



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:12 PM UTC

PDB ID : 9E15 / pdb_00009e15
Title : Alpha-Delta heterodimeric form of soluble hydrogenase I from *Pyrococcus furiosus*. Data processed and model refined in P1
Authors : Lanzilotta, W.N.; McTernan, P.M.; Adams, M.W.W.
Deposited on : 2024-10-21
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

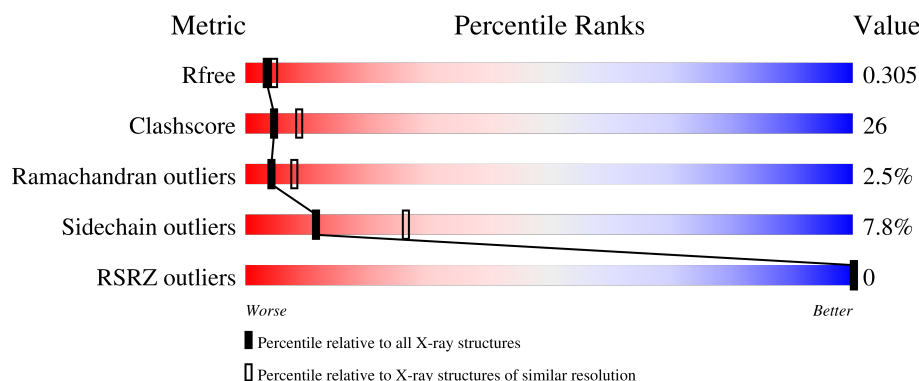
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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








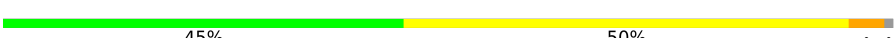


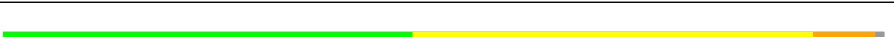
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	266	
1	C	266	
1	E	266	
1	G	266	
1	I	266	

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Mol	Chain	Length	Quality of chain
1	K	266	
1	M	266	
1	O	266	
2	B	424	
2	D	424	
2	F	424	
2	H	424	
2	J	424	
2	L	424	
2	N	424	
2	P	424	

