:E:233:TYR:CD1	1:E:267:LYS:HB2	2.25	0.72
1:B:287:LEU:HD11	1:B:308:TYR:N	2.05	0.72
1:D:393:GLN:C	1:D:394:LYS:HG2	2.14	0.72
1:B:190:ARG:CZ	1:B:190:ARG:HA	2.20	0.71
1:C:255:VAL:HG12	1:C:287:LEU:CD1	2.18	0.71
1:D:110:GLU:HG2	1:D:118:VAL:HB	1.70	0.71
1:E:87:THR:HG21	1:E:110:GLU:OE2	1.88	0.71
1:C:341:GLN:O	1:C:342:GLU:C	2.26	0.71
1:A:203:HIS:N	1:A:203:HIS:ND1	2.35	0.71
1:B:334:PHE:O	1:B:338:LEU:HD13	1.91	0.71
1:C:385:PHE:N	1:C:390:TRP:CE3	2.59	0.71
1:E:127:ILE:CD1	1:E:142:ILE:HD13	2.16	0.71
1:A:200:PRO:O	1:A:201:GLU:HB3	1.90	0.71
1:E:289:GLU:CD	1:E:317:ARG:HH12	1.98	0.71
1:B:345:LEU:O	1:B:378:VAL:HG22	1.91	0.71
1:C:235:THR:O	1:C:235:THR:CG2	2.38	0.71
1:D:339:ILE:HG21	1:D:345:LEU:CD2	2.16	0.71
1:F:188:ILE:N	1:F:188:ILE:HD12	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ILE:O	1:C:131:GLU:HG3	1.91	0.71
1:D:143:ILE:O	1:D:219:ILE:HA	1.89	0.71
1:D:223:TYR:CD1	1:D:312:PRO:HG3	2.26	0.71
1:F:388:ASP:O	1:F:389:ARG:C	2.31	0.71
1:A:251:LEU:HG	1:A:251:LEU:O	1.88	0.71
1:E:268:LEU:O	1:E:272:CYS:O	2.08	0.71
1:F:47:ASP:O	1:F:48:ALA:HB2	1.89	0.71
1:B:170:PRO:CG	1:B:191:THR:HG21	2.15	0.71
1:B:225:ASN:CA	1:B:225:ASN:N	2.53	0.71
1:C:232:HIS:CE1	1:C:260:THR:HG22	2.26	0.71
1:E:76:ILE:HD13	1:F:106:LEU:HD11	1.73	0.71
1:E:87:THR:HB	1:E:109:CYS:O	1.90	0.71
1:C:363:GLU:OE2	1:C:364:LEU:HD21	1.89	0.71
1:F:54:TRP:HB2	3:F:1620:HEM:CHC	2.20	0.71
1:A:191:THR:HG21	1:A:203:HIS:CB	2.19	0.70
1:D:338:LEU:HD13	1:D:346:CYS:SG	2.31	0.70
1:E:248:LEU:HD21	1:E:250:MET:O	1.91	0.70
1:A:132:ARG:O	1:C:74:PRO:CB	2.39	0.70
1:D:74:PRO:CB	1:D:76:ILE:O	2.39	0.70
1:D:358:VAL:O	1:D:362:GLN:HG2	1.91	0.70
1:F:387:SER:O	1:F:389:ARG:N	2.24	0.70
1:A:125:ARG:HG2	1:A:125:ARG:NH1	1.93	0.70
1:A:134:GLY:CA	1:C:76:ILE:HB	2.21	0.70
1:A:170:PRO:CA	1:A:191:THR:OG1	2.39	0.70
1:B:203:HIS:O	1:B:204:VAL:HG23	1.91	0.70
1:F:281:ASP:OD2	1:F:282:PRO:HD2	1.91	0.70
1:A:211:LYS:HD2	1:A:217:SER:HB2	1.73	0.70
1:C:291:GLU:OE1	1:C:291:GLU:HA	1.91	0.70
1:E:55:GLN:HB2	1:E:58:ARG:CG	2.21	0.70
1:E:176:GLU:CD	1:E:380:ASN:O	2.34	0.70
1:A:214:ILE:HB	1:A:217:SER:OG	1.91	0.70
1:B:169:MET:O	1:B:190:ARG:NH2	2.25	0.70
1:B:265:ALA:HB1	1:B:319:VAL:CG1	2.20	0.70
1:C:49:PRO:O	1:C:50:SER:C	2.35	0.70
1:D:228:ASN:OD1	1:D:259:GLY:HA3	1.91	0.70
1:A:156:LEU:O	1:A:160:VAL:HG23	1.91	0.70
1:F:156:LEU:HD23	1:F:184:LEU:CD2	2.20	0.70
1:F:228:ASN:OD1	1:F:228:ASN:C	2.35	0.70
1:D:221:ASP:OD2	1:D:222:GLN:N	2.25	0.70
1:E:289:GLU:OE2	1:E:317:ARG:HB3	1.91	0.70
1:B:137:LYS:HB2	1:B:140:ASP:OD2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:MET:O	1:E:190:ARG:HD2	1.92	0.70
1:F:226:ALA:O	1:F:230:LEU:HB2	1.91	0.70
1:C:201:GLU:HB2	1:C:209:ARG:NH2	2.03	0.70
1:D:230:LEU:HD23	3:D:1420:HEM:HBC2	1.73	0.70
1:D:249:ASP:OD2	1:D:368:GLN:CG	2.39	0.70
1:A:191:THR:HG22	1:A:203:HIS:HB3	1.74	0.69
1:C:110:GLU:CG	1:C:118:VAL:HG23	2.17	0.69
1:B:46:PRO:HD3	1:B:310:PHE:CD1	2.26	0.69
1:B:101:LEU:HD22	1:B:105:LEU:HD22	1.72	0.69
1:A:205:GLY:N	1:A:208:TRP:H	1.89	0.69
1:B:182:ARG:CZ	1:B:188:ILE:HD11	2.22	0.69
1:E:145:PRO:O	1:E:168:VAL:HG23	1.93	0.69
1:E:172:LYS:O	1:E:174:SER:N	2.25	0.69
1:A:249:ASP:OD2	1:A:368:GLN:HB3	1.92	0.69
1:C:382:MET:CE	1:D:176:GLU:HG3	2.20	0.69
1:D:311:ILE:CG2	1:D:317:ARG:HH12	2.01	0.69
1:E:320:VAL:HG11	1:E:323:TRP:CE2	2.28	0.69
1:B:169:MET:HE3	1:B:188:ILE:HG21	1.74	0.69
1:D:248:LEU:HD23	1:D:249:ASP:H	1.54	0.69
1:A:67:HIS:HB3	1:A:234:ASP:OD1	1.92	0.69
1:A:171:GLU:HB3	1:A:190:ARG:HB3	1.73	0.69
1:C:222:GLN:HB2	1:C:257:THR:HG21	1.74	0.69
1:E:92:ILE:CG2	1:E:95:ILE:HG23	2.20	0.69
1:E:345:LEU:C	1:E:378:VAL:HG13	2.17	0.69
1:A:173:MET:HE3	1:A:177:LYS:HD2	1.73	0.69
1:F:226:ALA:O	1:F:227:SER:C	2.33	0.69
1:A:210:LEU:HD22	1:A:214:ILE:CD1	2.21	0.69
1:B:327:ASN:H	1:B:327:ASN:ND2	1.85	0.69
1:C:142:ILE:HG22	1:C:143:ILE:N	2.07	0.69
1:C:384:LYS:HA	1:C:390:TRP:CG	2.28	0.69
1:C:384:LYS:O	1:C:386:LEU:N	2.26	0.69
1:D:134:GLY:HA3	1:F:76:ILE:O	1.93	0.69
1:D:283:GLU:HA	1:D:325:LYS:NZ	2.07	0.69
1:D:106:LEU:HD12	1:D:244:CYS:SG	2.32	0.69
1:D:384:LYS:O	1:D:385:PHE:CB	2.29	0.69
1:E:335:ALA:CB	1:E:385:PHE:HE1	2.06	0.69
1:B:335:ALA:CB	1:B:385:PHE:HE1	2.06	0.69
1:C:66:HIS:O	1:C:125:ARG:NH2	2.27	0.68
1:D:262:THR:HG23	1:D:316:ASP:HB3	1.75	0.68
1:D:281:ASP:OD1	1:D:288:ALA:HB2	1.94	0.68
1:F:229:PRO:HG3	1:F:314:VAL:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:SER:CB	1:B:206:VAL:HG23	2.24	0.68
1:D:102:LYS:HE3	1:D:366:GLU:HG3	1.73	0.68
1:F:133:ASP:HB2	1:F:135:THR:OG1	1.92	0.68
1:B:209:ARG:HA	1:B:212:ASN:ND2	2.08	0.68
1:C:290:PRO:C	1:C:292:GLU:N	2.52	0.68
1:E:193:THR:HG1	1:E:198:ASP:N	1.90	0.68
1:B:327:ASN:ND2	1:B:330:GLU:HB3	2.08	0.68
1:C:232:HIS:NE2	1:C:260:THR:HG22	2.08	0.68
1:D:192:PRO:O	1:D:193:THR:C	2.34	0.68
1:A:281:ASP:O	1:A:325:LYS:HA	1.93	0.68
1:A:399:GLU:O	1:A:399:GLU:HG2	1.92	0.68
1:D:201:GLU:O	1:D:201:GLU:OE2	2.11	0.68
1:D:300:THR:HG22	1:D:301:TYR:H	1.59	0.68
1:F:287:LEU:HD12	1:F:287:LEU:N	2.08	0.68
1:C:345:LEU:C	1:C:378:VAL:HG13	2.19	0.68
1:E:137:LYS:HB2	1:E:140:ASP:OD1	1.93	0.68
1:C:142:ILE:HG22	1:C:143:ILE:H	1.58	0.68
1:C:255:VAL:CB	1:C:287:LEU:CD1	2.62	0.68
1:D:252:VAL:HG22	1:D:278:ILE:HB	1.76	0.68
1:E:208:TRP:C	1:E:210:LEU:H	2.00	0.68
1:E:48:ALA:CB	1:E:224:ARG:NH2	2.51	0.68
1:B:225:ASN:N	1:B:225:ASN:C	2.51	0.68
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.76	0.68
1:C:110:GLU:OE2	1:C:121:ARG:NE	2.25	0.68
1:F:392:LEU:O	1:F:393:GLN:HG2	1.92	0.68
1:F:127:ILE:CD1	1:F:154:LEU:HD22	2.21	0.67
1:A:398:LYS:O	1:A:399:GLU:HB3	1.94	0.67
1:B:202:SER:HB3	1:B:206:VAL:HG23	1.76	0.67
1:E:174:SER:O	1:E:175:SER:CB	2.40	0.67
1:B:288:ALA:HB3	1:B:294:ASN:ND2	2.06	0.67
1:C:188:ILE:N	1:C:188:ILE:HD12	2.10	0.67
1:A:88:PRO:HG2	1:A:112:PHE:CD1	2.30	0.67
1:A:354:VAL:HG22	1:A:372:VAL:HG11	1.77	0.67
1:D:205:GLY:HA2	1:D:208:TRP:H	1.60	0.67
1:D:243:GLN:C	1:D:245:ASP:H	2.02	0.67
1:B:86:ASP:N	1:B:239:GLU:OE1	2.25	0.67
1:E:49:PRO:HA	1:E:313:THR:HG22	1.77	0.67
1:D:172:LYS:N	1:D:172:LYS:HD3	2.09	0.67
1:A:228:ASN:HB3	1:A:229:PRO:CD	2.24	0.67
1:B:126:MET:SD	1:B:220:LEU:HB3	2.34	0.67
1:C:104:GLU:CD	1:F:137:LYS:HD3	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ARG:HD2	1:D:93:ASN:HD21	1.60	0.67
1:D:221:ASP:O	1:D:225:ASN:HB3	1.95	0.67
1:E:81:LEU:HD21	1:E:157:ALA:HA	1.77	0.67
1:E:95:ILE:CG1	1:E:337:MET:CE	2.62	0.67
1:F:171:GLU:H	1:F:171:GLU:CD	2.02	0.67
1:A:91:ARG:HB3	1:A:91:ARG:NH1	2.09	0.67
1:B:46:PRO:O	1:B:47:ASP:OD1	2.13	0.67
1:B:399:GLU:O	1:B:399:GLU:OE2	2.13	0.67
1:C:129:ASP:O	1:C:133:ASP:HB2	1.95	0.67
1:D:143:ILE:HD11	1:D:214:ILE:HD12	1.76	0.67
1:F:336:ARG:HG3	1:F:385:PHE:HE1	1.60	0.67
1:A:137:LYS:HB2	1:A:140:ASP:OD2	1.95	0.67
1:F:232:HIS:CD2	1:F:260:THR:HG22	2.29	0.67
1:F:290:PRO:C	1:F:292:GLU:N	2.52	0.67
1:F:336:ARG:NH1	1:F:388:ASP:CA	2.57	0.67
1:A:205:GLY:N	1:A:208:TRP:HB2	2.10	0.66
1:A:331:ALA:O	1:A:351:GLY:HA3	1.95	0.66
1:D:283:GLU:HG2	1:D:325:LYS:HZ2	1.59	0.66
1:A:70:PRO:HG3	1:A:235:THR:HA	1.77	0.66
1:A:208:TRP:HD1	1:A:219:ILE:HD12	1.60	0.66
1:A:303:VAL:HG23	1:A:328:ASP:OD2	1.95	0.66
1:B:46:PRO:HG3	1:B:310:PHE:CE2	2.31	0.66
1:B:47:ASP:OD1	1:B:48:ALA:HA	1.70	0.66
1:B:164:ARG:HH21	1:B:166:ILE:CD1	2.08	0.66
1:B:367:GLY:H	1:C:216:ASN:ND2	1.91	0.66
1:D:363:GLU:HG3	1:D:364:LEU:HD12	1.77	0.66
1:E:95:ILE:HG13	1:E:337:MET:CE	2.01	0.66
1:A:205:GLY:H	1:A:208:TRP:HB2	1.60	0.66
1:D:102:LYS:HE3	1:D:366:GLU:CG	2.24	0.66
1:E:288:ALA:HB3	1:E:294:ASN:HD21	1.60	0.66
1:B:170:PRO:HD3	1:B:191:THR:HB	1.78	0.66
1:C:290:PRO:O	1:C:293:LEU:N	2.29	0.66
1:D:66:HIS:HD2	1:D:132:ARG:HD3	1.61	0.66
1:E:49:PRO:HG3	1:E:313:THR:CG2	2.23	0.66
1:E:376:ASP:OD1	1:E:381:TYR:HE1	1.78	0.66
1:F:288:ALA:CB	1:F:325:LYS:HD3	2.25	0.66
1:B:94:LYS:HD2	1:B:341:GLN:O	1.96	0.66
1:C:306:ILE:HG23	2:C:1310:PLP:H6	1.78	0.66
1:E:176:GLU:O	1:E:180:VAL:HG23	1.96	0.66
1:E:319:VAL:O	1:E:320:VAL:C	2.37	0.66
1:D:397:LEU:O	1:D:398:LYS:CD	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:ALA:CB	1:E:385:PHE:CE1	2.79	0.66
1:F:290:PRO:C	1:F:292:GLU:H	2.04	0.66
1:A:249:ASP:CG	1:A:368:GLN:HB3	2.21	0.66
1:C:191:THR:CG2	1:C:201:GLU:O	2.38	0.66
1:C:363:GLU:OE2	1:C:364:LEU:HD22	1.94	0.66
1:A:66:HIS:HD1	1:A:132:ARG:NH2	1.94	0.66
1:A:92:ILE:HG23	1:A:342:GLU:CD	2.21	0.66
1:D:205:GLY:O	1:D:206:VAL:C	2.37	0.66
1:E:198:ASP:HA	1:E:202:SER:CB	2.25	0.66
1:F:168:VAL:HG13	1:F:189:VAL:HG12	1.78	0.66
1:F:385:PHE:O	1:F:386:LEU:CB	2.40	0.66
1:F:393:GLN:O	1:F:394:LYS:CB	2.39	0.66
1:A:170:PRO:CD	1:A:203:HIS:NE2	2.58	0.66
1:A:248:LEU:HD22	1:A:250:MET:H	1.61	0.66
1:D:203:HIS:ND1	1:D:203:HIS:C	2.47	0.66
1:E:223:TYR:CD1	1:E:257:THR:HG22	2.30	0.66
1:F:177:LYS:HE3	1:F:380:ASN:CB	2.24	0.66
1:A:126:MET:HE1	1:A:222:GLN:HA	1.78	0.65
1:B:265:ALA:HB1	1:B:319:VAL:HG11	1.77	0.65
1:D:385:PHE:CD1	1:D:385:PHE:C	2.73	0.65
1:B:95:ILE:HG23	1:B:337:MET:CE	2.26	0.65
1:B:176:GLU:O	1:B:180:VAL:HG23	1.95	0.65
1:C:147:SER:OG	1:C:173:MET:HE2	1.96	0.65
1:D:171:GLU:O	1:D:172:LYS:HD2	1.94	0.65
1:E:95:ILE:O	1:E:95:ILE:HG12	1.95	0.65
1:E:207:ALA:O	1:E:210:LEU:CB	2.43	0.65
1:E:242:GLN:CA	1:E:242:GLN:HE21	2.09	0.65
1:A:256:GLY:HA3	2:A:1110:PLP:H5A1	1.77	0.65
1:A:390:TRP:CE2	1:A:394:LYS:HG3	2.31	0.65
1:D:110:GLU:HG2	1:D:118:VAL:CB	2.26	0.65
1:B:266:ARG:NH2	1:B:316:ASP:OD1	2.30	0.65
1:D:111:PHE:CB	1:D:377:SER:HB3	2.22	0.65
1:E:105:LEU:C	1:E:105:LEU:HD12	2.20	0.65
1:F:229:PRO:CG	1:F:314:VAL:HB	2.26	0.65
1:F:290:PRO:HB2	1:F:293:LEU:CG	2.18	0.65
1:A:80:ILE:HD12	1:A:83:LYS:CB	2.27	0.65
1:B:248:LEU:HD23	1:B:249:ASP:N	2.12	0.65
1:C:335:ALA:CB	1:C:385:PHE:CE1	2.80	0.65
1:D:95:ILE:HG23	1:D:337:MET:HE3	1.79	0.65
1:F:72:LYS:O	1:F:74:PRO:HD3	1.97	0.65
1:A:88:PRO:HG2	1:A:112:PHE:HD1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:NH1	1:C:137:LYS:HG2	2.10	0.65
1:C:55:GLN:HB2	1:C:58:ARG:HG3	1.79	0.65
1:D:105:LEU:HD12	1:D:370:CYS:O	1.97	0.65
1:A:103:CYS:SG	1:A:361:ALA:HB1	2.37	0.65
1:E:176:GLU:OE1	1:E:380:ASN:O	2.14	0.65
1:F:364:LEU:HD22	1:F:364:LEU:N	2.12	0.65
1:B:47:ASP:OD1	1:B:48:ALA:CB	2.45	0.64
1:C:59:PRO:HB2	1:C:62:GLU:CD	2.21	0.64
1:C:382:MET:HE2	1:D:176:GLU:CG	2.28	0.64
1:D:173:MET:HA	1:D:173:MET:HE3	0.71	0.64
1:E:394:LYS:CE	1:E:394:LYS:N	2.55	0.64
1:A:64:PRO:HG2	1:A:64:PRO:O	1.97	0.64
1:C:336:ARG:NH1	1:C:391:MET:HG3	2.12	0.64
1:F:247:LYS:N	1:F:247:LYS:HD2	2.12	0.64
1:E:205:GLY:C	1:E:207:ALA:H	2.04	0.64
1:E:248:LEU:CD2	1:E:250:MET:H	2.09	0.64
1:A:111:PHE:HB2	1:A:377:SER:HB3	1.78	0.64
1:D:224:ARG:NH1	1:D:224:ARG:HB3	2.11	0.64
1:A:159:ALA:HB1	1:B:340:ALA:O	1.98	0.64
1:C:350:ALA:CB	1:C:374:LEU:HD22	2.26	0.64
1:E:89:MET:HB2	1:E:243:GLN:CD	2.22	0.64
1:E:198:ASP:HB3	1:E:310:PHE:CE2	2.31	0.64
1:E:258:GLY:HA3	1:E:315:LEU:HB2	1.79	0.64
1:C:335:ALA:HB1	1:C:385:PHE:HZ	1.60	0.64
1:C:335:ALA:HB3	1:C:385:PHE:HE1	1.62	0.64
1:E:248:LEU:HD22	1:E:250:MET:H	1.63	0.64
1:F:393:GLN:HE21	1:F:394:LYS:H	1.46	0.64
1:B:161:ARG:HG2	1:B:161:ARG:NH1	2.08	0.64
1:E:89:MET:SD	1:E:108:LYS:HG2	2.37	0.64
1:A:221:ASP:O	1:A:225:ASN:HB2	1.97	0.64
1:E:310:PHE:O	1:E:312:PRO:HD3	1.98	0.64
1:B:122:ILE:HG22	1:B:228:ASN:HA	1.80	0.64
1:B:399:GLU:CD	1:B:399:GLU:C	2.63	0.64
1:D:219:ILE:HG22	1:D:221:ASP:N	2.13	0.64
1:A:125:ARG:HH11	1:A:125:ARG:CG	2.03	0.63
1:A:221:ASP:H	1:A:225:ASN:HD22	1.45	0.63
1:C:166:ILE:HG22	1:C:167:ILE:N	2.13	0.63
1:A:260:THR:O	1:A:264:ILE:HG13	1.99	0.63
1:C:255:VAL:CG1	1:C:258:GLY:HA2	2.29	0.63
1:D:361:ALA:HA	1:D:364:LEU:HD13	1.79	0.63
1:A:232:HIS:HA	1:A:236:THR:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:CYS:O	1:B:378:VAL:HG13	1.98	0.63
1:C:173:MET:N	1:C:173:MET:O	2.30	0.63
1:D:177:LYS:O	1:D:180:VAL:HG23	1.98	0.63
1:D:216:ASN:HD22	1:E:366:GLU:HB3	1.63	0.63
1:D:249:ASP:HB3	1:D:369:ARG:O	1.98	0.63
1:A:77:LEU:N	1:A:77:LEU:HD23	2.13	0.63
1:A:399:GLU:O	1:A:400:GLU:CB	2.45	0.63
1:D:249:ASP:O	1:D:250:MET:C	2.37	0.63
1:E:48:ALA:HB3	1:E:224:ARG:NH2	2.14	0.63
1:C:255:VAL:HG13	1:C:258:GLY:HA2	1.81	0.63
1:F:230:LEU:HA	3:F:1620:HEM:CBC	2.29	0.63
1:B:320:VAL:HG21	1:B:323:TRP:CZ2	2.33	0.63
1:B:384:LYS:O	1:B:385:PHE:CB	2.37	0.63
1:D:89:MET:SD	1:D:106:LEU:HB3	2.38	0.63
1:E:137:LYS:NZ	1:E:140:ASP:OD1	2.32	0.63
1:E:140:ASP:O	1:E:141:THR:CB	2.45	0.63
1:F:314:VAL:HG23	1:F:314:VAL:O	1.99	0.63
1:B:156:LEU:C	1:B:156:LEU:CD1	2.71	0.63
1:C:174:SER:C	1:C:176:GLU:H	2.06	0.63
1:C:388:ASP:O	1:C:392:LEU:HD12	1.98	0.63
1:C:229:PRO:HB3	3:C:1320:HEM:HBC1	1.81	0.63
1:E:49:PRO:O	1:E:50:SER:O	2.17	0.63
1:F:205:GLY:O	1:F:207:ALA:N	2.32	0.63
1:C:128:GLU:C	1:C:130:ALA:H	2.07	0.62
1:C:143:ILE:CG2	1:C:219:ILE:HG12	2.29	0.62
1:D:125:ARG:HH12	1:D:230:LEU:HB3	1.63	0.62
1:E:314:VAL:O	1:E:315:LEU:CB	2.28	0.62
1:F:237:ALA:HB1	1:F:267:LYS:HG2	1.80	0.62
1:F:316:ASP:OD1	1:F:318:THR:CB	2.47	0.62
1:B:95:ILE:HD13	1:B:338:LEU:HD12	1.81	0.62
1:D:128:GLU:CD	1:D:161:ARG:HH22	2.06	0.62
1:F:137:LYS:HB2	1:F:140:ASP:OD1	1.99	0.62
1:B:150:THR:HB	1:B:222:GLN:HE22	1.65	0.62
1:C:104:GLU:OE1	1:C:369:ARG:HD3	1.99	0.62
1:C:224:ARG:HD2	1:C:224:ARG:C	2.23	0.62
1:C:269:LYS:C	1:C:273:PRO:HD3	2.25	0.62
1:D:393:GLN:O	1:D:393:GLN:CG	2.48	0.62
1:E:198:ASP:CA	1:E:202:SER:HB2	2.29	0.62
1:F:239:GLU:O	1:F:240:ILE:C	2.40	0.62
1:F:246:GLY:C	1:F:247:LYS:HD2	2.24	0.62
1:A:289:GLU:OE2	1:A:317:ARG:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:O	1:A:295:GLN:HB2	1.98	0.62
1:B:101:LEU:CD2	1:B:105:LEU:HD22	2.29	0.62
1:B:228:ASN:OD1	1:B:259:GLY:HA3	1.98	0.62
1:C:361:ALA:O	1:C:362:GLN:C	2.36	0.62
1:E:95:ILE:HD11	1:E:337:MET:HE2	1.80	0.62
1:E:205:GLY:C	1:E:207:ALA:N	2.55	0.62
1:E:253:ALA:HB3	1:E:261:ILE:HD13	1.80	0.62
1:F:101:LEU:H	1:F:101:LEU:HD12	1.65	0.62
1:F:146:THR:HG21	1:F:150:THR:HB	1.79	0.62
1:A:297:GLU:HA	1:A:297:GLU:OE2	1.99	0.62
1:B:47:ASP:OD1	1:B:48:ALA:HB2	1.99	0.62
1:C:80:ILE:HG12	1:D:344:LEU:HD23	1.81	0.62
1:C:121:ARG:HH12	1:C:235:THR:CG2	2.12	0.62
1:C:331:ALA:O	1:C:335:ALA:HB2	2.00	0.62
1:D:171:GLU:C	1:D:172:LYS:HD3	2.24	0.62
1:F:47:ASP:O	1:F:48:ALA:CB	2.48	0.62
1:F:316:ASP:OD1	1:F:318:THR:N	2.32	0.62
1:A:283:GLU:CB	1:A:298:GLN:OE1	2.39	0.62
1:C:121:ARG:NH1	1:C:236:THR:OG1	2.32	0.62
1:C:209:ARG:O	1:C:213:GLU:HG2	1.98	0.62
1:D:63:SER:HA	3:D:1420:HEM:HMB3	1.82	0.62
1:D:102:LYS:HB3	1:D:366:GLU:HG3	1.81	0.62
1:F:221:ASP:OD2	1:F:224:ARG:HG3	2.00	0.62
1:B:225:ASN:H	1:B:314:VAL:HG12	1.64	0.62
1:E:95:ILE:CD1	1:E:337:MET:HE3	2.30	0.62
1:E:177:LYS:HA	1:E:180:VAL:CG2	2.30	0.62
1:F:95:ILE:HG23	1:F:337:MET:HE3	1.82	0.62
1:B:210:LEU:HD22	1:B:214:ILE:HD11	1.79	0.62
1:B:384:LYS:HB3	1:B:390:TRP:NE1	2.14	0.62
1:E:145:PRO:CB	1:E:204:VAL:HG12	2.29	0.62
1:F:144:GLU:HG2	1:F:146:THR:HG22	1.82	0.62
1:A:206:VAL:O	1:A:210:LEU:HB2	2.00	0.62
1:B:248:LEU:HD23	1:B:249:ASP:H	1.63	0.62
1:D:83:LYS:HA	1:D:83:LYS:HE3	1.82	0.62
1:E:373:ILE:N	1:E:373:ILE:HD12	2.14	0.62
1:A:391:MET:HE3	1:A:397:LEU:HD11	1.80	0.62
1:B:387:SER:CB	1:B:389:ARG:HH21	2.13	0.62
1:D:146:THR:O	1:D:167:ILE:HG23	2.00	0.62
1:D:205:GLY:N	1:D:208:TRP:H	1.96	0.62
1:E:170:PRO:HD2	1:E:203:HIS:CE1	2.35	0.62
1:D:253:ALA:CB	1:D:373:ILE:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:THR:O	1:F:239:GLU:HG3	2.00	0.61
1:F:336:ARG:HG3	1:F:385:PHE:CE1	2.35	0.61
1:A:247:LYS:HD2	1:A:247:LYS:N	2.15	0.61
1:E:77:LEU:HD22	1:E:77:LEU:N	2.14	0.61
1:F:126:MET:SD	1:F:220:LEU:HB3	2.40	0.61
1:F:275:CYS:SG	1:F:276:ARG:N	2.74	0.61
1:C:229:PRO:HB2	3:C:1320:HEM:HAC	1.82	0.61
1:D:144:GLU:CG	1:D:146:THR:HG22	2.31	0.61
1:D:247:LYS:HD2	1:D:247:LYS:N	2.15	0.61
1:E:137:LYS:HZ1	1:E:140:ASP:CG	2.08	0.61
1:F:214:ILE:HG22	1:F:217:SER:OG	2.00	0.61
1:F:336:ARG:HH12	1:F:388:ASP:N	1.98	0.61
1:A:205:GLY:O	1:A:209:ARG:N	2.32	0.61
1:B:52:CYS:SG	1:B:53:THR:N	2.74	0.61
1:C:76:ILE:HD13	1:D:106:LEU:HD11	1.83	0.61
1:C:264:ILE:HD12	1:C:373:ILE:HD11	1.82	0.61
1:E:125:ARG:HH11	1:E:125:ARG:CG	2.12	0.61
1:E:232:HIS:HA	1:E:236:THR:HB	1.83	0.61
1:E:390:TRP:O	1:E:391:MET:HB2	1.98	0.61
1:A:266:ARG:O	1:A:270:GLU:HG2	2.00	0.61
1:A:381:TYR:CD1	1:A:381:TYR:N	2.69	0.61
1:C:119:LYS:HD3	1:C:150:THR:HG23	1.82	0.61
1:C:373:ILE:HG22	1:C:375:PRO:HD3	1.82	0.61
1:D:92:ILE:HA	1:D:342:GLU:OE1	2.01	0.61
1:F:99:PHE:HE1	1:F:337:MET:HE1	1.66	0.61
1:D:88:PRO:HG2	1:D:109:CYS:HB2	1.82	0.61
1:D:126:MET:HG2	1:D:227:SER:HB2	1.83	0.61
1:E:320:VAL:HG21	1:E:323:TRP:CZ2	2.36	0.61
1:F:336:ARG:NH2	1:F:388:ASP:HB3	2.16	0.61
1:F:366:GLU:CD	1:F:366:GLU:H	2.08	0.61
1:E:207:ALA:HB1	1:E:219:ILE:CD1	2.30	0.61
1:E:340:ALA:O	1:F:159:ALA:HB1	2.00	0.61
1:E:383:THR:O	1:E:383:THR:HG22	2.00	0.61
1:F:336:ARG:NH1	1:F:388:ASP:HA	2.16	0.61
1:A:226:ALA:HA	3:A:1120:HEM:HMD2	1.83	0.61
1:C:331:ALA:HB2	1:C:352:SER:OG	2.01	0.61
1:E:123:SER:O	1:E:127:ILE:HG13	2.01	0.61
1:F:87:THR:HG21	1:F:110:GLU:HA	1.81	0.61
1:A:170:PRO:HD3	1:A:191:THR:HG1	1.65	0.60
1:C:388:ASP:O	1:C:392:LEU:CB	2.49	0.60
1:D:54:TRP:CE3	1:D:266:ARG:HD3	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:GLU:CB	1:E:154:LEU:HD12	2.20	0.60
1:F:176:GLU:HB3	1:F:177:LYS:HD2	1.83	0.60
1:F:303:VAL:CG2	1:F:328:ASP:HA	2.31	0.60
1:C:76:ILE:O	1:C:78:PRO:HD3	2.01	0.60
1:C:223:TYR:CD1	1:C:257:THR:HG22	2.36	0.60
1:D:110:GLU:HG2	1:D:118:VAL:CG2	2.31	0.60
1:E:213:GLU:O	1:E:215:PRO:HD3	2.01	0.60
1:E:291:GLU:HA	1:E:291:GLU:OE2	2.00	0.60
1:A:315:LEU:HD12	1:A:316:ASP:N	2.16	0.60
1:C:255:VAL:HG11	1:C:287:LEU:CD1	2.31	0.60
1:C:156:LEU:C	1:C:156:LEU:HD13	2.26	0.60
1:E:265:ALA:HB1	1:E:319:VAL:HB	1.84	0.60
1:F:141:THR:HA	1:F:164:ARG:O	2.02	0.60
1:F:242:GLN:HA	1:F:242:GLN:NE2	2.13	0.60
1:C:260:THR:HG23	2:C:1310:PLP:O1P	2.01	0.60
1:D:47:ASP:N	1:D:313:THR:HG22	2.17	0.60
1:E:397:LEU:HD11	1:F:390:TRP:CD1	2.37	0.60
1:C:320:VAL:HG11	1:C:323:TRP:CE2	2.36	0.60
1:D:243:GLN:C	1:D:245:ASP:N	2.52	0.60
1:E:77:LEU:N	1:E:77:LEU:CD2	2.64	0.60
1:E:144:GLU:HG3	1:E:146:THR:O	2.02	0.60
1:F:174:SER:O	1:F:178:VAL:HG23	2.02	0.60
1:F:249:ASP:O	1:F:250:MET:HB2	2.02	0.60
1:E:49:PRO:CA	1:E:313:THR:HG22	2.32	0.60
1:A:80:ILE:CD1	1:A:83:LYS:CB	2.79	0.60
1:A:102:LYS:HG2	1:A:366:GLU:CD	2.26	0.60
1:B:208:TRP:CD1	1:B:219:ILE:HD12	2.36	0.60
1:A:91:ARG:HH11	1:A:91:ARG:CB	2.13	0.60
1:A:188:ILE:HG22	1:A:190:ARG:CD	2.32	0.60
1:B:188:ILE:HD13	1:B:188:ILE:H	1.67	0.60
1:C:86:ASP:H	1:C:239:GLU:CD	2.09	0.60
1:E:288:ALA:HB3	1:E:294:ASN:OD1	2.02	0.60
1:A:91:ARG:NH1	1:A:91:ARG:CB	2.65	0.60
1:B:288:ALA:CB	1:B:294:ASN:HD21	2.11	0.60
1:C:92:ILE:HA	1:C:342:GLU:OE2	2.01	0.60
1:D:286:ILE:HA	1:D:294:ASN:HD22	1.62	0.60
1:E:225:ASN:OD1	1:E:227:SER:N	2.35	0.60
1:E:320:VAL:HG11	1:E:323:TRP:CD1	2.37	0.60
1:F:45:ARG:CA	1:F:47:ASP:H	2.14	0.60
1:F:287:LEU:HA	1:F:317:ARG:HH21	1.66	0.60
1:A:149:ASN:HA	1:A:152:ILE:HD12	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ILE:HG23	1:D:136:LEU:HD21	1.84	0.59
1:E:49:PRO:HA	1:E:313:THR:CG2	2.32	0.59
1:E:102:LYS:CD	1:E:365:GLN:HG2	2.31	0.59
1:E:176:GLU:N	1:E:177:LYS:H	2.00	0.59
1:F:230:LEU:O	1:F:233:TYR:HB3	2.02	0.59
1:A:66:HIS:ND1	1:A:132:ARG:NH2	2.50	0.59
1:B:210:LEU:HD22	1:B:214:ILE:CD1	2.32	0.59
1:C:169:MET:HE2	1:C:190:ARG:NE	2.16	0.59
1:B:292:GLU:OE2	1:B:292:GLU:N	2.29	0.59
1:C:291:GLU:C	1:C:291:GLU:CD	2.70	0.59
1:C:389:ARG:NH2	1:D:175:SER:OG	2.30	0.59
1:D:325:LYS:NZ	1:D:325:LYS:HB3	2.17	0.59
1:E:87:THR:HG21	1:E:110:GLU:CD	2.26	0.59
1:E:98:LYS:HD2	1:E:98:LYS:O	2.01	0.59
1:F:92:ILE:HG12	1:F:105:LEU:O	2.02	0.59
1:F:236:THR:O	1:F:240:ILE:HD12	2.02	0.59
1:F:290:PRO:CB	1:F:293:LEU:HG	2.23	0.59
1:A:379:ARG:O	1:A:380:ASN:C	2.37	0.59
1:B:101:LEU:HD13	1:B:358:VAL:HA	1.83	0.59
1:C:211:LYS:NZ	1:C:211:LYS:CB	2.65	0.59
1:C:226:ALA:HA	3:C:1320:HEM:CMD	2.33	0.59
1:C:384:LYS:HA	1:C:390:TRP:CD1	2.37	0.59
1:C:390:TRP:HA	1:C:393:GLN:HG2	1.85	0.59
1:E:288:ALA:HB3	1:E:294:ASN:ND2	2.17	0.59
1:E:294:ASN:ND2	1:E:294:ASN:H	2.00	0.59
1:F:254:SER:CA	1:F:280:VAL:HB	2.32	0.59
1:A:192:PRO:C	1:A:193:THR:HG22	2.27	0.59
1:A:252:VAL:HG22	1:A:278:ILE:HB	1.84	0.59
1:B:144:GLU:HG3	1:B:146:THR:HG22	1.84	0.59
1:C:361:ALA:O	1:C:363:GLU:N	2.34	0.59
1:D:211:LYS:HE2	1:D:219:ILE:HG13	1.85	0.59
1:D:219:ILE:CG2	1:D:220:LEU:N	2.63	0.59
1:D:233:TYR:CE1	1:D:267:LYS:HB2	2.37	0.59
1:F:170:PRO:HB2	1:F:173:MET:HE3	1.85	0.59
1:F:287:LEU:H	1:F:287:LEU:CD1	2.12	0.59
1:F:336:ARG:NH1	1:F:388:ASP:N	2.50	0.59
1:B:287:LEU:HD23	1:B:310:PHE:O	1.97	0.59
1:B:335:ALA:HB3	1:B:385:PHE:HE1	1.68	0.59
1:F:350:ALA:O	1:F:354:VAL:HG23	2.02	0.59
1:B:95:ILE:CG2	1:B:337:MET:HE3	2.32	0.59
1:C:253:ALA:HB3	1:C:261:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:VAL:O	1:E:207:ALA:HB3	2.03	0.59
1:F:249:ASP:O	1:F:250:MET:CB	2.50	0.59
1:F:264:ILE:CG2	1:F:268:LEU:HD12	2.32	0.59
1:B:249:ASP:HB2	1:B:369:ARG:O	2.03	0.59
1:C:287:LEU:O	1:C:323:TRP:CZ3	2.56	0.59
1:E:49:PRO:N	1:E:313:THR:HG21	2.17	0.59
1:F:96:GLY:O	1:F:101:LEU:HD13	2.03	0.59
1:F:346:CYS:SG	1:F:350:ALA:CB	2.91	0.59
1:A:366:GLU:C	1:A:367:GLY:CA	2.70	0.59
