Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 08:39 AM EDT

PDB ID	:	1M54
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 (i) symbol.

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

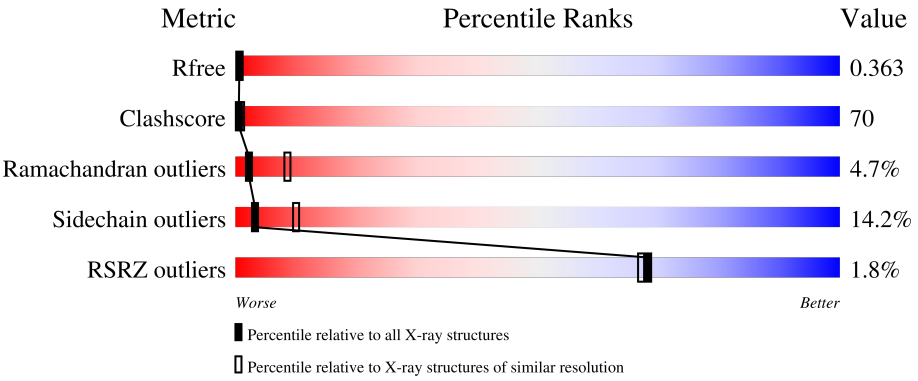
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	3% 28% 53% 13%
1	B	363	2% 32% 52% 9%
1	C	363	% 24% 62% 7% 5%
1	D	363	% 23% 59% 10% 5%
1	E	363	2% 27% 55% 10%

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Mol	Chain	Length	Quality of chain
1	F	363	2% 23% 56% 13% 5%

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 (i)

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.

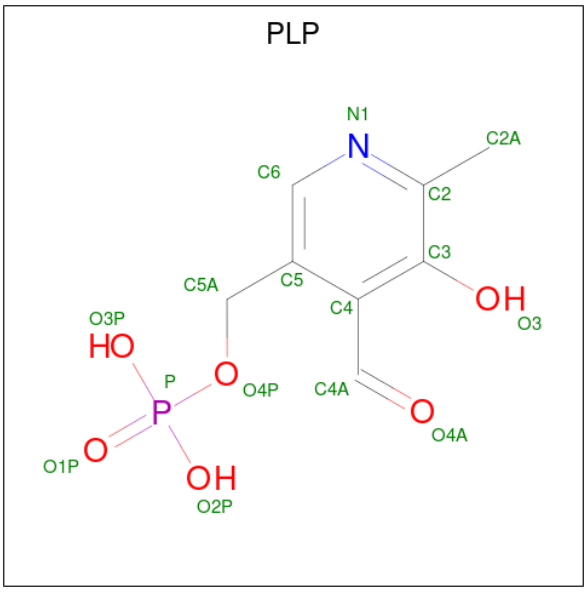
- Molecule 1 is a protein called CYSTATHIONINE BETA-SYNTHASE.

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:

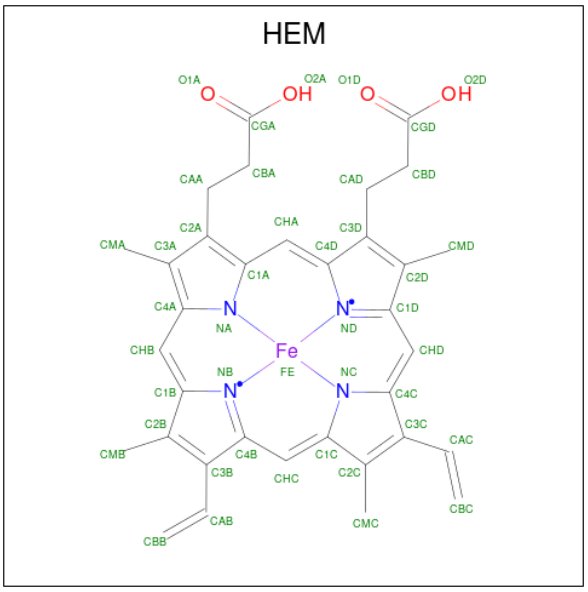
Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	ILE	engineered mutation	UNP P35520
B	44	MET	ILE	engineered mutation	UNP P35520
C	44	MET	ILE	engineered mutation	UNP P35520
D	44	MET	ILE	engineered mutation	UNP P35520
E	44	MET	ILE	engineered mutation	UNP P35520
F	44	MET	ILE	engineered mutation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

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

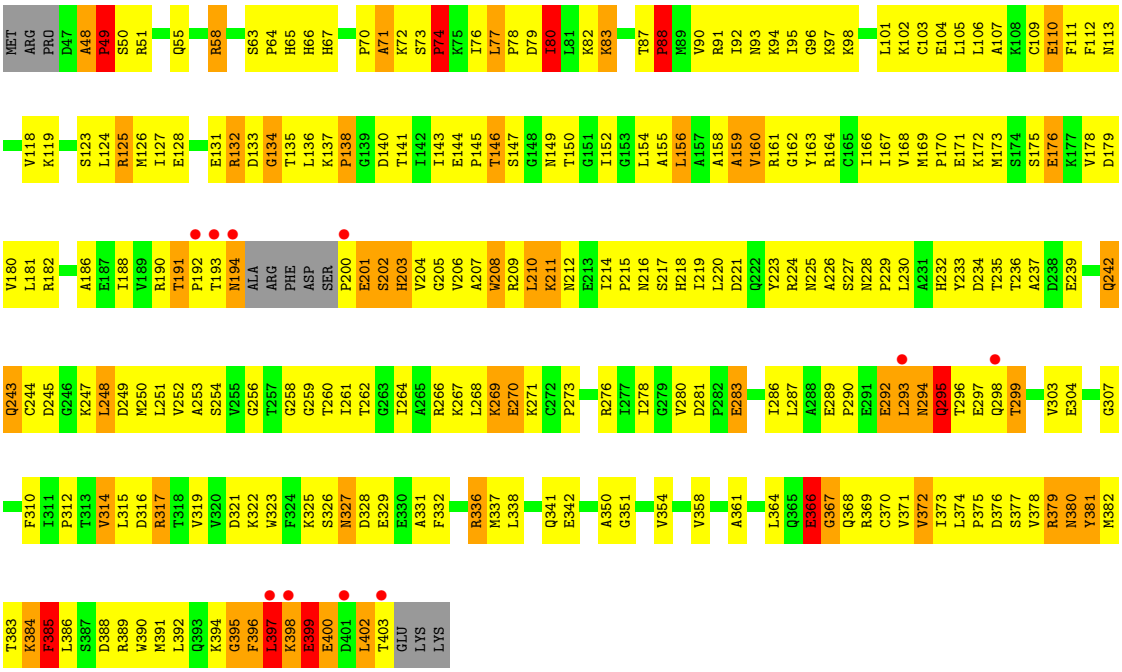
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	12	Total	O	0	0
			12	12		
4	C	14	Total	O	0	0
			14	14		
4	D	26	Total	O	0	0
			26	26		
4	E	24	Total	O	0	0
			24	24		
4	F	16	Total	O	0	0
			16	16		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

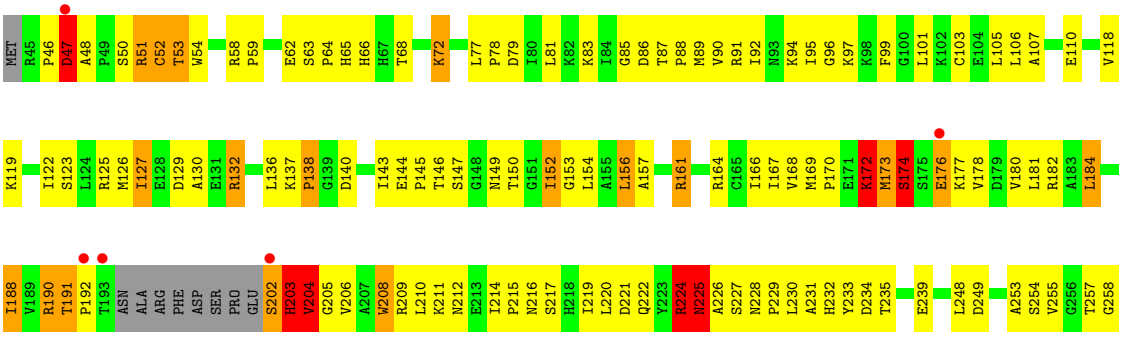
• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

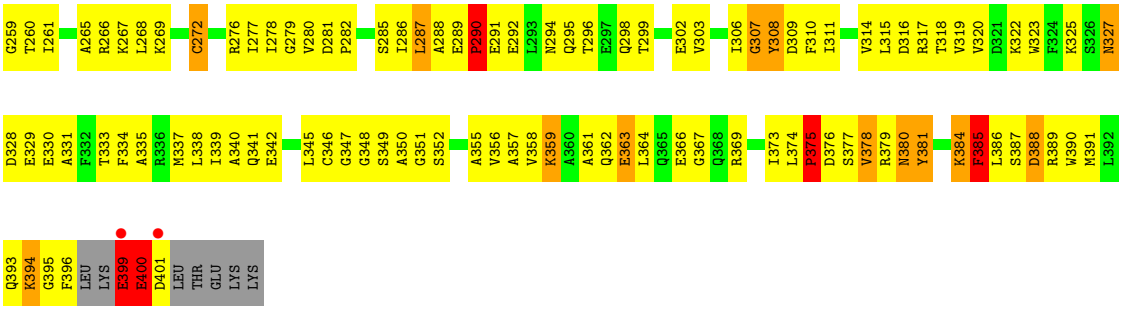
Chain A:



• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

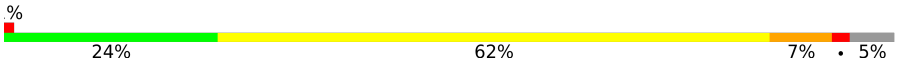
Chain B:

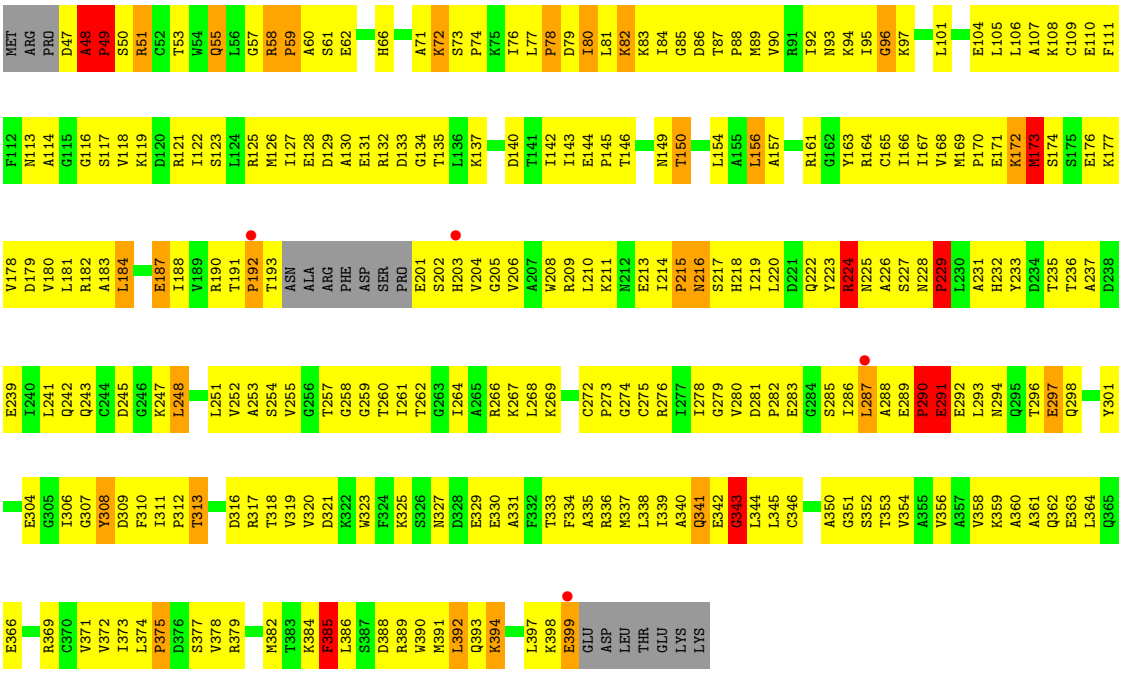




• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

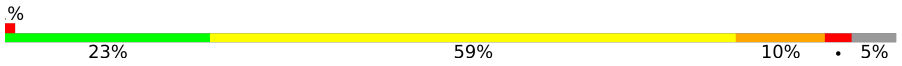
Chain C:

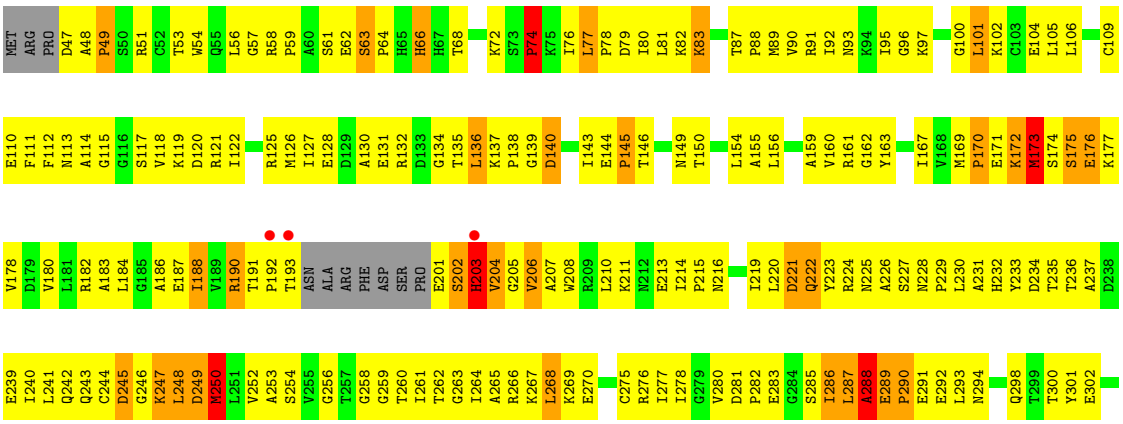


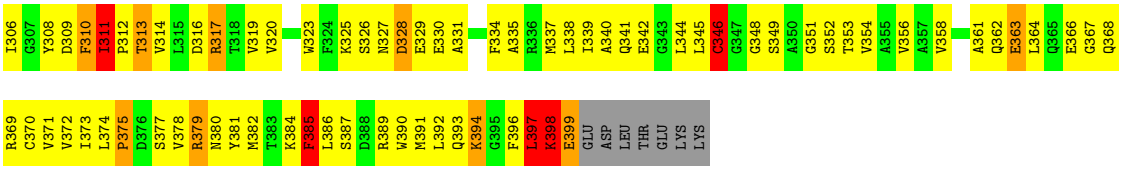


• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain D:

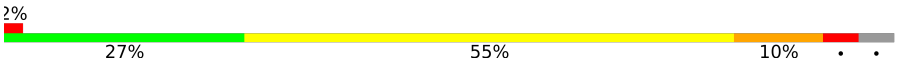


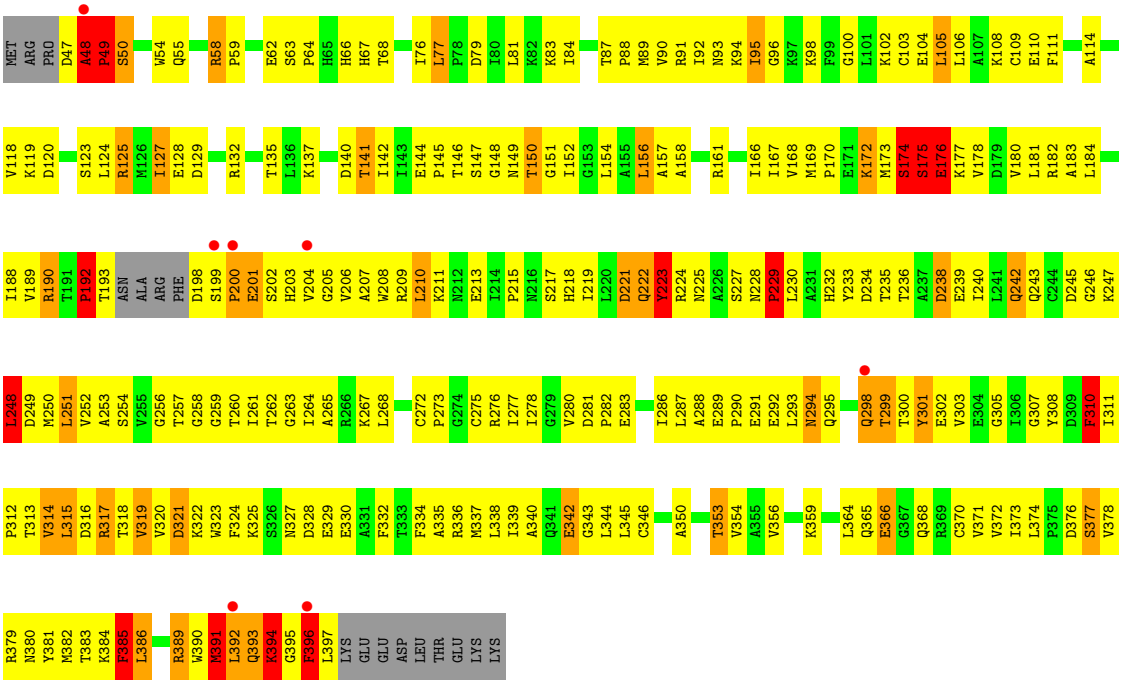




• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

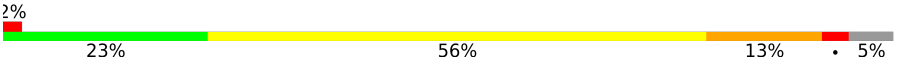
Chain E:

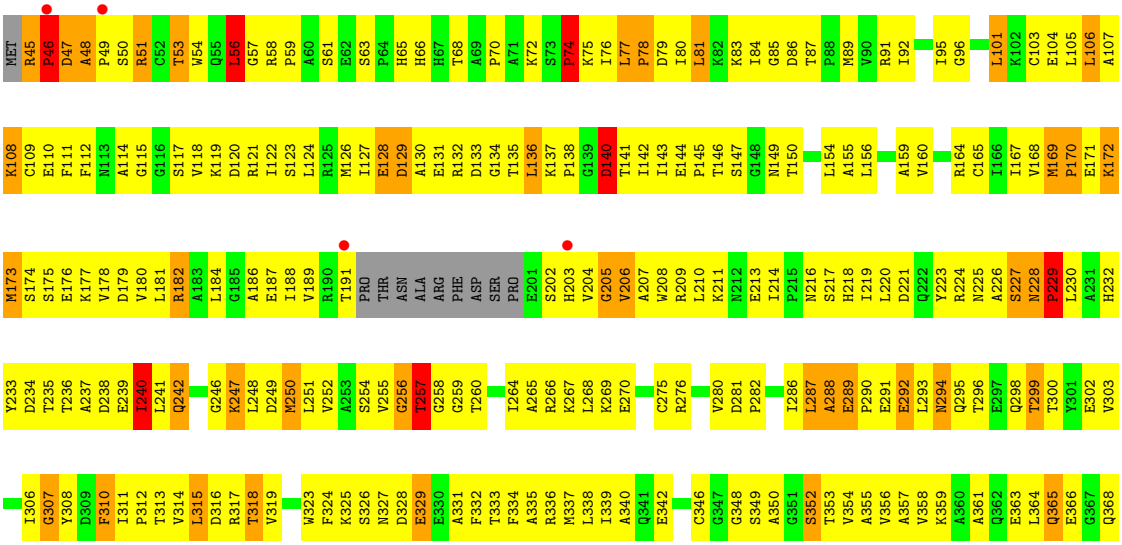


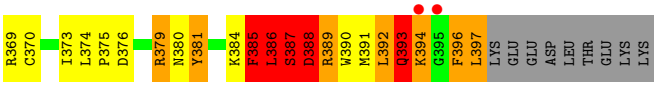


• Molecule 1: CYSTATHIONINE BETA-SYNTHASE

Chain F:






R369
C370
I373
L374
P375
D376
R379
N380
Y381
K384
F385
L386
S387
D388
R389
W390
M391
L392
Q393
K394
G395
F396
L397
LYS
GLU
GLU
ASP
LEU
THR
GLU
LYS
LYS

4 Data and refinement statistics (i)

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 47.14 – 2.89	Depositor EDS
% Data completeness (in resolution range)	83.3 (50.00-2.90) 92.2 (47.14-2.89)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.365 0.280 , 0.363	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)	0.31 , 12.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.81	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.81	8/2744 (0.3%)	1.11	16/3709 (0.4%)
1	B	1.88	2/2705 (0.1%)	1.25	21/3655 (0.6%)
1	C	0.69	3/2696 (0.1%)	1.23	21/3643 (0.6%)
1	D	0.62	1/2696 (0.0%)	1.10	21/3643 (0.6%)
1	E	0.68	3/2700 (0.1%)	1.13	24/3651 (0.7%)
1	F	0.62	1/2682 (0.0%)	1.23	21/3624 (0.6%)
All	All	0.99	18/16223 (0.1%)	1.17	124/21925 (0.6%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	ASP	C-O	76.62	2.69	1.23
1	B	225	ASN	N-CA	53.58	2.53	1.46
1	A	367	GLY	N-CA	22.28	1.79	1.46
1	C	173	MET	N-CA	18.61	1.83	1.46
1	E	176	GLU	N-CA	13.47	1.73	1.46
1	F	129	ASP	N-CA	8.84	1.64	1.46
1	E	329	GLU	N-CA	7.81	1.61	1.46
1	A	161	ARG	N-CA	7.36	1.61	1.46
1	D	367	GLY	N-CA	7.04	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	380	ASN	N-CA	6.91	1.60	1.46
1	E	394	LYS	N-CA	6.51	1.59	1.46
1	A	399	GLU	C-N	6.27	1.48	1.34
1	A	159	ALA	C-N	-6.16	1.19	1.34
1	A	71	ALA	CA-CB	5.86	1.64	1.52
1	A	160	VAL	N-CA	-5.72	1.34	1.46
1	C	229	PRO	CA-C	-5.46	1.42	1.52
1	C	192	PRO	N-CA	5.44	1.56	1.47
1	A	273	PRO	N-CA	5.13	1.55	1.47

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	225	ASN	N-CA-CB	28.34	161.61	110.60
1	B	289	GLU	C-N-CD	-20.15	76.27	120.60
1	C	48	ALA	C-N-CD	-19.43	77.85	120.60
1	B	224	ARG	C-N-CA	-18.00	76.71	121.70
1	E	176	GLU	N-CA-CB	17.69	142.44	110.60
1	F	46	PRO	CA-N-CD	-17.21	87.40	111.50
1	C	290	PRO	CA-N-CD	-17.14	87.50	111.50
1	C	289	GLU	C-N-CD	-15.99	85.42	120.60
1	B	401	ASP	CA-C-O	-14.84	88.94	120.10
1	B	225	ASN	N-CA-C	-14.47	71.93	111.00
1	A	367	GLY	N-CA-C	14.45	149.23	113.10
1	F	45	ARG	C-N-CA	13.40	178.30	122.00
1	F	45	ARG	C-N-CD	-13.40	91.12	120.60
1	B	289	GLU	C-N-CA	13.25	177.66	122.00
1	C	290	PRO	N-CA-CB	12.82	118.69	103.30
1	F	46	PRO	N-CA-CB	12.82	118.69	103.30
1	C	48	ALA	C-N-CA	12.33	173.78	122.00
1	A	366	GLU	CB-CA-C	12.25	134.90	110.40
1	C	289	GLU	C-N-CA	12.06	172.66	122.00
1	C	290	PRO	N-CD-CG	11.95	121.12	103.20
1	F	45	ARG	O-C-N	11.78	143.48	121.10
1	F	129	ASP	N-CA-C	-11.76	79.24	111.00
1	F	46	PRO	N-CD-CG	11.54	120.50	103.20
1	F	229	PRO	CA-N-CD	-11.45	95.47	111.50
1	F	128	GLU	N-CA-CB	-10.47	91.76	110.60
1	B	47	ASP	CB-CA-C	-10.08	90.24	110.40
1	A	74	PRO	CA-N-CD	-9.92	97.61	111.50
1	F	310	PHE	CB-CA-C	-9.85	90.71	110.40
1	B	47	ASP	C-N-CA	-9.68	97.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	394	LYS	N-CA-CB	-9.61	93.31	110.60
1	A	161	ARG	N-CA-C	-9.37	85.71	111.00
1	C	173	MET	N-CA-C	-9.34	85.78	111.00
1	D	289	GLU	CA-C-N	9.19	142.83	117.10
1	E	221	ASP	CA-C-N	-9.18	97.00	117.20
1	A	204	VAL	C-N-CA	-9.12	103.14	122.30
1	C	192	PRO	N-CA-C	9.06	135.66	112.10
1	E	48	ALA	C-N-CD	-8.84	101.14	120.60
1	B	381	TYR	N-CA-CB	-8.39	95.50	110.60
1	E	229	PRO	CA-N-CD	-8.13	100.11	111.50
1	E	200	PRO	CA-N-CD	-8.06	100.21	111.50
1	C	172	LYS	C-N-CA	-8.04	101.61	121.70
1	A	204	VAL	N-CA-C	-8.00	89.40	111.00
1	D	74	PRO	CA-N-CD	-7.95	100.37	111.50
1	B	400	GLU	O-C-N	-7.95	109.98	122.70
1	B	399	GLU	CB-CA-C	-7.87	94.66	110.40
1	B	400	GLU	C-N-CA	-7.81	102.17	121.70
1	A	379	ARG	C-N-CA	-7.64	102.59	121.70
1	F	45	ARG	CA-C-N	-7.45	96.23	117.10
1	F	310	PHE	CB-CG-CD1	-7.25	115.73	120.80
1	F	229	PRO	CA-C-N	-7.23	101.29	117.20
1	D	222	GLN	N-CA-C	-7.20	91.55	111.00
1	E	394	LYS	N-CA-C	7.14	130.28	111.00
1	B	401	ASP	CA-CB-CG	-7.05	97.88	113.40
1	E	221	ASP	C-N-CA	7.00	139.21	121.70
1	A	88	PRO	CA-N-CD	-6.95	101.77	111.50
1	D	287	LEU	N-CA-C	-6.94	92.26	111.00
1	D	289	GLU	N-CA-C	6.93	129.71	111.00
1	C	229	PRO	CA-N-CD	-6.91	101.83	111.50
1	E	176	GLU	N-CA-C	-6.76	92.74	111.00
1	D	287	LEU	C-N-CA	-6.76	104.80	121.70
1	D	367	GLY	N-CA-C	6.73	129.93	113.10
1	E	222	GLN	CA-C-N	-6.73	102.39	117.20
1	C	192	PRO	CA-N-CD	-6.73	102.08	111.50
1	B	290	PRO	CA-N-CD	-6.67	102.17	111.50
1	B	400	GLU	CA-C-N	6.59	131.69	117.20
1	D	288	ALA	C-N-CA	-6.53	105.38	121.70
1	E	329	GLU	N-CA-C	-6.53	93.38	111.00
1	D	221	ASP	CA-C-N	-6.51	102.87	117.20
1	A	204	VAL	CA-C-N	6.50	129.21	116.20
1	C	173	MET	N-CA-CB	6.50	122.31	110.60
1	D	310	PHE	CB-CA-C	-6.46	97.48	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	96	GLY	N-CA-C	-6.46	96.94	113.10
1	C	49	PRO	CA-N-CD	-6.43	102.50	111.50
1	E	221	ASP	O-C-N	6.40	132.94	122.70
1	F	81	LEU	CB-CA-C	6.40	122.36	110.20
1	E	192	PRO	CA-N-CD	-6.39	102.55	111.50
1	E	49	PRO	N-CA-C	6.38	128.68	112.10
1	F	128	GLU	N-CA-C	6.31	128.04	111.00
1	D	289	GLU	O-C-N	-6.28	109.16	121.10
1	A	203	HIS	CA-CB-CG	-6.21	103.04	113.60
1	C	341	GLN	N-CA-C	-6.17	94.33	111.00
1	D	250	MET	N-CA-C	6.13	127.56	111.00
1	F	56	LEU	CA-C-N	-6.12	103.97	116.20
1	D	145	PRO	CA-N-CD	-6.05	103.03	111.50
1	F	140	ASP	N-CA-C	6.02	127.25	111.00
1	A	399	GLU	N-CA-C	5.99	127.17	111.00
1	D	203	HIS	CA-CB-CG	-5.97	103.45	113.60
1	C	341	GLN	C-N-CA	-5.97	106.78	121.70
1	D	204	VAL	N-CA-C	-5.95	94.94	111.00
1	D	289	GLU	CA-C-O	-5.91	107.68	120.10
1	A	273	PRO	N-CA-C	5.88	127.38	112.10
1	C	375	PRO	N-CA-C	5.87	127.36	112.10
1	E	229	PRO	CA-C-N	-5.76	104.52	117.20
1	B	375	PRO	CA-N-CD	-5.71	103.50	111.50
1	E	175	SER	C-N-CA	-5.71	107.44	121.70
1	B	172	LYS	C-N-CA	5.69	135.92	121.70
1	D	385	PHE	N-CA-CB	5.67	120.81	110.60
1	D	290	PRO	CA-N-CD	-5.67	103.57	111.50
1	D	206	VAL	N-CA-C	-5.58	95.93	111.00
1	E	48	ALA	C-N-CA	5.56	145.37	122.00
1	C	392	LEU	CB-CA-C	-5.56	99.63	110.20
1	E	105	LEU	CB-CA-C	-5.50	99.74	110.20
1	E	314	VAL	N-CA-C	-5.49	96.17	111.00
1	B	172	LYS	CA-C-N	-5.49	105.13	117.20
1	B	203	HIS	CA-CB-CG	5.43	122.83	113.60
1	E	223	TYR	CB-CG-CD1	-5.43	117.74	121.00
1	D	203	HIS	CB-CA-C	-5.42	99.56	110.40
1	F	65	HIS	N-CA-C	5.42	125.62	111.00
1	C	229	PRO	CA-C-N	-5.38	105.36	117.20
1	A	293	LEU	CB-CA-C	-5.38	99.99	110.20
1	F	229	PRO	O-C-N	5.34	131.24	122.70
1	E	222	GLN	O-C-N	5.30	131.18	122.70
1	B	290	PRO	N-CA-C	-5.25	98.46	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	240	ILE	CB-CA-C	5.20	121.99	111.60
1	A	74	PRO	CB-CA-C	-5.19	99.01	112.00
1	E	298	GLN	N-CA-C	5.19	125.01	111.00
1	B	381	TYR	N-CA-C	5.18	124.98	111.00
1	A	370	CYS	C-N-CA	-5.16	108.81	121.70
1	C	343	GLY	N-CA-C	5.15	125.96	113.10
1	A	397	LEU	N-CA-C	5.14	124.88	111.00
1	F	128	GLU	C-N-CA	-5.13	108.88	121.70
1	D	385	PHE	CB-CG-CD1	5.10	124.37	120.80
1	C	59	PRO	N-CA-C	5.06	125.27	112.10
1	E	310	PHE	CB-CG-CD2	-5.05	117.27	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLU	Peptide
1	B	400	GLU	Mainchain
1	C	224	ARG	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2698	0	2721	365	0
1	B	2660	0	2678	317	0
1	C	2651	0	2678	413	0
1	D	2651	0	2679	442	1
1	E	2654	0	2676	454	1
1	F	2637	0	2668	403	0
2	A	15	0	7	3	0
2	B	15	0	7	1	0
2	C	15	0	7	5	0
2	D	15	0	7	6	0
2	E	15	0	7	5	0
2	F	15	0	7	4	0
3	A	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	30	5	0
3	C	43	0	30	9	0
3	D	43	0	30	7	0
3	E	43	0	30	5	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	2294	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 70.