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
3	SF4	A	501	-	-	X	-
3	SF4	C	501	-	-	X	-
3	SF4	C	502	-	-	X	-
3	SF4	C	503	-	-	X	-
3	SF4	E	501	-	-	X	-
3	SF4	E	503	-	-	X	-
3	SF4	G	501	-	-	X	-
3	SF4	G	503	-	-	X	-
3	SF4	I	501	-	-	X	-
3	SF4	K	501	-	-	X	-
3	SF4	K	502	-	-	X	-
3	SF4	K	503	-	-	X	-
3	SF4	M	502	-	-	X	-
3	SF4	M	503	-	-	X	-
3	SF4	O	501	-	-	X	-
4	FCO	B	501	-	-	X	-
4	FCO	D	501	-	-	X	-
4	FCO	F	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FCO	H	501	-	-	X	-
4	FCO	J	501	-	-	X	-
4	FCO	L	501	-	-	X	-
4	FCO	N	501	-	-	X	-
4	FCO	P	501	-	-	X	-
5	NI	H	502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 43445 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 Sulfhydrogenase 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	2	0
			2015	1296	328	371	20			
1	C	256	Total	C	N	O	S	0	1	0
			2008	1290	327	371	20			
1	E	256	Total	C	N	O	S	0	0	0
			2003	1287	327	369	20			
1	G	256	Total	C	N	O	S	0	0	0
			2003	1287	327	369	20			
1	I	256	Total	C	N	O	S	0	2	0
			2018	1298	330	370	20			
1	K	256	Total	C	N	O	S	0	0	0
			2003	1287	327	369	20			
1	M	256	Total	C	N	O	S	0	1	0
			2009	1292	328	369	20			
1	O	256	Total	C	N	O	S	0	1	0
			2009	1292	328	369	20			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP E7FHU4
A	-8	HIS	-	expression tag	UNP E7FHU4
A	-7	HIS	-	expression tag	UNP E7FHU4
A	-6	HIS	-	expression tag	UNP E7FHU4
A	-5	HIS	-	expression tag	UNP E7FHU4
A	-4	HIS	-	expression tag	UNP E7FHU4
A	-3	HIS	-	expression tag	UNP E7FHU4
A	-2	HIS	-	expression tag	UNP E7FHU4
A	-1	HIS	-	expression tag	UNP E7FHU4
A	0	HIS	-	expression tag	UNP E7FHU4
C	-9	MET	-	initiating methionine	UNP E7FHU4
C	-8	HIS	-	expression tag	UNP E7FHU4
C	-7	HIS	-	expression tag	UNP E7FHU4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	expression tag	UNP E7FHU4
C	-5	HIS	-	expression tag	UNP E7FHU4
C	-4	HIS	-	expression tag	UNP E7FHU4
C	-3	HIS	-	expression tag	UNP E7FHU4
C	-2	HIS	-	expression tag	UNP E7FHU4
C	-1	HIS	-	expression tag	UNP E7FHU4
C	0	HIS	-	expression tag	UNP E7FHU4
E	-9	MET	-	initiating methionine	UNP E7FHU4
E	-8	HIS	-	expression tag	UNP E7FHU4
E	-7	HIS	-	expression tag	UNP E7FHU4
E	-6	HIS	-	expression tag	UNP E7FHU4
E	-5	HIS	-	expression tag	UNP E7FHU4
E	-4	HIS	-	expression tag	UNP E7FHU4
E	-3	HIS	-	expression tag	UNP E7FHU4
E	-2	HIS	-	expression tag	UNP E7FHU4
E	-1	HIS	-	expression tag	UNP E7FHU4
E	0	HIS	-	expression tag	UNP E7FHU4
G	-9	MET	-	initiating methionine	UNP E7FHU4
G	-8	HIS	-	expression tag	UNP E7FHU4
G	-7	HIS	-	expression tag	UNP E7FHU4
G	-6	HIS	-	expression tag	UNP E7FHU4
G	-5	HIS	-	expression tag	UNP E7FHU4
G	-4	HIS	-	expression tag	UNP E7FHU4
G	-3	HIS	-	expression tag	UNP E7FHU4
G	-2	HIS	-	expression tag	UNP E7FHU4
G	-1	HIS	-	expression tag	UNP E7FHU4
G	0	HIS	-	expression tag	UNP E7FHU4
I	-9	MET	-	initiating methionine	UNP E7FHU4
I	-8	HIS	-	expression tag	UNP E7FHU4
I	-7	HIS	-	expression tag	UNP E7FHU4
I	-6	HIS	-	expression tag	UNP E7FHU4
I	-5	HIS	-	expression tag	UNP E7FHU4
I	-4	HIS	-	expression tag	UNP E7FHU4
I	-3	HIS	-	expression tag	UNP E7FHU4
I	-2	HIS	-	expression tag	UNP E7FHU4
I	-1	HIS	-	expression tag	UNP E7FHU4
I	0	HIS	-	expression tag	UNP E7FHU4
K	-9	MET	-	initiating methionine	UNP E7FHU4
K	-8	HIS	-	expression tag	UNP E7FHU4
K	-7	HIS	-	expression tag	UNP E7FHU4
K	-6	HIS	-	expression tag	UNP E7FHU4
K	-5	HIS	-	expression tag	UNP E7FHU4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	HIS	-	expression tag	UNP E7FHU4
K	-3	HIS	-	expression tag	UNP E7FHU4
K	-2	HIS	-	expression tag	UNP E7FHU4
K	-1	HIS	-	expression tag	UNP E7FHU4
K	0	HIS	-	expression tag	UNP E7FHU4
M	-9	MET	-	initiating methionine	UNP E7FHU4
M	-8	HIS	-	expression tag	UNP E7FHU4
M	-7	HIS	-	expression tag	UNP E7FHU4
M	-6	HIS	-	expression tag	UNP E7FHU4
M	-5	HIS	-	expression tag	UNP E7FHU4
M	-4	HIS	-	expression tag	UNP E7FHU4
M	-3	HIS	-	expression tag	UNP E7FHU4
M	-2	HIS	-	expression tag	UNP E7FHU4
M	-1	HIS	-	expression tag	UNP E7FHU4
M	0	HIS	-	expression tag	UNP E7FHU4
O	-9	MET	-	initiating methionine	UNP E7FHU4
O	-8	HIS	-	expression tag	UNP E7FHU4
O	-7	HIS	-	expression tag	UNP E7FHU4
O	-6	HIS	-	expression tag	UNP E7FHU4
O	-5	HIS	-	expression tag	UNP E7FHU4
O	-4	HIS	-	expression tag	UNP E7FHU4
O	-3	HIS	-	expression tag	UNP E7FHU4
O	-2	HIS	-	expression tag	UNP E7FHU4
O	-1	HIS	-	expression tag	UNP E7FHU4
O	0	HIS	-	expression tag	UNP E7FHU4