1:D:145:PRO:HG3	1:D:207:ALA:HB3	1.84	0.59
1:E:222:GLN:HE21	1:E:257:THR:CG2	2.16	0.59
1:F:396:PHE:O	1:F:396:PHE:HD2	1.82	0.59
1:C:336:ARG:CZ	1:C:391:MET:HG3	2.32	0.58
1:D:58:ARG:HD2	1:D:62:GLU:OE1	2.03	0.58
1:D:236:THR:O	1:D:240:ILE:HG13	2.02	0.58
1:D:320:VAL:HG11	1:D:323:TRP:NE1	2.18	0.58
1:E:93:ASN:HD21	1:F:79:ASP:HB3	1.68	0.58
1:A:137:LYS:HB2	1:A:140:ASP:CG	2.29	0.58
1:A:378:VAL:O	1:A:381:TYR:N	2.33	0.58
1:D:68:THR:O	1:D:234:ASP:HB3	2.03	0.58
1:D:248:LEU:HD23	1:D:249:ASP:N	2.14	0.58
1:F:299:THR:CG2	1:F:300:THR:OG1	2.51	0.58
1:C:156:LEU:C	1:C:156:LEU:CD1	2.76	0.58
1:C:264:ILE:O	1:C:268:LEU:HB2	2.03	0.58
1:D:61:SER:HB2	1:F:242:GLN:HE22	1.67	0.58
1:E:242:GLN:HE21	1:E:242:GLN:HA	1.67	0.58
1:C:269:LYS:O	1:C:273:PRO:CG	2.47	0.58
1:D:102:LYS:HE3	1:D:366:GLU:CD	2.28	0.58
1:E:389:ARG:NH2	1:F:175:SER:OG	2.36	0.58
1:A:94:LYS:NZ	1:A:341:GLN:HA	2.19	0.58
1:A:110:GLU:HG2	1:A:118:VAL:HG23	1.84	0.58
1:A:131:GLU:CG	1:A:136:LEU:HD23	2.32	0.58
1:A:191:THR:HG23	1:A:203:HIS:CG	2.39	0.58
1:A:205:GLY:C	1:A:207:ALA:N	2.60	0.58
1:C:86:ASP:N	1:C:239:GLU:OE1	2.33	0.58
1:C:135:THR:HG22	1:C:218:HIS:CE1	2.39	0.58
1:F:169:MET:CE	1:F:178:VAL:HG22	2.33	0.58
1:F:387:SER:O	1:F:388:ASP:C	2.47	0.58
1:B:46:PRO:CD	1:B:310:PHE:CD1	2.87	0.58
1:B:126:MET:O	1:B:127:ILE:C	2.47	0.58
1:C:346:CYS:O	1:C:378:VAL:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PRO:HD3	1:B:191:THR:CB	2.33	0.58
1:B:378:VAL:HG12	1:B:385:PHE:HE2	1.69	0.58
1:C:122:ILE:HG21	1:C:228:ASN:OD1	2.02	0.58
1:D:286:ILE:HD12	1:D:286:ILE:N	2.18	0.58
1:F:122:ILE:HD12	1:F:122:ILE:C	2.28	0.58
1:F:191:THR:HG21	4:F:1622:HOH:O	2.04	0.58
1:A:103:CYS:O	1:A:104:GLU:C	2.44	0.58
1:A:385:PHE:N	1:A:390:TRP:CE3	2.72	0.58
1:B:202:SER:O	1:B:203:HIS:ND1	2.36	0.58
1:C:171:GLU:HA	1:C:190:ARG:HE	1.68	0.58
1:D:56:LEU:CD1	1:D:270:GLU:HG2	2.34	0.58
1:D:169:MET:O	1:D:170:PRO:O	2.22	0.58
1:D:287:LEU:HD11	1:D:308:TYR:H	1.69	0.58
1:B:169:MET:HG3	1:B:169:MET:O	2.04	0.58
1:B:362:GLN:O	1:B:363:GLU:C	2.43	0.58
1:D:282:PRO:HA	1:D:326:SER:OG	2.04	0.58
1:F:252:VAL:HG12	1:F:353:THR:HG23	1.86	0.58
1:F:286:ILE:O	1:F:291:GLU:OE2	2.22	0.58
1:F:294:ASN:N	1:F:294:ASN:ND2	2.39	0.58
1:A:244:CYS:O	1:A:369:ARG:NH2	2.33	0.57
1:C:95:ILE:C	1:C:97:LYS:H	2.12	0.57
1:C:204:VAL:O	1:C:205:GLY:C	2.47	0.57
1:A:106:LEU:HD11	1:A:369:ARG:HD3	1.85	0.57
1:A:147:SER:HA	1:A:169:MET:HE2	1.86	0.57
1:C:76:ILE:HD13	1:D:106:LEU:CD1	2.33	0.57
1:C:85:GLY:HA2	1:C:121:ARG:NH2	2.19	0.57
1:C:382:MET:HB3	1:D:176:GLU:HG3	1.86	0.57
1:D:280:VAL:HG22	1:D:356:VAL:HG21	1.85	0.57
1:E:108:LYS:HE2	1:E:243:GLN:OE1	2.04	0.57
1:E:127:ILE:CD1	1:E:142:ILE:CD1	2.78	0.57
1:E:188:ILE:HG22	1:E:189:VAL:N	2.19	0.57
1:E:207:ALA:C	1:E:210:LEU:HB2	2.26	0.57
1:E:338:LEU:HD21	1:E:354:VAL:HG21	1.86	0.57
1:F:288:ALA:HB2	1:F:325:LYS:NZ	2.19	0.57
1:B:46:PRO:CG	1:B:310:PHE:CE2	2.87	0.57
1:C:301:TYR:OH	1:C:307:GLY:HA3	2.03	0.57
1:D:289:GLU:O	1:D:290:PRO:C	2.31	0.57
1:E:54:TRP:HB2	3:E:1520:HEM:CHC	2.34	0.57
1:F:335:ALA:HB1	1:F:385:PHE:CZ	2.39	0.57
1:F:336:ARG:HH12	1:F:388:ASP:HB3	1.67	0.57
1:A:91:ARG:NH1	1:B:78:PRO:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HG13	1:B:123:SER:N	2.19	0.57
1:C:90:VAL:HG22	1:D:77:LEU:HD13	1.85	0.57
1:C:166:ILE:HG22	1:C:167:ILE:H	1.68	0.57
1:E:125:ARG:HH12	1:E:230:LEU:HB3	1.69	0.57
1:E:313:THR:O	1:E:314:VAL:HG13	2.04	0.57
1:E:397:LEU:HD13	1:F:390:TRP:HB2	1.83	0.57
1:F:86:ASP:N	1:F:239:GLU:OE1	2.35	0.57
1:F:335:ALA:O	1:F:339:ILE:HG13	2.04	0.57
1:D:76:ILE:HG22	1:D:77:LEU:N	2.20	0.57
1:D:78:PRO:CD	1:D:82:LYS:HG3	2.35	0.57
1:E:322:LYS:HG2	1:E:323:TRP:N	2.20	0.57
1:D:89:MET:HE3	1:D:244:CYS:SG	2.45	0.57
1:E:382:MET:SD	1:E:386:LEU:HD12	2.44	0.57
1:F:179:ASP:HA	1:F:182:ARG:NH1	2.19	0.57
1:B:357:ALA:O	1:B:361:ALA:N	2.34	0.57
1:C:214:ILE:O	1:C:215:PRO:O	2.23	0.57
1:C:224:ARG:HD2	1:C:225:ASN:HA	1.84	0.57
1:C:283:GLU:OE2	1:C:296:THR:HG21	2.05	0.57
1:C:388:ASP:O	1:C:392:LEU:HB2	2.04	0.57
1:D:306:ILE:HG22	2:D:1410:PLP:H6	1.86	0.57
1:D:390:TRP:CZ2	1:D:394:LYS:HE2	2.39	0.57
1:E:49:PRO:CG	1:E:313:THR:HG22	2.29	0.57
1:E:221:ASP:OD2	1:E:223:TYR:HB2	2.04	0.57
1:A:147:SER:HB3	1:A:169:MET:HB2	1.86	0.57
1:B:63:SER:HA	3:B:1220:HEM:HMB3	1.87	0.57
1:C:128:GLU:C	1:C:130:ALA:N	2.60	0.57
1:C:379:ARG:O	1:C:379:ARG:HG2	2.04	0.57
1:E:154:LEU:O	1:E:158:ALA:HB2	2.05	0.57
1:A:83:LYS:HA	1:A:83:LYS:HZ1	1.69	0.57
1:A:128:GLU:O	1:A:132:ARG:HD3	2.05	0.57
1:A:251:LEU:HD22	1:A:264:ILE:CG2	2.35	0.57
1:B:350:ALA:CB	1:B:374:LEU:HD22	2.35	0.57
1:D:131:GLU:HA	1:D:136:LEU:HB3	1.85	0.57
1:A:170:PRO:CD	1:A:203:HIS:CE1	2.88	0.57
1:A:188:ILE:CG2	1:A:190:ARG:CD	2.83	0.57
1:C:174:SER:C	1:C:176:GLU:N	2.61	0.57
1:C:360:ALA:O	1:C:363:GLU:HG3	2.04	0.57
1:C:388:ASP:O	1:C:392:LEU:CG	2.53	0.57
1:D:390:TRP:CE2	1:D:394:LYS:HE2	2.40	0.57
1:E:287:LEU:HD21	1:E:312:PRO:HD2	1.86	0.57
1:C:286:ILE:HG13	1:C:308:TYR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LYS:CB	1:F:66:HIS:CE1	2.78	0.56
1:F:203:HIS:HA	4:F:1622:HOH:O	2.04	0.56
1:B:329:GLU:HG2	1:B:396:PHE:HD2	1.70	0.56
1:C:92:ILE:HB	1:C:105:LEU:HB3	1.87	0.56
1:C:170:PRO:HG3	1:C:203:HIS:CE1	2.39	0.56
1:C:282:PRO:O	1:C:325:LYS:NZ	2.37	0.56
1:F:208:TRP:CD1	1:F:219:ILE:HD12	2.40	0.56
1:A:192:PRO:O	1:A:193:THR:C	2.45	0.56
1:B:335:ALA:HB1	1:B:385:PHE:HE1	1.70	0.56
1:B:350:ALA:O	1:B:351:GLY:C	2.47	0.56
1:C:101:LEU:HD12	1:C:362:GLN:HG2	1.87	0.56
1:C:137:LYS:HB2	1:C:140:ASP:CG	2.30	0.56
1:C:144:GLU:HB2	1:C:154:LEU:CD1	2.35	0.56
1:D:287:LEU:CD1	1:D:308:TYR:H	2.18	0.56
1:D:390:TRP:O	1:D:391:MET:C	2.48	0.56
1:E:199:SER:HB2	1:E:201:GLU:H	1.70	0.56
1:A:315:LEU:HD12	1:A:316:ASP:H	1.69	0.56
1:C:335:ALA:CB	1:C:385:PHE:CZ	2.89	0.56
1:E:208:TRP:CZ3	1:E:219:ILE:HD12	2.40	0.56
1:E:343:GLY:CA	1:F:156:LEU:HD21	2.35	0.56
1:A:155:ALA:HA	1:A:158:ALA:HB3	1.88	0.56
1:A:201:GLU:O	1:A:202:SER:HB3	2.05	0.56
1:C:286:ILE:O	1:C:288:ALA:N	2.36	0.56
1:C:361:ALA:C	1:C:363:GLU:N	2.61	0.56
1:E:95:ILE:HD11	1:E:337:MET:CE	2.35	0.56
1:E:261:ILE:HG23	1:E:262:THR:N	2.21	0.56
1:F:233:TYR:O	1:F:237:ALA:HB3	2.05	0.56
1:F:288:ALA:HB3	1:F:325:LYS:HZ3	1.70	0.56
1:A:200:PRO:O	1:A:201:GLU:CB	2.49	0.56
1:B:209:ARG:HA	1:B:212:ASN:HD22	1.70	0.56
1:D:131:GLU:HG3	1:D:136:LEU:HD23	1.87	0.56
1:D:310:PHE:O	1:D:311:ILE:HD12	2.03	0.56
1:E:91:ARG:HH21	1:F:78:PRO:HA	1.71	0.56
1:A:90:VAL:HG22	1:B:77:LEU:HB2	1.88	0.56
1:A:127:ILE:HG23	1:A:136:LEU:CD2	2.36	0.56
1:B:64:PRO:O	1:B:65:HIS:CG	2.59	0.56
1:C:51:ARG:HD3	3:C:1320:HEM:O2A	2.05	0.56
1:D:74:PRO:HB3	1:D:76:ILE:O	2.05	0.56
1:E:89:MET:CE	1:E:240:ILE:HA	2.36	0.56
1:F:63:SER:HA	3:F:1620:HEM:HMB3	1.87	0.56
1:A:169:MET:O	1:A:190:ARG:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:C	1:A:314:VAL:HG22	2.30	0.56
1:B:203:HIS:C	1:B:204:VAL:CG2	2.77	0.56
1:C:59:PRO:O	1:C:60:ALA:C	2.49	0.56
1:C:192:PRO:C	1:C:193:THR:OG1	2.47	0.56
1:C:251:LEU:HD23	1:C:251:LEU:C	2.31	0.56
1:D:48:ALA:HB1	1:D:49:PRO:CD	2.35	0.56
1:D:72:LYS:O	1:D:74:PRO:HD3	2.06	0.56
1:D:125:ARG:NH1	1:D:230:LEU:HB3	2.21	0.56
1:D:130:ALA:HB3	1:D:136:LEU:HD22	1.86	0.56
1:D:213:GLU:O	1:D:215:PRO:HD3	2.05	0.56
1:D:372:VAL:O	1:D:372:VAL:HG12	2.05	0.56
1:E:316:ASP:OD2	1:E:318:THR:CB	2.54	0.56
1:F:111:PHE:CD2	1:F:346:CYS:HB3	2.41	0.56
1:F:254:SER:CB	1:F:306:ILE:HG21	2.34	0.56
1:F:308:TYR:HD2	1:F:310:PHE:O	1.88	0.56
1:A:179:ASP:OD1	1:B:389:ARG:NH2	2.39	0.56
1:C:122:ILE:HG13	1:C:123:SER:N	2.21	0.56
1:D:349:SER:HB2	1:D:375:PRO:HG2	1.88	0.56
1:B:268:LEU:O	1:B:272:CYS:O	2.24	0.56
1:C:143:ILE:HG21	1:C:219:ILE:HG12	1.86	0.56
1:C:361:ALA:HA	1:C:364:LEU:HD23	1.88	0.56
1:F:149:ASN:OD1	1:F:380:ASN:ND2	2.39	0.56
1:A:221:ASP:N	1:A:225:ASN:HD22	2.03	0.55
1:D:173:MET:CE	1:D:173:MET:CA	2.40	0.55
1:E:394:LYS:N	1:E:394:LYS:HZ2	2.04	0.55
1:F:144:GLU:CD	1:F:145:PRO:HD2	2.31	0.55
1:F:176:GLU:O	1:F:180:VAL:CG2	2.50	0.55
1:A:106:LEU:HD11	1:A:369:ARG:CD	2.36	0.55
1:E:250:MET:N	1:E:275:CYS:SG	2.80	0.55
1:F:338:LEU:HD11	1:F:354:VAL:HG21	1.88	0.55
1:A:336:ARG:NH1	1:A:388:ASP:OD2	2.40	0.55
1:B:97:LYS:C	1:B:99:PHE:H	2.14	0.55
1:B:348:GLY:O	1:B:349:SER:C	2.48	0.55
1:B:366:GLU:HB3	1:C:216:ASN:ND2	2.20	0.55
1:C:268:LEU:O	1:C:272:CYS:CA	2.54	0.55
1:A:78:PRO:HB3	1:B:91:ARG:HH21	1.71	0.55
1:C:255:VAL:HG11	1:C:287:LEU:HD12	1.88	0.55
1:E:198:ASP:HB3	1:E:310:PHE:HZ	1.65	0.55
1:E:346:CYS:O	1:E:378:VAL:CG1	2.53	0.55
1:F:289:GLU:HB2	1:F:323:TRP:CD1	2.40	0.55
1:A:194:ASN:N	1:A:200:PRO:CD	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:VAL:O	1:C:107:ALA:N	2.39	0.55
1:E:89:MET:HE1	1:E:240:ILE:HA	1.89	0.55
1:B:287:LEU:HD11	1:B:308:TYR:HB2	1.89	0.55
1:C:77:LEU:CB	1:D:90:VAL:HG22	2.33	0.55
1:C:255:VAL:HG12	1:C:287:LEU:HD13	1.86	0.55
1:C:353:THR:HG21	1:C:372:VAL:HG13	1.88	0.55
1:C:363:GLU:CD	1:C:364:LEU:HD22	2.32	0.55
1:D:126:MET:HB3	1:D:220:LEU:HD22	1.88	0.55
1:D:329:GLU:HG3	1:D:396:PHE:HD2	1.71	0.55
1:E:68:THR:HG21	1:E:132:ARG:HH12	1.71	0.55
1:E:83:LYS:O	1:E:83:LYS:HG3	2.07	0.55
1:F:137:LYS:O	1:F:140:ASP:HB2	2.06	0.55
1:A:126:MET:O	1:A:220:LEU:HD22	2.07	0.55
1:C:59:PRO:HG2	1:C:62:GLU:CD	2.31	0.55
1:C:382:MET:HB3	1:D:176:GLU:CG	2.37	0.55
1:E:183:ALA:HB1	1:F:339:ILE:HG21	1.89	0.55
1:F:81:LEU:CD2	1:F:84:ILE:HD11	2.35	0.55
1:A:188:ILE:CG2	1:A:190:ARG:HD3	2.37	0.55
1:A:226:ALA:O	1:A:230:LEU:HG	2.06	0.55
1:C:211:LYS:NZ	1:C:219:ILE:HD12	2.21	0.55
1:D:191:THR:O	1:D:191:THR:HG22	2.07	0.55
1:D:231:ALA:O	1:D:235:THR:OG1	2.22	0.55
1:E:90:VAL:HG22	1:F:77:LEU:HG	1.89	0.55
1:E:95:ILE:CD1	1:E:337:MET:CE	2.85	0.55
1:E:364:LEU:HD12	1:E:368:GLN:CD	2.32	0.55
1:A:191:THR:C	1:A:193:THR:N	2.59	0.55
1:E:92:ILE:HG21	1:E:95:ILE:HG23	1.88	0.55
1:E:252:VAL:HB	1:E:372:VAL:HG22	1.89	0.55
1:B:146:THR:HG21	1:B:222:GLN:HE21	1.71	0.55
1:B:257:THR:N	2:B:1210:PLP:O3P	2.37	0.55
1:C:211:LYS:HA	1:C:217:SER:CB	2.37	0.55
1:D:156:LEU:CA	1:D:184:LEU:HD13	2.37	0.55
1:E:172:LYS:HG3	1:E:173:MET:N	2.21	0.55
1:E:261:ILE:HG23	1:E:262:THR:H	1.72	0.55
1:A:248:LEU:HD21	1:A:371:VAL:H	1.73	0.54
1:B:400:GLU:O	1:B:400:GLU:HG2	2.05	0.54
1:D:219:ILE:HG22	1:D:221:ASP:H	1.71	0.54
1:D:250:MET:CE	1:D:276:ARG:HB2	2.37	0.54
1:F:115:GLY:HA3	1:F:120:ASP:OD2	2.07	0.54
1:F:299:THR:HG22	1:F:300:THR:CB	2.36	0.54
1:B:325:LYS:HB3	1:B:325:LYS:HZ2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:GLU:HG2	1:D:118:VAL:HG23	1.88	0.54
1:D:113:ASN:O	1:D:114:ALA:C	2.49	0.54
1:D:176:GLU:O	1:D:180:VAL:HG23	2.07	0.54
1:F:80:ILE:O	1:F:81:LEU:C	2.49	0.54
1:B:106:LEU:HD11	1:B:369:ARG:HD3	1.88	0.54
1:D:223:TYR:HD1	1:D:312:PRO:HG3	1.71	0.54
1:E:233:TYR:CE1	1:E:267:LYS:HD3	2.43	0.54
1:F:103:CYS:HB2	1:F:368:GLN:O	2.07	0.54
1:F:136:LEU:HD21	1:F:142:ILE:HD11	1.90	0.54
1:A:276:ARG:HH21	1:A:321:ASP:HB3	1.72	0.54
1:D:137:LYS:O	1:D:140:ASP:HB2	2.07	0.54
1:D:373:ILE:C	1:D:374:LEU:HD23	2.32	0.54
3:D:1420:HEM:HBB2	3:D:1420:HEM:HMB2	1.90	0.54
1:E:208:TRP:C	1:E:210:LEU:N	2.66	0.54
1:D:117:SER:OG	1:D:120:ASP:OD1	2.25	0.54
1:D:205:GLY:C	1:D:208:TRP:H	2.14	0.54
1:E:177:LYS:HA	1:E:180:VAL:HG23	1.89	0.54
1:E:281:ASP:OD2	1:E:282:PRO:HD2	2.07	0.54
1:E:290:PRO:HB3	1:E:292:GLU:OE2	2.08	0.54
1:E:396:PHE:O	1:F:389:ARG:NH2	2.40	0.54
1:F:127:ILE:CD1	1:F:154:LEU:CD2	2.82	0.54
1:F:248:LEU:CD1	1:F:268:LEU:HD21	2.38	0.54
1:A:80:ILE:HD11	1:A:83:LYS:HB2	1.87	0.54
1:A:110:GLU:HG2	1:A:118:VAL:HA	1.90	0.54
1:C:78:PRO:O	1:D:91:ARG:HB3	2.07	0.54
1:C:113:ASN:O	1:C:114:ALA:C	2.51	0.54
1:C:291:GLU:CD	1:C:291:GLU:O	2.51	0.54
1:D:53:THR:O	1:D:58:ARG:NH2	2.26	0.54
1:D:233:TYR:CZ	1:D:267:LYS:HE3	2.42	0.54
1:E:54:TRP:HB2	3:E:1520:HEM:C4B	2.42	0.54
1:A:83:LYS:HA	1:A:83:LYS:HZ2	1.69	0.54
1:A:126:MET:CG	1:A:220:LEU:HB3	2.38	0.54
1:C:174:SER:OG	1:C:176:GLU:HB3	2.08	0.54
1:D:95:ILE:HG12	1:D:337:MET:HG2	1.89	0.54
1:E:213:GLU:N	1:E:213:GLU:OE2	2.41	0.54
1:F:144:GLU:HG3	1:F:146:THR:HG22	1.86	0.54
1:F:381:TYR:N	1:F:381:TYR:CD1	2.76	0.54
1:A:96:GLY:C	1:A:98:LYS:H	2.16	0.54
1:B:68:THR:HG22	1:B:234:ASP:CB	2.38	0.54
1:B:211:LYS:HD2	1:B:219:ILE:HG13	1.89	0.54
1:C:88:PRO:HB2	1:D:77:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:CG2	1:C:143:ILE:H	2.21	0.54
1:C:179:ASP:OD2	1:D:389:ARG:NH2	2.40	0.54
1:E:48:ALA:H	1:E:313:THR:CG2	2.06	0.54
1:A:66:HIS:HD1	1:A:132:ARG:HH22	1.56	0.54
1:A:176:GLU:O	1:A:180:VAL:HG23	2.08	0.54
1:C:211:LYS:HB2	1:C:211:LYS:HZ2	1.73	0.54
1:E:222:GLN:HE21	1:E:257:THR:HG21	1.73	0.54
1:F:45:ARG:HA	1:F:47:ASP:H	1.73	0.54
1:F:89:MET:SD	1:F:106:LEU:HB3	2.48	0.54
1:F:168:VAL:HG22	1:F:189:VAL:CB	2.33	0.54
1:F:331:ALA:HB2	1:F:352:SER:OG	2.07	0.54
1:A:66:HIS:CE1	1:C:71:ALA:HA	2.42	0.54
1:A:124:LEU:O	1:A:128:GLU:HG3	2.06	0.54
1:B:123:SER:OG	1:B:154:LEU:N	2.41	0.54
1:C:121:ARG:HH22	1:C:239:GLU:CD	2.15	0.54
1:D:177:LYS:HG2	1:D:380:ASN:OD1	2.08	0.54
1:D:221:ASP:OD2	1:D:221:ASP:C	2.51	0.54
1:E:248:LEU:HD22	1:E:275:CYS:SG	2.48	0.54
1:F:391:MET:HE3	1:F:392:LEU:CD2	2.38	0.54
1:A:72:LYS:O	1:A:74:PRO:HD3	2.08	0.53
1:A:94:LYS:HZ2	1:A:341:GLN:HA	1.71	0.53
1:C:276:ARG:NH2	1:C:321:ASP:HB3	2.23	0.53
1:D:145:PRO:HG3	1:D:207:ALA:CB	2.37	0.53
1:E:176:GLU:CA	1:E:396:PHE:CZ	2.87	0.53
1:E:254:SER:HB2	1:E:353:THR:HG23	1.91	0.53
1:F:250:MET:HE1	1:F:364:LEU:HD21	1.88	0.53
1:A:188:ILE:HD12	1:A:188:ILE:N	2.22	0.53
1:A:296:THR:HG23	1:A:298:GLN:HB3	1.90	0.53
1:B:146:THR:O	1:B:146:THR:HG23	2.08	0.53
1:E:332:PHE:HE1	1:E:390:TRP:CH2	2.25	0.53
1:F:251:LEU:CD1	1:F:264:ILE:HG21	2.38	0.53
1:A:258:GLY:HA3	1:A:315:LEU:HB2	1.90	0.53
1:C:92:ILE:HA	1:C:342:GLU:CD	2.34	0.53
1:C:172:LYS:O	1:C:173:MET:CA	2.56	0.53
1:D:91:ARG:CG	1:D:93:ASN:HD21	2.21	0.53
1:D:287:LEU:HD11	1:D:308:TYR:N	2.23	0.53
1:E:201:GLU:O	1:E:201:GLU:CD	2.47	0.53
1:F:361:ALA:HA	1:F:364:LEU:HD23	1.90	0.53
1:A:92:ILE:HG23	1:A:342:GLU:HG3	1.88	0.53
1:B:173:MET:O	1:B:174:SER:O	2.27	0.53
1:B:352:SER:O	1:B:356:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:MET:C	1:C:128:GLU:H	2.17	0.53
1:C:255:VAL:CG1	1:C:287:LEU:HD12	2.37	0.53
1:E:124:LEU:O	1:E:128:GLU:HB2	2.09	0.53
1:E:311:ILE:HD13	1:E:317:ARG:HE	1.72	0.53
1:D:364:LEU:HD12	1:D:364:LEU:N	2.24	0.53
1:E:111:PHE:HB3	1:E:376:ASP:C	2.34	0.53
1:E:149:ASN:HA	1:E:152:ILE:HD13	1.90	0.53
1:A:155:ALA:HB2	1:A:186:ALA:HB2	1.90	0.53
1:A:398:LYS:CD	1:A:398:LYS:H	2.21	0.53
1:B:327:ASN:HD21	1:B:330:GLU:CB	2.21	0.53
1:C:117:SER:CB	1:C:149:ASN:HB3	2.38	0.53
1:F:56:LEU:HD22	1:F:269:LYS:HB3	1.87	0.53
1:F:168:VAL:HG13	1:F:189:VAL:CG1	2.38	0.53
1:B:131:GLU:OE1	1:B:163:TYR:OH	2.25	0.53
1:B:379:ARG:HB3	1:B:379:ARG:CZ	2.38	0.53
1:D:92:ILE:HG23	1:D:342:GLU:CD	2.34	0.53
1:D:250:MET:CB	1:D:364:LEU:HD21	2.29	0.53
1:D:282:PRO:HD3	1:D:306:ILE:HD12	1.90	0.53
1:F:78:PRO:HB2	1:F:79:ASP:OD2	2.09	0.53
1:A:232:HIS:O	1:A:237:ALA:N	2.37	0.53
1:C:224:ARG:CG	1:C:224:ARG:O	2.57	0.53
1:D:210:LEU:HD22	1:D:214:ILE:HD11	1.90	0.53
1:D:320:VAL:HG11	1:D:323:TRP:CE2	2.44	0.53
1:E:324:PHE:CE2	1:E:359:LYS:HE3	2.44	0.53
1:C:79:ASP:O	1:C:80:ILE:C	2.51	0.53
1:D:79:ASP:OD1	1:D:81:LEU:HB2	2.09	0.53
1:E:257:THR:OG1	2:E:1510:PLP:O3P	2.24	0.53
1:A:232:HIS:HA	1:A:236:THR:CB	2.39	0.53
1:B:349:SER:HB3	2:B:1210:PLP:H2A3	1.90	0.53
1:B:379:ARG:NH1	1:B:379:ARG:CB	2.72	0.53
1:C:85:GLY:O	1:C:86:ASP:HB3	2.09	0.53
1:C:341:GLN:O	1:C:342:GLU:HB3	2.08	0.53
1:E:288:ALA:HA	1:E:323:TRP:CD2	2.44	0.53
1:F:54:TRP:CE3	1:F:266:ARG:NE	2.77	0.53
1:F:111:PHE:CE1	1:F:112:PHE:CE1	2.96	0.53
1:F:364:LEU:H	1:F:364:LEU:CD2	2.18	0.53
1:B:281:ASP:OD1	1:B:288:ALA:HB2	2.09	0.52
1:B:384:LYS:HB3	1:B:390:TRP:CD1	2.44	0.52
1:C:95:ILE:HD11	1:C:337:MET:O	2.09	0.52
1:C:389:ARG:O	1:C:393:GLN:HG2	2.09	0.52
1:D:170:PRO:HD3	1:D:203:HIS:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ASN:OD1	1:D:228:ASN:C	2.52	0.52
1:F:80:ILE:HG13	1:F:114:ALA:HB1	1.90	0.52
1:F:146:THR:HG21	1:F:150:THR:CG2	2.38	0.52
1:F:389:ARG:HG2	1:F:390:TRP:H	1.74	0.52
1:A:76:ILE:C	1:A:77:LEU:HD23	2.33	0.52
1:B:327:ASN:HD21	1:B:330:GLU:HB3	1.73	0.52
1:C:253:ALA:O	1:C:280:VAL:N	2.39	0.52
1:D:378:VAL:O	1:D:381:TYR:N	2.42	0.52
1:E:176:GLU:O	1:E:180:VAL:CG2	2.56	0.52
1:F:167:ILE:O	1:F:188:ILE:HA	2.09	0.52
1:D:156:LEU:HA	1:D:184:LEU:HD13	1.90	0.52
1:E:119:LYS:HG3	1:E:150:THR:N	2.24	0.52
1:E:144:GLU:OE2	1:E:145:PRO:HD2	2.09	0.52
1:E:193:THR:O	1:E:193:THR:HG23	2.08	0.52
1:E:232:HIS:CD2	1:E:260:THR:HA	2.44	0.52
1:B:156:LEU:C	1:B:156:LEU:HD12	2.33	0.52
1:C:280:VAL:HG13	1:C:356:VAL:HG21	1.92	0.52
1:D:54:TRP:CD2	1:D:266:ARG:HD3	2.44	0.52
1:D:87:THR:HB	1:D:109:CYS:O	2.10	0.52
1:D:266:ARG:HG2	1:D:319:VAL:HG11	1.91	0.52
1:D:306:ILE:HG22	2:D:1410:PLP:C6	2.40	0.52
1:E:268:LEU:HD23	1:E:277:ILE:CD1	2.39	0.52
1:B:85:GLY:O	1:B:86:ASP:HB3	2.09	0.52
1:C:334:PHE:HA	1:C:337:MET:HB2	1.91	0.52
1:E:228:ASN:HB3	1:E:229:PRO:CD	2.39	0.52
1:E:283:GLU:HG2	1:E:325:LYS:HE3	1.92	0.52
1:F:256:GLY:O	1:F:257:THR:HB	2.09	0.52
1:A:152:ILE:HA	1:A:181:LEU:HD21	1.91	0.52
1:A:290:PRO:HD2	1:A:293:LEU:CG	2.38	0.52
1:B:228:ASN:HB3	1:B:229:PRO:CD	2.39	0.52
1:F:155:ALA:HA	1:F:165:CYS:SG	2.50	0.52
1:F:288:ALA:CB	1:F:325:LYS:HZ3	2.22	0.52
1:B:110:GLU:HG3	1:B:118:VAL:HA	1.92	0.52
1:C:77:LEU:CD2	1:C:83:LYS:HB2	2.37	0.52
1:C:81:LEU:HD21	1:C:157:ALA:HA	1.92	0.52
1:D:117:SER:C	1:D:119:LYS:N	2.67	0.52
1:E:103:CYS:HB2	1:E:368:GLN:O	2.10	0.52
1:E:249:ASP:CG	1:E:368:GLN:HE21	2.18	0.52
1:A:193:THR:O	1:A:193:THR:CG2	2.30	0.52
1:A:262:THR:CG2	1:A:316:ASP:HB3	2.40	0.52
1:B:72:LYS:HZ3	1:B:72:LYS:CA	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASN:H	1:C:342:GLU:CD	2.17	0.52
1:C:104:GLU:OE2	1:F:137:LYS:HD3	2.09	0.52
1:C:382:MET:HE2	1:D:176:GLU:HA	1.92	0.52
1:D:386:LEU:O	1:D:386:LEU:HD13	2.10	0.52
1:A:144:GLU:CD	1:A:145:PRO:HD2	2.35	0.52
1:A:226:ALA:HA	3:A:1120:HEM:CMD	2.40	0.52
1:A:379:ARG:HH21	1:A:380:ASN:CG	2.18	0.52
1:B:150:THR:HG21	1:B:222:GLN:NE2	2.24	0.52
1:B:192:PRO:O	1:B:202:SER:N	2.43	0.52
1:E:59:PRO:HD2	1:E:62:GLU:OE1	2.09	0.52
1:E:335:ALA:O	1:E:339:ILE:HG13	2.10	0.52
1:F:241:LEU:HD21	1:F:268:LEU:CD2	2.39	0.52
1:B:68:THR:HG22	1:B:234:ASP:HB3	1.91	0.52
1:C:329:GLU:O	1:C:333:THR:HG23	2.10	0.52
1:D:100:GLY:O	1:D:101:LEU:C	2.53	0.52
1:D:201:GLU:O	1:D:202:SER:HB2	2.10	0.52
1:F:282:PRO:CG	1:F:307:GLY:HA3	2.40	0.52
1:F:327:ASN:OD1	1:F:329:GLU:N	2.42	0.52
1:D:300:THR:HG22	1:D:301:TYR:N	2.24	0.51
1:E:247:LYS:O	1:E:248:LEU:HB2	2.10	0.51
1:E:248:LEU:HD23	1:E:249:ASP:N	2.26	0.51
1:E:316:ASP:C	1:E:318:THR:H	2.18	0.51
1:A:146:THR:HG21	1:A:150:THR:HB	1.92	0.51
1:A:219:ILE:HG22	1:A:219:ILE:O	2.09	0.51
1:B:170:PRO:CG	1:B:191:THR:CG2	2.82	0.51
1:C:142:ILE:CG2	1:C:143:ILE:N	2.74	0.51
1:E:168:VAL:O	1:E:203:HIS:NE2	2.43	0.51
1:E:299:THR:HG22	1:E:300:THR:CA	2.38	0.51
1:F:210:LEU:HA	1:F:213:GLU:OE1	2.10	0.51
1:A:92:ILE:HG23	1:A:342:GLU:CG	2.40	0.51
1:B:51:ARG:CG	1:B:51:ARG:O	2.57	0.51
1:C:89:MET:HB2	1:C:243:GLN:OE1	2.11	0.51
1:E:228:ASN:C	1:E:228:ASN:OD1	2.52	0.51
1:F:119:LYS:O	1:F:120:ASP:C	2.54	0.51
1:C:72:LYS:N	1:C:72:LYS:HD2	2.25	0.51
1:D:280:VAL:HG11	1:D:352:SER:HB3	1.92	0.51
1:E:76:ILE:HD11	1:F:369:ARG:HH11	1.74	0.51
1:E:299:THR:HG22	1:E:300:THR:H	1.69	0.51
1:A:125:ARG:HH12	1:A:230:LEU:HB3	1.74	0.51
1:B:46:PRO:CD	1:B:310:PHE:CG	2.88	0.51
1:B:50:SER:O	1:B:51:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:O	1:B:51:ARG:HG2	2.11	0.51
1:B:140:ASP:OD1	1:B:216:ASN:HB3	2.10	0.51
1:D:221:ASP:O	1:D:225:ASN:CB	2.59	0.51
1:D:237:ALA:CB	1:D:264:ILE:HA	2.38	0.51
1:D:258:GLY:O	1:D:262:THR:OG1	2.19	0.51
1:E:110:GLU:HG2	1:E:118:VAL:HG23	1.91	0.51
1:F:137:LYS:HB2	1:F:140:ASP:CG	2.36	0.51
1:F:146:THR:HG21	1:F:150:THR:CB	2.40	0.51
1:D:229:PRO:CG	1:D:314:VAL:HB	2.40	0.51
1:E:92:ILE:HG22	1:E:95:ILE:HG23	1.85	0.51
1:E:264:ILE:O	1:E:265:ALA:C	2.52	0.51
1:E:289:GLU:CD	1:E:317:ARG:NH1	2.64	0.51
1:E:382:MET:O	1:E:386:LEU:HB3	2.11	0.51
1:E:394:LYS:HZ2	1:E:394:LYS:CA	2.23	0.51
1:F:79:ASP:OD2	1:F:79:ASP:N	2.43	0.51
1:F:316:ASP:OD1	1:F:318:THR:OG1	2.26	0.51
1:A:251:LEU:CD2	1:A:264:ILE:CG2	2.88	0.51
1:B:46:PRO:O	1:B:47:ASP:C	2.51	0.51
1:B:178:VAL:HA	1:B:181:LEU:HD12	1.93	0.51
1:D:173:MET:HE3	1:D:173:MET:C	2.33	0.51
1:E:125:ARG:CG	1:E:125:ARG:NH1	2.73	0.51
1:E:144:GLU:OE1	1:E:146:THR:HG22	2.11	0.51
1:F:232:HIS:HA	1:F:236:THR:HB	1.92	0.51
1:F:288:ALA:CB	1:F:325:LYS:CD	2.88	0.51
1:A:104:GLU:HB3	1:A:369:ARG:HG2	1.92	0.51
1:A:110:GLU:C	1:A:112:PHE:H	2.18	0.51
1:A:281:ASP:OD1	1:A:325:LYS:HE3	2.11	0.51
1:B:286:ILE:HD12	1:B:287:LEU:HD23	1.92	0.51
1:C:59:PRO:CG	1:C:62:GLU:CD	2.83	0.51
1:C:356:VAL:O	1:C:359:LYS:HB2	2.10	0.51
1:D:78:PRO:HG3	1:D:82:LYS:HZ2	1.74	0.51
1:D:83:LYS:HE3	1:D:83:LYS:CA	2.40	0.51
1:D:249:ASP:C	1:D:275:CYS:HG	2.17	0.51
1:E:49:PRO:O	1:E:50:SER:C	2.52	0.51
1:E:169:MET:HG3	1:E:190:ARG:HD2	1.92	0.51
1:F:288:ALA:CB	1:F:325:LYS:NZ	2.74	0.51
1:F:303:VAL:HG22	1:F:328:ASP:OD2	2.10	0.51
1:F:316:ASP:OD1	1:F:316:ASP:C	2.54	0.51