All (2294) 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:D:398:LYS:HZ2	1:D:398:LYS:CB	0.86	1.32
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: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:E:94:LYS:O	1:E:95:ILE:HG22	1.44	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:310:PHE:C	1:D:311:ILE:HG13	1.47	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:E:95:ILE:CG1	1:E:337:MET:HE3	1.78	1.14
1:D:397:LEU:O	1:D:398:LYS:HB2	1.39	1.13
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: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:B:399:GLU:O	1:B:399:GLU:CD	1.87	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: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:398:LYS:HZ2	1:D:398:LYS:HB3	1.10	1.10
1:C:382:MET:HE2	1:D:176:GLU:HG3	1.29	1.09
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:95:ILE:HG13	1:E:337:MET:HE3	1.08	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:D:171:GLU:C	1:D:172:LYS:HD2	1.76	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
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: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:F:289:GLU:O	1:F:290:PRO:C	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:290:PRO:O	1:C:291:GLU:C	1.98	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:D:173:MET:CE	1:D:173:MET:CA	2.40	1.00
1:F:56:LEU:HD12	1:F:57:GLY:H	1.27	1.00
1:C:190:ARG:C	1:C:192:PRO:HD3	1.83	0.99
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:D:173:MET:HA	1:D:173:MET:HE3	1.00	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:173:MET:CA	1:D:173:MET:HE3	1.93	0.97
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:C:59:PRO:CD	1:C:62:GLU:OE2	2.13	0.97
1:D:398:LYS:HB2	1:D:398:LYS:HZ1	1.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:95:ILE:HG23	1:A:337:MET:HE3	1.51	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:201:GLU:O	1:D:201:GLU:CD	2.07	0.92
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:170:PRO:HA	1:A:191:THR:OG1	1.73	0.89
1:D:171:GLU:C	1:D:172:LYS:CD	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:397:LEU:O	1:D:398:LYS:CE	2.24	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:C:173:MET:N	1:C:173:MET:C	2.30	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
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:E:172:LYS:O	1:E:173:MET:C	2.14	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:E:95:ILE:HG13	1:E:337:MET:CE	2.01	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:F:250:MET:HE3	1:F:364:LEU:HD21	1.57	0.84
1:D:253:ALA:HB2	1:D:373:ILE:HD12	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ILE:HG22	1:F:268:LEU:HD12	1.60	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: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: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: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
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:B:72:LYS:HZ3	1:B:72:LYS:HA	1.44	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:C:172:LYS:C	1:C:173:MET:CA	2.49	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:F:135:THR:O	1:F:136:LEU:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:SER:C	1:E:176:GLU:CA	2.50	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:382:MET:HE2	1:D:176:GLU:CG	2.11	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
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:384:LYS:O	1:F:385:PHE:C	2.18	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:C:47:ASP:CG	1:C:48:ALA:H	1.86	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:E:176:GLU:N	1:E:176:GLU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:PRO:HA	1:C:168:VAL:HB	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: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
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:E:95:ILE:CG1	1:E:337:MET:CE	2.62	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:F:299:THR:CG2	1:F:300:THR:N	2.41	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:171:GLU:OE1	1:D:190:ARG:HD3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:95:ILE:HD11	1:E:337:MET:HE2	1.69	0.74
1:E:281:ASP:O	1:E:325:LYS:HA	1.88	0.74
1:E:286:ILE:HG13	1:E:286:ILE:O	1.86	0.74
1:E:199:SER:OG	1:E:201:GLU:C	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:173:MET:HE2	1:D:174:SER:H	1.54	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: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: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: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:A:193:THR:O	1:A:193:THR:CG2	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:203:HIS:C	1:B:204:VAL:HG23	2.10	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: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:205:GLY:C	1:D:207:ALA:N	2.35	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
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: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:224:ARG:C	1:B:225:ASN:CA	2.58	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:F:294:ASN:N	1:F:294:ASN:ND2	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:C:164:ARG:HE	1:C:187:GLU:CD	1.96	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: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: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:A:205:GLY:O	1:A:206:VAL:C	2.21	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:A:83:LYS:HA	1:A:83:LYS:HZ1	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:89:MET:HE1	1:E:240:ILE:HA	1.75	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:C:388:ASP:C	1:C:392:LEU:HD12	2.14	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
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: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: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: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:D:137:LYS:HD3	1:E:104:GLU:CD	2.14	0.68
1:E:48:ALA:CB	1:E:224:ARG:NH2	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:C:272:CYS:O	1:C:273:PRO:C	2.31	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:C:366:GLU:CD	1:C:366:GLU:H	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:GLY:HA2	1:D:208:TRP:H	1.60	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:95:ILE:HG23	1:D:337:MET:HE3	1.77	0.67
1:D:172:LYS:N	1:D:172:LYS:HD3	2.09	0.67
1:D:393:GLN:C	1:D:394:LYS:HG2	2.14	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: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:C:341:GLN:O	1:C:342:GLU:C	2.26	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:E:289:GLU:CD	1:E:317:ARG:HH12	1.98	0.67
1:F:232:HIS:CD2	1:F:260:THR:HG22	2.29	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:E:95:ILE:O	1:E:95:ILE:HG12	1.95	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:F:388:ASP:O	1:F:389:ARG:C	2.31	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: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:176:GLU:CD	1:E:380:ASN:O	2.34	0.66
1:E:288:ALA:HB3	1:E:294:ASN:HD21	1.60	0.66
1:B:95:ILE:HG23	1:B:337:MET:CE	2.26	0.66
1:B:170:PRO:HD3	1:B:191:THR:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:193:THR:HG1	1:E:198:ASP:N	1.92	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:D:397:LEU:O	1:D:398:LYS:CD	2.44	0.66
1:E:335:ALA:CB	1:E:385:PHE:CE1	2.79	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: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: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:B:265:ALA:HB1	1:B:319:VAL:HG11	1.77	0.65
1:B:176:GLU:O	1:B:180:VAL:HG23	1.95	0.65
1:D:171:GLU:O	1:D:172:LYS:HD2	1.94	0.65
1:E:207:ALA:O	1:E:210:LEU:CB	2.43	0.65
1:C:49:PRO:O	1:C:50:SER:C	2.35	0.65
1:E:242:GLN:CA	1:E:242:GLN:HE21	2.09	0.65
1:F:228:ASN:OD1	1:F:228:ASN:C	2.35	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: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: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:B:95:ILE:HG23	1:B:337:MET:HE3	1.79	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:D:310:PHE:C	1:D:311:ILE:CG1	2.33	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:E:345:LEU:C	1:E:378:VAL:HG13	2.17	0.64
1:F:247:LYS:N	1:F:247:LYS:HD2	2.12	0.64
1:E:248:LEU:CD2	1:E:250:MET:H	2.09	0.64
1:F:226:ALA:O	1:F:227:SER:C	2.33	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: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:C:173:MET:N	1:C:173:MET:O	2.30	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:C:290:PRO:C	1:C:292:GLU:N	2.52	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:173:MET:HA	1:D:173:MET:HE2	1.70	0.63
1:D:192:PRO:O	1:D:193:THR:C	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:346:CYS:O	1:B:378:VAL:HG13	1.98	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:C:345:LEU:C	1:C:378:VAL:HG13	2.19	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:A:379:ARG:O	1:A:380:ASN:C	2.37	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:225:ASN:N	1:B:225:ASN:C	2.51	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: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:243:GLN:C	1:D:245:ASP:H	2.02	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: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:E:208:TRP:C	1:E:210:LEU:H	2.00	0.62
1:A:289:GLU:OE2	1:A:317:ARG:HB3	1.99	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:GLN:C	1:D:245:ASP:N	2.52	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:104:GLU:CD	1:F:137:LYS:HD3	2.19	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: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:177:LYS:HA	1:E:180:VAL:CG2	2.30	0.62
1:F:290:PRO:C	1:F:292:GLU:N	2.52	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:F:290:PRO:C	1:F:292:GLU:H	2.04	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
1:F:171:GLU:H	1:F:171:GLU:CD	2.02	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:319:VAL:O	1:E:320:VAL:C	2.37	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:92:ILE:HG23	1:A:342:GLU:CD	2.21	0.61
1:A:205:GLY:O	1:A:209:ARG:N	2.32	0.61
1:A:249:ASP:CG	1:A:368:GLN:HB3	2.21	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:D:205:GLY:O	1:D:206:VAL:C	2.37	0.61
1:F:288:ALA:HB2	1:F:325:LYS:HZ2	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:D:398:LYS:NZ	1:D:398:LYS:HB3	1.85	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:D:203:HIS:ND1	1:D:203:HIS:C	2.47	0.61
1:D:385:PHE:CD1	1:D:385:PHE:C	2.73	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: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
1:E:144:GLU:CB	1:E:154:LEU:HD12	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:105:LEU:C	1:E:105:LEU:HD12	2.20	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: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:B:208:TRP:CD1	1:B:219:ILE:HD12	2.36	0.60
1:E:205:GLY:C	1:E:207:ALA:H	2.04	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:59:PRO:HB2	1:C:62:GLU:CD	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:MET:HB2	1:E:243:GLN:CD	2.22	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:B:292:GLU:OE2	1:B:292:GLU:N	2.29	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: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: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: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: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:C:253:ALA:HB3	1:C:261:ILE:HD12	1.85	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:137:LYS:HZ1	1:E:140:ASP:CG	2.05	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:D:249:ASP:O	1:D:250:MET:C	2.37	0.58
1:F:299:THR:CG2	1:F:300:THR:OG1	2.51	0.58
1:C:174:SER:C	1:C:176:GLU:H	2.06	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: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:B:156:LEU:C	1:B:156:LEU:CD1	2.71	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:E:205:GLY:C	1:E:207:ALA:N	2.55	0.58
1:F:169:MET:CE	1:F:178:VAL:HG22	2.33	0.58
1:B:46:PRO:CD	1:B:310:PHE:CD1	2.87	0.58
1:C:361:ALA:O	1:C:362:GLN:C	2.36	0.58
1:C:346:CYS:O	1:C:378:VAL:HG12	2.03	0.58
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:191:THR:HG21	4:F:1622:HOH:O	2.04	0.58
1:A:385:PHE:N	1:A:390:TRP:CE3	2.72	0.58
1:B:122:ILE:HG13	1:B:123:SER:N	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:CD1	1:D:270:GLU:HG2	2.34	0.58
1:D:128:GLU:CD	1:D:161:ARG:HH22	2.06	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:C:224:ARG:HD2	1:C:224:ARG:C	2.23	0.58
1:C:269:LYS:C	1:C:273:PRO:HD3	2.25	0.58
1:D:282:PRO:HA	1:D:326:SER:OG	2.04	0.58
1:F:239:GLU:O	1:F:240:ILE:C	2.40	0.58
1:F:246:GLY:C	1:F:247:LYS:HD2	2.24	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:A:244:CYS:O	1:A:369:ARG:NH2	2.33	0.57
1:C:128:GLU:C	1:C:130:ALA:H	2.07	0.57
1:A:106:LEU:HD11	1:A:369:ARG:HD3	1.85	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: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: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
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:D:171:GLU:C	1:D:172:LYS:HD3	2.24	0.57
1:E:322:LYS:HG2	1:E:323:TRP:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:325:LYS:HB3	1:B:325:LYS:HZ2	1.70	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: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
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:F:208:TRP:CD1	1:F:219:ILE:HD12	2.40	0.56
1:A:201:GLU:O	1:A:202:SER:HB3	2.05	0.56
1:B:335:ALA:HB1	1:B:385:PHE:HE1	1.70	0.56
1:C:101:LEU:HD12	1:C:362:GLN:HG2	1.87	0.56
1:C:144:GLU:HB2	1:C:154:LEU:CD1	2.35	0.56
1:C:282:PRO:O	1:C:325:LYS:NZ	2.37	0.56
1:D:287:LEU:CD1	1:D:308:TYR:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:366:GLU:CD	1:F:366:GLU:H	2.08	0.56
1:A:155:ALA:HA	1:A:158:ALA:HB3	1.88	0.56
1:C:286:ILE:O	1:C:288:ALA:N	2.36	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: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
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:F:311:ILE:O	1:F:311:ILE:CG2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:C	1:C:156:LEU:HD13	2.26	0.55
1:D:258:GLY:O	1:D:262:THR:OG1	2.19	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: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:A:102:LYS:HG2	1:A:366:GLU:CD	2.26	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
1:C:86:ASP:H	1:C:239:GLU:CD	2.09	0.55
1:C:90:VAL:O	1:C:107:ALA:N	2.39	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: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: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:191:THR:C	1:A:193:THR:N	2.59	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:B:400:GLU:O	1:B:400:GLU:HG2	2.05	0.55
1:E:87:THR:HG21	1:E:110:GLU:CD	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:128:GLU:C	1:C:130:ALA:N	2.60	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:D:219:ILE:HG22	1:D:221:ASP:H	1.71	0.54
1:D:250:MET:HE2	1:D:276:ARG:HB2	1.90	0.54
1:D:250:MET:CE	1:D:276:ARG:HB2	2.37	0.54
1:E:149:ASN:HD22	2:E:1510:PLP:H2A1	1.70	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:D:110:GLU:HG2	1:D:118:VAL:HG23	1.88	0.54
1:D:176:GLU:O	1:D:180:VAL:HG23	2.07	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
3:D:1420:HEM:HBB2	3:D:1420:HEM:HMB2	1.90	0.54
1:F:122:ILE:HD12	1:F:122:ILE:C	2.28	0.54
1:D:117:SER:OG	1:D:120:ASP:OD1	2.25	0.54
1:E:177:LYS:HA	1:E:180:VAL:HG23	1.89	0.54
1:E:262:THR:HG1	1:E:315:LEU:HA	1.72	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:A:366:GLU:C	1:A:367:GLY:CA	2.70	0.54
1:C:78:PRO:O	1:D:91:ARG:HB3	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:TRP:HB2	3:E:1520:HEM:C4B	2.42	0.54
1:A:126:MET:CG	1:A:220:LEU:HB3	2.38	0.54
1:B:327:ASN:N	1:B:327:ASN:ND2	2.45	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:137:LYS:HB2	1:A:140:ASP:CG	2.29	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
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:156:LEU:C	1:C:156:LEU:CD1	2.76	0.54
1:E:222:GLN:HE21	1:E:257:THR:HG21	1.73	0.54
1:E:394:LYS:N	1:E:394:LYS:HZ2	2.06	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:D:102:LYS:HE3	1:D:366:GLU:CD	2.28	0.54
1:D:177:LYS:HG2	1:D:380:ASN:OD1	2.08	0.54
1:E:248:LEU:HD22	1:E:275:CYS:SG	2.48	0.54
1:A:72:LYS:O	1:A:74:PRO:HD3	2.08	0.53
1:A:94:LYS:HZ1	1:A:341:GLN:HA	1.71	0.53
1:A:205:GLY:C	1:A:207:ALA:N	2.60	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:387:SER:O	1:F:388:ASP:C	2.47	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:126:MET:O	1:B:127:ILE:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:A:103:CYS:O	1:A:104:GLU:C	2.44	0.53
1:C:104:GLU:OE2	1:F:137:LYS:HD3	2.09	0.53
1:D:364:LEU:HD12	1:D:364:LEU:N	2.24	0.53
1:E:149:ASN:HA	1:E:152:ILE:HD13	1.90	0.53
1:E:193:THR:O	1:E:193:THR:HG23	2.08	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:362:GLN:O	1:B:363:GLU:C	2.43	0.53
1:B:379:ARG:HB3	1:B:379:ARG:CZ	2.38	0.53
1:C:95:ILE:C	1:C:97:LYS:H	2.12	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:204:VAL:O	1:C:205:GLY:C	2.47	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:207:ALA:C	1:E:210:LEU:HB2	2.26	0.53
1:E:324:PHE:CE2	1:E:359:LYS:HE3	2.44	0.53
1:C:211:LYS:HB2	1:C:211:LYS:HZ2	1.74	0.53
1:D:79:ASP:OD1	1:D:81:LEU:HB2	2.09	0.53
1:D:289:GLU:O	1:D:290:PRO:C	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:F:169:MET:HE3	1:F:178:VAL:HG22	1.91	0.52
1:C:192:PRO:C	1:C:193:THR:OG1	2.47	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:232:HIS:CD2	1:E:260:THR:HA	2.44	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:174:SER:C	1:C:176:GLU:N	2.61	0.52
1:C:334:PHE:HA	1:C:337:MET:HB2	1.91	0.52
1:C:361:ALA:C	1:C:363:GLU:N	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:47:ASP:CG	1:C:48:ALA:N	2.61	0.52
1:F:155:ALA:HA	1:F:165:CYS:SG	2.50	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:E:103:CYS:HB2	1:E:368:GLN:O	2.10	0.52
1:F:79:ASP:OD2	1:F:79:ASP:N	2.43	0.52
1:A:262:THR:CG2	1:A:316:ASP:HB3	2.40	0.52
1:D:386:LEU:O	1:D:386:LEU:HD13	2.10	0.52
1:A:226:ALA:HA	3:A:1120:HEM:CMD	2.40	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:B:350:ALA:O	1:B:351:GLY:C	2.47	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:A:192:PRO:O	1:A:193:THR:C	2.45	0.52
1:B:68:THR:HG22	1:B:234:ASP:HB3	1.91	0.52
1:C:137:LYS:HB2	1:C:140:ASP:CG	2.30	0.52
1:C:329:GLU:O	1:C:333:THR:HG23	2.10	0.52
1:D:201:GLU:O	1:D:202:SER:HB2	2.10	0.52
1:D:390:TRP:O	1:D:391:MET:C	2.48	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: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:72:LYS:HA	1:B:72:LYS:NZ	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:HIS:C	1:B:204:VAL:CG2	2.77	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
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:C:251:LEU:HD23	1:C:251:LEU:C	2.31	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:E:110:GLU:HG2	1:E:118:VAL:HG23	1.91	0.51