- Molecule 2 is a protein called Sulfhydrogenase 1 subunit alpha.

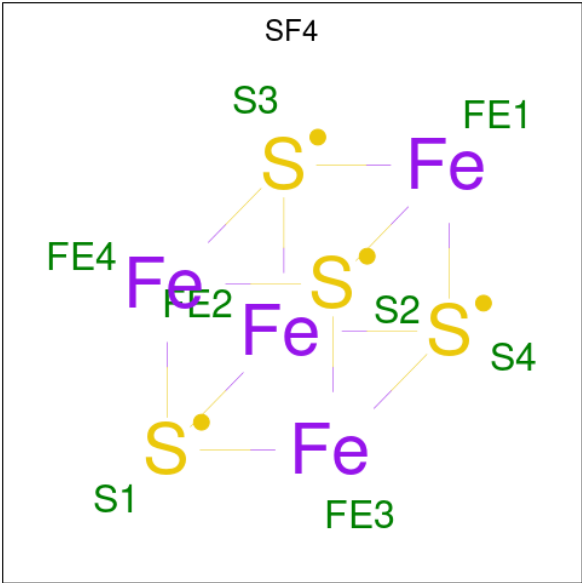
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	3	0
			3349	2158	559	617	15			
2	D	419	Total	C	N	O	S	0	1	0
			3332	2145	556	616	15			
2	F	419	Total	C	N	O	S	0	3	0
			3343	2153	557	618	15			
2	H	420	Total	C	N	O	S	0	0	0
			3330	2143	555	617	15			
2	J	419	Total	C	N	O	S	0	1	0
			3331	2145	555	616	15			
2	L	421	Total	C	N	O	S	0	1	0
			3342	2151	558	618	15			
2	N	421	Total	C	N	O	S	0	1	0
			3342	2151	558	618	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	419	Total	C	N	O	S	0	0	0
			3325	2140	554	616	15			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



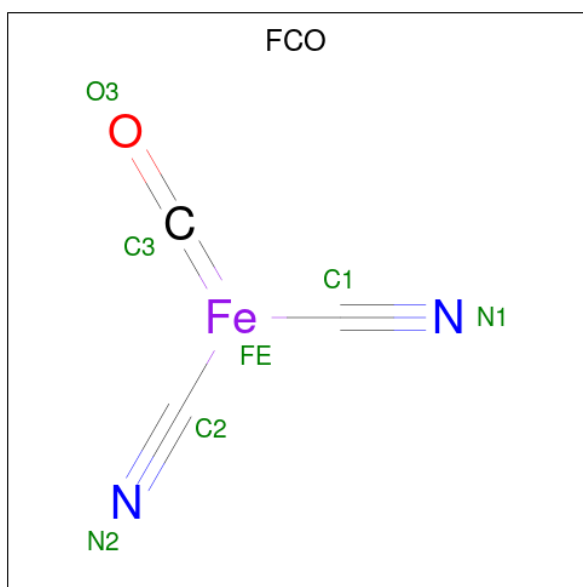
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is CARBONMONOXIDE-(DICYANO) IRON (CCD ID: FCO) (formula: $\text{C}_3\text{FeN}_2\text{O}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	D	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	F	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	H	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	N	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
4	P	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