1:A:281:ASP:HB3	1:A:325:LYS:HD2	1.92	0.51
1:A:390:TRP:C	1:A:392:LEU:N	2.68	0.51
1:B:95:ILE:CD1	1:B:338:LEU:HD12	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:O	1:B:173:MET:HG2	2.10	0.51
1:C:233:TYR:CE1	1:C:267:LYS:HE3	2.46	0.51
1:D:95:ILE:HG12	1:D:337:MET:HE3	1.93	0.51
1:D:173:MET:HE2	1:D:177:LYS:HZ2	1.76	0.51
1:D:302:GLU:HB2	1:D:328:ASP:OD1	2.11	0.51
1:F:51:ARG:HD3	3:F:1620:HEM:O2D	2.10	0.51
1:F:101:LEU:H	1:F:101:LEU:CD1	2.23	0.51
1:F:205:GLY:O	1:F:206:VAL:C	2.54	0.51
1:A:102:LYS:CG	1:A:366:GLU:OE2	2.56	0.51
1:B:329:GLU:HG2	1:B:396:PHE:CD2	2.46	0.51
1:B:388:ASP:HA	1:B:391:MET:HB2	1.93	0.51
1:C:88:PRO:HA	4:C:1328:HOH:O	2.11	0.51
1:C:232:HIS:CG	1:C:260:THR:HA	2.46	0.51
1:D:290:PRO:O	1:D:291:GLU:C	2.54	0.51
1:E:125:ARG:O	1:E:129:ASP:N	2.44	0.51
1:E:232:HIS:NE2	1:E:260:THR:HG22	2.26	0.51
1:A:66:HIS:CD2	1:C:72:LYS:H	2.29	0.50
1:A:170:PRO:CD	1:A:191:THR:HG1	2.25	0.50
1:A:203:HIS:CG	1:A:203:HIS:O	2.64	0.50
1:B:126:MET:O	1:B:129:ASP:N	2.44	0.50
1:B:278:ILE:HD13	1:B:322:LYS:HB2	1.93	0.50
1:D:346:CYS:HA	1:D:377:SER:HA	1.92	0.50
1:E:68:THR:CG2	1:E:132:ARG:HH22	2.24	0.50
1:E:89:MET:HB2	1:E:243:GLN:OE1	2.10	0.50
1:F:119:LYS:HG3	1:F:149:ASN:HB2	1.93	0.50
1:F:167:ILE:N	1:F:187:GLU:O	2.40	0.50
1:F:179:ASP:HA	1:F:182:ARG:HH12	1.76	0.50
1:D:223:TYR:HD1	1:D:312:PRO:CG	2.24	0.50
1:A:228:ASN:OD1	1:A:259:GLY:HA3	2.12	0.50
1:B:118:VAL:HG13	1:B:119:LYS:N	2.26	0.50
1:C:166:ILE:C	1:C:167:ILE:HG13	2.36	0.50
1:D:385:PHE:C	1:D:385:PHE:HD1	2.20	0.50
1:E:105:LEU:C	1:E:105:LEU:CD1	2.76	0.50
1:F:281:ASP:O	1:F:325:LYS:HA	2.11	0.50
1:A:136:LEU:HD21	1:A:163:TYR:CE1	2.46	0.50
1:A:190:ARG:O	1:A:192:PRO:HD2	2.06	0.50
1:B:92:ILE:HB	1:B:105:LEU:HB3	1.93	0.50
1:B:386:LEU:O	1:B:386:LEU:HD13	2.11	0.50
1:C:340:ALA:O	1:C:341:GLN:HG2	2.12	0.50
1:D:236:THR:HG21	1:D:264:ILE:HD11	1.92	0.50
1:E:49:PRO:N	1:E:313:THR:CG2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:PHE:HE1	1:F:112:PHE:CE1	2.30	0.50
1:F:288:ALA:HB1	1:F:325:LYS:HD3	1.91	0.50
1:B:177:LYS:O	1:B:180:VAL:HB	2.11	0.50
1:B:233:TYR:CE2	1:B:267:LYS:NZ	2.80	0.50
1:B:286:ILE:HA	1:B:294:ASN:OD1	2.11	0.50
1:C:223:TYR:O	1:C:313:THR:HG23	2.11	0.50
1:E:102:LYS:CD	1:E:365:GLN:HA	2.41	0.50
1:F:172:LYS:HD3	1:F:172:LYS:H	1.76	0.50
1:A:170:PRO:CD	1:A:191:THR:OG1	2.60	0.50
1:C:85:GLY:HA2	1:C:121:ARG:CZ	2.42	0.50
1:C:229:PRO:HB2	3:C:1320:HEM:CAC	2.42	0.50
1:D:51:ARG:HD3	3:D:1420:HEM:O2D	2.12	0.50
1:E:288:ALA:HB3	1:E:294:ASN:CG	2.36	0.50
1:A:125:ARG:HH12	1:A:230:LEU:CB	2.23	0.50
1:A:133:ASP:HA	1:C:74:PRO:HB2	1.93	0.50
1:E:291:GLU:OE2	1:E:291:GLU:CA	2.59	0.50
1:F:118:VAL:O	1:F:121:ARG:HB2	2.11	0.50
1:A:103:CYS:HB3	1:A:364:LEU:HB3	1.92	0.50
1:A:248:LEU:CD2	1:A:249:ASP:H	2.25	0.50
1:A:289:GLU:HA	1:A:290:PRO:C	2.36	0.50
1:A:327:ASN:OD1	1:A:329:GLU:N	2.44	0.50
1:E:119:LYS:O	1:E:123:SER:HB2	2.11	0.50
1:F:223:TYR:HD1	1:F:312:PRO:HG3	1.75	0.50
1:A:169:MET:HG2	1:A:188:ILE:HG23	1.94	0.50
1:B:276:ARG:O	1:B:277:ILE:HG12	2.12	0.50
1:B:296:THR:C	1:B:298:GLN:H	2.20	0.50
1:C:226:ALA:HA	3:C:1320:HEM:HMD2	1.94	0.50
1:D:127:ILE:O	1:D:131:GLU:HG3	2.12	0.50
1:F:226:ALA:O	1:F:228:ASN:N	2.45	0.50
1:A:376:ASP:C	1:A:376:ASP:OD2	2.54	0.49
1:B:66:HIS:HE1	1:B:132:ARG:NE	2.09	0.49
1:B:137:LYS:HB2	1:B:140:ASP:CG	2.37	0.49
1:B:202:SER:O	1:B:203:HIS:CG	2.65	0.49
1:B:205:GLY:O	1:B:209:ARG:HD3	2.12	0.49
1:B:328:ASP:O	1:B:331:ALA:HB3	2.12	0.49
1:C:224:ARG:O	1:C:224:ARG:HG2	2.11	0.49
1:E:222:GLN:C	1:E:223:TYR:CG	2.90	0.49
1:E:238:ASP:OD2	1:E:238:ASP:N	2.44	0.49
1:E:310:PHE:O	1:E:312:PRO:CD	2.59	0.49
1:F:225:ASN:OD1	1:F:225:ASN:C	2.55	0.49
1:A:131:GLU:OE1	1:A:163:TYR:OH	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ASN:O	1:A:295:GLN:CB	2.60	0.49
1:C:90:VAL:HG22	1:D:77:LEU:HD12	1.91	0.49
1:C:95:ILE:HD11	1:C:337:MET:C	2.37	0.49
1:D:177:LYS:O	1:D:180:VAL:CG2	2.60	0.49
1:F:336:ARG:NH1	1:F:388:ASP:HB3	2.26	0.49
1:C:125:ARG:HG2	1:C:231:ALA:HB2	1.93	0.49
1:D:88:PRO:CG	1:D:112:PHE:HD1	2.24	0.49
1:D:256:GLY:H	2:D:1410:PLP:H5A1	1.77	0.49
1:E:302:GLU:OE1	1:E:302:GLU:HA	2.11	0.49
1:E:395:GLY:O	1:E:396:PHE:HB2	2.11	0.49
1:F:248:LEU:HD13	1:F:268:LEU:HD21	1.94	0.49
1:F:255:VAL:HG21	1:F:323:TRP:CH2	2.47	0.49
1:A:382:MET:HB3	1:B:176:GLU:HG3	1.95	0.49
1:B:126:MET:HG2	1:B:227:SER:HB2	1.94	0.49
1:C:89:MET:O	1:D:77:LEU:HD12	2.12	0.49
1:C:223:TYR:CE1	1:C:257:THR:HG22	2.48	0.49
1:C:233:TYR:CD1	1:C:267:LYS:HB2	2.47	0.49
1:D:155:ALA:CB	1:D:186:ALA:HB2	2.42	0.49
1:D:261:ILE:HD11	1:D:277:ILE:CG2	2.42	0.49
1:E:55:GLN:OE1	1:E:55:GLN:HA	2.13	0.49
1:E:177:LYS:O	1:E:181:LEU:HG	2.12	0.49
1:A:232:HIS:O	1:A:237:ALA:HB2	2.12	0.49
1:B:280:VAL:CG2	1:B:356:VAL:HG21	2.41	0.49
1:B:316:ASP:C	1:B:318:THR:H	2.19	0.49
1:B:384:LYS:HA	1:B:390:TRP:CG	2.48	0.49
1:C:339:ILE:HA	1:C:344:LEU:O	2.13	0.49
1:C:361:ALA:C	1:C:363:GLU:H	2.20	0.49
1:F:328:ASP:O	1:F:329:GLU:C	2.54	0.49
1:F:357:ALA:O	1:F:358:VAL:C	2.53	0.49
1:A:119:LYS:HG3	1:A:149:ASN:HB2	1.94	0.49
1:C:117:SER:HB2	1:C:149:ASN:HB3	1.94	0.49
1:E:320:VAL:CG1	1:E:323:TRP:NE1	2.72	0.49
1:F:129:ASP:OD1	1:F:227:SER:OG	2.30	0.49
1:F:204:VAL:HB	1:F:208:TRP:HZ3	1.77	0.49
1:B:335:ALA:HB1	1:B:385:PHE:CE1	2.47	0.49
1:B:373:ILE:O	1:B:375:PRO:HD2	2.12	0.49
1:E:144:GLU:HG2	1:E:151:GLY:HA2	1.93	0.49
1:F:118:VAL:O	1:F:118:VAL:HG22	2.13	0.49
1:F:255:VAL:CG1	1:F:258:GLY:HA2	2.42	0.49
1:A:188:ILE:CG2	1:A:190:ARG:HD2	2.42	0.49
1:A:248:LEU:HD22	1:A:249:ASP:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HA	1:B:184:LEU:CD2	2.42	0.49
1:D:56:LEU:HD11	1:D:270:GLU:HA	1.94	0.49
1:D:261:ILE:O	1:D:265:ALA:CB	2.61	0.49
1:E:76:ILE:CD1	1:F:106:LEU:HD11	2.41	0.49
1:E:311:ILE:HD13	1:E:317:ARG:NE	2.27	0.49
1:E:336:ARG:HA	1:E:339:ILE:CD1	2.30	0.49
1:E:394:LYS:N	1:E:394:LYS:NZ	2.60	0.49
1:F:117:SER:HB3	1:F:376:ASP:HB3	1.94	0.49
1:F:176:GLU:HG3	1:F:380:ASN:HA	1.95	0.49
1:F:303:VAL:HG21	1:F:328:ASP:HA	1.94	0.49
1:B:384:LYS:HB3	1:B:390:TRP:CD2	2.48	0.49
1:D:205:GLY:N	1:D:207:ALA:H	2.11	0.49
1:E:315:LEU:HD12	1:E:316:ASP:N	2.27	0.49
1:A:251:LEU:HD22	1:A:264:ILE:HG21	1.95	0.49
1:A:322:LYS:CG	1:A:323:TRP:N	2.75	0.49
1:C:82:LYS:N	1:C:82:LYS:CD	2.75	0.49
1:C:156:LEU:HA	1:C:184:LEU:HD22	1.95	0.49
1:C:215:PRO:O	1:C:216:ASN:C	2.55	0.49
1:C:286:ILE:C	1:C:286:ILE:HD12	2.37	0.49
1:C:316:ASP:O	1:C:319:VAL:HG22	2.13	0.49
1:D:348:GLY:O	1:D:351:GLY:N	2.44	0.49
1:E:208:TRP:CH2	1:E:219:ILE:HD12	2.48	0.49
1:E:245:ASP:O	1:E:247:LYS:N	2.43	0.49
1:C:81:LEU:HD12	1:C:161:ARG:CZ	2.42	0.48
1:C:232:HIS:HA	1:C:236:THR:HB	1.94	0.48
1:D:105:LEU:HD11	1:D:372:VAL:CG2	2.43	0.48
1:D:308:TYR:HD2	1:D:312:PRO:HD3	1.78	0.48
3:D:1420:HEM:HBD2	3:D:1420:HEM:HHA	1.95	0.48
1:E:68:THR:CG2	1:E:132:ARG:HH12	2.26	0.48
1:E:125:ARG:NH1	1:E:230:LEU:HB3	2.28	0.48
1:A:107:ALA:HA	1:A:372:VAL:O	2.13	0.48
1:A:248:LEU:HD11	1:A:371:VAL:HB	1.94	0.48
1:B:79:ASP:OD1	1:B:81:LEU:HB2	2.13	0.48
1:B:230:LEU:HD23	3:B:1220:HEM:HBC2	1.95	0.48
1:C:316:ASP:OD2	1:C:318:THR:CB	2.60	0.48
1:D:89:MET:CG	1:D:106:LEU:HB3	2.43	0.48
1:D:254:SER:HA	1:D:280:VAL:HB	1.96	0.48
1:F:282:PRO:HA	1:F:326:SER:O	2.13	0.48
1:F:333:THR:OG1	1:F:334:PHE:N	2.45	0.48
1:A:137:LYS:O	1:A:138:PRO:C	2.55	0.48
1:A:154:LEU:O	1:A:158:ALA:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:PHE:CD2	1:B:386:LEU:N	2.81	0.48
1:C:156:LEU:HA	1:C:184:LEU:CD2	2.43	0.48
1:C:229:PRO:HB3	3:C:1320:HEM:CBC	2.43	0.48
1:D:330:GLU:HG3	1:D:331:ALA:N	2.28	0.48
1:A:395:GLY:O	1:A:396:PHE:CG	2.66	0.48
1:C:156:LEU:HD13	1:C:156:LEU:O	2.13	0.48
1:D:349:SER:OG	1:D:375:PRO:HB2	2.13	0.48
1:E:63:SER:HA	3:E:1520:HEM:HMB3	1.94	0.48
1:E:137:LYS:NZ	1:E:140:ASP:CG	2.70	0.48
1:F:85:GLY:O	1:F:86:ASP:HB3	2.12	0.48
1:F:251:LEU:HD13	1:F:264:ILE:HG21	1.96	0.48
1:A:110:GLU:C	1:A:112:PHE:N	2.70	0.48
1:B:110:GLU:HG2	1:B:118:VAL:HG23	1.94	0.48
1:B:373:ILE:O	1:B:375:PRO:CD	2.61	0.48
1:C:47:ASP:CG	1:C:48:ALA:N	2.61	0.48
1:C:232:HIS:CD2	1:C:260:THR:HA	2.48	0.48
1:E:312:PRO:O	1:E:314:VAL:O	2.31	0.48
1:E:364:LEU:N	1:E:364:LEU:HD22	2.28	0.48
1:B:50:SER:O	1:B:51:ARG:C	2.55	0.48
1:C:59:PRO:CB	1:C:62:GLU:CG	2.64	0.48
1:D:80:ILE:O	1:D:80:ILE:HG13	2.12	0.48
1:E:105:LEU:HD12	1:E:370:CYS:O	2.14	0.48
1:F:329:GLU:O	1:F:333:THR:HG23	2.13	0.48
1:A:268:LEU:O	1:A:269:LYS:C	2.56	0.48
1:B:46:PRO:CG	1:B:310:PHE:CD2	2.95	0.48
1:B:290:PRO:O	1:B:291:GLU:C	2.57	0.48
1:C:190:ARG:O	1:C:192:PRO:HD2	2.00	0.48
1:C:384:LYS:O	1:C:385:PHE:C	2.57	0.48
1:D:110:GLU:CG	1:D:118:VAL:HB	2.43	0.48
1:D:226:ALA:O	1:D:227:SER:C	2.57	0.48
1:D:261:ILE:HD11	1:D:277:ILE:HG22	1.96	0.48
1:E:334:PHE:O	1:E:338:LEU:HD12	2.14	0.48
1:F:258:GLY:HA3	1:F:315:LEU:HB2	1.95	0.48
1:A:126:MET:SD	1:A:220:LEU:HB3	2.54	0.48
1:A:230:LEU:O	1:A:233:TYR:HB3	2.14	0.48
1:B:66:HIS:CE1	1:B:132:ARG:NE	2.81	0.48
1:B:122:ILE:CG2	1:B:228:ASN:HA	2.43	0.48
1:C:94:LYS:NZ	1:D:159:ALA:O	2.35	0.48
1:C:282:PRO:O	1:C:285:SER:HB3	2.13	0.48
1:D:252:VAL:HG12	1:D:353:THR:HG23	1.95	0.48
1:D:349:SER:HB3	2:D:1410:PLP:N1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:VAL:O	1:E:182:ARG:HG3	2.13	0.48
1:F:54:TRP:HB2	3:F:1620:HEM:C4B	2.48	0.48
1:A:103:CYS:SG	1:A:103:CYS:O	2.71	0.48
1:B:280:VAL:HG22	1:B:356:VAL:HG21	1.96	0.48
1:C:126:MET:C	1:C:128:GLU:N	2.71	0.48
1:C:183:ALA:O	1:D:340:ALA:HB2	2.14	0.48
1:D:127:ILE:O	1:D:136:LEU:HD23	2.14	0.48
1:D:391:MET:SD	1:D:396:PHE:HB2	2.53	0.48
1:E:67:HIS:HA	1:E:234:ASP:OD2	2.13	0.48
1:E:81:LEU:HD12	1:E:161:ARG:CZ	2.42	0.48
1:E:262:THR:O	1:E:263:GLY:C	2.57	0.48
1:A:253:ALA:HB2	1:A:373:ILE:HD12	1.96	0.48
1:A:261:ILE:HG23	1:A:262:THR:N	2.29	0.48
1:D:204:VAL:O	1:D:204:VAL:HG22	2.13	0.48
1:D:265:ALA:HB1	1:D:319:VAL:HB	1.96	0.48
1:E:125:ARG:HH12	1:E:230:LEU:CB	2.26	0.48
1:E:327:ASN:HD21	1:E:330:GLU:HB2	1.78	0.48
1:E:389:ARG:O	1:E:390:TRP:C	2.55	0.48
1:F:101:LEU:HD12	1:F:101:LEU:N	2.28	0.48
1:F:165:CYS:O	1:F:186:ALA:HA	2.14	0.48
1:B:254:SER:HB3	1:B:306:ILE:CG2	2.44	0.47
1:B:347:GLY:HA3	1:B:381:TYR:CD1	2.48	0.47
1:D:91:ARG:HG2	1:D:93:ASN:ND2	2.29	0.47
1:E:192:PRO:O	1:E:193:THR:C	2.56	0.47
1:E:316:ASP:C	1:E:318:THR:N	2.72	0.47
1:F:202:SER:HA	4:F:1635:HOH:O	2.14	0.47
1:F:394:LYS:NZ	1:F:394:LYS:CA	2.73	0.47
1:A:276:ARG:HD2	4:A:1127:HOH:O	2.14	0.47
1:B:379:ARG:CB	1:B:379:ARG:HH11	2.27	0.47
1:C:247:LYS:N	1:C:247:LYS:CD	2.75	0.47
1:C:286:ILE:C	1:C:288:ALA:H	2.21	0.47
1:D:106:LEU:O	1:D:371:VAL:HA	2.15	0.47
1:D:115:GLY:N	1:D:120:ASP:OD2	2.46	0.47
1:D:205:GLY:C	1:D:207:ALA:H	2.17	0.47
1:F:299:THR:HG22	1:F:300:THR:CA	2.42	0.47
1:F:350:ALA:HB1	1:F:374:LEU:HD22	1.96	0.47
1:A:132:ARG:HB2	1:A:132:ARG:NH1	2.25	0.47
1:A:147:SER:CB	1:A:169:MET:HB2	2.44	0.47
1:B:96:GLY:O	1:B:101:LEU:HB2	2.13	0.47
1:B:156:LEU:HA	1:B:184:LEU:HD22	1.95	0.47
1:C:388:ASP:O	1:C:392:LEU:CD1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:GLU:O	1:D:201:GLU:CG	2.63	0.47
1:D:398:LYS:O	1:D:399:GLU:C	2.56	0.47
1:E:188:ILE:CG2	1:E:189:VAL:N	2.77	0.47
1:E:392:LEU:H	1:E:392:LEU:HD12	1.79	0.47
1:F:167:ILE:CD1	1:F:181:LEU:HD13	2.39	0.47
1:A:292:GLU:N	1:A:292:GLU:OE1	2.47	0.47
1:B:287:LEU:HD21	1:B:308:TYR:C	2.39	0.47
1:C:226:ALA:HA	3:C:1320:HEM:HMD1	1.96	0.47
1:C:384:LYS:HD2	1:C:390:TRP:NE1	2.29	0.47
1:D:373:ILE:O	1:D:374:LEU:HD23	2.14	0.47
1:F:104:GLU:OE2	1:F:106:LEU:HD21	2.14	0.47
1:F:265:ALA:HB1	1:F:319:VAL:O	2.14	0.47
1:A:221:ASP:H	1:A:225:ASN:ND2	2.11	0.47
1:A:251:LEU:CD2	1:A:264:ILE:HG21	2.45	0.47
1:B:81:LEU:C	1:B:83:LYS:H	2.20	0.47
1:B:101:LEU:HD12	1:B:362:GLN:HE21	1.80	0.47
1:B:153:GLY:O	1:B:156:LEU:HB3	2.15	0.47
1:C:59:PRO:CB	1:C:62:GLU:CD	2.87	0.47
1:D:223:TYR:CD1	1:D:312:PRO:CG	2.95	0.47
1:D:398:LYS:NZ	1:D:398:LYS:HB3	1.85	0.47
1:E:148:GLY:O	1:E:149:ASN:C	2.57	0.47
1:A:95:ILE:CD1	1:A:338:LEU:HD23	2.42	0.47
1:A:96:GLY:C	1:A:98:LYS:N	2.72	0.47
1:A:232:HIS:HD2	1:A:259:GLY:O	1.97	0.47
1:A:262:THR:O	1:A:266:ARG:HG3	2.14	0.47
1:C:135:THR:HG22	1:C:218:HIS:NE2	2.29	0.47
1:E:199:SER:HG	1:E:202:SER:HA	1.80	0.47
1:F:188:ILE:N	1:F:188:ILE:CD1	2.75	0.47
1:F:255:VAL:O	1:F:306:ILE:HG22	2.14	0.47
1:A:94:LYS:HE3	1:A:341:GLN:CB	2.45	0.47
1:A:143:ILE:HG12	1:A:166:ILE:HD12	1.97	0.47
1:A:232:HIS:CD2	1:A:260:THR:HG22	2.50	0.47
1:A:267:LYS:HD2	1:A:271:LYS:CD	2.44	0.47
1:B:231:ALA:O	1:B:235:THR:OG1	2.31	0.47
1:D:224:ARG:HG3	1:D:313:THR:HG21	1.96	0.47
1:D:331:ALA:O	1:D:351:GLY:HA3	2.15	0.47
1:D:335:ALA:O	1:D:338:LEU:HB2	2.15	0.47
1:D:384:LYS:HD2	1:D:390:TRP:NE1	2.29	0.47
1:D:397:LEU:C	1:D:398:LYS:HZ1	2.23	0.47
1:E:169:MET:HG3	1:E:190:ARG:CD	2.45	0.47
1:E:243:GLN:O	1:E:245:ASP:OD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:GLU:OE1	1:E:342:GLU:HA	2.14	0.47
1:E:381:TYR:HB2	1:E:385:PHE:HE2	1.80	0.47
1:F:264:ILE:O	1:F:265:ALA:C	2.57	0.47
1:F:266:ARG:HG2	1:F:319:VAL:HG11	1.96	0.47
1:A:233:TYR:O	1:A:237:ALA:HB3	2.15	0.47
1:A:298:GLN:O	1:A:299:THR:C	2.58	0.47
1:B:150:THR:C	1:B:152:ILE:H	2.23	0.47
1:B:286:ILE:HA	1:B:294:ASN:CG	2.39	0.47
1:F:107:ALA:HB1	1:F:374:LEU:HD11	1.97	0.47
1:F:119:LYS:C	1:F:121:ARG:N	2.69	0.47
1:F:232:HIS:NE2	1:F:260:THR:HG22	2.30	0.47
1:B:287:LEU:CD1	1:B:308:TYR:N	2.76	0.47
1:B:394:LYS:HA	1:B:394:LYS:HE3	1.96	0.47
1:C:278:ILE:HG22	1:C:279:GLY:N	2.29	0.47
1:C:311:ILE:HD13	1:C:317:ARG:NH1	2.30	0.47
1:D:61:SER:CB	1:F:242:GLN:HE22	2.28	0.47
1:D:126:MET:HG2	1:D:225:ASN:ND2	2.30	0.47
1:D:205:GLY:HA2	1:D:208:TRP:N	2.27	0.47
1:D:316:ASP:C	1:D:316:ASP:OD2	2.56	0.47
1:A:297:GLU:OE2	1:A:297:GLU:CA	2.61	0.47
1:C:82:LYS:N	1:C:82:LYS:HD3	2.30	0.47
1:D:76:ILE:HG22	1:D:77:LEU:H	1.79	0.47
1:D:177:LYS:O	1:D:180:VAL:HB	2.15	0.47
1:D:378:VAL:HG23	1:D:379:ARG:N	2.30	0.47
1:E:91:ARG:NH2	1:F:78:PRO:HA	2.30	0.47
1:F:46:PRO:O	1:F:47:ASP:O	2.33	0.47
1:A:63:SER:HB2	3:A:1120:HEM:HAB	1.97	0.46
1:A:202:SER:HG	1:A:203:HIS:H	1.59	0.46
1:B:72:LYS:NZ	1:B:86:ASP:OD1	2.48	0.46
1:D:364:LEU:HD12	1:D:364:LEU:H	1.79	0.46
1:E:105:LEU:HA	1:E:370:CYS:HB3	1.97	0.46
1:E:137:LYS:HB2	1:E:137:LYS:HZ2	1.80	0.46
1:E:268:LEU:O	1:E:272:CYS:C	2.57	0.46
1:F:169:MET:HE2	1:F:173:MET:HG3	1.98	0.46
1:F:391:MET:HE3	1:F:392:LEU:HD21	1.96	0.46
1:A:78:PRO:HB3	1:B:91:ARG:NH2	2.30	0.46
1:A:264:ILE:CD1	1:A:373:ILE:HD11	2.45	0.46
1:D:285:SER:O	1:D:294:ASN:ND2	2.48	0.46
1:E:397:LEU:HD11	1:F:390:TRP:HD1	1.79	0.46
1:A:137:LYS:CB	1:A:140:ASP:OD2	2.62	0.46
1:B:147:SER:HB3	1:B:167:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ILE:CD1	1:D:106:LEU:HD11	2.45	0.46
1:C:90:VAL:HA	1:D:77:LEU:HD12	1.96	0.46
1:C:306:ILE:CG2	2:C:1310:PLP:H6	2.43	0.46
1:D:64:PRO:CD	3:D:1420:HEM:HMB3	2.45	0.46
1:D:104:GLU:OE1	1:D:369:ARG:HD3	2.14	0.46
1:D:115:GLY:CA	1:D:120:ASP:OD2	2.63	0.46
1:D:130:ALA:HB3	1:D:136:LEU:CD2	2.45	0.46
1:F:224:ARG:HA	1:F:313:THR:OG1	2.16	0.46
1:F:355:ALA:O	1:F:359:LYS:HE2	2.15	0.46
1:B:149:ASN:O	1:B:152:ILE:HB	2.16	0.46
1:A:83:LYS:O	1:A:83:LYS:HE3	2.15	0.46
1:A:254:SER:HB3	1:A:280:VAL:HB	1.98	0.46
1:A:262:THR:HG23	1:A:316:ASP:HB3	1.96	0.46
1:C:80:ILE:CG1	1:D:344:LEU:HD23	2.44	0.46
1:D:88:PRO:O	1:D:109:CYS:N	2.45	0.46
1:D:139:GLY:HA2	1:D:162:GLY:O	2.15	0.46
1:D:177:LYS:O	1:D:180:VAL:CB	2.63	0.46
1:D:228:ASN:HB3	1:D:229:PRO:CD	2.46	0.46
1:D:233:TYR:O	1:D:267:LYS:NZ	2.43	0.46
1:D:372:VAL:HG12	1:D:374:LEU:HD21	1.96	0.46
1:F:119:LYS:NZ	2:F:1610:PLP:O3	2.49	0.46
1:F:128:GLU:O	1:F:132:ARG:NH1	2.47	0.46
1:A:94:LYS:HE3	1:A:341:GLN:HB3	1.98	0.46
1:A:215:PRO:O	1:A:216:ASN:HB2	2.16	0.46
1:D:241:LEU:O	1:D:246:GLY:N	2.49	0.46
1:E:68:THR:HG21	1:E:132:ARG:HH22	1.80	0.46
1:A:266:ARG:HG2	1:A:319:VAL:HG11	1.97	0.46
1:A:382:MET:HA	1:A:382:MET:HE3	1.97	0.46
1:C:187:GLU:C	1:C:188:ILE:HD12	2.39	0.46
1:C:208:TRP:HD1	1:C:211:LYS:HZ1	1.62	0.46
1:C:248:LEU:CD2	1:C:371:VAL:HG23	2.41	0.46
1:D:91:ARG:HG2	1:D:93:ASN:HD21	1.80	0.46
1:D:156:LEU:HD13	1:D:156:LEU:C	2.40	0.46
1:D:190:ARG:HH11	1:D:190:ARG:HA	1.80	0.46
1:D:397:LEU:C	1:D:398:LYS:NZ	2.74	0.46
1:E:89:MET:HE2	1:E:243:GLN:OE1	2.16	0.46
1:F:45:ARG:HA	1:F:47:ASP:N	2.29	0.46
1:F:204:VAL:HB	1:F:208:TRP:CZ3	2.51	0.46
1:F:288:ALA:HB2	1:F:325:LYS:CD	2.46	0.46
1:F:288:ALA:HB2	1:F:325:LYS:HZ2	1.79	0.46
1:A:292:GLU:CD	1:A:292:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:THR:O	1:B:239:GLU:HG3	2.16	0.46
1:B:281:ASP:OD1	1:B:287:LEU:C	2.59	0.46
1:C:81:LEU:O	1:C:84:ILE:HG13	2.16	0.46
1:C:92:ILE:CG2	1:C:96:GLY:H	2.28	0.46
1:C:316:ASP:OD2	1:C:318:THR:OG1	2.28	0.46
1:D:144:GLU:HG2	1:D:146:THR:CG2	2.46	0.46
1:D:293:LEU:HB3	1:D:325:LYS:HD3	1.98	0.46
1:E:141:THR:O	1:E:217:SER:HA	2.16	0.46
1:F:324:PHE:CG	1:F:356:VAL:HG13	2.51	0.46
1:F:348:GLY:O	1:F:349:SER:C	2.57	0.46
1:A:71:ALA:HB1	1:C:66:HIS:CE1	2.50	0.46
1:A:95:ILE:HG13	1:A:342:GLU:HG2	1.97	0.46
1:A:188:ILE:HG22	1:A:190:ARG:HD3	1.96	0.46
1:B:339:ILE:HG23	1:B:345:LEU:HD23	1.97	0.46
1:C:339:ILE:HG21	1:D:183:ALA:HB1	1.96	0.46
1:D:325:LYS:HB3	1:D:325:LYS:HZ3	1.80	0.46
1:F:95:ILE:CD1	1:F:338:LEU:HD23	2.46	0.46
1:F:129:ASP:O	1:F:132:ARG:N	2.48	0.46
1:F:241:LEU:HD21	1:F:268:LEU:HD21	1.98	0.46
1:A:267:LYS:O	1:A:270:GLU:HG3	2.16	0.46
1:B:137:LYS:O	1:B:138:PRO:C	2.58	0.46
1:C:132:ARG:C	1:C:134:GLY:H	2.24	0.46
1:D:329:GLU:HG3	1:D:396:PHE:CD2	2.50	0.46
1:E:156:LEU:HA	1:E:184:LEU:HD22	1.98	0.46
1:E:169:MET:HA	1:E:203:HIS:NE2	2.31	0.46
1:E:342:GLU:HB3	1:E:344:LEU:HG	1.98	0.46
1:F:83:LYS:HB3	1:F:114:ALA:HB2	1.98	0.46
1:F:95:ILE:HD13	1:F:338:LEU:HD23	1.96	0.46
1:A:182:ARG:HG2	1:A:188:ILE:HD13	1.98	0.45
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.79	0.45
1:E:63:SER:HB2	3:E:1520:HEM:CBB	2.46	0.45
1:F:223:TYR:O	1:F:314:VAL:HG22	2.16	0.45
1:F:296:THR:HG23	1:F:298:GLN:HB2	1.97	0.45
1:A:95:ILE:CD1	1:A:342:GLU:HG2	2.46	0.45
1:A:143:ILE:HD12	1:A:217:SER:HB3	1.97	0.45
1:A:190:ARG:H	1:A:190:ARG:HG2	1.44	0.45
1:A:379:ARG:HH21	1:A:380:ASN:ND2	2.14	0.45
1:B:127:ILE:HD12	1:B:157:ALA:HB3	1.98	0.45
1:B:150:THR:CB	1:B:222:GLN:HE22	2.29	0.45
1:D:338:LEU:CD2	1:D:344:LEU:HD12	2.35	0.45
1:E:175:SER:O	1:E:176:GLU:CA	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:SER:H	1:E:202:SER:CB	2.21	0.45
1:F:176:GLU:HG2	1:F:380:ASN:C	2.40	0.45
1:F:391:MET:C	1:F:392:LEU:HG	2.41	0.45
1:A:79:ASP:N	1:A:79:ASP:OD2	2.49	0.45
1:A:244:CYS:O	1:A:245:ASP:CB	2.61	0.45
1:B:91:ARG:HH11	1:C:137:LYS:HG2	1.77	0.45
1:B:253:ALA:O	1:B:279:GLY:HA2	2.17	0.45
1:C:385:PHE:CA	1:C:391:MET:HG2	2.30	0.45
1:D:81:LEU:C	1:D:83:LYS:H	2.24	0.45
1:D:224:ARG:HA	1:D:313:THR:HG23	1.97	0.45
1:E:111:PHE:CE2	1:E:346:CYS:HB3	2.51	0.45
1:E:250:MET:HA	1:E:276:ARG:O	2.17	0.45
1:E:288:ALA:HB1	1:E:293:LEU:HD12	1.97	0.45
1:E:382:MET:HE3	1:F:176:GLU:OE2	2.16	0.45
1:F:46:PRO:O	1:F:47:ASP:HB2	2.15	0.45
1:F:211:LYS:O	1:F:214:ILE:O	2.34	0.45
1:A:402:LEU:O	1:A:403:THR:OG1	2.20	0.45
1:B:208:TRP:O	1:B:212:ASN:ND2	2.50	0.45
1:C:281:ASP:O	1:C:325:LYS:HA	2.16	0.45
1:D:128:GLU:O	1:D:132:ARG:HB2	2.17	0.45
1:D:354:VAL:HG22	1:D:372:VAL:HG11	1.97	0.45
1:E:79:ASP:OD1	1:E:81:LEU:HB2	2.16	0.45
1:E:350:ALA:HB2	1:E:374:LEU:HB3	1.98	0.45
1:F:48:ALA:HB3	1:F:49:PRO:CD	2.46	0.45
1:D:232:HIS:HA	1:D:236:THR:HB	1.98	0.45
1:D:264:ILE:O	1:D:268:LEU:HB2	2.16	0.45
1:D:327:ASN:HB3	1:D:330:GLU:HG2	1.98	0.45
1:E:149:ASN:OD1	1:E:380:ASN:ND2	2.50	0.45
1:E:161:ARG:HG2	1:E:161:ARG:HH11	1.81	0.45
1:E:253:ALA:HB3	1:E:261:ILE:CD1	2.46	0.45
1:F:394:LYS:HZ2	1:F:394:LYS:C	2.25	0.45
1:A:55:GLN:HB3	1:A:58:ARG:HG2	1.98	0.45
1:A:254:SER:CB	1:A:280:VAL:HB	2.47	0.45
1:A:287:LEU:HD21	1:A:310:PHE:O	2.17	0.45
1:B:221:ASP:OD2	1:B:221:ASP:C	2.60	0.45
1:C:169:MET:HE2	1:C:190:ARG:CD	2.46	0.45
1:C:233:TYR:O	1:C:237:ALA:HB3	2.16	0.45
1:D:138:PRO:HA	1:D:163:TYR:HE2	1.82	0.45
1:D:385:PHE:HD1	1:D:385:PHE:O	1.98	0.45
1:F:251:LEU:HD23	1:F:251:LEU:C	2.41	0.45
1:A:203:HIS:HB2	1:A:206:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:HA	1:B:342:GLU:OE1	2.17	0.45
1:B:281:ASP:OD2	1:B:282:PRO:HD2	2.16	0.45
1:D:224:ARG:HB3	1:D:224:ARG:CZ	2.47	0.45
1:D:364:LEU:H	1:D:364:LEU:CD1	2.29	0.45
1:E:338:LEU:CD2	1:E:354:VAL:HG21	2.45	0.45
1:F:167:ILE:HD12	1:F:181:LEU:CD1	2.39	0.45
1:A:78:PRO:CB	1:B:91:ARG:HH21	2.29	0.45
1:A:137:LYS:HB2	1:A:140:ASP:OD1	2.17	0.45
1:C:169:MET:SD	1:C:190:ARG:HD3	2.57	0.45
1:C:188:ILE:N	1:C:188:ILE:CD1	2.79	0.45
1:C:388:ASP:O	1:C:392:LEU:N	2.50	0.45
1:D:384:LYS:HE2	1:D:384:LYS:HB3	1.76	0.45
1:F:235:THR:O	1:F:236:THR:C	2.60	0.45
1:F:358:VAL:HG23	1:F:359:LYS:N	2.32	0.45
1:A:155:ALA:CB	1:A:186:ALA:HB2	2.47	0.45
1:B:103:CYS:HB3	1:B:364:LEU:HB3	1.99	0.45
1:C:84:ILE:HA	1:C:113:ASN:OD1	2.16	0.45
1:F:99:PHE:CE1	1:F:337:MET:HE1	2.50	0.45
1:F:127:ILE:O	1:F:131:GLU:HG3	2.17	0.45
1:F:136:LEU:HD12	1:F:136:LEU:HA	1.65	0.45
1:F:140:ASP:O	1:F:141:THR:CB	2.65	0.45
1:F:181:LEU:HA	1:F:184:LEU:HD12	1.98	0.45
1:F:342:GLU:HA	4:F:1630:HOH:O	2.17	0.45
1:C:178:VAL:HG12	1:C:182:ARG:NH1	2.33	0.45
1:E:174:SER:HB2	1:E:175:SER:H	1.59	0.45
1:F:89:MET:CG	1:F:106:LEU:HD12	2.47	0.45