1:E:394:LYS:HZ2	1:E:394:LYS:CA	2.22	0.51
1:F:146:THR:HG21	1:F:150:THR:CB	2.40	0.51
1:C:382:MET:CE	1:D:176:GLU:HG3	2.20	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:382:MET:O	1:E:386:LEU:HB3	2.11	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:178:VAL:HA	1:B:181:LEU:HD12	1.93	0.51
1:D:173:MET:HE2	1:D:174:SER:N	2.24	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: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:149:ASN:ND2	2:C:1310:PLP:H2A1	2.25	0.51
1:C:356:VAL:O	1:C:359:LYS:HB2	2.10	0.51
1:D:83:LYS:HE3	1:D:83:LYS:CA	2.40	0.51
1:E:169:MET:HG3	1:E:190:ARG:HD2	1.92	0.51
1:F:144:GLU:CD	1:F:145:PRO:HD2	2.31	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:387:SER:O	1:F:387:SER:OG	2.24	0.51
1:A:281:ASP:HB3	1:A:325:LYS:HD2	1.92	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: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:A:102:LYS:CG	1:A:366:GLU:OE2	2.56	0.51
1:B:97:LYS:C	1:B:99:PHE:H	2.14	0.51
1:B:329:GLU:HG2	1:B:396:PHE:CD2	2.46	0.51
1:B:348:GLY:O	1:B:349:SER:C	2.48	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: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: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:A:223:TYR:C	1:A:314:VAL:HG22	2.30	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: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:B:399:GLU:CD	1:B:399:GLU:C	2.63	0.50
1:C:59:PRO:HG2	1:C:62:GLU:CD	2.31	0.50
1:C:59:PRO:O	1:C:60:ALA:C	2.49	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:364:LEU:HD12	1:E:368:GLN:CD	2.32	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:C:291:GLU:C	1:C:291:GLU:CD	2.70	0.50
1:D:51:ARG:HD3	3:D:1420:HEM:O2D	2.12	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: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:C:226:ALA:HA	3:C:1320:HEM:HMD2	1.94	0.50
1:D:113:ASN:O	1:D:114:ALA:C	2.49	0.50
1:D:127:ILE:O	1:D:131:GLU:HG3	2.12	0.50
1:F:80:ILE:O	1:F:81:LEU:C	2.49	0.50
1:F:226:ALA:O	1:F:228:ASN:N	2.45	0.50
1:B:66:HIS:HE1	1:B:132:ARG:NE	2.09	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:D:373:ILE:C	1:D:374:LEU:HD23	2.32	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:PRO:CG	1:D:112:PHE:HD1	2.24	0.49
1:D:205:GLY:C	1:D:208:TRP:H	2.14	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:C:291:GLU:CD	1:C:291:GLU:O	2.51	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:384:LYS:HA	1:B:390:TRP:CG	2.48	0.49
1:C:113:ASN:O	1:C:114:ALA:C	2.51	0.49
1:C:339:ILE:HA	1:C:344:LEU:O	2.13	0.49
1:A:96:GLY:C	1:A:98:LYS:H	2.16	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:C:121:ARG:HH22	1:C:239:GLU:CD	2.15	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
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:221:ASP:OD2	1:D:221:ASP:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:192:PRO:C	1:A:193:THR:HG22	2.27	0.49
1:B:384:LYS:HB3	1:B:390:TRP:CD2	2.48	0.49
1:C:363:GLU:CD	1:C:364:LEU:HD22	2.32	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: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:C	1:E:210:LEU:N	2.66	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:92:ILE:HA	1:C:342:GLU:CD	2.34	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
1:D:330:GLU:HG3	1:D:331:ALA:N	2.28	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:126:MET:C	1:C:128:GLU:H	2.17	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:E:201:GLU:O	1:E:201:GLU:CD	2.47	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: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:E:111:PHE:HB3	1:E:376:ASP:C	2.34	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: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: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: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: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:B:46:PRO:CG	1:B:310:PHE:CD2	2.95	0.48
1:B:95:ILE:CG2	1:B:337:MET:HE3	2.42	0.48
1:C:79:ASP:O	1:C:80:ILE:C	2.51	0.48
1:C:190:ARG:O	1:C:192:PRO:HD2	2.00	0.48
1:D:92:ILE:HG23	1:D:342:GLU:CD	2.34	0.48
1:D:110:GLU:CG	1:D:118:VAL:HB	2.43	0.48
1:D:261:ILE:HD11	1:D:277:ILE:HG22	1.96	0.48
1:E:149:ASN:ND2	2:E:1510:PLP:H2A1	2.28	0.48
1:E:334:PHE:O	1:E:338:LEU:HD12	2.14	0.48
1:F:95:ILE:HG23	1:F:337:MET:HE3	1.96	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:76:ILE:C	1:A:77:LEU:HD23	2.33	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:C:94:LYS:NZ	1:D:159:ALA:O	2.35	0.48
1:D:204:VAL:O	1:D:204:VAL:HG22	2.13	0.48
1:D:228:ASN:OD1	1:D:228:ASN:C	2.52	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: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: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: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: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:A:170:PRO:HD3	1:A:191:THR:HG1	1.79	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
1:D:201:GLU:O	1:D:201:GLU:CG	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:C	1:D:119:LYS:N	2.67	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: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:D:223:TYR:CD1	1:D:312:PRO:CG	2.95	0.47
1:E:249:ASP:CG	1:E:368:GLN:HE21	2.18	0.47
1:E:264:ILE:O	1:E:265:ALA:C	2.52	0.47
1:A:95:ILE:CD1	1:A:338:LEU:HD23	2.42	0.47
1:A:144:GLU:CD	1:A:145:PRO:HD2	2.35	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:B:72:LYS:HZ3	1:B:72:LYS:CA	2.21	0.47
1:C:135:THR:HG22	1:C:218:HIS:NE2	2.29	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:A:379:ARG:HH21	1:A:380:ASN:CG	2.18	0.47
1:B:231:ALA:O	1:B:235:THR:OG1	2.31	0.47
1:C:93:ASN:H	1:C:342:GLU:CD	2.17	0.47
1:D:100:GLY:O	1:D:101:LEU:C	2.53	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: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
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: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:B:156:LEU:C	1:B:156:LEU:HD12	2.33	0.47
1:E:95:ILE:CD1	1:E:337:MET:HE3	2.43	0.47
1:F:107:ALA:HB1	1:F:374:LEU:HD11	1.97	0.47
1:F:232:HIS:NE2	1:F:260:THR:HG22	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:249:ASP:O	1:D:275:CYS:SG	2.71	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:E:228:ASN:C	1:E:228:ASN:OD1	2.52	0.47
1:F:46:PRO:O	1:F:47:ASP:O	2.33	0.47
1:F:119:LYS:O	1:F:120:ASP:C	2.54	0.47
1:A:63:SER:HB2	3:A:1120:HEM:HAB	1.97	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: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:316:ASP:C	1:E:318:THR:H	2.18	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:A:149:ASN:ND2	2:A:1110:PLP:H2A1	2.30	0.46
1:B:147:SER:HB3	1:B:167:ILE:CG2	2.45	0.46
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:A:110:GLU:C	1:A:112:PHE:H	2.18	0.46
1:B:46:PRO:O	1:B:47:ASP:C	2.51	0.46
1:B:149:ASN:O	1:B:152:ILE:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:GLY:C	1:D:207:ALA:H	2.17	0.46
1:D:334:PHE:CE2	1:D:337:MET:HE1	2.50	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:A:382:MET:HA	1:A:382:MET:HE3	1.98	0.46
1:A:390:TRP:C	1:A:392:LEU:N	2.68	0.46
1:B:393:GLN:OE1	1:B:393:GLN:HA	2.16	0.46
1:C:59:PRO:CG	1:C:62:GLU:CD	2.83	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:372:VAL:HG12	1:D:374:LEU:HD21	1.96	0.46
1:E:49:PRO:O	1:E:50:SER:C	2.52	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:F:316:ASP:OD1	1:F:316:ASP:C	2.54	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:A:289:GLU:HA	1:A:290:PRO:C	2.36	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: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:160:VAL:O	1:D:160:VAL:CG1	2.63	0.46
1:D:190:ARG:HH11	1:D:190:ARG:HA	1.80	0.46
1:D:290:PRO:O	1:D:291:GLU:C	2.54	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:205:GLY:O	1:F:206:VAL:C	2.54	0.46
1:F:288:ALA:HB2	1:F:325:LYS:CD	2.46	0.46
1:B:235:THR:O	1:B:239:GLU:HG3	2.16	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: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:137:LYS:HB2	1:F:140:ASP:CG	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:ALA:HB3	1:F:325:LYS:HZ3	1.81	0.46
1:F:324:PHE:CG	1:F:356:VAL:HG13	2.51	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:166:ILE:C	1:C:167:ILE:HG13	2.36	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:D:329:GLU:HG3	1:D:396:PHE:CD2	2.50	0.46
1:E:105:LEU:C	1:E:105:LEU:CD1	2.76	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:F:149:ASN:ND2	2:F:1610:PLP:H2A1	2.31	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:D:385:PHE:C	1:D:385:PHE:HD1	2.20	0.45
1:E:175:SER:O	1:E:176:GLU:CA	2.64	0.45
1:E:199:SER:H	1:E:202:SER:CB	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:E:294:ASN:CG	2.36	0.45
1:E:288:ALA:HB1	1:E:293:LEU:HD12	1.97	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:208:TRP:HD1	1:C:211:LYS:HZ1	1.63	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:B:296:THR:C	1:B:298:GLN:H	2.20	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: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:C:127:ILE:O	1:C:127:ILE:HG22	2.16	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:A:203:HIS:HB2	1:A:206:VAL:HB	1.99	0.45
1:B:92:ILE:HA	1:B:342:GLU:OE1	2.17	0.45
1:B:137:LYS:HB2	1:B:140:ASP:CG	2.37	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:222:GLN:C	1:E:223:TYR:CG	2.90	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:F:328:ASP:O	1:F:329:GLU:C	2.54	0.45
1:A:78:PRO:CB	1:B:91:ARG:HH21	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HB2	1:A:140:ASP:OD1	2.17	0.45
1:C:95:ILE:HD11	1:C:337:MET:C	2.37	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:225:ASN:OD1	1:F:225:ASN:C	2.55	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:B:316:ASP:C	1:B:318:THR:H	2.19	0.45
1:C:84:ILE:HA	1:C:113:ASN:OD1	2.16	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:A:376:ASP:C	1:A:376:ASP:OD2	2.54	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: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:C:361:ALA:C	1:C:363:GLU:H	2.20	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:F:332:PHE:HB3	1:F:391:MET:HE2	1.98	0.44
1:F:357:ALA:O	1:F:358:VAL:C	2.53	0.44
1:A:191:THR:HG21	1:A:203:HIS:HB3	1.85	0.44
1:B:378:VAL:HG12	1:B:385:PHE:CE2	2.51	0.44
1:E:338:LEU:HD21	1:E:354:VAL:HG11	1.99	0.44
1:F:70:PRO:HG3	1:F:235:THR:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:PRO:HB2	3:A:1120:HEM:HAC	1.98	0.44
1:C:49:PRO:O	1:C:50:SER:O	2.34	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:C:286:ILE:C	1:C:286:ILE:HD12	2.37	0.44
1:D:89:MET:HE3	1:D:371:VAL:HG22	1.99	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:C:215:PRO:O	1:C:216:ASN:C	2.55	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:B:334:PHE:CD2	1:B:337:MET:HE2	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:C	1:A:112:PHE:N	2.70	0.44
1:A:137:LYS:O	1:A:138:PRO:C	2.55	0.44
1:A:221:ASP:HB3	1:A:224:ARG:HB2	2.00	0.44
1:B:81:LEU:C	1:B:83:LYS:H	2.20	0.44
1:B:232:HIS:CD2	1:B:260:THR:HA	2.53	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:137:LYS:NZ	1:E:140:ASP:CG	2.70	0.44
1:E:201:GLU:HB2	1:E:205:GLY:HA2	1.96	0.44
1:F:140:ASP:O	1:F:141:THR:HB	2.17	0.44
1:F:149:ASN:HD21	2:F:1610:PLP:H2A1	1.82	0.44
1:F:250:MET:HE1	1:F:364:LEU:HD21	1.97	0.44
1:A:251:LEU:HD22	1:A:264:ILE:HG22	1.99	0.43
1:A:332:PHE:HB3	1:A:391:MET:HE2	2.00	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:398:LYS:H	1:A:398:LYS:HD2	1.82	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
1:C:80:ILE:HD13	1:C:80:ILE:HA	1.74	0.43
1:C:126:MET:C	1:C:128:GLU:N	2.71	0.43
1:E:63:SER:HB2	3:E:1520:HEM:HBB2	1.99	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:B:50:SER:O	1:B:51:ARG:C	2.55	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:285:SER:O	1:C:294:ASN:OD1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:LYS:C	1:F:121:ARG:N	2.69	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:268:LEU:O	1:A:269:LYS:C	2.56	0.43
1:B:282:PRO:CG	1:B:307:GLY:HA3	2.48	0.43
1:B:290:PRO:O	1:B:291:GLU:C	2.57	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:272:CYS:O	1:C:274:GLY:N	2.51	0.43
1:C:338:LEU:HD11	1:C:354:VAL:HG21	2.01	0.43
1:C:384:LYS:O	1:C:385:PHE:C	2.57	0.43
1:D:56:LEU:HD22	1:D:269:LYS:HB3	2.01	0.43
1:D:226:ALA:O	1:D:227:SER:C	2.57	0.43
1:E:88:PRO:HG2	1:E:109:CYS:HB2	1.99	0.43
1:F:117:SER:O	1:F:120:ASP:OD1	2.37	0.43
1:A:96:GLY:C	1:A:98:LYS:N	2.72	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:D:233:TYR:O	1:D:267:LYS:NZ	2.43	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: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
1:D:56:LEU:HD13	1:D:270:GLU:HG2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:O	1:D:266:ARG:HG3	2.19	0.43
1:E:262:THR:O	1:E:263:GLY:C	2.57	0.43
1:E:316:ASP:C	1:E:318:THR:N	2.72	0.43
1:E:386:LEU:HD23	1:E:386:LEU:HA	1.80	0.43
1:E:389:ARG:O	1:E:390:TRP:C	2.55	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:C:89:MET:SD	1:C:106:LEU:HB3	2.59	0.43
1:D:160:VAL:O	1:D:160:VAL:HG12	2.17	0.43
1:D:233:TYR:HD1	1:D:263:GLY:O	2.02	0.43
1:D:316:ASP:C	1:D:316:ASP:OD2	2.56	0.43
1:E:192:PRO:O	1:E:193:THR:C	2.56	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:95:ILE:HG23	1:B:337:MET:HE1	1.97	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: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
1:C:272:CYS:SG	1:C:275:CYS:HB2	2.59	0.43
1:C:286:ILE:C	1:C:288:ALA:H	2.21	0.43
1:D:309:ASP:OD1	1:D:310:PHE:N	2.52	0.43
1:D:398:LYS:O	1:D:399:GLU:C	2.56	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: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:B:261:ILE:HD11	1:B:320:VAL:HG13	2.01	0.42
1:B:287:LEU:HD21	1:B:308:TYR:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:PHE:HE2	1:E:374:LEU:HD12	1.84	0.42
1:E:137:LYS:HB2	1:E:137:LYS:HZ2	1.83	0.42
1:E:267:LYS:HG3	1:E:267:LYS:O	2.19	0.42
1:F:251:LEU:HD11	1:F:264:ILE:HG21	2.01	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:C:59:PRO:CB	1:C:62:GLU:CD	2.87	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:C:393:GLN:HG3	1:C:394:LYS:HZ3	1.83	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:148:GLY:O	1:E:149:ASN:C	2.57	0.42
1:E:150:THR:CB	1:E:222:GLN:OE1	2.68	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:214:ILE:O	1:A:217:SER:OG	2.30	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:C:81:LEU:CD1	1:C:161:ARG:CZ	2.98	0.42
1:C:118:VAL:N	1:C:375:PRO:O	2.52	0.42
1:C:187:GLU:C	1:C:188:ILE:HD12	2.39	0.42
1:C:343:GLY:O	1:D:80:ILE:HG21	2.19	0.42
1:C:389:ARG:HH22	1:D:175:SER:HG	1.62	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:E:103:CYS:HA	1:E:368:GLN:O	2.18	0.42
1:E:277:ILE:O	1:E:321:ASP:HB2	2.19	0.42
1:E:305:GLY:HA3	2:E:1510:PLP:H2A3	2.00	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: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:183:ALA:O	1:F:340:ALA:HB2	2.20	0.42
1:F:264:ILE:O	1:F:265:ALA:C	2.57	0.42
1:F:364:LEU:HD12	1:F:368:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:298:GLN:O	1:A:299:THR:C	2.58	0.42
1:B:90:VAL:O	1:B:107:ALA:N	2.52	0.42
1:B:150:THR:C	1:B:152:ILE:H	2.23	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:HA	1:B:294:ASN:CG	2.39	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
1:D:156:LEU:HD13	1:D:156:LEU:C	2.40	0.42
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:E:346:CYS:N	1:E:378:VAL:HG13	2.34	0.42
1:F:89:MET:HE2	1:F:108:LYS:HG2	2.01	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:348:GLY:O	1:F:349:SER:C	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:GLN:CA	1:E:242:GLN:NE2	2.80	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:E:166:ILE:O	1:E:167:ILE:HD12	2.20	0.42
1:E:268:LEU:O	1:E:272:CYS:C	2.57	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: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:F:59:PRO:C	1:F:61:SER:N	2.73	0.42
1:F:334:PHE:CE2	1:F:337:MET:HE1	2.54	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:E:93:ASN:ND2	1:F:79:ASP:HB3	2.32	0.41
1:F:91:ARG:HD3	1:F:104:GLU:OE2	2.20	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:HG2	1:A:209:ARG:O	2.21	0.41
1:B:176:GLU:O	1:B:180:VAL:CG2	2.64	0.41
1:B:316:ASP:OD2	1:B:318:THR:HB	2.20	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:C:82:LYS:HD3	1:C:82:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:249:ASP:C	1:D:275:CYS:HG	2.22	0.41
1:E:176:GLU:HA	1:E:396:PHE:CD1	2.52	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:D:95:ILE:HG12	1:D:337:MET:HE3	2.02	0.41
1:E:66:HIS:O	1:E:125:ARG:NH2	2.53	0.41
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:83:LYS:HA	1:A:83:LYS:HZ2	1.82	0.41
1:B:281:ASP:OD1	1:B:287:LEU:C	2.59	0.41
1:C:87:THR:OG1	1:C:108:LYS:HE3	2.20	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:A:146:THR:O	1:A:146:THR:CG2	2.69	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:A:292:GLU:H	1:A:292:GLU:CD	2.24	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:221:ASP:O	1:D:225:ASN:N	2.42	0.41
1:D:235:THR:H	1:D:235:THR:HG1	1.68	0.41
1:D:261:ILE:O	1:D:265:ALA:HB2	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:137:LYS:O	1:B:138:PRO:C	2.58	0.41
1:C:59:PRO:CB	1:C:62:GLU:OE2	2.68	0.41
1:C:132:ARG:C	1:C:134:GLY:H	2.24	0.41
1:C:261:ILE:HG23	1:C:262:THR:N	2.36	0.41
1:C:291:GLU:OE1	1:C:291:GLU:CA	2.61	0.41
1:D:76:ILE:CG2	1:D:77:LEU:N	2.84	0.41
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:394:LYS:HZ2	1:E:394:LYS:C	2.24	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: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: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:248:LEU:HD13	1:C:275:CYS:SG	2.61	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:176:GLU:HG2	1:F:380:ASN:C	2.40	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:F:391:MET:C	1:F:392:LEU:HG	2.41	0.41
1:A:392:LEU:HD22	1:A:398:LYS:HB3	2.03	0.41
1:C:316:ASP:OD2	1:C:318:THR:OG1	2.28	0.41
1:C:345:LEU:O	1:C:378:VAL:HG13	2.21	0.41
1:D:81:LEU:C	1:D:83:LYS:H	2.24	0.41
1:D:256:GLY:N	2:D:1410:PLP:H5A1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:PRO:CD	1:A:191:THR:HG1	2.34	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:B:52:CYS:HB2	3:B:1220:HEM:C4D	2.56	0.40
1:B:87:THR:HB	1:B:88:PRO:HD2	2.02	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:F:290:PRO:O	1:F:292:GLU:N	2.54	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: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:D:173:MET:CA	1:D:173:MET:HE2	2.36	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:F:251:LEU:HD23	1:F:251:LEU:C	2.41	0.40
1:B:221:ASP:C	1:B:221:ASP:OD2	2.60	0.40
1:B:226:ALA:HB1	1:B:230:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:235:THR:O	1:F:236:THR:C	2.60	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 10
1	B	341/363 (94%)	276 (81%)	54 (16%)	11 (3%)	4 16
1	C	342/363 (94%)	284 (83%)	43 (13%)	15 (4%)	2 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	342/363 (94%)	274 (80%)	52 (15%)	16 (5%)	2 8
1	E	343/363 (94%)	271 (79%)	54 (16%)	18 (5%)	2 6
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 8