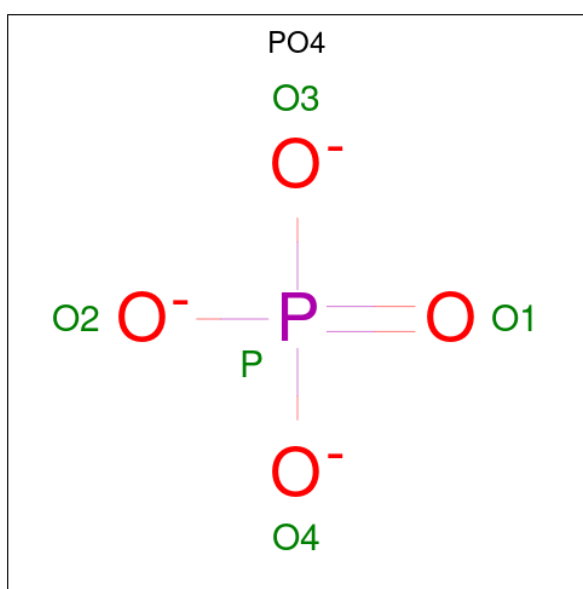
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		
5	F	1	Total	Ni	0	0
			1	1		
5	H	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	1	Total	Ni	0	0
			1	1		
5	L	1	Total	Ni	0	0
			1	1		
5	N	1	Total	Ni	0	0
			1	1		
5	P	1	Total	Ni	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		
6	J	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	O	P	0	0
			5	4	1		
6	P	1	Total	O	P	0	0
			5	4	1		
6	P	1	Total	O	P	0	0
			5	4	1		
6	P	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Mg	0	0
			1	1		
7	P	1	Total	Mg	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	37	Total	O	0	0
			37	37		
8	C	36	Total	O	0	0
			36	36		
8	D	27	Total	O	0	0
			27	27		
8	E	22	Total	O	0	0
			22	22		
8	F	29	Total	O	0	0
			29	29		
8	G	15	Total	O	0	0
			15	15		
8	H	40	Total	O	0	0
			40	40		
8	I	16	Total	O	0	0
			16	16		
8	J	25	Total	O	0	0
			25	25		
8	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	23	Total 23	O 23	0	0
8	M	11	Total 11	O 11	0	0
8	N	18	Total 18	O 18	0	0
8	O	13	Total 13	O 13	0	0
8	P	31	Total 31	O 31	0	0

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.

Chain A:

50% 40% 5%

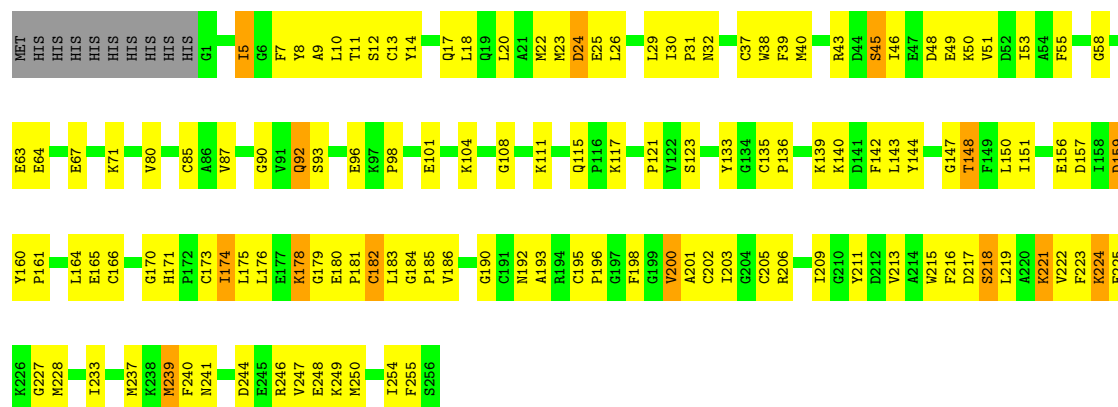
Residue IDs: MET, HIS, HIS, HIS, HIS, HIS, HIS, HIS, HIS, G1, R4, F7, L10, T11, S12, C13, Y14, G15, C16, Q19, L20, M23, D24, E25, L26, L27, Q28, L29, I30, P31, N32, A33, V36, C37, W38, F39, M40, I41, D42, R43, D44, S45, I46, E47, K50, V51, A54, F55, I56, E57, C58.