1:F:233:TYR:CE1	1:F:267:LYS:HE2	2.52	0.45
1:F:302:GLU:HB2	1:F:328:ASP:OD1	2.16	0.45
1:F:396:PHE:CD2	1:F:396:PHE:C	2.95	0.45
1:B:81:LEU:C	1:B:83:LYS:N	2.74	0.44
1:B:385:PHE:CD2	1:B:386:LEU:HB2	2.52	0.44
1:C:169:MET:O	1:C:190:ARG:HA	2.17	0.44
1:D:83:LYS:HA	1:D:83:LYS:CE	2.47	0.44
1:D:121:ARG:CD	1:D:236:THR:OG1	2.65	0.44
1:D:320:VAL:CG1	1:D:323:TRP:NE1	2.80	0.44
1:F:210:LEU:HD23	1:F:210:LEU:O	2.17	0.44
1:A:191:THR:HG21	1:A:203:HIS:HB3	1.85	0.44
1:B:104:GLU:CD	1:C:137:LYS:HD3	2.42	0.44
1:B:378:VAL:HG12	1:B:385:PHE:CE2	2.51	0.44
1:C:132:ARG:C	1:C:134:GLY:N	2.75	0.44
1:E:338:LEU:HD21	1:E:354:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:PRO:HG3	1:F:235:THR:HA	1.99	0.44
1:F:169:MET:HE3	1:F:178:VAL:HG22	1.98	0.44
1:C:166:ILE:CG2	1:C:167:ILE:N	2.79	0.44
1:C:211:LYS:NZ	1:C:211:LYS:HB2	2.29	0.44
1:D:144:GLU:CB	1:D:146:THR:HG22	2.48	0.44
1:D:221:ASP:OD2	1:D:223:TYR:CA	2.63	0.44
1:D:233:TYR:CD1	1:D:267:LYS:HB2	2.51	0.44
1:F:111:PHE:CE2	1:F:346:CYS:HB3	2.53	0.44
1:F:361:ALA:CA	1:F:364:LEU:HD23	2.47	0.44
1:A:59:PRO:O	1:A:60:ALA:C	2.58	0.44
1:A:229:PRO:HB2	3:A:1120:HEM:HAC	1.98	0.44
1:A:378:VAL:O	1:A:379:ARG:C	2.60	0.44
1:C:49:PRO:O	1:C:50:SER:O	2.34	0.44
1:C:111:PHE:HB3	1:C:376:ASP:C	2.42	0.44
1:C:113:ASN:O	1:C:116:GLY:N	2.50	0.44
1:C:228:ASN:CB	1:C:229:PRO:CD	2.96	0.44
1:C:337:MET:O	1:C:341:GLN:HG3	2.18	0.44
1:D:205:GLY:H	1:D:208:TRP:H	1.63	0.44
1:D:393:GLN:O	1:D:394:LYS:CG	2.49	0.44
1:E:102:LYS:HD2	1:E:365:GLN:HA	1.99	0.44
1:E:206:VAL:O	1:E:206:VAL:HG12	2.16	0.44
1:E:265:ALA:HB2	1:E:277:ILE:HG21	1.98	0.44
1:E:299:THR:HG22	1:E:300:THR:HG22	1.87	0.44
1:F:144:GLU:OE2	1:F:145:PRO:HD2	2.17	0.44
1:A:80:ILE:HD11	1:A:83:LYS:CB	2.47	0.44
1:A:119:LYS:O	1:A:123:SER:HB2	2.16	0.44
1:B:229:PRO:C	3:B:1220:HEM:HBC1	2.43	0.44
1:C:80:ILE:O	1:C:81:LEU:C	2.61	0.44
1:C:127:ILE:O	1:C:127:ILE:HG22	2.16	0.44
1:E:111:PHE:HB3	1:E:377:SER:N	2.33	0.44
1:E:205:GLY:O	1:E:207:ALA:N	2.50	0.44
1:E:350:ALA:HA	1:E:353:THR:OG1	2.18	0.44
1:F:294:ASN:HD22	1:F:294:ASN:H	1.56	0.44
1:B:287:LEU:CD1	1:B:308:TYR:H	2.30	0.44
1:B:316:ASP:C	1:B:318:THR:N	2.75	0.44
1:D:345:LEU:C	1:D:378:VAL:HG13	2.13	0.44
1:E:242:GLN:HE21	1:E:242:GLN:C	2.26	0.44
1:A:95:ILE:HD11	1:A:338:LEU:HA	2.00	0.44
1:A:136:LEU:HD21	1:A:163:TYR:CZ	2.52	0.44
1:C:233:TYR:CZ	1:C:267:LYS:HE3	2.52	0.44
1:D:122:ILE:HD13	1:D:228:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:LEU:O	1:D:394:LYS:N	2.45	0.44
1:E:49:PRO:CA	1:E:313:THR:CG2	2.91	0.44
1:E:90:VAL:CG1	1:E:91:ARG:N	2.81	0.44
1:E:228:ASN:OD1	1:E:259:GLY:HA3	2.18	0.44
1:F:47:ASP:HB3	1:F:311:ILE:O	2.17	0.44
1:F:143:ILE:HD12	1:F:217:SER:HB3	1.99	0.44
1:F:172:LYS:H	1:F:172:LYS:CD	2.29	0.44
1:A:188:ILE:HG22	1:A:190:ARG:HD2	2.00	0.44
1:A:373:ILE:HG22	1:A:375:PRO:HD3	2.00	0.44
1:A:383:THR:HG23	1:B:176:GLU:OE2	2.17	0.44
1:B:72:LYS:HA	1:B:72:LYS:NZ	2.23	0.44
1:F:257:THR:CG2	1:F:259:GLY:H	2.31	0.44
1:A:66:HIS:NE2	1:C:71:ALA:CA	2.77	0.44
1:A:221:ASP:HB3	1:A:224:ARG:HB2	2.00	0.44
1:B:232:HIS:CD2	1:B:260:THR:HA	2.53	0.44
1:B:262:THR:O	1:B:263:GLY:C	2.60	0.44
1:C:111:PHE:HB2	1:C:377:SER:HB3	2.00	0.44
1:C:333:THR:OG1	1:C:334:PHE:N	2.51	0.44
1:D:144:GLU:HB3	1:D:146:THR:HG22	2.00	0.44
1:E:201:GLU:HB2	1:E:205:GLY:HA2	1.96	0.44
1:E:394:LYS:HZ2	1:E:394:LYS:C	2.26	0.44
1:F:140:ASP:O	1:F:141:THR:HB	2.17	0.44
1:A:229:PRO:C	3:A:1120:HEM:HBC1	2.43	0.43
1:A:251:LEU:HD22	1:A:264:ILE:HG22	1.99	0.43
1:B:119:LYS:O	1:B:123:SER:HB2	2.17	0.43
1:B:125:ARG:HG3	1:B:227:SER:HB3	2.00	0.43
1:C:126:MET:HG2	1:C:220:LEU:HD22	1.99	0.43
1:C:191:THR:HA	1:C:192:PRO:HD2	1.55	0.43
1:C:269:LYS:O	1:C:273:PRO:HD3	2.18	0.43
1:C:310:PHE:O	1:C:312:PRO:HD3	2.18	0.43
1:D:150:THR:O	1:D:154:LEU:HG	2.17	0.43
1:E:252:VAL:HA	1:E:278:ILE:HB	1.99	0.43
1:E:379:ARG:HA	1:E:382:MET:HG2	2.00	0.43
1:F:81:LEU:HD12	1:F:160:VAL:HG11	1.99	0.43
1:F:122:ILE:HD12	1:F:123:SER:N	2.33	0.43
1:A:81:LEU:C	1:A:83:LYS:H	2.26	0.43
1:A:350:ALA:O	1:A:351:GLY:C	2.58	0.43
1:A:398:LYS:H	1:A:398:LYS:HD2	1.82	0.43
1:B:72:LYS:HZ1	1:B:86:ASP:CG	2.26	0.43
1:B:287:LEU:HD11	1:B:308:TYR:H	1.83	0.43
1:B:358:VAL:O	1:B:362:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ILE:HD13	1:C:80:ILE:HA	1.74	0.43
1:D:95:ILE:CG2	1:D:337:MET:HE3	2.48	0.43
1:E:63:SER:HB2	3:E:1520:HEM:HBB2	1.99	0.43
1:E:363:GLU:C	1:E:364:LEU:HD22	2.43	0.43
1:A:67:HIS:HA	1:A:234:ASP:OD2	2.18	0.43
1:A:248:LEU:CD2	1:A:249:ASP:N	2.81	0.43
1:C:81:LEU:HD12	1:C:161:ARG:NH1	2.33	0.43
1:C:164:ARG:NE	1:C:187:GLU:OE1	2.47	0.43
1:C:214:ILE:C	1:C:215:PRO:O	2.61	0.43
1:C:285:SER:O	1:C:294:ASN:OD1	2.36	0.43
1:C:286:ILE:C	1:C:288:ALA:N	2.76	0.43
1:D:97:LYS:HD2	4:D:1437:HOH:O	2.19	0.43
1:D:121:ARG:HD3	1:D:236:THR:OG1	2.18	0.43
1:D:397:LEU:O	1:D:398:LYS:HE3	2.16	0.43
1:F:314:VAL:HG12	3:F:1620:HEM:CMD	2.49	0.43
1:F:332:PHE:HB3	1:F:391:MET:CE	2.48	0.43
1:A:48:ALA:HB3	1:A:49:PRO:HD3	2.00	0.43
1:A:327:ASN:OD1	1:A:327:ASN:C	2.60	0.43
1:B:282:PRO:CG	1:B:307:GLY:HA3	2.48	0.43
1:B:303:VAL:HG23	1:B:328:ASP:OD2	2.18	0.43
1:C:166:ILE:O	1:C:167:ILE:HG13	2.19	0.43
1:C:338:LEU:HD11	1:C:354:VAL:HG21	2.01	0.43
1:D:56:LEU:HD22	1:D:269:LYS:HB3	2.01	0.43
1:D:169:MET:C	1:D:170:PRO:O	2.61	0.43
1:D:283:GLU:CD	1:D:296:THR:HG21	2.44	0.43
1:E:56:LEU:C	1:E:58:ARG:H	2.26	0.43
1:E:88:PRO:HG2	1:E:109:CYS:HB2	1.99	0.43
1:E:229:PRO:C	3:E:1520:HEM:HBC1	2.44	0.43
1:F:117:SER:O	1:F:120:ASP:OD1	2.37	0.43
1:B:177:LYS:HE3	1:B:380:ASN:HB2	2.01	0.43
1:B:188:ILE:HD13	1:B:188:ILE:N	2.33	0.43
1:D:78:PRO:CG	1:D:82:LYS:HG3	2.49	0.43
1:E:105:LEU:O	1:E:105:LEU:CD1	2.62	0.43
1:E:110:GLU:HG2	1:E:118:VAL:CB	2.48	0.43
1:E:176:GLU:HB3	1:E:396:PHE:CE1	2.54	0.43
1:F:108:LYS:CE	1:F:239:GLU:OE2	2.66	0.43
1:F:177:LYS:HE3	1:F:380:ASN:CG	2.43	0.43
1:A:87:THR:HB	1:A:109:CYS:O	2.18	0.43
1:A:141:THR:HG23	1:A:164:ARG:HB3	2.00	0.43
1:A:227:SER:HA	1:A:230:LEU:HD12	2.00	0.43
1:C:143:ILE:O	1:C:143:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:CYS:O	1:C:274:GLY:N	2.51	0.43
1:D:56:LEU:HD13	1:D:270:GLU:HG2	1.99	0.43
1:D:175:SER:C	1:D:177:LYS:N	2.74	0.43
1:E:124:LEU:O	1:E:125:ARG:C	2.61	0.43
1:F:173:MET:HA	1:F:173:MET:HE2	2.00	0.43
1:F:299:THR:HG22	1:F:300:THR:H	1.72	0.43
1:A:78:PRO:HD2	1:A:82:LYS:HG3	2.00	0.43
1:A:254:SER:HA	1:A:280:VAL:HB	2.01	0.43
1:A:350:ALA:HB1	1:A:374:LEU:HD22	2.01	0.43
1:B:329:GLU:HG3	1:B:396:PHE:HE2	1.83	0.43
1:C:101:LEU:HD11	1:C:358:VAL:CA	2.45	0.43
1:C:168:VAL:HG11	1:C:203:HIS:O	2.18	0.43
1:C:228:ASN:HB3	1:C:229:PRO:CD	2.49	0.43
1:C:306:ILE:HG23	2:C:1310:PLP:C6	2.48	0.43
1:C:327:ASN:O	1:C:330:GLU:HB3	2.17	0.43
1:D:117:SER:HB2	1:D:149:ASN:HB3	2.00	0.43
1:D:121:ARG:HH22	1:D:239:GLU:CD	2.26	0.43
1:D:173:MET:HE2	1:D:174:SER:H	1.84	0.43
1:D:262:THR:O	1:D:266:ARG:HG3	2.19	0.43
1:E:386:LEU:HD23	1:E:386:LEU:HA	1.80	0.43
1:F:105:LEU:HD12	1:F:370:CYS:O	2.18	0.43
1:A:170:PRO:CD	1:A:203:HIS:HE2	2.28	0.43
1:A:232:HIS:O	1:A:237:ALA:CB	2.66	0.43
1:B:169:MET:HE3	1:B:188:ILE:CG2	2.47	0.43
1:B:226:ALA:C	1:B:228:ASN:N	2.76	0.43
1:C:89:MET:SD	1:C:106:LEU:HB3	2.59	0.43
1:D:233:TYR:HD1	1:D:263:GLY:O	2.02	0.43
1:F:136:LEU:HD13	1:F:218:HIS:CD2	2.54	0.43
1:A:66:HIS:NE2	1:C:72:LYS:N	2.61	0.43
1:B:54:TRP:CE2	1:B:266:ARG:HG2	2.54	0.43
1:B:59:PRO:O	1:B:60:ALA:C	2.61	0.43
1:B:97:LYS:C	1:B:99:PHE:N	2.77	0.43
1:B:143:ILE:HD12	1:B:217:SER:OG	2.18	0.43
1:E:147:SER:HB3	1:E:169:MET:HB3	2.01	0.43
1:E:268:LEU:HD23	1:E:277:ILE:HD11	2.01	0.43
1:E:364:LEU:HD12	1:E:368:GLN:NE2	2.34	0.43
1:F:176:GLU:CG	1:F:380:ASN:O	2.59	0.43
1:F:181:LEU:O	1:F:184:LEU:HB2	2.19	0.43
1:F:287:LEU:O	1:F:288:ALA:C	2.61	0.43
1:A:77:LEU:HG	1:B:89:MET:O	2.18	0.43
1:B:222:GLN:HB2	1:B:257:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PRO:C	1:B:325:LYS:HZ1	2.27	0.43
1:C:224:ARG:C	1:C:224:ARG:CD	2.84	0.43
1:C:272:CYS:SG	1:C:275:CYS:HB2	2.59	0.43
1:D:202:SER:O	1:D:203:HIS:C	2.60	0.43
1:D:309:ASP:OD1	1:D:310:PHE:N	2.52	0.43
1:E:210:LEU:O	1:E:211:LYS:C	2.62	0.43
1:E:211:LYS:HA	1:E:217:SER:OG	2.19	0.43
1:E:283:GLU:CG	1:E:325:LYS:HB3	2.43	0.43
1:E:373:ILE:N	1:E:373:ILE:CD1	2.82	0.43
1:F:119:LYS:CG	1:F:149:ASN:HB2	2.49	0.43
1:F:303:VAL:HG11	1:F:331:ALA:CB	2.49	0.43
1:F:327:ASN:OD1	1:F:327:ASN:C	2.61	0.43
1:A:97:LYS:HD3	1:A:97:LYS:HA	1.58	0.42
1:A:248:LEU:HD22	1:A:249:ASP:H	1.84	0.42
1:A:260:THR:HG23	2:A:1110:PLP:O1P	2.19	0.42
1:A:336:ARG:HH12	1:A:388:ASP:CG	2.27	0.42
1:B:261:ILE:HD11	1:B:320:VAL:HG13	2.01	0.42
1:B:391:MET:SD	1:B:396:PHE:HD1	2.40	0.42
1:D:64:PRO:HD3	3:D:1420:HEM:HMB3	2.01	0.42
1:E:111:PHE:HE2	1:E:374:LEU:HD12	1.84	0.42
1:F:251:LEU:HD11	1:F:264:ILE:HG21	2.01	0.42
1:F:293:LEU:C	1:F:294:ASN:HD22	2.24	0.42
1:F:346:CYS:SG	1:F:350:ALA:HB1	2.58	0.42
1:F:365:GLN:HE21	1:F:365:GLN:HB3	1.71	0.42
1:A:191:THR:HA	1:A:192:PRO:HD2	1.95	0.42
1:A:316:ASP:OD2	1:A:316:ASP:C	2.63	0.42
1:C:87:THR:HB	1:C:109:CYS:O	2.19	0.42
1:C:211:LYS:NZ	1:C:211:LYS:HB3	2.32	0.42
1:D:169:MET:SD	1:D:188:ILE:HD13	2.60	0.42
1:D:254:SER:OG	2:D:1410:PLP:H6	2.19	0.42
1:E:68:THR:O	1:E:234:ASP:HB3	2.19	0.42
1:E:150:THR:CB	1:E:222:GLN:OE1	2.68	0.42
1:E:232:HIS:HD2	1:E:259:GLY:C	2.27	0.42
1:E:260:THR:O	1:E:264:ILE:HG13	2.19	0.42
1:E:389:ARG:O	1:E:392:LEU:HG	2.19	0.42
1:A:208:TRP:CD1	1:A:219:ILE:HD12	2.48	0.42
1:A:224:ARG:CZ	1:A:224:ARG:HB3	2.49	0.42
1:B:62:GLU:O	1:B:63:SER:HB2	2.19	0.42
1:B:83:LYS:O	1:B:83:LYS:HG3	2.19	0.42
1:B:175:SER:C	1:B:177:LYS:N	2.76	0.42
1:C:81:LEU:CD1	1:C:161:ARG:CZ	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:VAL:N	1:C:375:PRO:O	2.52	0.42
1:C:343:GLY:O	1:D:80:ILE:HG21	2.19	0.42
1:D:128:GLU:HG3	1:D:161:ARG:NH1	2.34	0.42
1:D:345:LEU:HD23	1:D:345:LEU:HA	1.67	0.42
1:D:378:VAL:O	1:D:379:ARG:C	2.62	0.42
1:E:103:CYS:HA	1:E:368:GLN:O	2.18	0.42
1:E:267:LYS:O	1:E:267:LYS:HG3	2.19	0.42
1:E:277:ILE:O	1:E:321:ASP:HB2	2.19	0.42
1:A:192:PRO:C	1:A:194:ASN:N	2.75	0.42
1:A:228:ASN:HB3	1:A:229:PRO:HD2	2.00	0.42
1:A:378:VAL:HG23	1:A:379:ARG:N	2.35	0.42
1:A:383:THR:C	1:A:384:LYS:HG2	2.44	0.42
1:B:347:GLY:O	1:B:348:GLY:C	2.61	0.42
1:B:373:ILE:C	1:B:375:PRO:HD3	2.44	0.42
1:C:53:THR:HB	1:C:58:ARG:NH2	2.35	0.42
1:C:106:LEU:HD21	1:D:76:ILE:HD13	2.01	0.42
1:E:102:LYS:HB3	1:E:366:GLU:OE1	2.19	0.42
1:E:126:MET:C	1:E:128:GLU:N	2.76	0.42
1:E:183:ALA:O	1:F:340:ALA:HB2	2.20	0.42
1:F:364:LEU:HD12	1:F:368:GLN:NE2	2.34	0.42
1:A:77:LEU:HG	1:B:90:VAL:HG22	2.02	0.42
1:A:104:GLU:O	1:A:369:ARG:HA	2.20	0.42
1:A:167:ILE:CD1	1:A:181:LEU:HD22	2.50	0.42
1:A:268:LEU:O	1:A:270:GLU:N	2.52	0.42
1:B:169:MET:HE1	1:B:178:VAL:HG22	2.01	0.42
1:C:95:ILE:O	1:C:97:LYS:N	2.53	0.42
1:C:140:ASP:O	1:C:163:TYR:HB3	2.20	0.42
1:C:167:ILE:CD1	1:C:181:LEU:HD22	2.50	0.42
1:D:387:SER:OG	1:D:389:ARG:NH2	2.52	0.42
1:E:207:ALA:CB	1:E:219:ILE:HD11	2.35	0.42
1:E:245:ASP:OD2	1:E:245:ASP:N	2.50	0.42
1:E:294:ASN:ND2	1:E:294:ASN:N	2.67	0.42
1:A:78:PRO:HG2	1:A:79:ASP:OD2	2.20	0.42
1:B:90:VAL:O	1:B:107:ALA:N	2.52	0.42
1:B:190:ARG:O	1:B:192:PRO:HD3	2.20	0.42
1:B:229:PRO:O	3:B:1220:HEM:HBC1	2.19	0.42
1:B:286:ILE:HD11	1:B:309:ASP:C	2.45	0.42
1:C:316:ASP:OD2	1:C:318:THR:HB	2.20	0.42
1:D:88:PRO:HG3	1:D:112:PHE:CD1	2.54	0.42
1:D:101:LEU:HD12	1:D:362:GLN:NE2	2.35	0.42
1:D:155:ALA:HB1	1:D:186:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:HD11	1:F:76:ILE:HG21	2.01	0.42
1:E:301:TYR:CD1	1:E:301:TYR:N	2.86	0.42
1:F:135:THR:HG22	1:F:136:LEU:H	1.84	0.42
1:F:336:ARG:NH1	1:F:388:ASP:CB	2.74	0.42
1:F:391:MET:HE3	1:F:392:LEU:HD23	2.02	0.42
1:B:95:ILE:HD13	1:B:338:LEU:CD1	2.49	0.42
1:B:257:THR:O	1:B:314:VAL:CG2	2.67	0.42
1:B:265:ALA:O	1:B:269:LYS:HG3	2.20	0.42
1:B:282:PRO:HD3	1:B:306:ILE:HD12	2.00	0.42
1:C:171:GLU:O	1:C:190:ARG:NH2	2.52	0.42
1:D:83:LYS:HE3	1:D:83:LYS:C	2.45	0.42
1:D:91:ARG:HD3	1:D:93:ASN:HD21	1.81	0.42
1:E:233:TYR:CZ	1:E:267:LYS:HD3	2.54	0.42
1:A:242:GLN:NE2	1:C:61:SER:HB2	2.24	0.42
1:B:254:SER:HB3	1:B:306:ILE:HG22	2.02	0.42
1:C:80:ILE:HG12	1:D:344:LEU:CD2	2.50	0.42
1:D:105:LEU:HD11	1:D:372:VAL:HG21	2.00	0.42
1:F:334:PHE:O	1:F:335:ALA:C	2.62	0.42
1:A:94:LYS:HB3	1:A:341:GLN:OE1	2.20	0.42
1:A:217:SER:O	1:A:218:HIS:CG	2.73	0.42
1:B:145:PRO:HA	1:B:168:VAL:HB	2.01	0.42
1:B:222:GLN:O	1:B:314:VAL:HG11	2.20	0.42
1:C:241:LEU:HD21	1:C:268:LEU:HD12	2.02	0.42
1:C:296:THR:O	1:C:298:GLN:N	2.52	0.42
1:D:68:THR:H	1:D:234:ASP:CG	2.27	0.42
1:D:348:GLY:O	1:D:349:SER:C	2.63	0.42
1:E:166:ILE:O	1:E:167:ILE:HD12	2.20	0.42
1:B:291:GLU:O	1:B:292:GLU:C	2.63	0.42
1:B:302:GLU:OE1	1:B:394:LYS:HD2	2.19	0.42
1:C:73:SER:HA	1:C:74:PRO:HD2	1.89	0.42
1:C:178:VAL:CG1	1:C:182:ARG:NH1	2.83	0.42
1:E:95:ILE:HG23	1:E:95:ILE:O	2.19	0.42
1:E:156:LEU:C	1:E:156:LEU:HD12	2.44	0.42
1:E:276:ARG:HE	1:E:276:ARG:HB3	1.42	0.42
1:E:280:VAL:HG22	1:E:356:VAL:HG11	2.02	0.42
1:A:64:PRO:O	1:A:65:HIS:CG	2.73	0.41
1:A:170:PRO:HD3	1:A:191:THR:OG1	2.19	0.41
1:A:178:VAL:O	1:A:182:ARG:HG3	2.20	0.41
1:B:130:ALA:CB	1:B:136:LEU:HB2	2.50	0.41
1:B:331:ALA:O	1:B:351:GLY:HA3	2.20	0.41
1:D:229:PRO:C	3:D:1420:HEM:HBC1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:MET:HE2	1:D:276:ARG:HB2	2.01	0.41
1:E:93:ASN:ND2	1:F:79:ASP:HB3	2.32	0.41
1:E:119:LYS:O	1:E:120:ASP:C	2.63	0.41
1:F:91:ARG:HD3	1:F:104:GLU:OE2	2.20	0.41
1:F:231:ALA:C	1:F:233:TYR:N	2.76	0.41
1:F:255:VAL:HG13	1:F:258:GLY:HA2	2.00	0.41
1:F:389:ARG:HG2	1:F:390:TRP:N	2.35	0.41
1:A:209:ARG:O	1:A:209:ARG:HG2	2.21	0.41
1:B:176:GLU:O	1:B:180:VAL:CG2	2.64	0.41
1:B:210:LEU:C	1:B:212:ASN:N	2.76	0.41
1:B:316:ASP:OD2	1:B:318:THR:HB	2.20	0.41
1:C:55:GLN:C	1:C:57:GLY:N	2.78	0.41
1:D:288:ALA:HA	1:D:323:TRP:CE3	2.54	0.41
1:E:154:LEU:O	1:E:158:ALA:CB	2.68	0.41
1:E:169:MET:HG2	1:E:188:ILE:CG2	2.50	0.41
1:E:248:LEU:HD23	1:E:249:ASP:H	1.85	0.41
1:E:257:THR:O	1:E:312:PRO:HB2	2.21	0.41
1:E:260:THR:HG23	2:E:1510:PLP:O1P	2.20	0.41
1:F:335:ALA:CB	1:F:385:PHE:CZ	3.03	0.41
1:A:144:GLU:HB2	1:A:154:LEU:HD13	2.02	0.41
1:A:158:ALA:O	1:A:162:GLY:N	2.53	0.41
1:A:281:ASP:HB3	1:A:325:LYS:CD	2.49	0.41
1:B:255:VAL:HG21	1:B:323:TRP:CH2	2.55	0.41
1:B:286:ILE:HD12	1:B:286:ILE:C	2.45	0.41
1:B:360:ALA:C	1:B:362:GLN:H	2.26	0.41
1:C:82:LYS:HD3	1:C:82:LYS:H	1.85	0.41
1:C:235:THR:O	1:C:239:GLU:CG	2.63	0.41
1:D:236:THR:CG2	1:D:264:ILE:HD11	2.49	0.41
1:E:176:GLU:HA	1:E:396:PHE:CD1	2.52	0.41
1:E:230:LEU:O	1:E:231:ALA:C	2.63	0.41
1:F:101:LEU:CD2	1:F:105:LEU:HD22	2.49	0.41
1:F:168:VAL:CG2	1:F:189:VAL:HB	2.38	0.41
1:F:241:LEU:HD21	1:F:268:LEU:HD23	2.01	0.41
1:A:228:ASN:CB	1:A:229:PRO:CD	2.96	0.41
1:C:206:VAL:O	1:C:210:LEU:HG	2.20	0.41
1:C:264:ILE:CD1	1:C:373:ILE:HD11	2.49	0.41
1:C:268:LEU:O	1:C:272:CYS:C	2.63	0.41
1:C:348:GLY:O	1:C:349:SER:C	2.64	0.41
1:D:54:TRP:CG	1:D:266:ARG:HH11	2.38	0.41
1:D:85:GLY:C	1:D:87:THR:N	2.77	0.41
1:E:66:HIS:O	1:E:125:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LEU:CD1	1:F:76:ILE:CD1	2.91	0.41
1:E:235:THR:O	1:E:239:GLU:HG3	2.20	0.41
1:A:58:ARG:O	1:A:59:PRO:C	2.62	0.41
1:B:55:GLN:O	1:B:56:LEU:C	2.61	0.41
1:C:87:THR:OG1	1:C:108:LYS:HE3	2.20	0.41
1:D:173:MET:HE2	1:D:177:LYS:NZ	2.34	0.41
1:E:121:ARG:C	1:E:123:SER:N	2.78	0.41
1:E:201:GLU:O	1:E:201:GLU:CG	2.67	0.41
1:E:272:CYS:HA	1:E:273:PRO:HD2	1.88	0.41
1:E:322:LYS:NZ	1:E:323:TRP:O	2.52	0.41
1:E:346:CYS:N	1:E:378:VAL:HG13	2.34	0.41
1:A:188:ILE:HG21	1:A:190:ARG:HD3	2.01	0.41
1:A:228:ASN:HB3	1:A:229:PRO:HD3	2.02	0.41
1:B:203:HIS:O	1:B:204:VAL:CG2	2.63	0.41
1:B:287:LEU:HD11	1:B:308:TYR:CA	2.50	0.41
1:C:90:VAL:HG21	1:D:80:ILE:HD13	2.01	0.41
1:D:54:TRP:CZ3	1:D:266:ARG:HD3	2.54	0.41
1:D:160:VAL:O	1:D:160:VAL:CG1	2.63	0.41
1:D:221:ASP:O	1:D:225:ASN:N	2.42	0.41
1:D:261:ILE:O	1:D:265:ALA:HB2	2.20	0.41
1:D:336:ARG:O	1:D:337:MET:C	2.62	0.41
1:F:130:ALA:O	1:F:135:THR:HB	2.19	0.41
1:F:242:GLN:HE21	1:F:242:GLN:CA	2.14	0.41
1:C:177:LYS:HA	1:C:180:VAL:HG23	2.03	0.41
1:C:177:LYS:NZ	1:C:304:GLU:OE2	2.34	0.41
1:C:264:ILE:HG22	1:C:268:LEU:HD22	2.02	0.41
1:C:342:GLU:HG3	1:C:342:GLU:O	2.21	0.41
1:C:366:GLU:CD	1:C:366:GLU:N	2.73	0.41
1:D:72:LYS:NZ	1:F:63:SER:O	2.46	0.41
1:D:143:ILE:CD1	1:D:214:ILE:HD12	2.46	0.41
1:D:302:GLU:OE2	1:D:394:LYS:HE3	2.21	0.41
1:E:198:ASP:HA	1:E:202:SER:OG	2.20	0.41
1:F:146:THR:HG21	1:F:150:THR:HG22	2.01	0.41
1:F:226:ALA:HA	3:F:1620:HEM:HMD2	2.01	0.41
1:F:316:ASP:O	1:F:319:VAL:HG22	2.20	0.41
1:A:77:LEU:N	1:A:77:LEU:CD2	2.83	0.41
1:A:337:MET:O	1:A:341:GLN:HB2	2.21	0.41
1:A:393:GLN:C	1:A:395:GLY:H	2.29	0.41
1:C:59:PRO:CB	1:C:62:GLU:OE2	2.68	0.41
1:C:261:ILE:HG23	1:C:262:THR:N	2.36	0.41
1:D:76:ILE:CG2	1:D:77:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:HG21	1:D:228:ASN:ND2	2.35	0.41
1:E:48:ALA:HB2	1:E:224:ARG:NH2	2.18	0.41
1:E:126:MET:C	1:E:128:GLU:H	2.29	0.41
1:F:79:ASP:O	1:F:80:ILE:C	2.64	0.41
1:F:119:LYS:O	1:F:121:ARG:N	2.54	0.41
1:A:92:ILE:O	1:A:92:ILE:HG22	2.20	0.41
1:A:113:ASN:O	1:A:114:ALA:C	2.63	0.41
1:A:194:ASN:O	1:A:200:PRO:CD	2.57	0.41
1:A:232:HIS:CA	1:A:236:THR:HB	2.49	0.41
1:A:239:GLU:O	1:A:243:GLN:HB2	2.21	0.41
1:B:64:PRO:HD2	3:B:1220:HEM:HMB3	2.03	0.41
1:B:126:MET:CG	1:B:227:SER:HB2	2.51	0.41
1:B:150:THR:CB	1:B:222:GLN:NE2	2.84	0.41
1:B:210:LEU:C	1:B:212:ASN:H	2.29	0.41
1:B:226:ALA:C	1:B:228:ASN:H	2.29	0.41
1:B:299:THR:O	1:B:299:THR:HG22	2.21	0.41
1:B:327:ASN:ND2	1:B:330:GLU:OE2	2.53	0.41
1:C:92:ILE:N	1:C:105:LEU:O	2.41	0.41
1:C:127:ILE:HD11	1:C:154:LEU:HA	2.03	0.41
1:C:215:PRO:C	1:C:217:SER:N	2.72	0.41
1:C:248:LEU:HD13	1:C:275:CYS:SG	2.61	0.41
1:D:249:ASP:O	1:D:275:CYS:SG	2.71	0.41
1:E:110:GLU:HG2	1:E:118:VAL:HB	2.03	0.41
1:E:308:TYR:CE2	1:E:310:PHE:HE1	2.38	0.41
1:F:226:ALA:HB2	3:F:1620:HEM:C2D	2.56	0.41
1:F:232:HIS:CD2	1:F:260:THR:HA	2.56	0.41
1:A:381:TYR:O	1:A:382:MET:C	2.64	0.41
1:A:392:LEU:HD22	1:A:398:LYS:HB3	2.03	0.41
1:B:156:LEU:C	1:B:156:LEU:HD13	2.46	0.41
1:D:256:GLY:N	2:D:1410:PLP:H5A1	2.36	0.41
1:E:58:ARG:O	1:E:59:PRO:C	2.62	0.41
1:E:146:THR:HA	1:E:203:HIS:CE1	2.55	0.41
1:E:256:GLY:HA2	1:E:307:GLY:H	1.86	0.41
1:F:145:PRO:HB3	1:F:207:ALA:CB	2.51	0.41
1:F:292:GLU:H	1:F:292:GLU:HG3	1.69	0.41
1:F:315:LEU:HD12	1:F:316:ASP:H	1.84	0.41
1:A:143:ILE:O	1:A:219:ILE:HG12	2.21	0.40
1:A:188:ILE:HG21	1:A:190:ARG:CD	2.51	0.40
1:A:194:ASN:H	1:A:200:PRO:CD	2.26	0.40
1:A:311:ILE:O	1:A:312:PRO:C	2.64	0.40
1:B:52:CYS:HB2	3:B:1220:HEM:C4D	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:HB	1:B:88:PRO:HD2	2.02	0.40
1:B:276:ARG:C	1:B:277:ILE:HG12	2.45	0.40
1:B:318:THR:O	1:B:318:THR:HG22	2.21	0.40
1:C:121:ARG:NH2	1:C:239:GLU:OE2	2.55	0.40
1:C:252:VAL:HG12	1:C:353:THR:HG23	2.03	0.40
1:D:88:PRO:HG3	1:D:112:PHE:HD1	1.86	0.40
1:E:89:MET:HB2	1:E:243:GLN:NE2	2.35	0.40
1:E:102:LYS:HG2	1:E:366:GLU:OE1	2.21	0.40
1:E:110:GLU:HG2	1:E:118:VAL:CG2	2.51	0.40
1:E:233:TYR:CE1	1:E:267:LYS:HB2	2.55	0.40
1:E:251:LEU:HA	1:E:371:VAL:O	2.22	0.40
1:F:53:THR:HG23	3:F:1620:HEM:CHB	2.51	0.40
1:F:230:LEU:HA	3:F:1620:HEM:HBC2	2.02	0.40
1:A:235:THR:O	1:A:239:GLU:HG3	2.22	0.40
1:B:85:GLY:O	1:B:86:ASP:CB	2.69	0.40
1:B:94:LYS:CD	1:B:341:GLN:HB3	2.45	0.40
1:C:281:ASP:O	1:C:325:LYS:HD2	2.21	0.40
1:C:353:THR:CG2	1:C:372:VAL:HG13	2.51	0.40
1:D:125:ARG:HD2	1:D:125:ARG:HA	1.90	0.40
1:D:282:PRO:HG3	1:D:306:ILE:HG13	2.03	0.40
1:E:92:ILE:HG22	1:E:94:LYS:O	2.21	0.40
1:E:106:LEU:HD13	1:F:76:ILE:HG23	2.02	0.40
1:E:248:LEU:CD2	1:E:250:MET:O	2.65	0.40
1:F:56:LEU:HD22	1:F:269:LYS:CB	2.50	0.40
1:F:205:GLY:C	1:F:207:ALA:N	2.78	0.40
1:A:94:LYS:HE2	1:A:341:GLN:O	2.21	0.40
1:A:101:LEU:CD2	1:A:105:LEU:HD22	2.50	0.40
1:A:276:ARG:NH2	1:A:321:ASP:HB3	2.34	0.40
1:C:316:ASP:C	1:C:318:THR:N	2.78	0.40
1:C:345:LEU:O	1:C:378:VAL:HG13	2.21	0.40
1:D:318:THR:C	1:D:320:VAL:H	2.29	0.40
1:D:392:LEU:C	1:D:394:LYS:N	2.80	0.40
1:E:114:ALA:HA	1:F:112:PHE:CZ	2.57	0.40
1:E:382:MET:O	1:E:386:LEU:CB	2.69	0.40
1:F:70:PRO:HG2	1:F:238:ASP:HB3	2.04	0.40
1:B:122:ILE:O	1:B:123:SER:C	2.63	0.40
1:B:226:ALA:HB1	1:B:230:LEU:CD1	2.51	0.40
1:B:228:ASN:OD1	1:B:228:ASN:C	2.63	0.40
1:B:287:LEU:HD21	1:B:308:TYR:HB3	2.02	0.40
1:C:176:GLU:O	1:C:180:VAL:HG23	2.21	0.40
1:C:309:ASP:O	1:C:310:PHE:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:THR:H	1:D:235:THR:HG1	1.68	0.40
1:D:242:GLN:OE1	1:D:242:GLN:HA	2.22	0.40
1:F:168:VAL:HA	1:F:189:VAL:O	2.22	0.40
1:F:380:ASN:HB2	1:F:381:TYR:CE1	2.56	0.40
1:A:326:SER:OG	1:A:327:ASN:N	2.54	0.40
1:B:58:ARG:HA	1:B:59:PRO:HD3	1.93	0.40
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.78	0.40
1:B:315:LEU:HD12	1:B:316:ASP:N	2.36	0.40
1:B:393:GLN:OE1	1:B:393:GLN:HA	2.16	0.40
1:D:110:GLU:HG3	1:D:118:VAL:HA	2.04	0.40
1:E:105:LEU:HA	1:E:370:CYS:O	2.22	0.40
1:E:106:LEU:CD1	1:F:76:ILE:HG21	2.52	0.40
1:E:272:CYS:SG	1:E:275:CYS:HB2	2.62	0.40
1:E:320:VAL:CG1	1:E:323:TRP:CD1	3.04	0.40
1:F:232:HIS:CD2	1:F:260:THR:CG2	3.03	0.40
1:F:316:ASP:C	1:F:318:THR:H	2.29	0.40