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

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Mol	Chain	Res	Type
1	E	50	SER
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

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Mol	Chain	Res	Type
1	E	248	LEU
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	294/304 (97%)	245 (83%)	49 (17%)	2 6
1	B	289/304 (95%)	247 (86%)	42 (14%)	3 9
1	C	288/304 (95%)	260 (90%)	28 (10%)	8 25
1	D	288/304 (95%)	249 (86%)	39 (14%)	4 11
1	E	289/304 (95%)	248 (86%)	41 (14%)	3 10
1	F	286/304 (94%)	239 (84%)	47 (16%)	2 7
All	All	1734/1824 (95%)	1488 (86%)	246 (14%)	3 10

All (246) 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	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	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	194	ASN
1	A	201	GLU
1	A	202	SER
1	A	208	TRP
1	A	210	LEU
1	A	211	LYS
1	A	212	ASN
1	A	242	GLN
1	A	243	GLN
1	A	248	LEU
1	A	270	GLU
1	A	283	GLU
1	A	292	GLU
1	A	294	ASN
1	A	295	GLN
1	A	314	VAL
1	A	317	ARG
1	A	327	ASN
1	A	336	ARG
1	A	372	VAL
1	A	381	TYR
1	A	384	LYS

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Mol	Chain	Res	Type
1	A	385	PHE
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	132	ARG
1	B	138	PRO
1	B	152	ILE
1	B	156	LEU
1	B	161	ARG
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	208	TRP
1	B	215	PRO
1	B	224	ARG
1	B	225	ASN
1	B	272	CYS
1	B	287	LEU
1	B	290	PRO
1	B	308	TYR
1	B	309	ASP
1	B	311	ILE
1	B	317	ARG
1	B	327	ASN
1	B	359	LYS
1	B	363	GLU
1	B	375	PRO
1	B	376	ASP
1	B	377	SER

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Mol	Chain	Res	Type
1	B	378	VAL
1	B	380	ASN
1	B	384	LYS
1	B	385	PHE
1	B	388	ASP
1	B	394	LYS
1	B	399	GLU
1	C	49	PRO
1	C	55	GLN
1	C	58	ARG
1	C	72	LYS
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	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	287	LEU
1	C	290	PRO
1	C	291	GLU
1	C	297	GLU
1	C	308	TYR
1	C	313	THR
1	C	385	PHE
1	C	394	LYS
1	C	399	GLU
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

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Mol	Chain	Res	Type
1	D	136	LEU
1	D	140	ASP
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	202	SER
1	D	203	HIS
1	D	247	LYS
1	D	248	LEU
1	D	249	ASP
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	328	ASP
1	D	341	GLN
1	D	346	CYS
1	D	363	GLU
1	D	379	ARG
1	D	382	MET
1	D	385	PHE
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	125	ARG
1	E	127	ILE
1	E	135	THR
1	E	150	THR
1	E	156	LEU
1	E	172	LYS

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Mol	Chain	Res	Type
1	E	174	SER
1	E	176	GLU
1	E	190	ARG
1	E	192	PRO
1	E	200	PRO
1	E	201	GLU
1	E	209	ARG
1	E	210	LEU
1	E	229	PRO
1	E	238	ASP
1	E	242	GLN
1	E	248	LEU
1	E	251	LEU
1	E	294	ASN
1	E	295	GLN
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
1	E	385	PHE
1	E	386	LEU
1	E	389	ARG
1	E	391	MET
1	E	392	LEU
1	E	394	LYS
1	E	396	PHE
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	74	PRO
1	F	75	LYS
1	F	77	LEU
1	F	78	PRO
1	F	101	LEU

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Mol	Chain	Res	Type
1	F	106	LEU
1	F	108	LYS
1	F	138	PRO
1	F	140	ASP
1	F	169	MET
1	F	170	PRO
1	F	172	LYS
1	F	182	ARG
1	F	209	ARG
1	F	227	SER
1	F	228	ASN
1	F	229	PRO
1	F	242	GLN
1	F	247	LYS
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	318	THR
1	F	329	GLU
1	F	352	SER
1	F	365	GLN
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	396	PHE
1	F	397	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	225	ASN
1	A	242	GLN
1	A	393	GLN
1	B	66	HIS
1	B	212	ASN
1	B	222	GLN
1	B	232	HIS
1	B	294	ASN
1	B	295	GLN
1	B	327	ASN
1	B	362	GLN
1	B	365	GLN
1	C	55	GLN
1	C	66	HIS
1	C	216	ASN
1	C	222	GLN
1	D	55	GLN
1	D	93	ASN
1	D	212	ASN
1	D	216	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	149	ASN
1	F	203	HIS
1	F	216	ASN
1	F	218	HIS
1	F	242	GLN
1	F	294	ASN
1	F	365	GLN
1	F	380	ASN
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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	HEM	C	1320	1	27,50,50	2.33	12 (44%)	17,82,82	1.82	4 (23%)
2	PLP	E	1510	1	15,15,16	1.64	4 (26%)	20,22,23	1.33	3 (15%)
2	PLP	D	1410	1	15,15,16	1.62	4 (26%)	20,22,23	1.41	3 (15%)
2	PLP	B	1210	1	15,15,16	2.51	6 (40%)	20,22,23	2.24	8 (40%)
2	PLP	F	1610	1	15,15,16	1.37	4 (26%)	20,22,23	1.14	1 (5%)
3	HEM	A	1120	1	27,50,50	2.20	9 (33%)	17,82,82	1.74	5 (29%)
3	HEM	B	1220	1	27,50,50	2.13	9 (33%)	17,82,82	1.50	4 (23%)
3	HEM	E	1520	1	27,50,50	2.19	10 (37%)	17,82,82	1.57	4 (23%)
2	PLP	A	1110	1	15,15,16	1.52	3 (20%)	20,22,23	1.18	2 (10%)
3	HEM	F	1620	1	27,50,50	2.11	11 (40%)	17,82,82	2.00	7 (41%)
2	PLP	C	1310	1	15,15,16	1.55	4 (26%)	20,22,23	1.25	2 (10%)
3	HEM	D	1420	1	27,50,50	2.21	9 (33%)	17,82,82	1.67	4 (23%)