Chain C:

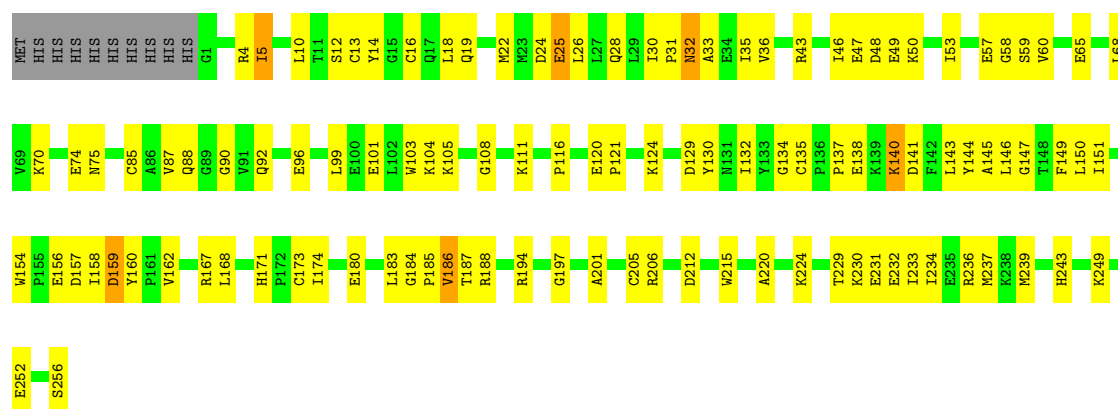
43% 45% 8%

Amino Acid	Category
K221	Basic
V222	Polar
F223	Aromatic
K224	Basic
E225	Acidic
M228	Non-polar
E232	Acidic
L233	Polar
R236	Basic
M237	Non-polar
K238	Basic
M239	Non-polar
F240	Aromatic
E245	Acidic
R246	Basic
V247	Polar
M250	Non-polar
K253	Basic
L254	Polar
F255	Aromatic
S256	Polar
S153	Polar
M154	Non-polar
P155	Polar
L158	Polar
D159	Acidic
Y160	Aromatic
V162	Polar
C163	Cysteine
L164	Polar
E165	Acidic
C166	Cysteine
R167	Basic
L168	Polar
M169	Non-polar
G170	Polar
H171	Polar
P172	Polar
C173	Cysteine
L174	Polar
L175	Polar
L176	Polar
E177	Acidic
K178	Basic
C182	Cysteine
L183	Polar
G184	Polar
P185	Polar
L186	Polar
T187	Polar
R188	Basic
A189	Polar
N192	Polar
A193	Polar
R194	Basic
C195	Cysteine
P196	Polar
G197	Polar
F198	Aromatic
G199	Polar
V200	Polar
A201	Polar
C202	Cysteine
C205	Cysteine
R206	Basic
G207	Polar
D212	Acidic
V213	Polar
A214	Polar
M215	Non-polar
F216	Aromatic
D217	Acidic
S218	Polar
L219	Polar
A220	Polar
I72	Polar
R73	Basic
K77	Basic
I78	Polar
C85	Cysteine
A86	Polar
V87	Polar
Q88	Polar
G89	Polar
G90	Polar
V91	Polar
Q92	Polar
S93	Polar
W94	Aromatic
S95	Polar
L99	Polar
L102	Polar
W103	Aromatic
K104	Basic
K105	Basic
V106	Polar
Y107	Aromatic
K111	Basic
V112	Polar
K113	Basic
F114	Aromatic
Q115	Polar
P116	Polar
K117	Basic
K118	Basic
A119	Polar
E120	Acidic
V121	Polar
V122	Polar
S123	Polar
K127	Basic
V128	Polar
D129	Acidic
Y130	Aromatic
C135	Cysteine
P136	Polar
P137	Polar
C138	Cysteine
K139	Basic
K140	Basic
D141	Acidic
F142	Aromatic
L143	Polar
T148	Polar
F149	Aromatic
G158	Polar
L150	Polar
MET	Start
HIS	Amino Acid
HIS	Amino Acid
HIS	Amino Acid
HIS	Amino Acid
HIS	Amino Acid
HIS	Amino Acid
HIS	Amino Acid
G1	Polar
I5	Polar
G6	Polar
F7	Polar
T11	Polar
S12	Polar
C13	Cysteine
Y14	Aromatic
Q17	Polar
L18	Polar
Q19	Polar
L20	Polar
A21	Polar
M22	Non-polar
M23	Non-polar
L26	Polar
L27	Polar
Q28	Polar
L29	Polar
I30	Polar
P31	Polar
I35	Polar
V36	Polar
C37	Cysteine
W38	Aromatic
F39	Aromatic
M40	Non-polar
I41	Polar
D42	Acidic
R43	Basic
D44	Acidic
S45	Polar
I46	Polar
E47	Acidic
D48	Acidic
V51	Polar
D52	Acidic
I53	Polar
I56	Polar
E57	Acidic
G58	Polar
S59	Polar