All (1) 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)
1:D:399:GLU:CD	1:E:173:MET:O[1_554]	1.97	0.23

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	348/363 (96%)	271 (78%)	62 (18%)	15 (4%)	2	8
1	B	341/363 (94%)	276 (81%)	54 (16%)	11 (3%)	3	13
1	C	342/363 (94%)	284 (83%)	43 (13%)	15 (4%)	2	8
1	D	342/363 (94%)	274 (80%)	52 (15%)	16 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	343/363 (94%)	271 (79%)	54 (16%)	18 (5%)	1	5
1	F	340/363 (94%)	268 (79%)	50 (15%)	22 (6%)	1	3
All	All	2056/2178 (94%)	1644 (80%)	315 (15%)	97 (5%)	2	7

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ALA
1	A	134	GLY
1	A	295	GLN
1	A	299	THR
1	A	385	PHE
1	A	399	GLU
1	A	400	GLU
1	B	173	MET
1	B	174	SER
1	B	225	ASN
1	B	290	PRO
1	B	307	GLY
1	C	48	ALA
1	C	49	PRO
1	C	51	ARG
1	C	173	MET
1	C	202	SER
1	C	215	PRO
1	C	216	ASN
1	C	290	PRO
1	C	291	GLU
1	C	297	GLU
1	C	343	GLY
1	C	385	PHE
1	D	170	PRO
1	D	173	MET
1	D	245	ASP
1	D	250	MET
1	D	288	ALA
1	D	346	CYS
1	D	398	LYS
1	E	48	ALA
1	E	49	PRO
1	E	50	SER