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
3	HEM	C	1320	1	-	0/6/54/54	-
2	PLP	E	1510	1	-	2/6/6/8	0/1/1/1
2	PLP	D	1410	1	-	2/6/6/8	0/1/1/1
2	PLP	B	1210	1	-	0/6/6/8	0/1/1/1
2	PLP	F	1610	1	-	0/6/6/8	0/1/1/1
3	HEM	A	1120	1	-	0/6/54/54	-
3	HEM	B	1220	1	-	0/6/54/54	-
3	HEM	E	1520	1	-	0/6/54/54	-
2	PLP	A	1110	1	-	2/6/6/8	0/1/1/1
3	HEM	F	1620	1	-	2/6/54/54	-
2	PLP	C	1310	1	-	1/6/6/8	0/1/1/1
3	HEM	D	1420	1	-	2/6/54/54	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	PLP	C3-C2	-5.93	1.35	1.40
3	C	1320	HEM	C3B-CAB	5.60	1.59	1.47
3	D	1420	HEM	C3B-CAB	5.25	1.58	1.47
3	E	1520	HEM	C3B-CAB	4.93	1.58	1.47
3	C	1320	HEM	C3C-CAC	4.71	1.57	1.47
3	A	1120	HEM	C3C-CAC	4.56	1.57	1.47
3	A	1120	HEM	C3B-CAB	4.53	1.57	1.47
3	B	1220	HEM	C3C-CAC	4.50	1.57	1.47
3	F	1620	HEM	C3C-CAC	4.16	1.56	1.47
3	B	1220	HEM	C3B-CAB	4.08	1.56	1.47
3	D	1420	HEM	C3C-CAC	4.08	1.56	1.47
2	B	1210	PLP	C2-N1	3.99	1.41	1.33
3	F	1620	HEM	C3B-CAB	3.99	1.56	1.47
3	C	1320	HEM	CBB-CAB	3.99	1.55	1.29
3	A	1120	HEM	CBB-CAB	3.98	1.55	1.29
3	E	1520	HEM	C3C-CAC	3.89	1.55	1.47
3	B	1220	HEM	CBB-CAB	3.85	1.54	1.29
3	E	1520	HEM	CBB-CAB	3.84	1.54	1.29
3	D	1420	HEM	CBB-CAB	3.83	1.54	1.29
2	B	1210	PLP	C4A-C4	-3.79	1.43	1.51
3	D	1420	HEM	CBC-CAC	3.74	1.54	1.29
3	F	1620	HEM	CBB-CAB	3.74	1.54	1.29
3	E	1520	HEM	CBC-CAC	3.67	1.53	1.29
3	C	1320	HEM	CBC-CAC	3.64	1.53	1.29
2	B	1210	PLP	C6-N1	3.57	1.42	1.34
3	B	1220	HEM	CBC-CAC	3.56	1.52	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1620	HEM	CBC-CAC	3.50	1.52	1.29
3	D	1420	HEM	C3C-C2C	-3.46	1.35	1.40
3	A	1120	HEM	CBC-CAC	3.40	1.51	1.29
2	D	1410	PLP	C2-N1	3.28	1.40	1.33
2	E	1510	PLP	C5-C4	3.20	1.44	1.40
2	A	1110	PLP	C5-C4	3.09	1.43	1.40
2	E	1510	PLP	C2-N1	2.90	1.39	1.33
3	A	1120	HEM	CMC-C2C	2.88	1.58	1.51
2	D	1410	PLP	C5-C4	2.87	1.43	1.40
3	E	1520	HEM	C3C-C2C	-2.87	1.36	1.40
2	A	1110	PLP	C2-N1	2.79	1.39	1.33
3	C	1320	HEM	CAA-C2A	2.78	1.56	1.52
2	C	1310	PLP	C2-N1	2.77	1.39	1.33
3	F	1620	HEM	CAA-C2A	2.71	1.56	1.52
2	F	1610	PLP	C2-N1	2.58	1.38	1.33
3	D	1420	HEM	CAD-C3D	2.58	1.56	1.52
3	E	1520	HEM	CMC-C2C	2.58	1.57	1.51
3	C	1320	HEM	CMC-C2C	2.56	1.57	1.51
3	A	1120	HEM	CAD-C3D	2.56	1.56	1.52
3	E	1520	HEM	C1D-ND	2.55	1.41	1.36
2	D	1410	PLP	C6-N1	2.55	1.39	1.34
3	C	1320	HEM	C1C-C2C	2.52	1.48	1.42
3	B	1220	HEM	C3C-C2C	-2.51	1.36	1.40
2	C	1310	PLP	C6-N1	2.50	1.39	1.34
3	F	1620	HEM	C1D-ND	2.50	1.41	1.36
3	C	1320	HEM	C3C-C2C	-2.48	1.36	1.40
3	F	1620	HEM	C3C-C2C	-2.46	1.37	1.40
2	E	1510	PLP	P-O3P	-2.44	1.45	1.54
3	C	1320	HEM	CAD-C3D	2.44	1.56	1.52
2	C	1310	PLP	C5-C4	2.42	1.43	1.40
2	E	1510	PLP	C6-N1	2.42	1.39	1.34
2	F	1610	PLP	P-O3P	-2.40	1.45	1.54
3	F	1620	HEM	CMC-C2C	2.38	1.57	1.51
3	A	1120	HEM	CAA-C2A	2.36	1.55	1.52
2	A	1110	PLP	C6-N1	2.36	1.39	1.34
3	C	1320	HEM	C4A-CHB	-2.36	1.34	1.41
3	B	1220	HEM	C1D-ND	2.34	1.41	1.36
3	A	1120	HEM	C4A-CHB	-2.34	1.34	1.41
3	D	1420	HEM	CMC-C2C	2.33	1.57	1.51
2	B	1210	PLP	C5A-C5	2.32	1.57	1.50
3	A	1120	HEM	C1C-C2C	2.29	1.47	1.42
3	B	1220	HEM	C1B-C2B	2.27	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1410	PLP	P-O3P	-2.27	1.46	1.54
3	E	1520	HEM	CMA-C3A	2.26	1.56	1.51
3	F	1620	HEM	C1C-C2C	2.24	1.47	1.42
2	F	1610	PLP	C6-N1	2.23	1.39	1.34
3	B	1220	HEM	CMC-C2C	2.23	1.56	1.51
3	B	1220	HEM	CAA-C2A	2.23	1.55	1.52
2	C	1310	PLP	C5A-C5	2.20	1.56	1.50
3	D	1420	HEM	C4A-CHB	-2.18	1.34	1.41
3	C	1320	HEM	C1D-ND	2.16	1.40	1.36
3	F	1620	HEM	CAD-C3D	2.15	1.56	1.52
3	D	1420	HEM	CMA-C3A	2.11	1.56	1.51
2	B	1210	PLP	P-O3P	-2.05	1.47	1.54
3	E	1520	HEM	C1C-C2C	2.03	1.47	1.42
3	E	1520	HEM	CAD-C3D	2.02	1.55	1.52
3	F	1620	HEM	CMA-C3A	2.02	1.55	1.51
3	C	1320	HEM	CMA-C3A	2.01	1.55	1.51
2	F	1610	PLP	C5-C4	2.00	1.42	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1210	PLP	C3-C4-C5	6.09	125.31	118.74
3	F	1620	HEM	CBA-CAA-C2A	4.29	120.39	112.49
3	C	1320	HEM	CBA-CAA-C2A	4.18	120.20	112.49
2	D	1410	PLP	O4P-C5A-C5	4.10	117.17	109.35
2	C	1310	PLP	O4P-C5A-C5	3.70	116.40	109.35
2	E	1510	PLP	O4P-C5A-C5	3.64	116.28	109.35
3	A	1120	HEM	CMC-C2C-C3C	3.63	131.47	124.68
2	B	1210	PLP	C5-C6-N1	-3.57	117.88	123.82
3	B	1220	HEM	CMC-C2C-C3C	3.30	130.86	124.68
3	A	1120	HEM	CBA-CAA-C2A	3.22	118.42	112.49
3	C	1320	HEM	CMC-C2C-C3C	3.21	130.69	124.68
3	E	1520	HEM	CMC-C2C-C3C	3.16	130.60	124.68
3	C	1320	HEM	CMB-C2B-C3B	3.16	130.59	124.68
3	D	1420	HEM	CMC-C2C-C3C	3.15	130.58	124.68
3	F	1620	HEM	CMC-C2C-C3C	3.13	130.53	124.68
3	D	1420	HEM	CMB-C2B-C3B	3.03	130.35	124.68
3	F	1620	HEM	CBD-CAD-C3D	2.98	117.96	112.48
2	B	1210	PLP	O4P-C5A-C5	2.86	114.81	109.35
3	D	1420	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
2	B	1210	PLP	C4A-C4-C5	-2.62	118.23	120.94
3	A	1120	HEM	CMA-C3A-C4A	-2.60	124.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1120	HEM	CMB-C2B-C3B	2.54	129.43	124.68
2	B	1210	PLP	O3-C3-C2	2.52	122.98	117.49
3	E	1520	HEM	CMA-C3A-C4A	-2.48	124.65	128.46
3	B	1220	HEM	CMA-C3A-C4A	-2.43	124.72	128.46
3	E	1520	HEM	CMB-C2B-C3B	2.43	129.23	124.68
2	B	1210	PLP	C4A-C4-C3	-2.39	116.45	120.50
3	F	1620	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
3	E	1520	HEM	CMD-C2D-C1D	-2.34	124.87	128.46
2	F	1610	PLP	O3P-P-O1P	2.30	119.67	110.68
3	D	1420	HEM	CMD-C2D-C1D	-2.28	124.96	128.46
3	F	1620	HEM	CMB-C2B-C3B	2.23	128.84	124.68
2	C	1310	PLP	O3P-P-O1P	2.21	119.35	110.68
2	E	1510	PLP	C5A-C5-C6	-2.21	115.73	119.37
2	B	1210	PLP	O3P-P-O1P	2.19	119.25	110.68
3	B	1220	HEM	CMD-C2D-C1D	-2.16	125.15	128.46
2	E	1510	PLP	O3P-P-O1P	2.14	119.08	110.68
3	F	1620	HEM	CMD-C2D-C1D	-2.14	125.18	128.46
2	A	1110	PLP	O3P-P-O1P	2.13	119.04	110.68
2	A	1110	PLP	O4P-C5A-C5	2.11	113.37	109.35
3	C	1320	HEM	CMD-C2D-C1D	-2.10	125.24	128.46
2	D	1410	PLP	O3P-P-O1P	2.09	118.87	110.68
2	B	1210	PLP	C6-N1-C2	2.07	123.01	119.17
3	A	1120	HEM	CMD-C2D-C1D	-2.07	125.28	128.46
3	F	1620	HEM	CAA-CBA-CGA	-2.05	109.23	112.67
3	B	1220	HEM	CMB-C2B-C3B	2.02	128.45	124.68
2	D	1410	PLP	C5A-C5-C6	-2.02	116.06	119.37

There are no chirality outliers.

All (11) 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	D	1420	HEM	C2D-C3D-CAD-CBD
3	D	1420	HEM	C4D-C3D-CAD-CBD
3	F	1620	HEM	C1A-C2A-CAA-CBA
3	F	1620	HEM	C3A-C2A-CAA-CBA
2	A	1110	PLP	C6-C5-C5A-O4P
2	C	1310	PLP	C4-C5-C5A-O4P

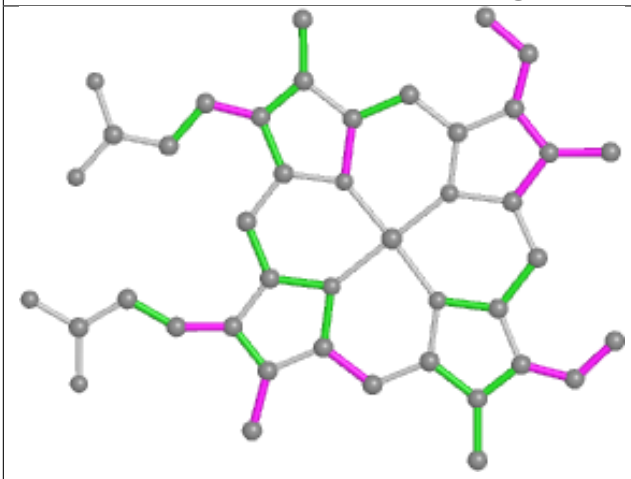
There are no ring outliers.

12 monomers are involved in 64 short contacts:

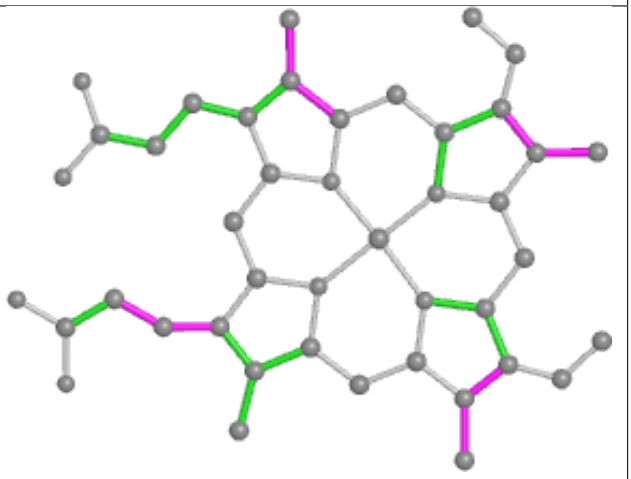
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1320	HEM	9	0
2	E	1510	PLP	5	0
2	D	1410	PLP	6	0
2	B	1210	PLP	1	0
2	F	1610	PLP	4	0
3	A	1120	HEM	4	0
3	B	1220	HEM	5	0
3	E	1520	HEM	5	0
2	A	1110	PLP	3	0
3	F	1620	HEM	10	0
2	C	1310	PLP	5	0
3	D	1420	HEM	7	0