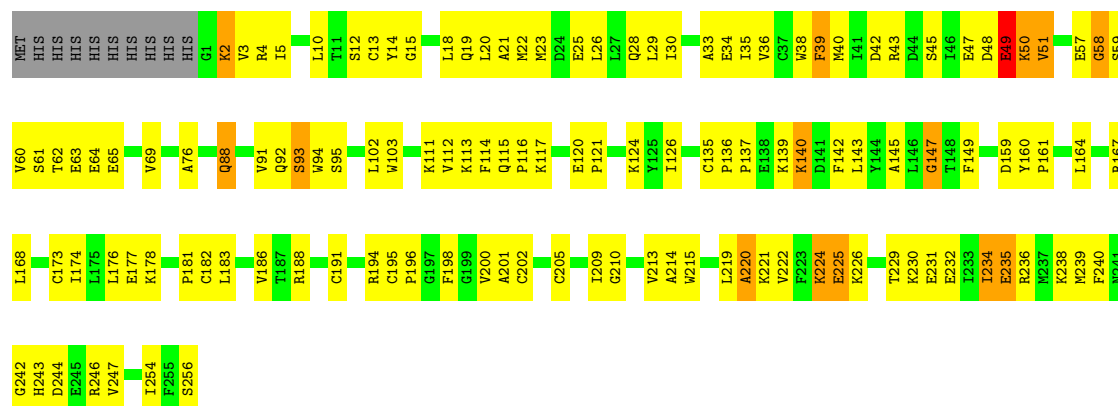
Chain E: 47% 44% 5% .



• Molecule 1: Sulfhydrogenase 1 subunit delta

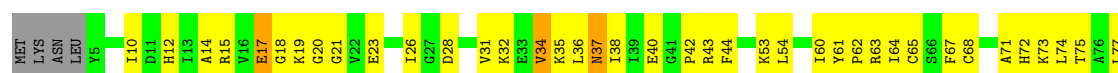


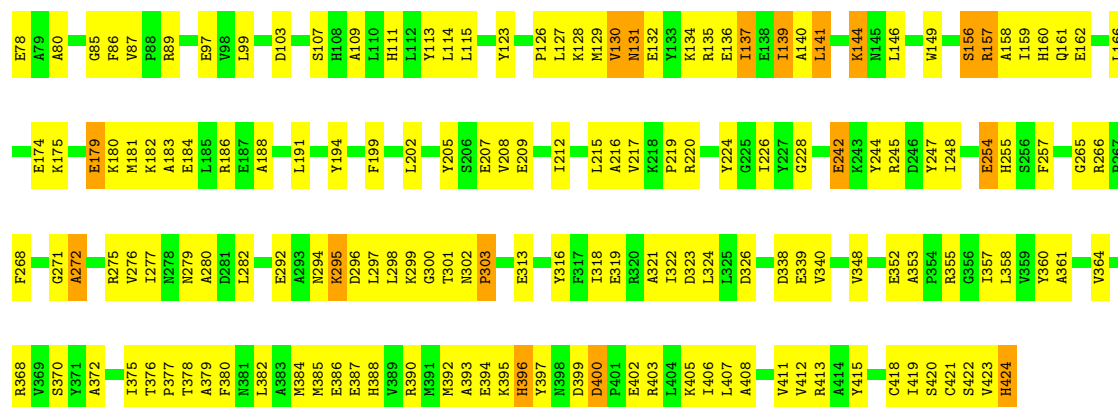
• Molecule 1: Sulfhydrogenase 1 subunit delta