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Mol	Chain	Res	Type
1	E	141	THR
1	E	174	SER
1	E	175	SER
1	E	223	TYR
1	E	299	THR
1	E	385	PHE
1	E	391	MET
1	E	393	GLN
1	E	396	PHE
1	F	46	PRO
1	F	48	ALA
1	F	74	PRO
1	F	136	LEU
1	F	173	MET
1	F	206	VAL
1	F	250	MET
1	F	257	THR
1	F	385	PHE
1	F	387	SER
1	F	388	ASP
1	F	393	GLN
1	F	394	LYS
1	A	395	GLY
1	A	396	PHE
1	B	204	VAL
1	B	385	PHE
1	B	395	GLY
1	C	259	GLY
1	D	101	LEU
1	D	385	PHE
1	D	394	LYS
1	D	397	LEU
1	E	100	GLY
1	E	176	GLU
1	F	205	GLY
1	F	386	LEU
1	A	49	PRO
1	B	172	LYS
1	C	57	GLY
1	C	96	GLY
1	D	96	GLY
1	E	248	LEU

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Mol	Chain	Res	Type
1	F	47	ASP
1	F	170	PRO
1	F	288	ALA
1	F	315	LEU
1	A	307	GLY
1	A	269	LYS
1	B	203	HIS
1	D	49	PRO
1	D	57	GLY
1	E	95	ILE
1	E	246	GLY
1	E	315	LEU
1	F	307	GLY
1	F	256	GLY
1	A	286	ILE
1	D	311	ILE
1	D	375	PRO
1	F	240	ILE
1	A	80	ILE
1	B	127	ILE
1	A	312	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/304 (97%)	246 (84%)	48 (16%)	2	8
1	B	289/304 (95%)	243 (84%)	46 (16%)	2	8
1	C	288/304 (95%)	254 (88%)	34 (12%)	5	17
1	D	288/304 (95%)	245 (85%)	43 (15%)	3	10
1	E	289/304 (95%)	245 (85%)	44 (15%)	3	9
1	F	286/304 (94%)	232 (81%)	54 (19%)	1	5
All	All	1734/1824 (95%)	1465 (84%)	269 (16%)	2	9

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	50	SER
1	A	51	ARG
1	A	55	GLN
1	A	58	ARG
1	A	73	SER
1	A	74	PRO
1	A	77	LEU
1	A	80	ILE
1	A	83	LYS
1	A	88	PRO
1	A	97	LYS
1	A	110	GLU
1	A	125	ARG
1	A	132	ARG
1	A	138	PRO
1	A	146	THR
1	A	156	LEU
1	A	172	LYS
1	A	173	MET
1	A	176	GLU
1	A	191	THR
1	A	201	GLU
1	A	202	SER
1	A	208	TRP
1	A	210	LEU
1	A	212	ASN
1	A	225	ASN
1	A	243	GLN
1	A	248	LEU
1	A	270	GLU
1	A	283	GLU
1	A	294	ASN
1	A	295	GLN
1	A	311	ILE
1	A	314	VAL
1	A	327	ASN
1	A	336	ARG
1	A	372	VAL
1	A	381	TYR
1	A	384	LYS
1	A	385	PHE

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Mol	Chain	Res	Type
1	A	386	LEU
1	A	389	ARG
1	A	397	LEU
1	A	398	LYS
1	A	399	GLU
1	A	402	LEU
1	B	47	ASP
1	B	51	ARG
1	B	52	CYS
1	B	53	THR
1	B	72	LYS
1	B	101	LEU
1	B	132	ARG
1	B	138	PRO
1	B	152	ILE
1	B	156	LEU
1	B	161	ARG
1	B	167	ILE
1	B	172	LYS
1	B	174	SER
1	B	176	GLU
1	B	184	LEU
1	B	188	ILE
1	B	190	ARG
1	B	191	THR
1	B	202	SER
1	B	204	VAL
1	B	215	PRO
1	B	224	ARG
1	B	225	ASN
1	B	267	LYS
1	B	272	CYS
1	B	287	LEU
1	B	290	PRO
1	B	309	ASP
1	B	311	ILE
1	B	317	ARG
1	B	319	VAL
1	B	320	VAL
1	B	325	LYS
1	B	327	ASN
1	B	359	LYS

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Mol	Chain	Res	Type
1	B	363	GLU
1	B	372	VAL
1	B	375	PRO
1	B	377	SER
1	B	378	VAL
1	B	380	ASN
1	B	384	LYS
1	B	385	PHE
1	B	394	LYS
1	B	399	GLU
1	C	49	PRO
1	C	55	GLN
1	C	58	ARG
1	C	78	PRO
1	C	80	ILE
1	C	82	LYS
1	C	150	THR
1	C	156	LEU
1	C	165	CYS
1	C	184	LEU
1	C	187	GLU
1	C	188	ILE
1	C	191	THR
1	C	192	PRO
1	C	211	LYS
1	C	224	ARG
1	C	227	SER
1	C	229	PRO
1	C	242	GLN
1	C	245	ASP
1	C	248	LEU
1	C	254	SER
1	C	255	VAL
1	C	268	LEU
1	C	273	PRO
1	C	287	LEU
1	C	290	PRO
1	C	291	GLU
1	C	313	THR
1	C	366	GLU
1	C	375	PRO
1	C	385	PHE

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Mol	Chain	Res	Type
1	C	394	LYS
1	C	399	GLU
1	D	51	ARG
1	D	59	PRO
1	D	63	SER
1	D	66	HIS
1	D	74	PRO
1	D	77	LEU
1	D	83	LYS
1	D	135	THR
1	D	136	LEU
1	D	145	PRO
1	D	169	MET
1	D	172	LYS
1	D	173	MET
1	D	175	SER
1	D	176	GLU
1	D	187	GLU
1	D	188	ILE
1	D	190	ARG
1	D	191	THR
1	D	202	SER
1	D	203	HIS
1	D	204	VAL
1	D	219	ILE
1	D	248	LEU
1	D	250	MET
1	D	268	LEU
1	D	286	ILE
1	D	292	GLU
1	D	298	GLN
1	D	311	ILE
1	D	313	THR
1	D	317	ARG
1	D	325	LYS
1	D	328	ASP
1	D	341	GLN
1	D	346	CYS
1	D	372	VAL
1	D	379	ARG
1	D	382	MET
1	D	385	PHE