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

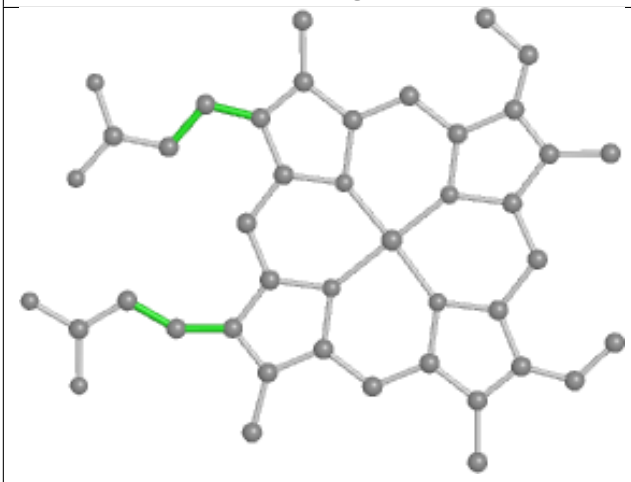
Ligand HEM C 1320



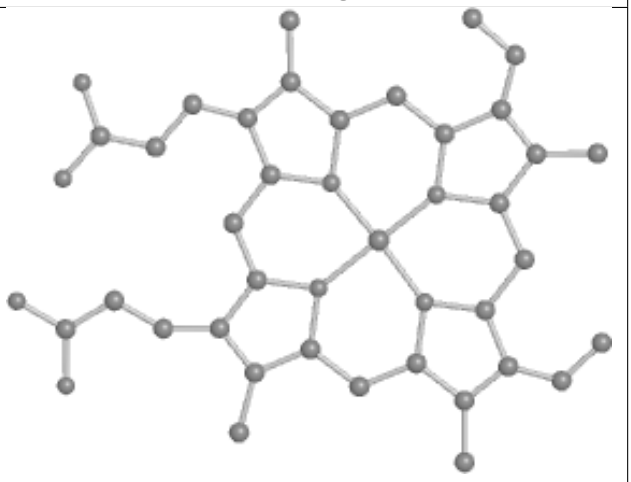
Bond lengths



Bond angles

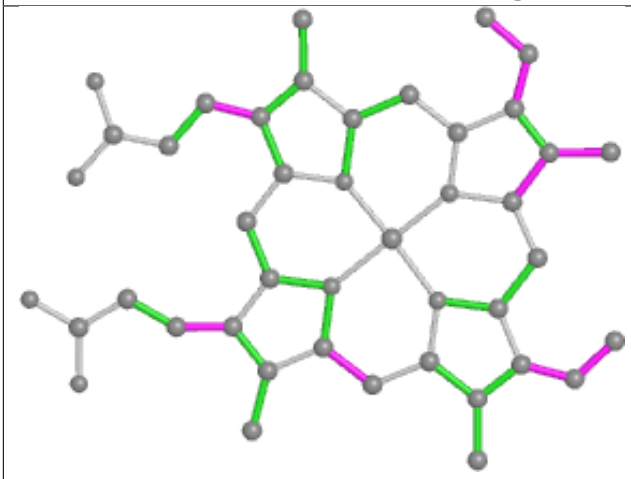


Torsions

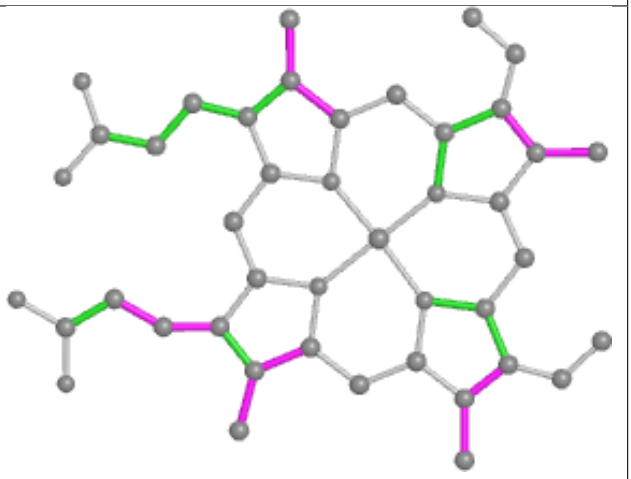


Rings

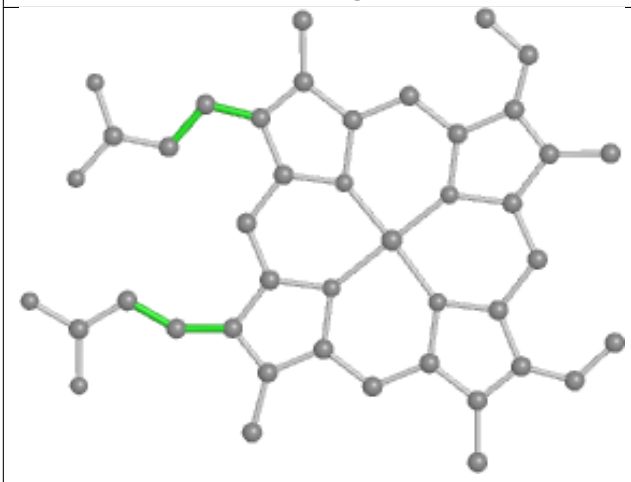
Ligand HEM A 1120



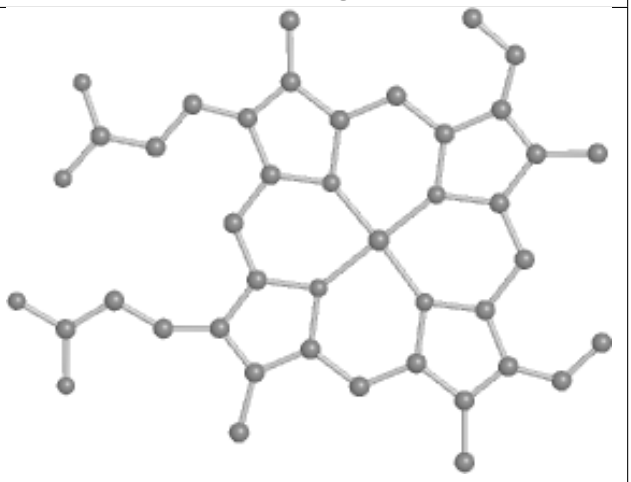
Bond lengths



Bond angles

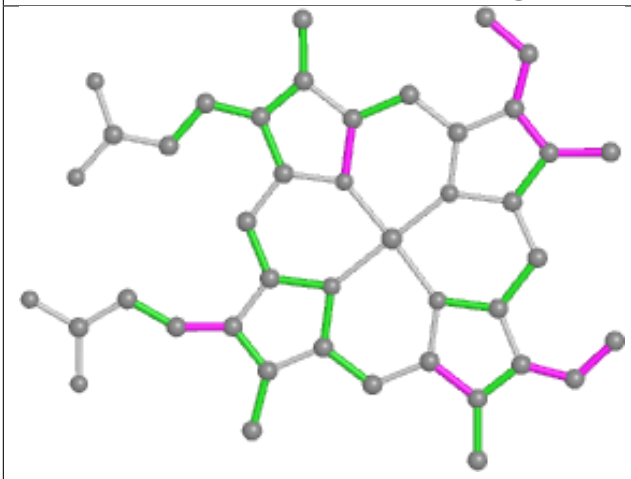


Torsions

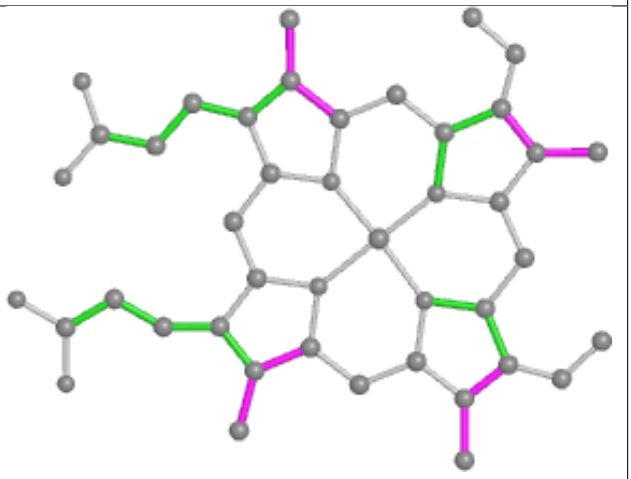


Rings

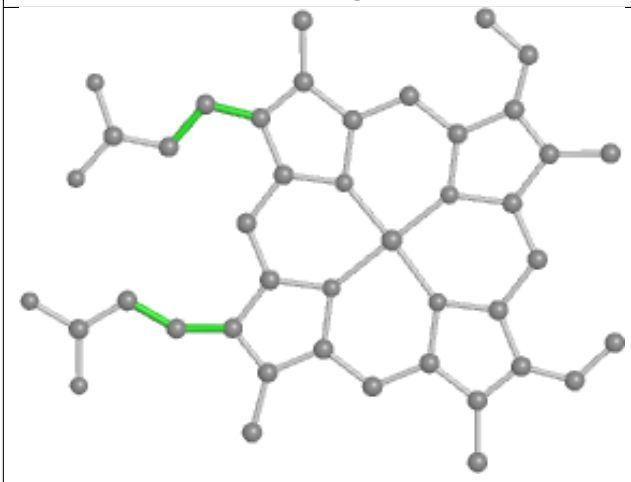
Ligand HEM B 1220



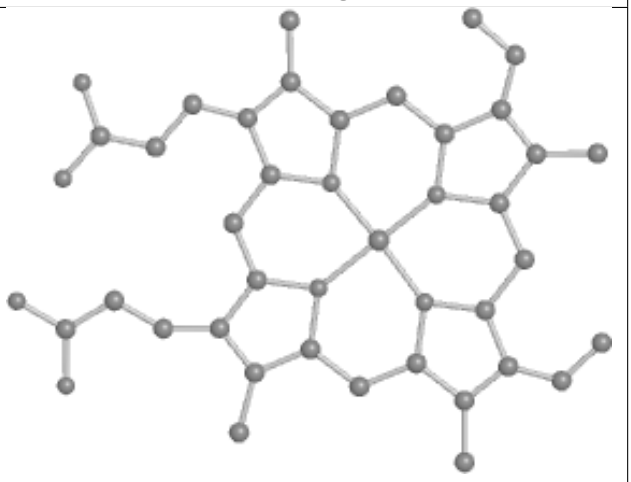
Bond lengths



Bond angles

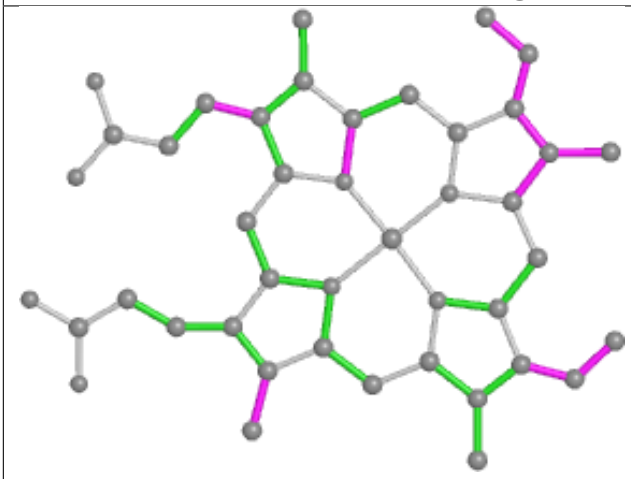


Torsions

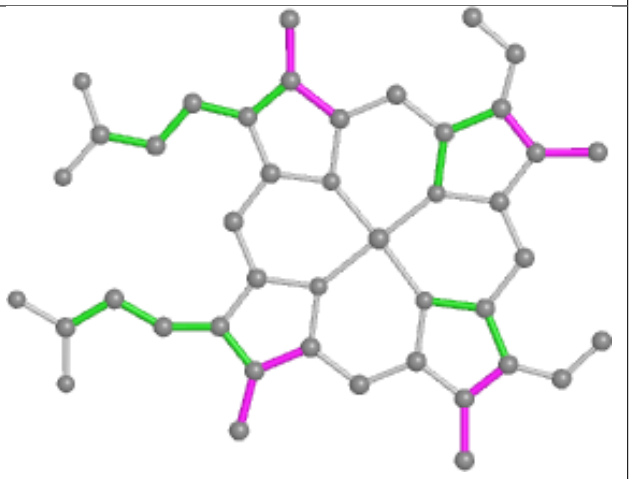


Rings

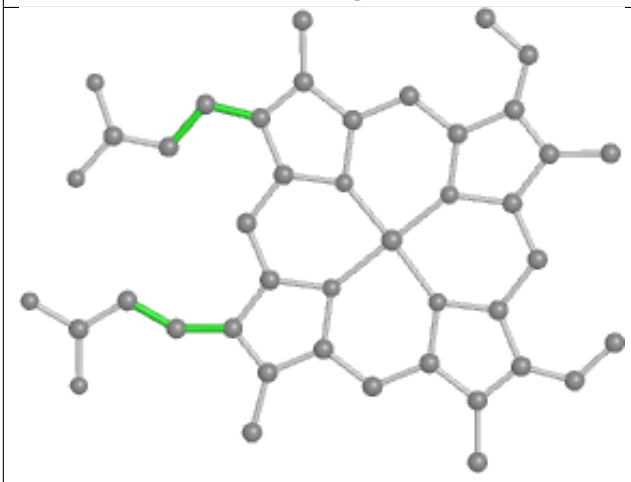
Ligand HEM E 1520



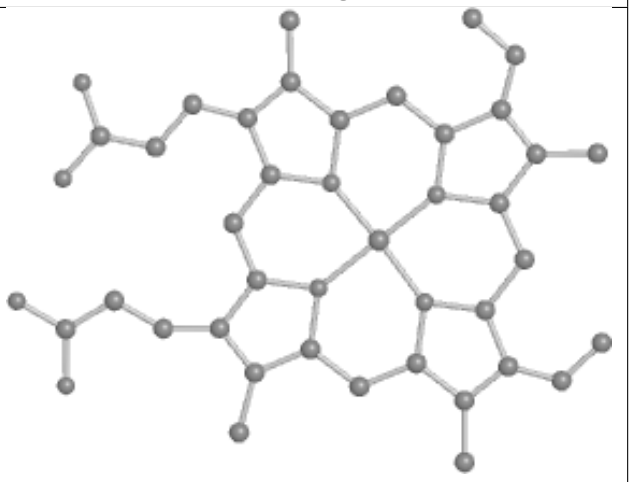
Bond lengths



Bond angles

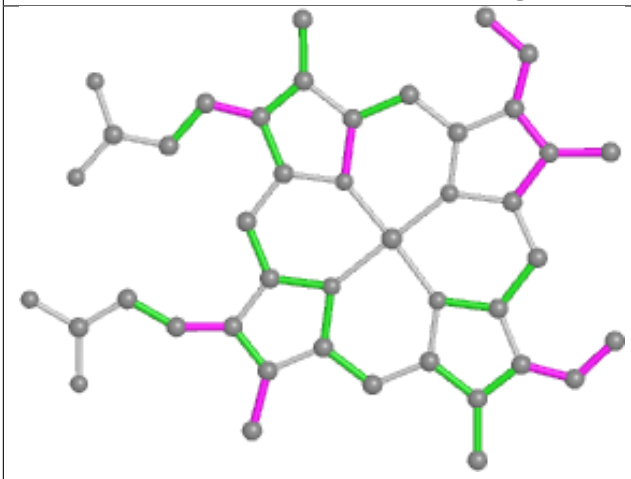


Torsions

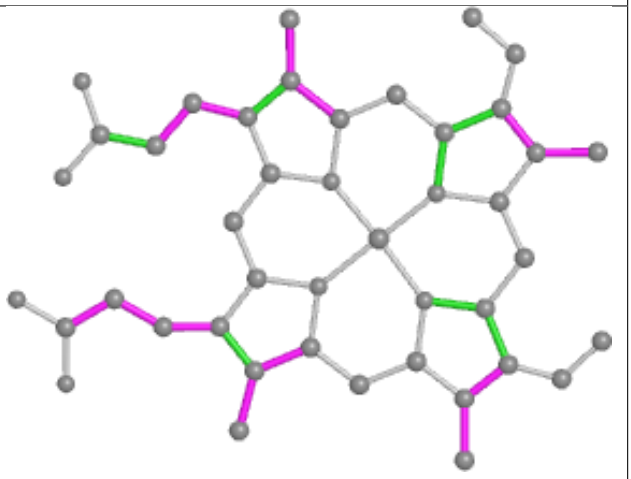


Rings

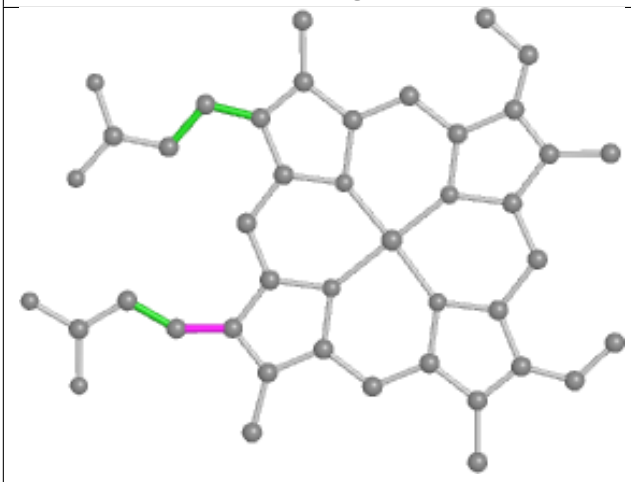
Ligand HEM F 1620



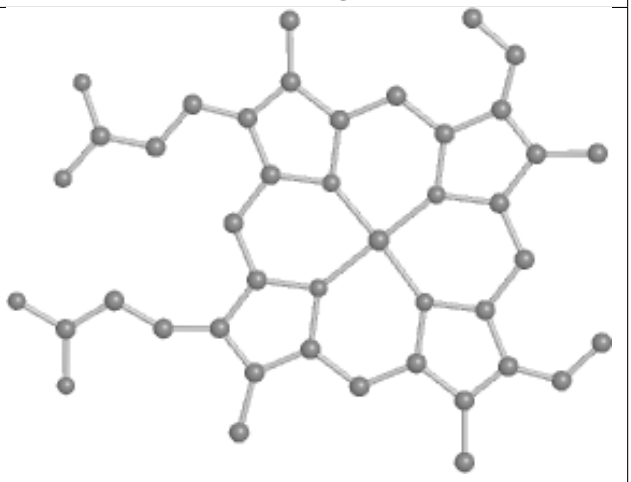
Bond lengths



Bond angles

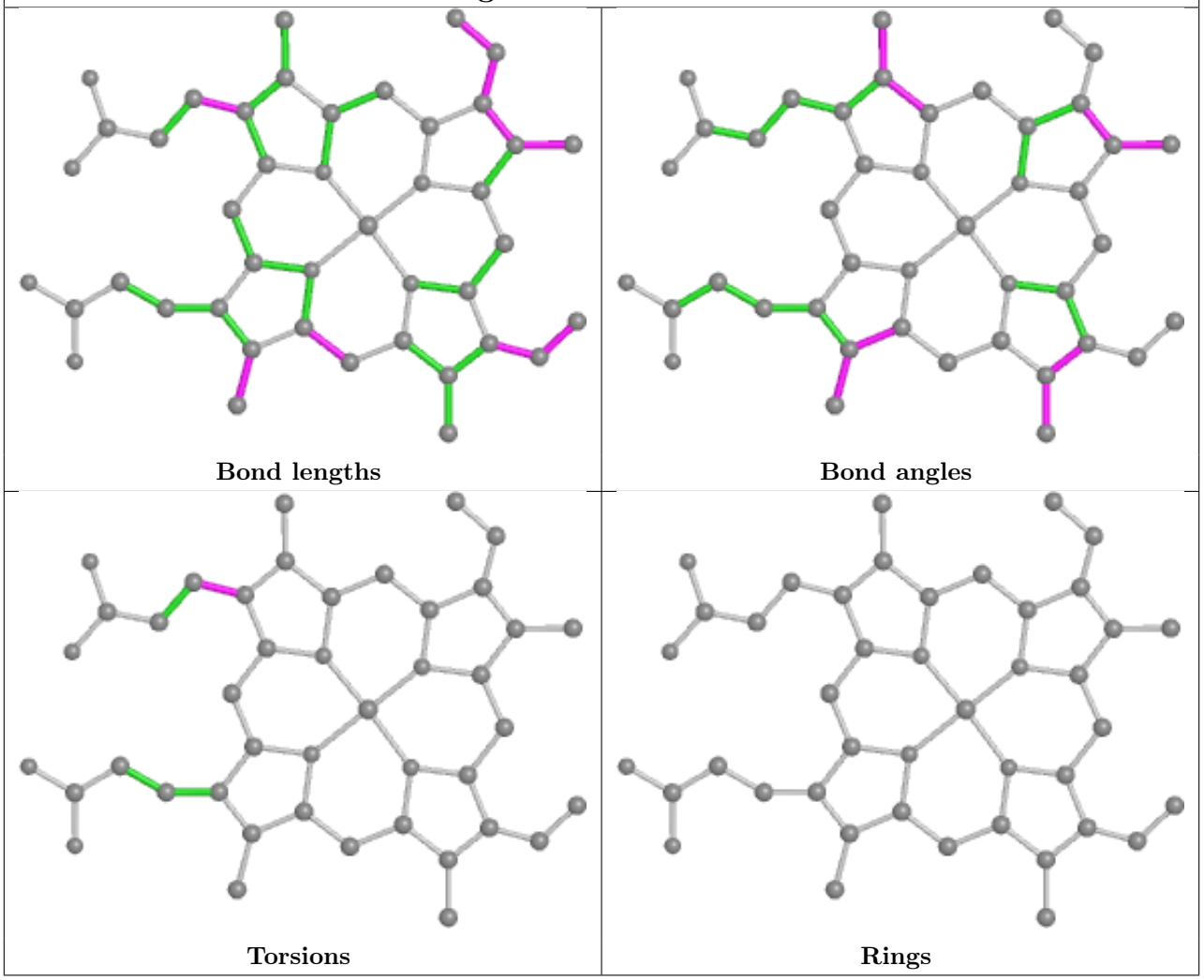


Torsions



Rings

Ligand HEM D 1420



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.27	10 (2%)	53	49	8, 24, 44, 61	0
1	B	347/363 (95%)	-0.30	7 (2%)	65	63	9, 23, 44, 74	0
1	C	346/363 (95%)	-0.32	4 (1%)	79	79	10, 24, 46, 60	0
1	D	346/363 (95%)	-0.27	3 (0%)	84	84	10, 24, 44, 59	0
1	E	347/363 (95%)	-0.21	7 (2%)	65	63	8, 26, 47, 61	0
1	F	344/363 (94%)	-0.24	6 (1%)	70	69	8, 26, 53, 70	0
All	All	2082/2178 (95%)	-0.27	37 (1%)	68	67	8, 24, 46, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	298	GLN	4.9
1	F	191	THR	4.0
1	A	298	GLN	3.8
1	D	203	HIS	3.7
1	F	394	LYS	3.6
1	E	48	ALA	3.6
1	A	200	PRO	3.5
1	A	192	PRO	3.4
1	E	199	SER	3.4
1	C	399	GLU	3.1
1	F	395	GLY	3.1
1	B	401	ASP	3.0
1	D	192	PRO	2.9
1	E	392	LEU	2.9
1	A	193	THR	2.8
1	C	203	HIS	2.7
1	E	204	VAL	2.7
1	A	397	LEU	2.7
1	C	287	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	193	THR	2.6
1	B	202	SER	2.6
1	F	203	HIS	2.5
1	E	200	PRO	2.4
1	D	193	THR	2.4
1	A	194	ASN	2.4
1	A	403	THR	2.3
1	B	47	ASP	2.3
1	B	176	GLU	2.3
1	A	293	LEU	2.2
1	A	401	ASP	2.2
1	B	192	PRO	2.2
1	C	192	PRO	2.1
1	E	396	PHE	2.1
1	B	399	GLU	2.1
1	A	398	LYS	2.1
1	F	49	PRO	2.1
1	F	46	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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
3	HEM	E	1520	43/43	0.89	0.22	36,44,46,46	0
3	HEM	F	1620	43/43	0.90	0.20	30,36,38,40	0
3	HEM	C	1320	43/43	0.92	0.18	28,35,39,39	0
3	HEM	A	1120	43/43	0.92	0.19	20,38,40,42	0
3	HEM	B	1220	43/43	0.92	0.18	27,35,38,40	0