• Molecule 1: Sulfhydrogenase 1 subunit delta

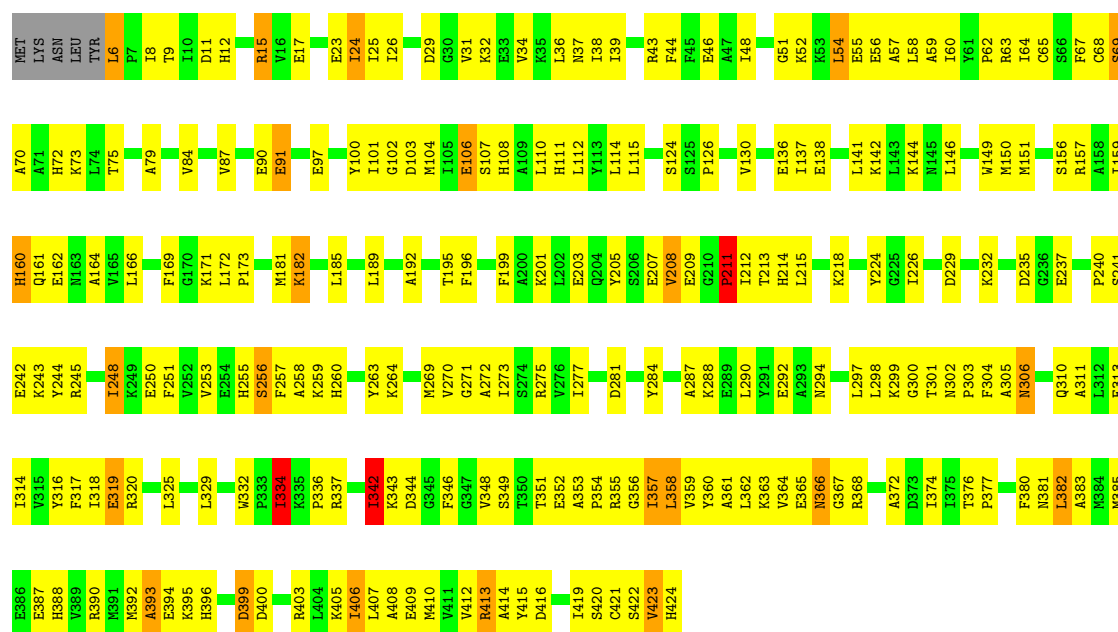






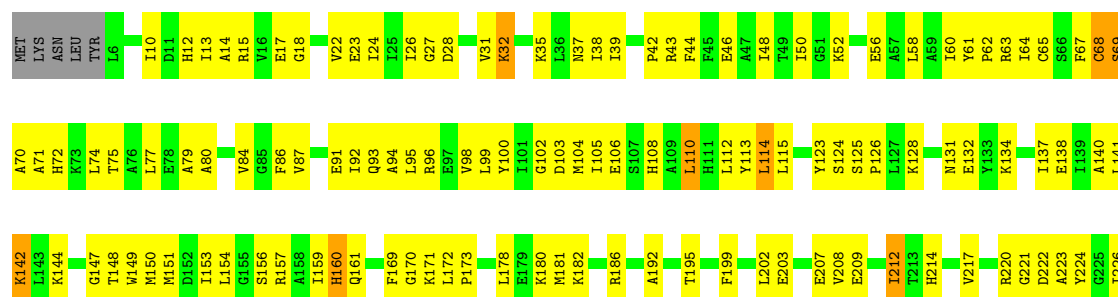
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain D: 44% 48% 5% ..