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Mol	Chain	Res	Type
1	D	397	LEU
1	D	398	LYS
1	D	399	GLU
1	E	49	PRO
1	E	58	ARG
1	E	64	PRO
1	E	77	LEU
1	E	119	LYS
1	E	125	ARG
1	E	127	ILE
1	E	135	THR
1	E	150	THR
1	E	156	LEU
1	E	167	ILE
1	E	170	PRO
1	E	172	LYS
1	E	174	SER
1	E	176	GLU
1	E	192	PRO
1	E	200	PRO
1	E	201	GLU
1	E	210	LEU
1	E	229	PRO
1	E	238	ASP
1	E	242	GLN
1	E	247	LYS
1	E	248	LEU
1	E	251	LEU
1	E	287	LEU
1	E	291	GLU
1	E	294	ASN
1	E	295	GLN
1	E	297	GLU
1	E	301	TYR
1	E	310	PHE
1	E	317	ARG
1	E	319	VAL
1	E	321	ASP
1	E	342	GLU
1	E	353	THR
1	E	366	GLU
1	E	377	SER

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Mol	Chain	Res	Type
1	E	385	PHE
1	E	386	LEU
1	E	391	MET
1	E	392	LEU
1	E	394	LYS
1	F	46	PRO
1	F	50	SER
1	F	51	ARG
1	F	53	THR
1	F	56	LEU
1	F	58	ARG
1	F	68	THR
1	F	74	PRO
1	F	75	LYS
1	F	77	LEU
1	F	78	PRO
1	F	101	LEU
1	F	106	LEU
1	F	108	LYS
1	F	138	PRO
1	F	140	ASP
1	F	156	LEU
1	F	169	MET
1	F	170	PRO
1	F	171	GLU
1	F	172	LYS
1	F	182	ARG
1	F	188	ILE
1	F	209	ARG
1	F	227	SER
1	F	228	ASN
1	F	229	PRO
1	F	242	GLN
1	F	255	VAL
1	F	257	THR
1	F	287	LEU
1	F	289	GLU
1	F	292	GLU
1	F	294	ASN
1	F	295	GLN
1	F	299	THR
1	F	306	ILE

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Mol	Chain	Res	Type
1	F	310	PHE
1	F	311	ILE
1	F	318	THR
1	F	352	SER
1	F	365	GLN
1	F	372	VAL
1	F	379	ARG
1	F	381	TYR
1	F	385	PHE
1	F	386	LEU
1	F	387	SER
1	F	388	ASP
1	F	389	ARG
1	F	392	LEU
1	F	393	GLN
1	F	394	LYS
1	F	397	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	225	ASN
1	A	242	GLN
1	A	243	GLN
1	A	393	GLN
1	B	66	HIS
1	B	212	ASN
1	B	218	HIS
1	B	222	GLN
1	B	232	HIS
1	B	294	ASN
1	B	295	GLN
1	B	327	ASN
1	B	341	GLN
1	B	362	GLN
1	B	365	GLN
1	C	55	GLN
1	C	66	HIS
1	C	216	ASN
1	C	218	HIS
1	C	222	GLN

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Mol	Chain	Res	Type
1	D	55	GLN
1	D	93	ASN
1	D	212	ASN
1	D	216	ASN
1	D	225	ASN
1	D	362	GLN
1	E	93	ASN
1	E	149	ASN
1	E	242	GLN
1	E	368	GLN
1	E	380	ASN
1	F	66	HIS
1	F	203	HIS
1	F	216	ASN
1	F	218	HIS
1	F	242	GLN
1	F	295	GLN
1	F	365	GLN
1	F	393	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	PLP	C	1310	-	15,15,16	1.61	4 (26%)	21,22,23	1.25	2 (9%)
2	PLP	F	1610	1	15,15,16	1.42	3 (20%)	21,22,23	1.14	3 (14%)
3	HEM	B	1220	1	50,50,50	1.82	10 (20%)	67,82,82	0.94	3 (4%)
3	HEM	C	1320	1	50,50,50	1.98	15 (30%)	67,82,82	1.03	3 (4%)
2	PLP	B	1210	-	15,15,16	2.56	6 (40%)	21,22,23	2.17	10 (47%)
3	HEM	D	1420	1	50,50,50	1.91	13 (26%)	67,82,82	1.03	3 (4%)
3	HEM	E	1520	1	50,50,50	1.89	12 (24%)	67,82,82	1.00	5 (7%)
3	HEM	F	1620	1	50,50,50	1.85	13 (26%)	67,82,82	1.06	6 (8%)
2	PLP	E	1510	1	15,15,16	1.68	4 (26%)	21,22,23	1.35	3 (14%)
2	PLP	A	1110	1	15,15,16	1.56	3 (20%)	21,22,23	1.20	2 (9%)
3	HEM	A	1120	1	50,50,50	1.93	16 (32%)	67,82,82	0.99	4 (5%)
2	PLP	D	1410	1	15,15,16	1.66	4 (26%)	21,22,23	1.42	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	1310	-	-	1/6/6/8	0/1/1/1
2	PLP	F	1610	1	-	0/6/6/8	0/1/1/1
3	HEM	B	1220	1	-	6/14/54/54	-
3	HEM	C	1320	1	-	2/14/54/54	-
2	PLP	B	1210	-	-	0/6/6/8	0/1/1/1
3	HEM	D	1420	1	-	8/14/54/54	-
3	HEM	E	1520	1	-	6/14/54/54	-
3	HEM	F	1620	1	-	9/14/54/54	-
2	PLP	E	1510	1	-	2/6/6/8	0/1/1/1
2	PLP	A	1110	1	-	2/6/6/8	0/1/1/1
3	HEM	A	1120	1	-	2/14/54/54	-
2	PLP	D	1410	1	-	2/6/6/8	0/1/1/1

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	PLP	C3-C2	-5.78	1.35	1.41
3	C	1320	HEM	CBB-CAB	5.29	1.55	1.30
3	A	1120	HEM	CBB-CAB	5.27	1.55	1.30
3	B	1220	HEM	CBB-CAB	5.10	1.54	1.30
3	E	1520	HEM	CBB-CAB	5.08	1.54	1.30
3	D	1420	HEM	CBB-CAB	5.07	1.54	1.30
3	D	1420	HEM	CBC-CAC	4.94	1.54	1.30
3	F	1620	HEM	CBB-CAB	4.93	1.54	1.30
3	E	1520	HEM	CBC-CAC	4.85	1.53	1.30
3	C	1320	HEM	CBC-CAC	4.80	1.53	1.30
3	B	1220	HEM	CBC-CAC	4.69	1.52	1.30
3	F	1620	HEM	CBC-CAC	4.60	1.52	1.30
3	C	1320	HEM	CAB-C3B	4.48	1.59	1.47
3	A	1120	HEM	CBC-CAC	4.46	1.51	1.30
2	B	1210	PLP	C2-N1	4.23	1.41	1.33
3	D	1420	HEM	CAB-C3B	4.22	1.58	1.47
3	E	1520	HEM	CAB-C3B	3.97	1.58	1.47
2	B	1210	PLP	C4A-C4	-3.93	1.43	1.51
3	C	1320	HEM	CAC-C3C	3.77	1.57	1.47
3	A	1120	HEM	CMC-C2C	3.74	1.58	1.50
2	B	1210	PLP	C6-N1	3.70	1.42	1.34
3	B	1220	HEM	FE-NA	3.70	2.07	1.95
3	A	1120	HEM	CAB-C3B	3.67	1.57	1.47
3	A	1120	HEM	CAC-C3C	3.66	1.57	1.47
3	B	1220	HEM	CAC-C3C	3.61	1.57	1.47
3	E	1520	HEM	FE-NA	3.53	2.06	1.95
2	D	1410	PLP	C2-N1	3.48	1.40	1.33
3	C	1320	HEM	FE-NA	3.43	2.06	1.95
3	E	1520	HEM	CMC-C2C	3.38	1.57	1.50
3	A	1120	HEM	FE-NA	3.38	2.06	1.95
3	C	1320	HEM	CMC-C2C	3.37	1.57	1.50
3	F	1620	HEM	CAC-C3C	3.35	1.56	1.47
3	D	1420	HEM	FE-NA	3.33	2.06	1.95
3	B	1220	HEM	CAB-C3B	3.32	1.56	1.47
3	D	1420	HEM	CAC-C3C	3.29	1.56	1.47
3	F	1620	HEM	CAB-C3B	3.25	1.56	1.47
3	F	1620	HEM	FE-NA	3.19	2.05	1.95
3	F	1620	HEM	CMC-C2C	3.15	1.57	1.50
3	E	1520	HEM	CAC-C3C	3.14	1.55	1.47
2	E	1510	PLP	C5-C4	3.10	1.44	1.40
3	F	1620	HEM	FE-NB	3.09	2.04	1.94
3	D	1420	HEM	CMC-C2C	3.09	1.57	1.50
2	E	1510	PLP	C2-N1	3.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1620	HEM	O1A-CGA	3.03	1.32	1.22
2	A	1110	PLP	C5-C4	3.00	1.43	1.40
3	E	1520	HEM	FE-NB	2.99	2.04	1.94
3	B	1220	HEM	CMC-C2C	2.97	1.56	1.50
2	A	1110	PLP	C2-N1	2.96	1.39	1.33
2	C	1310	PLP	C2-N1	2.93	1.39	1.33
3	A	1120	HEM	FE-NB	2.88	2.03	1.94
3	D	1420	HEM	O1A-CGA	2.81	1.31	1.22
2	D	1410	PLP	C5-C4	2.79	1.43	1.40
2	F	1610	PLP	C2-N1	2.73	1.38	1.33
3	E	1520	HEM	CMA-C3A	2.72	1.56	1.50
3	D	1420	HEM	FE-NB	2.70	2.03	1.94
3	C	1320	HEM	O1A-CGA	2.69	1.30	1.22
3	C	1320	HEM	FE-NB	2.66	2.03	1.94
3	E	1520	HEM	O1A-CGA	2.66	1.30	1.22
2	D	1410	PLP	C6-N1	2.64	1.39	1.34
2	C	1310	PLP	C6-N1	2.60	1.39	1.34
3	D	1420	HEM	CMA-C3A	2.57	1.56	1.50
3	A	1120	HEM	CMB-C2B	2.52	1.55	1.50
2	E	1510	PLP	P-O3P	-2.52	1.45	1.54
2	E	1510	PLP	C6-N1	2.51	1.39	1.34
3	B	1220	HEM	FE-NB	2.49	2.02	1.94
2	F	1610	PLP	P-O3P	-2.47	1.45	1.54
3	F	1620	HEM	CMA-C3A	2.47	1.55	1.50
3	C	1320	HEM	CMA-C3A	2.46	1.55	1.50
3	A	1120	HEM	CMA-C3A	2.45	1.55	1.50
2	A	1110	PLP	C6-N1	2.45	1.39	1.34
2	B	1210	PLP	C5A-C5	2.42	1.57	1.50
3	A	1120	HEM	O1A-CGA	2.42	1.30	1.22
3	B	1220	HEM	O1A-CGA	2.39	1.29	1.22
3	F	1620	HEM	CMB-C2B	2.37	1.55	1.50
3	C	1320	HEM	CMB-C2B	2.35	1.55	1.50
2	C	1310	PLP	C5-C4	2.34	1.43	1.40
2	D	1410	PLP	P-O3P	-2.34	1.46	1.54
3	E	1520	HEM	CMD-C2D	2.33	1.55	1.50
2	F	1610	PLP	C6-N1	2.32	1.39	1.34
3	F	1620	HEM	C4A-C3A	2.31	1.48	1.43
3	B	1220	HEM	CMA-C3A	2.30	1.55	1.50
2	C	1310	PLP	C5A-C5	2.29	1.56	1.50
3	C	1320	HEM	CHB-C4A	-2.22	1.34	1.39
3	A	1120	HEM	CHB-C4A	-2.20	1.34	1.39
3	C	1320	HEM	C4A-C3A	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1220	HEM	CMB-C2B	2.17	1.55	1.50
3	A	1120	HEM	CBD-CAD	2.15	1.59	1.51
2	B	1210	PLP	P-O3P	-2.11	1.47	1.54
3	C	1320	HEM	CMD-C2D	2.11	1.55	1.50
3	D	1420	HEM	CAD-C3D	2.10	1.56	1.51
3	A	1120	HEM	CAD-C3D	2.09	1.56	1.51
3	E	1520	HEM	FE-NC	2.09	2.02	1.95
3	D	1420	HEM	CBD-CAD	2.07	1.59	1.51
3	C	1320	HEM	FE-NC	2.06	2.02	1.95
3	D	1420	HEM	CMB-C2B	2.06	1.55	1.50
3	F	1620	HEM	FE-NC	2.06	2.02	1.95
3	A	1120	HEM	O2A-CGA	-2.05	1.24	1.30
3	E	1520	HEM	CMB-C2B	2.03	1.54	1.50
3	F	1620	HEM	CMD-C2D	2.02	1.54	1.50
3	C	1320	HEM	CAD-C3D	2.01	1.56	1.51
3	A	1120	HEM	FE-NC	2.01	2.01	1.95
3	A	1120	HEM	CMD-C2D	2.00	1.54	1.50
3	D	1420	HEM	CHB-C4A	-2.00	1.34	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1210	PLP	C3-C4-C5	5.61	125.31	118.59
2	D	1410	PLP	O4P-C5A-C5	4.17	117.17	109.36
2	C	1310	PLP	O4P-C5A-C5	3.76	116.40	109.36
2	E	1510	PLP	O4P-C5A-C5	3.70	116.28	109.36
2	B	1210	PLP	C5-C6-N1	-3.66	117.88	123.83
3	E	1520	HEM	O1A-CGA-CBA	-3.03	113.48	123.09
2	B	1210	PLP	O4P-C5A-C5	2.91	114.81	109.36
3	F	1620	HEM	CBA-CAA-C2A	2.84	120.39	112.53
3	B	1220	HEM	O1A-CGA-CBA	-2.78	114.29	123.09
3	C	1320	HEM	CBA-CAA-C2A	2.77	120.20	112.53
3	F	1620	HEM	O1A-CGA-CBA	-2.65	114.68	123.09
2	B	1210	PLP	C4A-C4-C5	-2.62	118.23	120.94
3	D	1420	HEM	O1A-CGA-CBA	-2.62	114.79	123.09
2	B	1210	PLP	O3-C3-C2	2.61	122.98	117.58
3	B	1220	HEM	CBB-CAB-C3B	-2.59	114.58	127.53
3	C	1320	HEM	O1A-CGA-CBA	-2.45	115.33	123.09
2	B	1210	PLP	C4A-C4-C3	-2.44	116.45	120.52
3	D	1420	HEM	C3B-C4B-NB	2.40	111.19	109.47
3	E	1520	HEM	C3B-C4B-NB	2.40	111.19	109.47
3	B	1220	HEM	C3B-C4B-NB	2.38	111.17	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1120	HEM	CBB-CAB-C3B	-2.36	115.75	127.53
3	A	1120	HEM	O1A-CGA-CBA	-2.34	115.66	123.09
3	E	1520	HEM	CBC-CAC-C3C	-2.33	115.90	127.53
2	F	1610	PLP	O3P-P-O1P	2.27	119.67	110.83
3	F	1620	HEM	CBB-CAB-C3B	-2.25	116.30	127.53
2	E	1510	PLP	C5A-C5-C6	-2.23	115.73	119.36
3	E	1520	HEM	CBB-CAB-C3B	-2.22	116.43	127.53
3	F	1620	HEM	CBC-CAC-C3C	-2.21	116.47	127.53
2	C	1310	PLP	O3P-P-O1P	2.18	119.35	110.83
2	B	1210	PLP	O3P-P-O1P	2.16	119.25	110.83
2	A	1110	PLP	O4P-C5A-C5	2.14	113.37	109.36
3	D	1420	HEM	CBC-CAC-C3C	-2.14	116.83	127.53
3	A	1120	HEM	CBA-CAA-C2A	2.13	118.42	112.53
2	E	1510	PLP	O3P-P-O1P	2.12	119.08	110.83
2	B	1210	PLP	C3-C2-N1	-2.11	118.30	120.96
2	A	1110	PLP	O3P-P-O1P	2.10	119.04	110.83
2	B	1210	PLP	C6-N1-C2	2.10	123.01	119.20
3	F	1620	HEM	C3B-C4B-NB	2.09	110.97	109.47
3	E	1520	HEM	CHC-C4B-NB	-2.08	122.19	124.42
3	A	1120	HEM	CHC-C4B-NB	-2.07	122.19	124.42
2	D	1410	PLP	O3P-P-O1P	2.06	118.87	110.83
3	C	1320	HEM	C3B-C4B-NB	2.06	110.94	109.47
2	B	1210	PLP	C2A-C2-N1	2.05	121.50	117.64
2	F	1610	PLP	C5-C6-N1	-2.05	120.50	123.83
3	F	1620	HEM	CHC-C4B-NB	-2.03	122.23	124.42
2	D	1410	PLP	C5A-C5-C6	-2.03	116.06	119.36
2	F	1610	PLP	O4P-C5A-C5	2.01	113.13	109.36

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1110	PLP	C4-C5-C5A-O4P
2	D	1410	PLP	C4-C5-C5A-O4P
2	D	1410	PLP	C6-C5-C5A-O4P
2	E	1510	PLP	C4-C5-C5A-O4P
2	E	1510	PLP	C6-C5-C5A-O4P
3	B	1220	HEM	C2B-C3B-CAB-CBB
3	B	1220	HEM	C4B-C3B-CAB-CBB
3	C	1320	HEM	C2C-C3C-CAC-CBC
3	E	1520	HEM	C2B-C3B-CAB-CBB
3	F	1620	HEM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	A	1120	HEM	C2B-C3B-CAB-CBB
3	F	1620	HEM	C2B-C3B-CAB-CBB
3	A	1120	HEM	C4B-C3B-CAB-CBB
3	C	1320	HEM	C4C-C3C-CAC-CBC
3	F	1620	HEM	C4C-C3C-CAC-CBC
3	D	1420	HEM	C4D-C3D-CAD-CBD
2	A	1110	PLP	C6-C5-C5A-O4P
3	F	1620	HEM	C3A-C2A-CAA-CBA
3	D	1420	HEM	C2D-C3D-CAD-CBD
3	B	1220	HEM	C2C-C3C-CAC-CBC
3	D	1420	HEM	C2C-C3C-CAC-CBC
3	E	1520	HEM	C2C-C3C-CAC-CBC
3	E	1520	HEM	C4B-C3B-CAB-CBB
3	F	1620	HEM	C4B-C3B-CAB-CBB
2	C	1310	PLP	C4-C5-C5A-O4P
3	E	1520	HEM	C4C-C3C-CAC-CBC
3	D	1420	HEM	CAA-CBA-CGA-O1A
3	D	1420	HEM	CAA-CBA-CGA-O2A
3	B	1220	HEM	CAA-CBA-CGA-O1A
3	B	1220	HEM	CAA-CBA-CGA-O2A
3	F	1620	HEM	CAA-CBA-CGA-O2A
3	F	1620	HEM	CAA-CBA-CGA-O1A
3	F	1620	HEM	C1A-C2A-CAA-CBA
3	E	1520	HEM	CAA-CBA-CGA-O2A
3	B	1220	HEM	C4C-C3C-CAC-CBC
3	D	1420	HEM	C4C-C3C-CAC-CBC
3	E	1520	HEM	CAA-CBA-CGA-O1A
3	D	1420	HEM	CAD-CBD-CGD-O2D
3	D	1420	HEM	CAD-CBD-CGD-O1D
3	F	1620	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

12 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1310	PLP	4	0
2	F	1610	PLP	2	0
3	B	1220	HEM	6	0
3	C	1320	HEM	9	0
2	B	1210	PLP	2	0
3	D	1420	HEM	8	0
3	E	1520	HEM	6	0

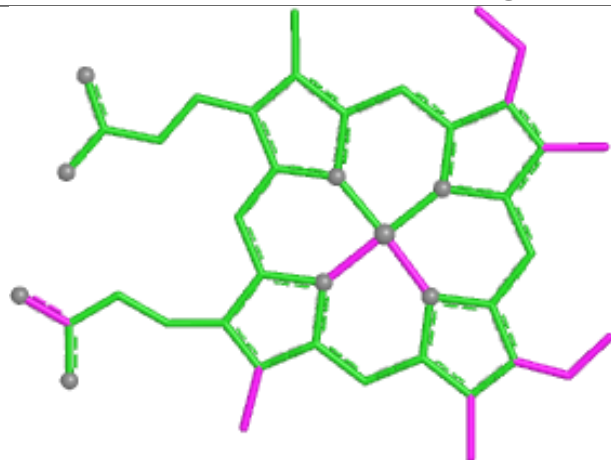
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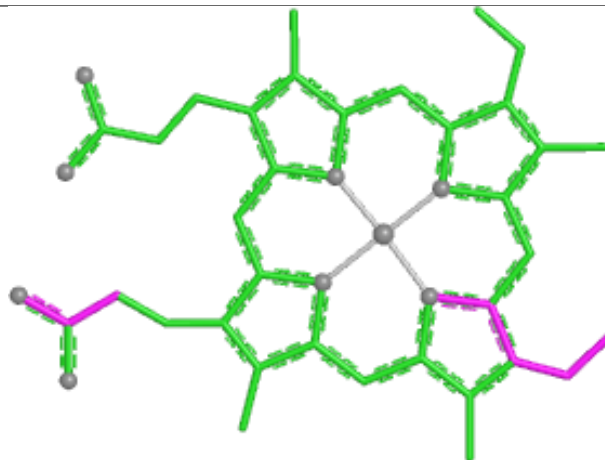
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1620	HEM	10	0
2	E	1510	PLP	2	0
2	A	1110	PLP	2	0
3	A	1120	HEM	6	0
2	D	1410	PLP	6	0

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

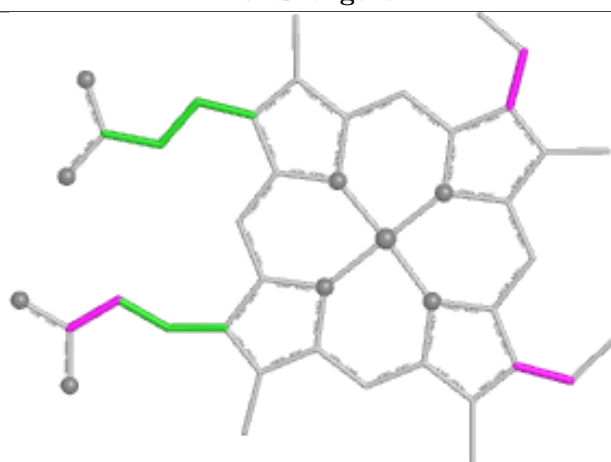
Ligand HEM B 1220



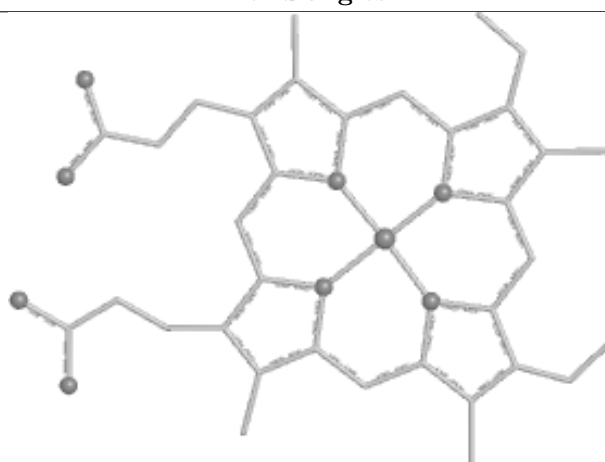
Bond lengths



Bond angles

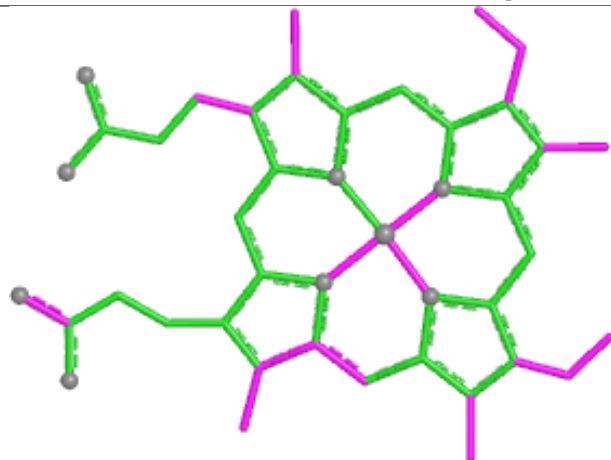


Torsions

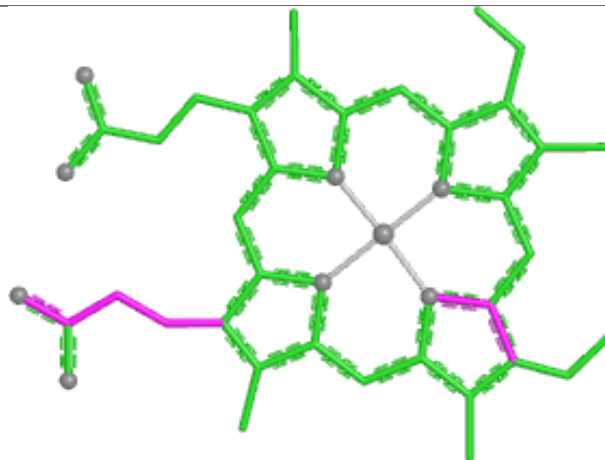


Rings

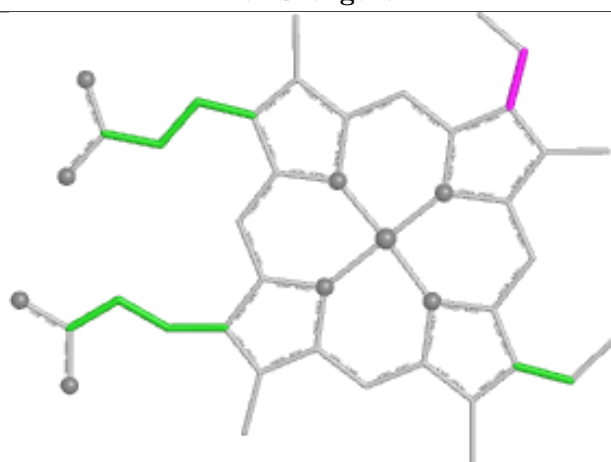
Ligand HEM C 1320



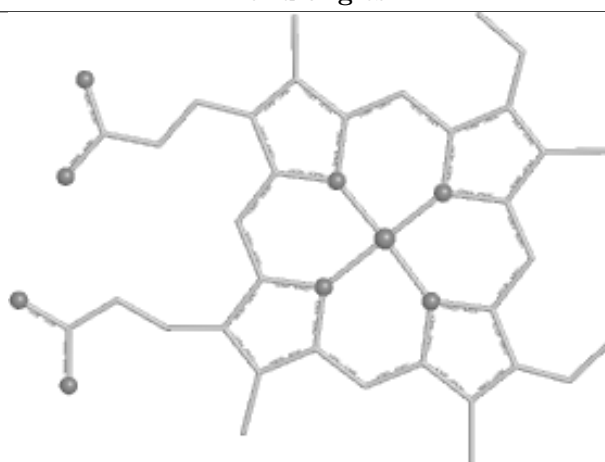
Bond lengths



Bond angles

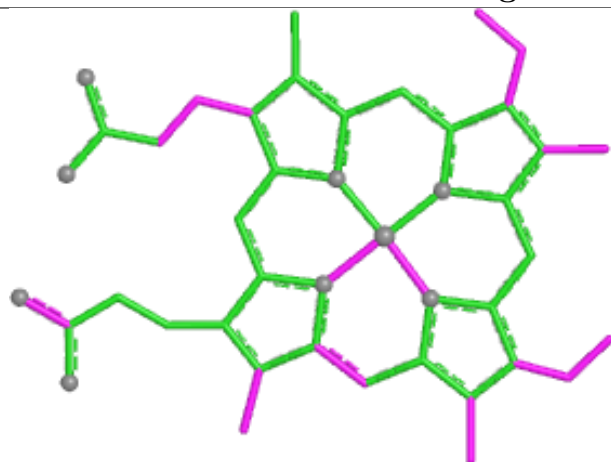


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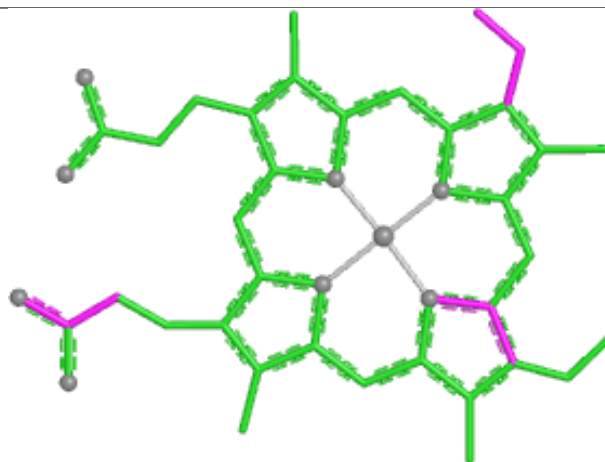