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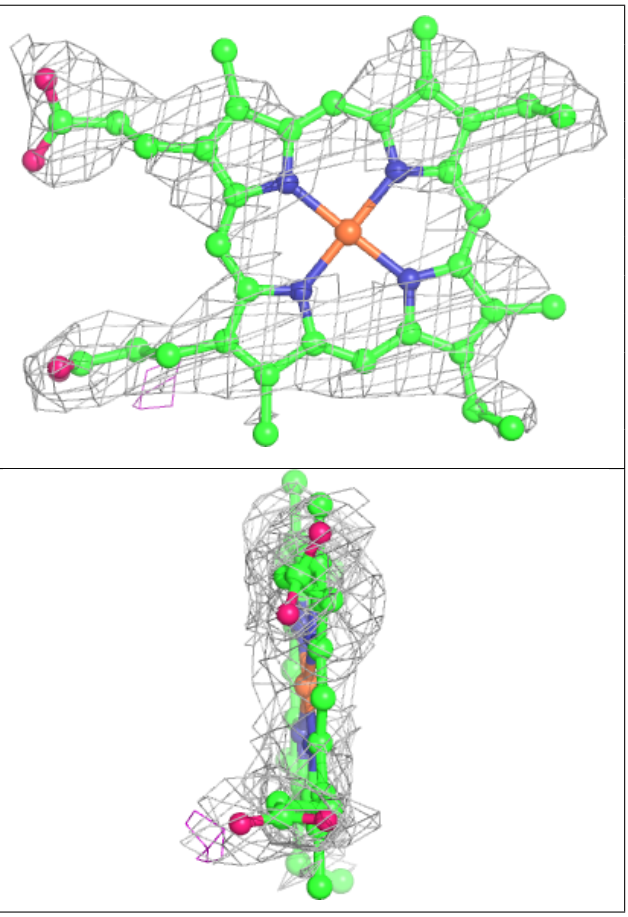
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	D	1420	43/43	0.93	0.16	27,32,34,35	0
2	PLP	D	1410	15/16	0.96	0.16	20,22,24,27	0
2	PLP	E	1510	15/16	0.96	0.17	20,23,26,27	0
2	PLP	A	1110	15/16	0.96	0.14	14,19,23,23	0
2	PLP	B	1210	15/16	0.96	0.16	14,21,22,22	0
2	PLP	C	1310	15/16	0.97	0.15	17,19,23,24	0
2	PLP	F	1610	15/16	0.98	0.12	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.

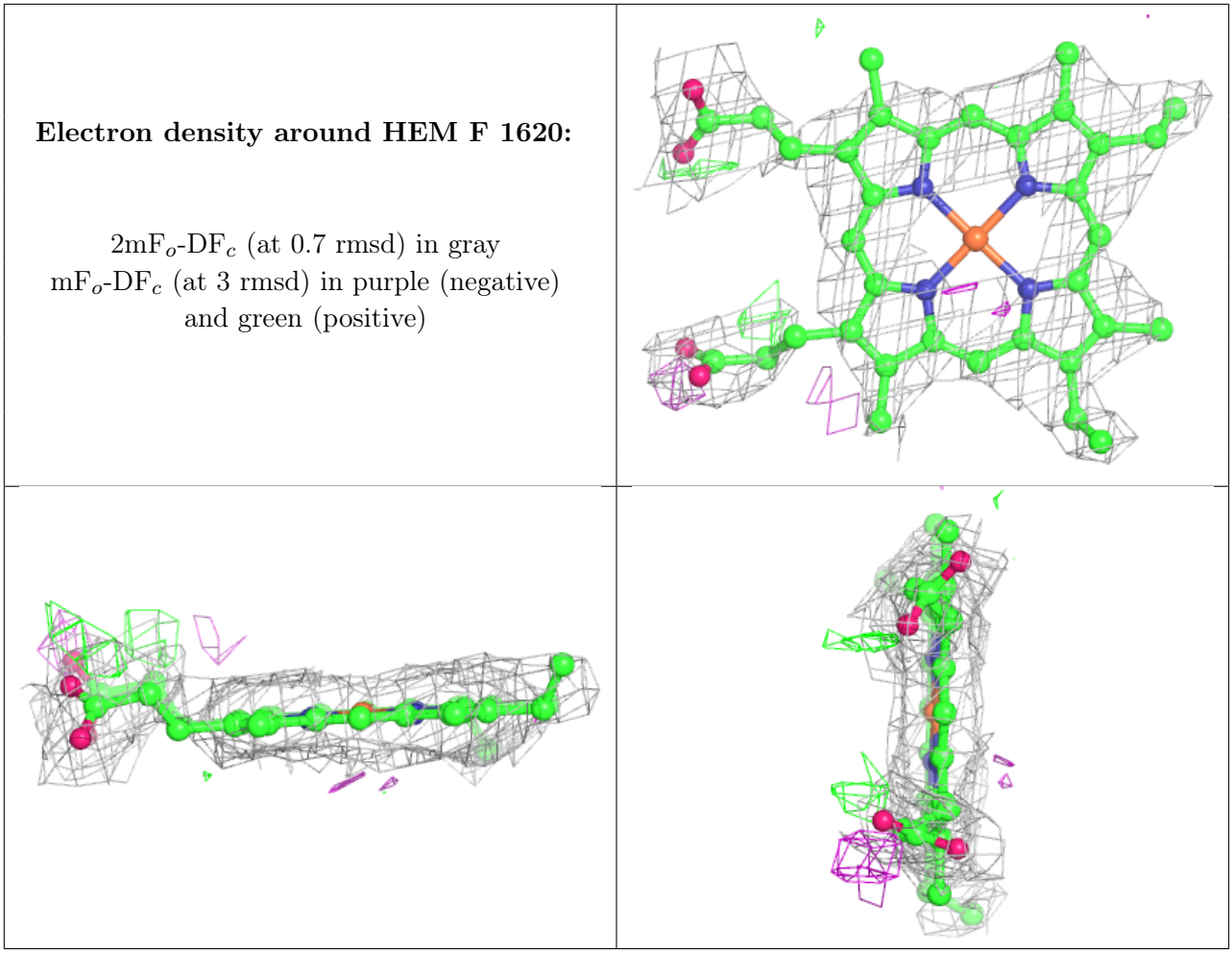
Electron density around HEM E 1520:

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



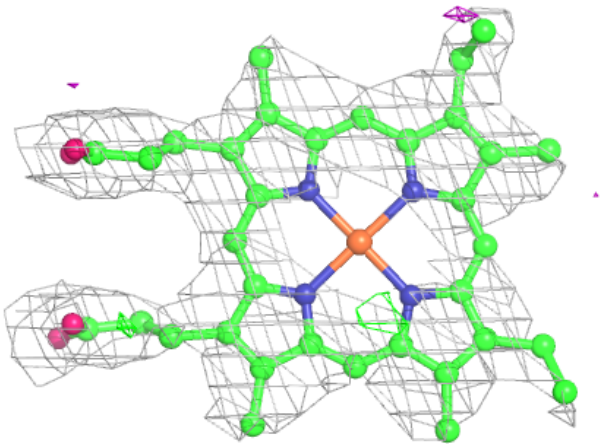
Electron density around HEM F 1620:

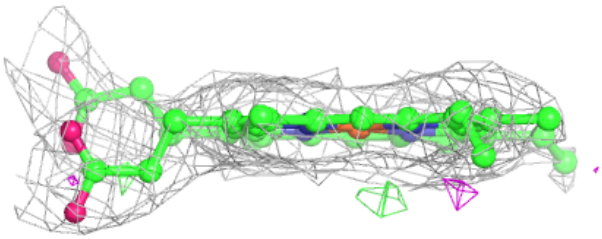
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

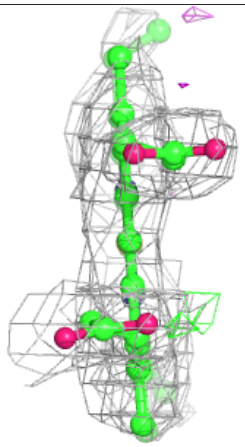


Electron density around HEM C 1320:

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

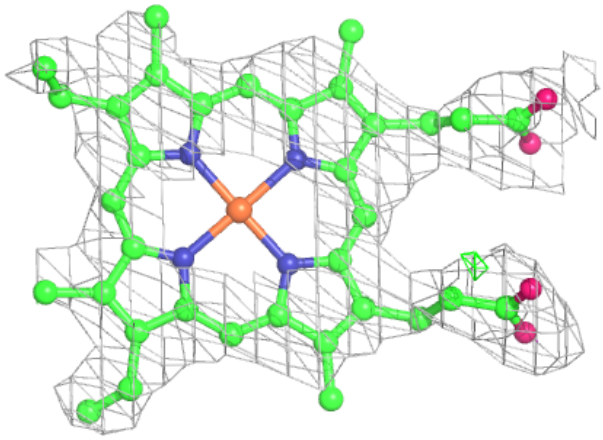


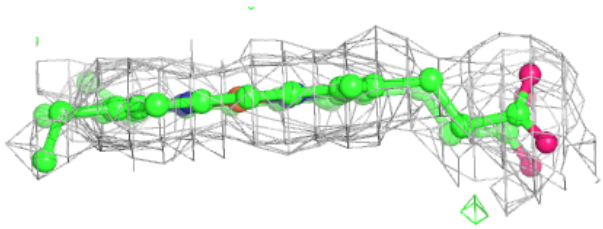


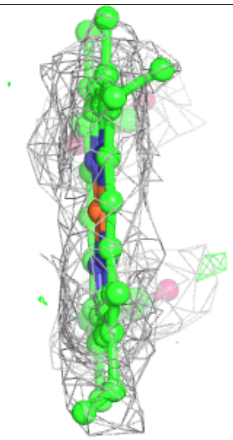


Electron density around HEM A 1120:

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

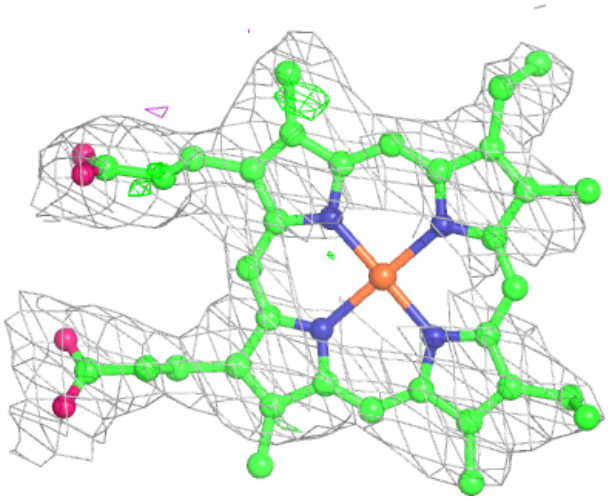


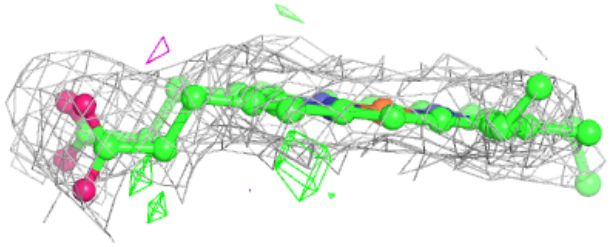


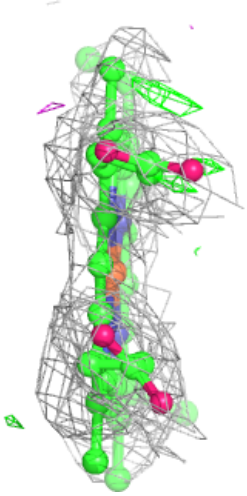


Electron density around HEM B 1220:

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

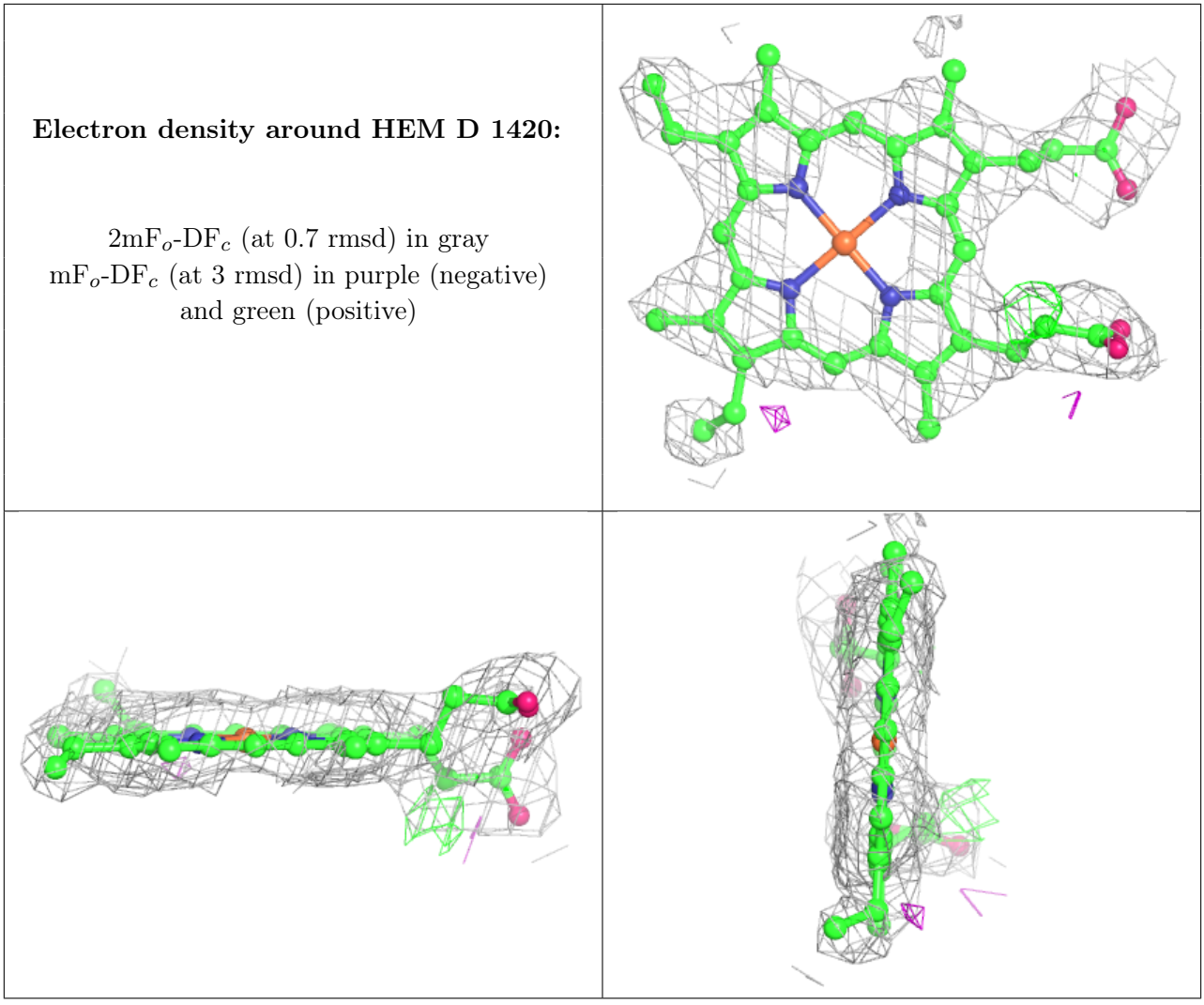






Electron density around HEM D 1420:

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



6.5 Other polymers

There are no such residues in this entry.