Rings

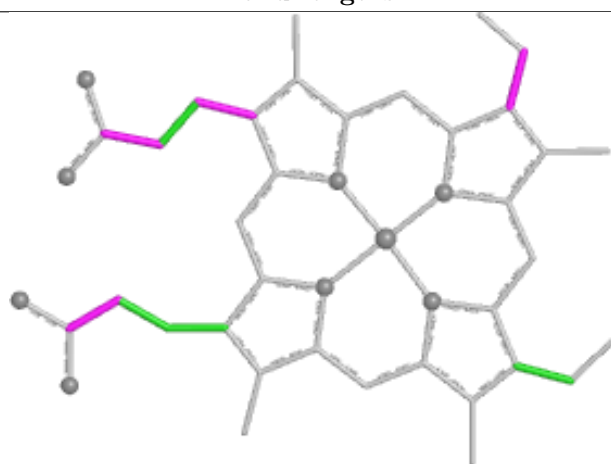
Ligand HEM D 1420



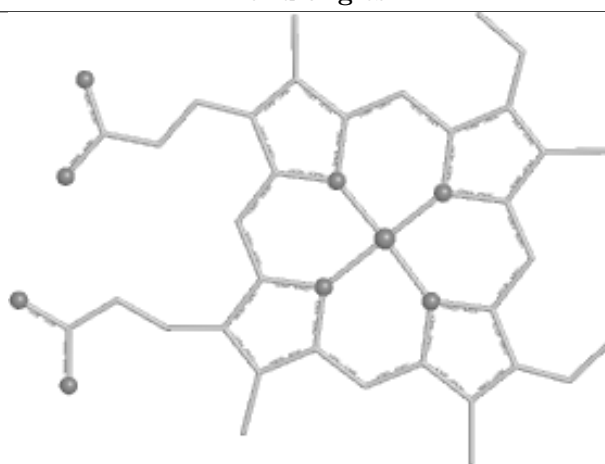
Bond lengths



Bond angles

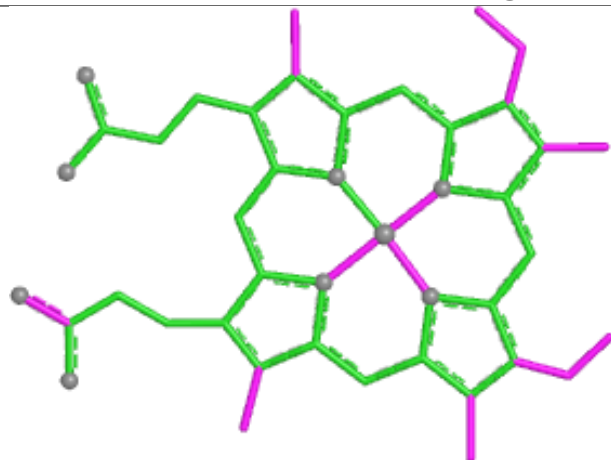


Torsions

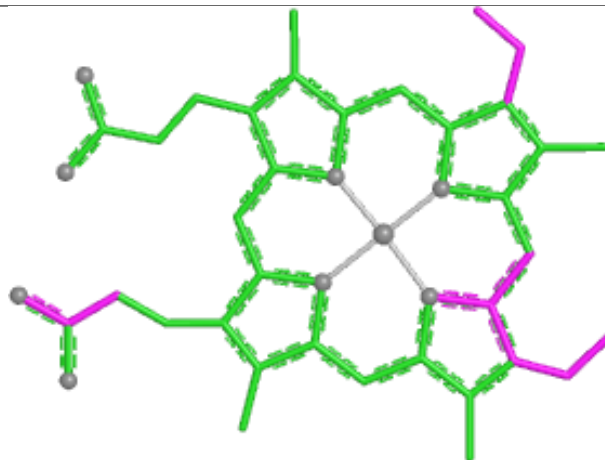


Rings

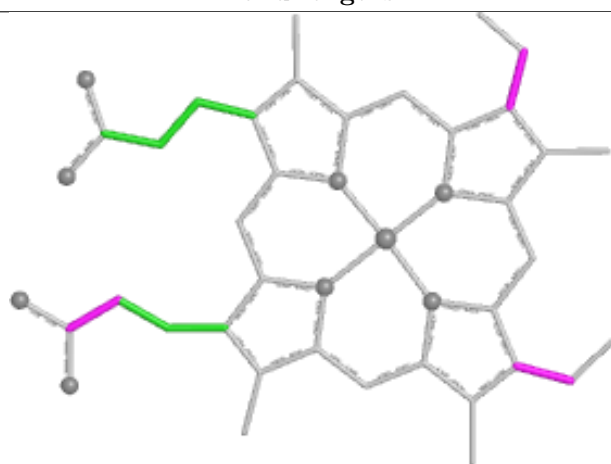
Ligand HEM E 1520



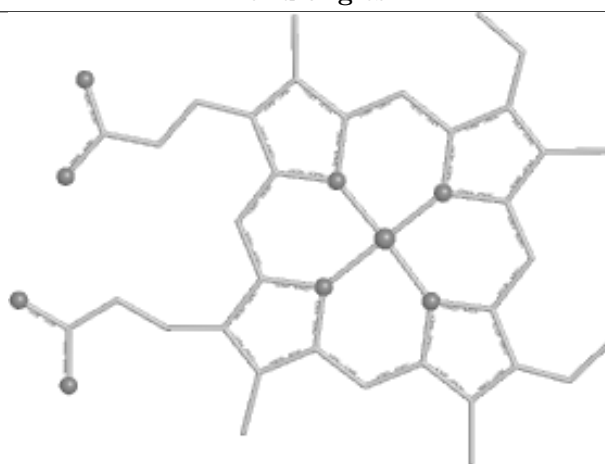
Bond lengths



Bond angles

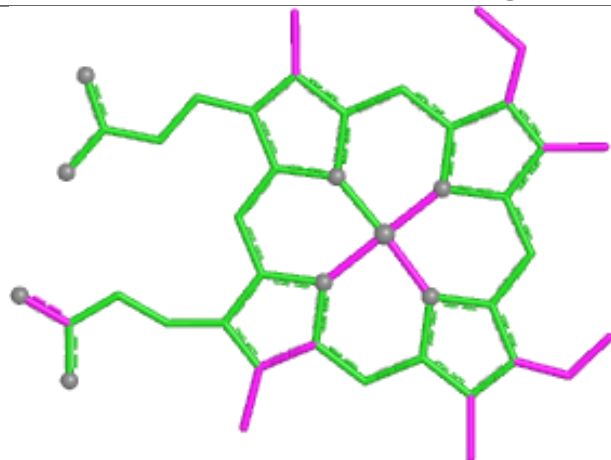


Torsions

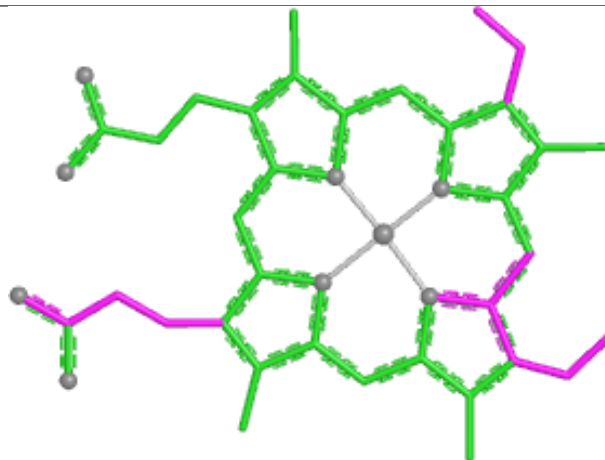


Rings

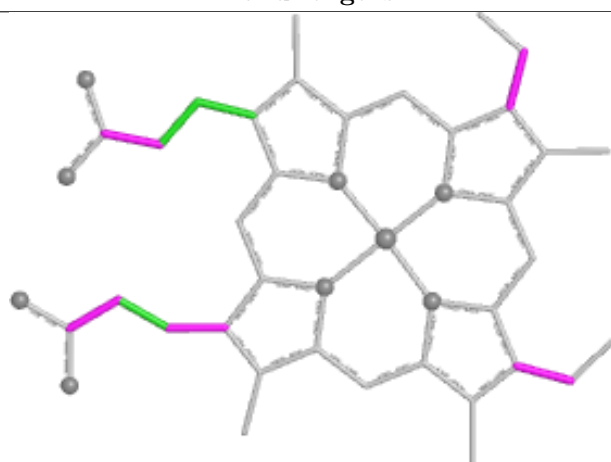
Ligand HEM F 1620



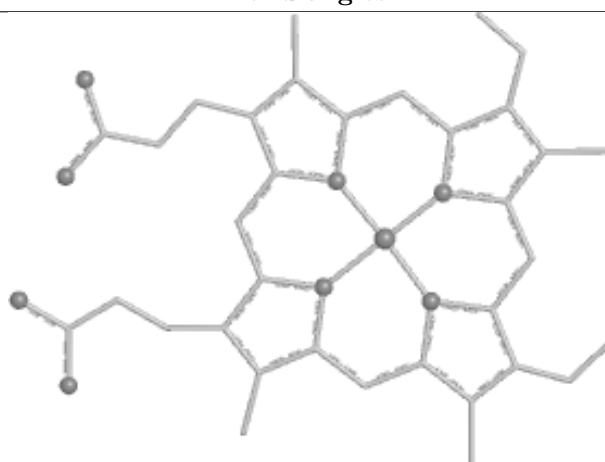
Bond lengths



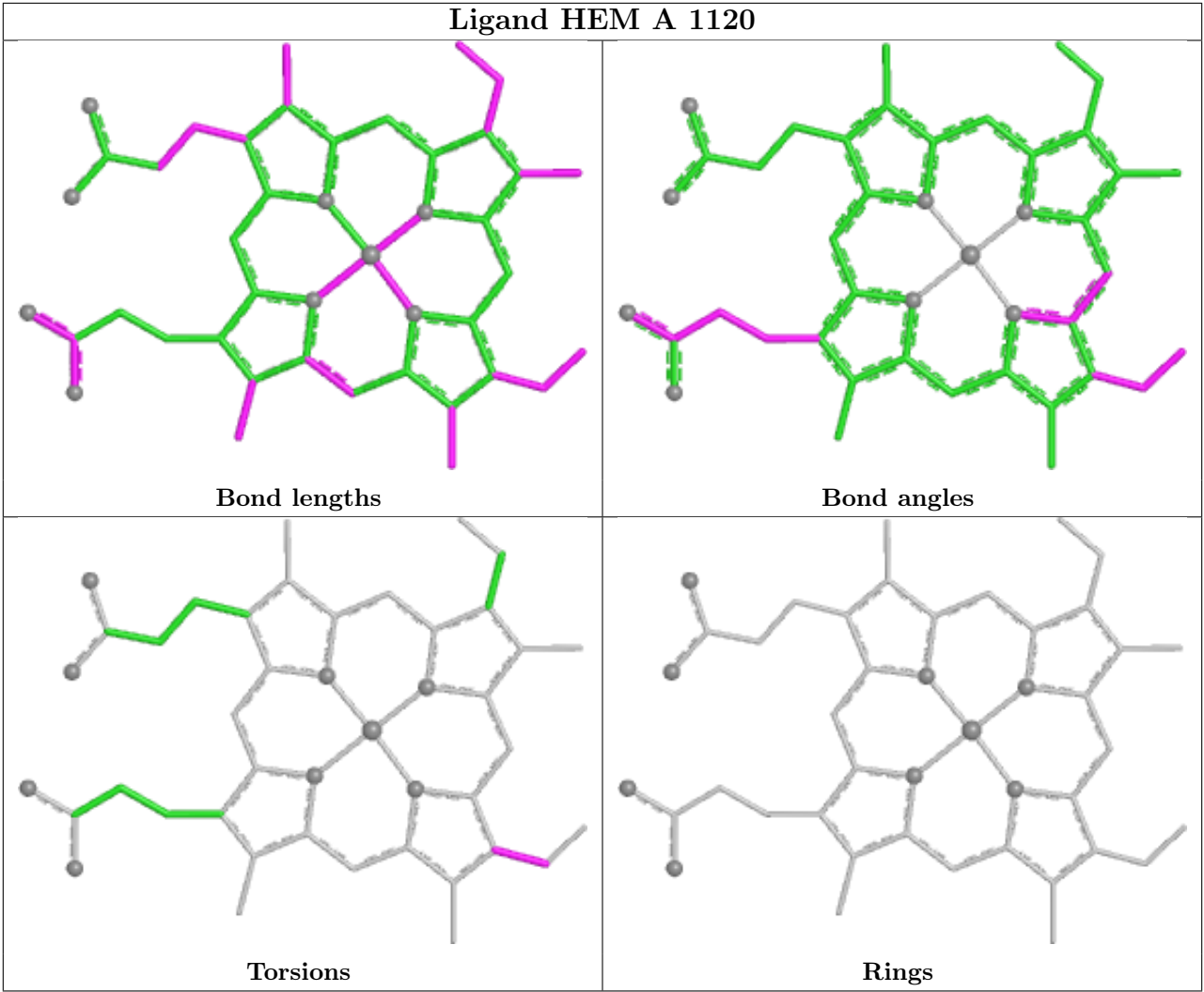
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	159:ALA	C	160:VAL	N	1.19

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/363 (96%)	-1.50	0 100 100	8, 24, 44, 61	0
1	B	347/363 (95%)	-1.54	0 100 100	9, 23, 44, 74	0
1	C	346/363 (95%)	-1.52	0 100 100	10, 24, 46, 60	0
1	D	346/363 (95%)	-1.51	0 100 100	10, 24, 44, 59	0
1	E	347/363 (95%)	-1.49	0 100 100	8, 26, 47, 61	0
1	F	344/363 (94%)	-1.49	0 100 100	8, 26, 53, 70	0
All	All	2082/2178 (95%)	-1.51	0 100 100	8, 24, 46, 74	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	B	1210	15/16	0.99	0.04	14,21,22,22	0

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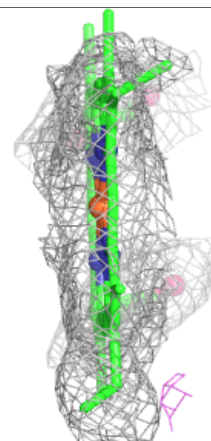
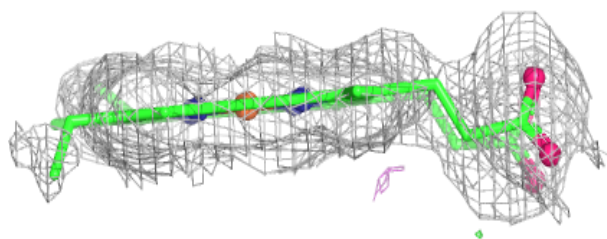
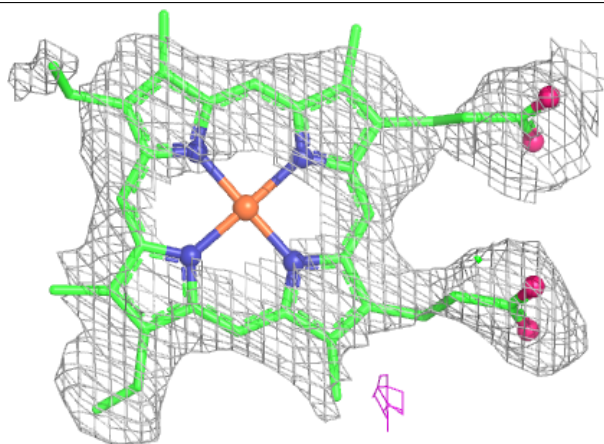
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PLP	C	1310	15/16	0.99	0.03	17,19,23,24	0
2	PLP	E	1510	15/16	0.99	0.04	20,23,26,27	0
3	HEM	A	1120	43/43	0.99	0.04	20,38,40,42	0
3	HEM	B	1220	43/43	0.99	0.04	27,35,38,40	0
3	HEM	C	1320	43/43	0.99	0.04	28,35,39,39	0
3	HEM	D	1420	43/43	0.99	0.04	27,32,34,35	0
3	HEM	E	1520	43/43	0.99	0.04	36,44,46,46	0
3	HEM	F	1620	43/43	0.99	0.04	30,36,38,40	0
2	PLP	D	1410	15/16	1.00	0.04	20,22,24,27	0
2	PLP	A	1110	15/16	1.00	0.03	14,19,23,23	0
2	PLP	F	1610	15/16	1.00	0.03	11,14,17,18	0

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

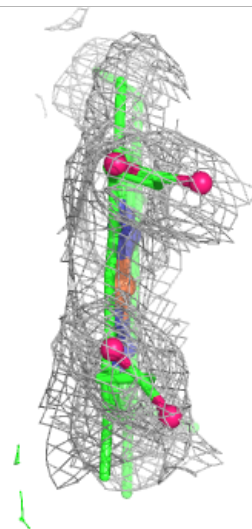
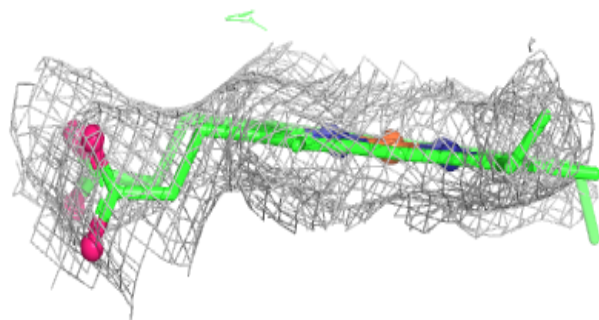
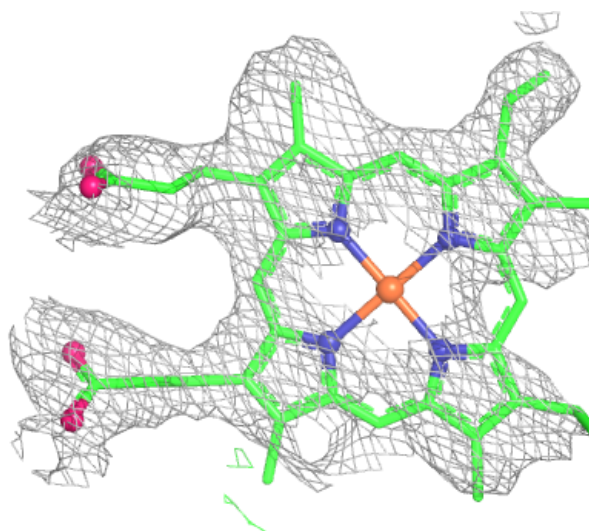
Electron density around HEM A 1120:

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



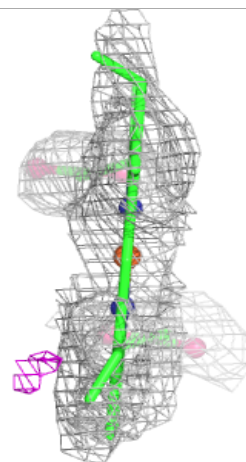
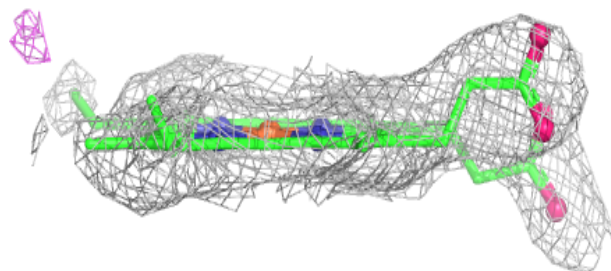
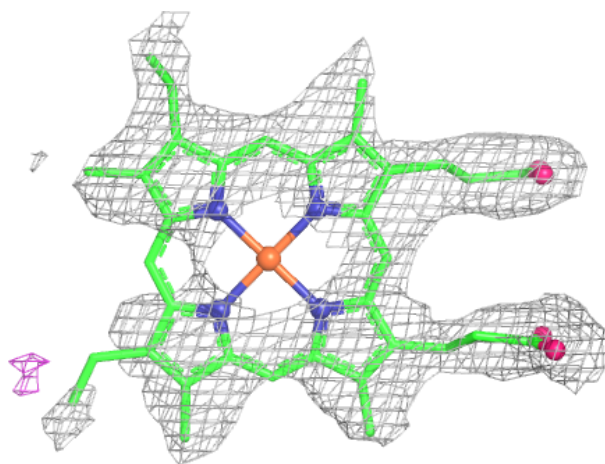
Electron density around HEM B 1220:

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



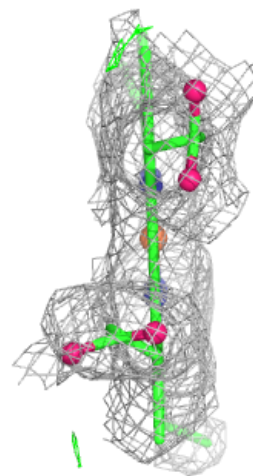
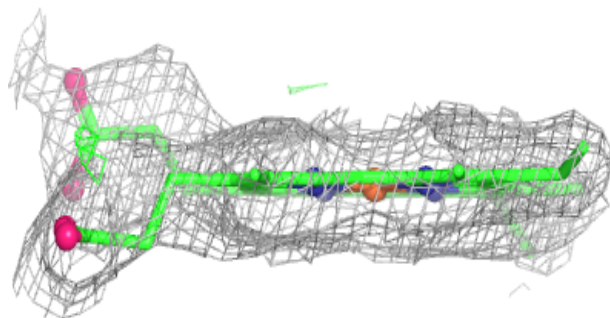
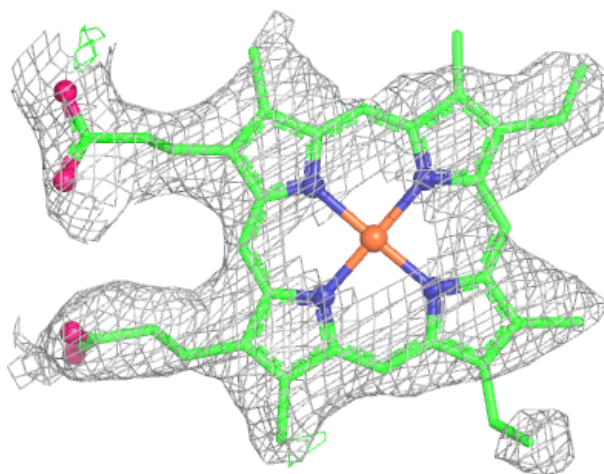
Electron density around HEM C 1320:

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



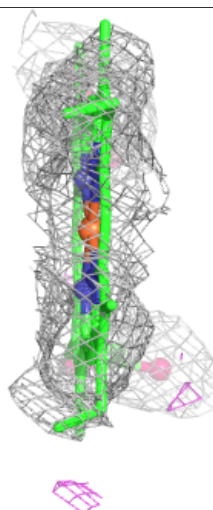
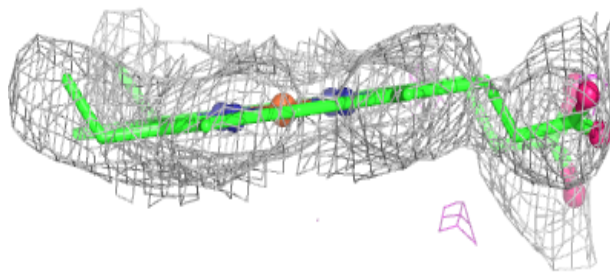
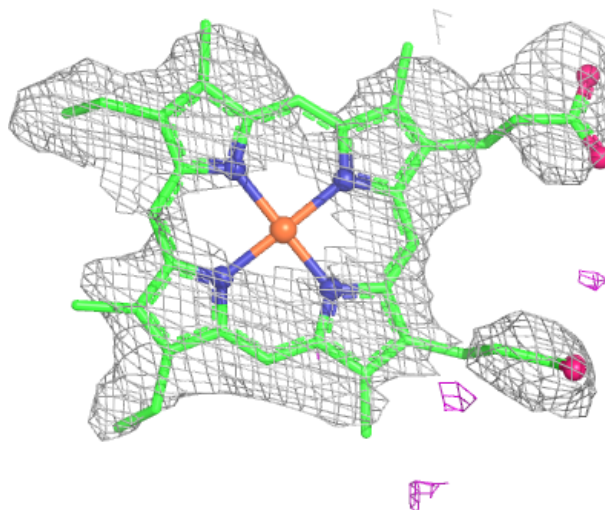
Electron density around HEM D 1420:

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



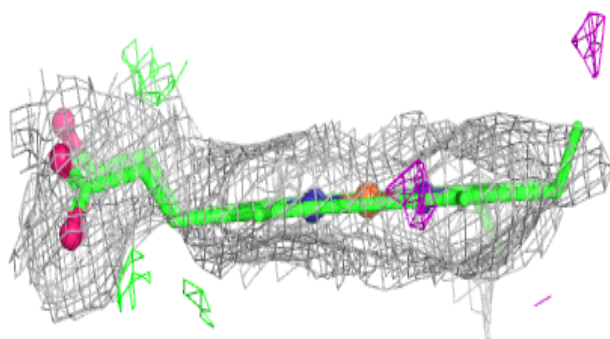
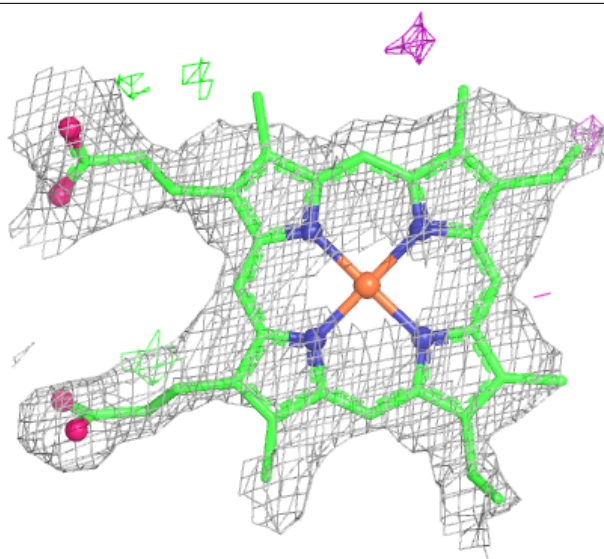
Electron density around HEM E 1520:

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



Electron density around HEM F 1620:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.