• Molecule 2: Sulfhydrogenase 1 subunit alpha

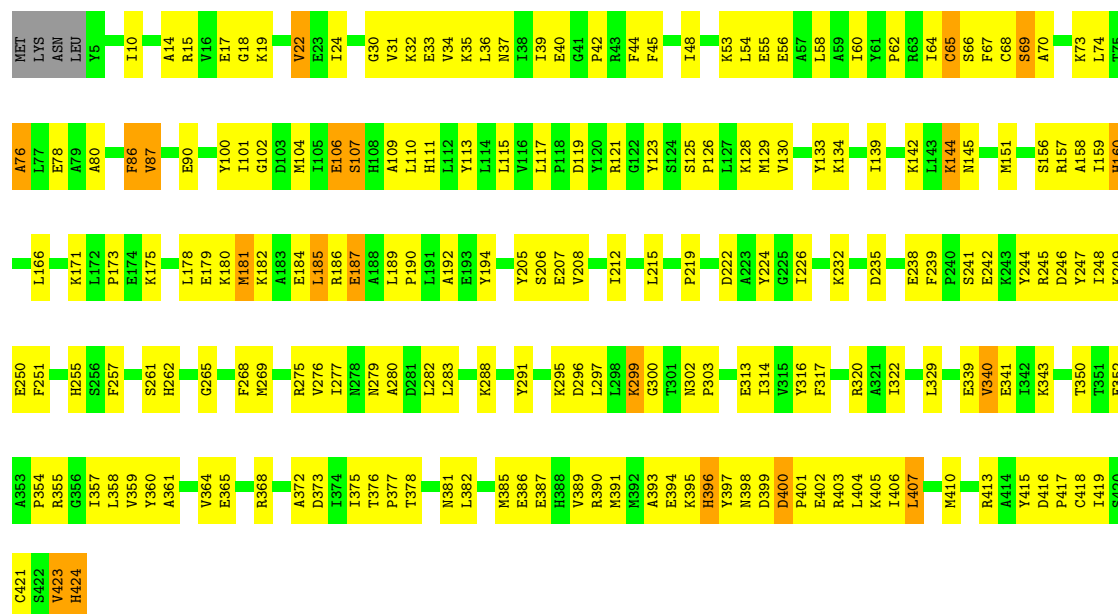
Chain F: 45% 50% ..





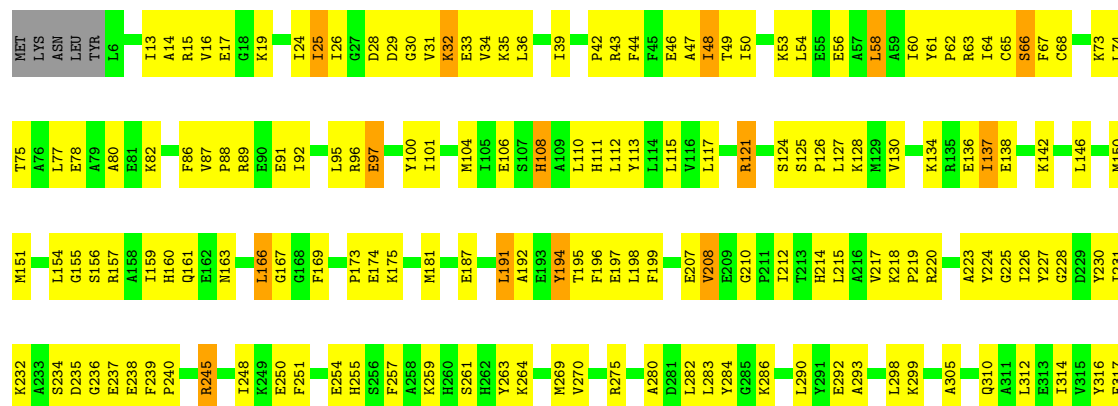
• Molecule 2: Sulfhydrogenase 1 subunit alpha

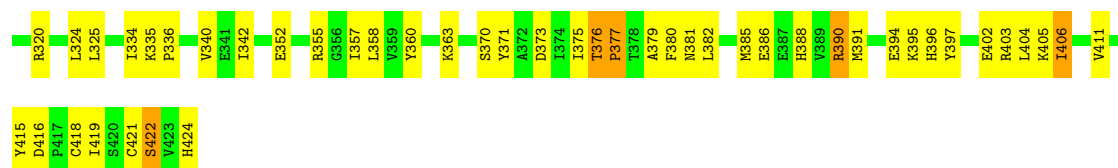
Chain H: 51% 43% 5% •



• Molecule 2: Sulfhydrogenase 1 subunit alpha

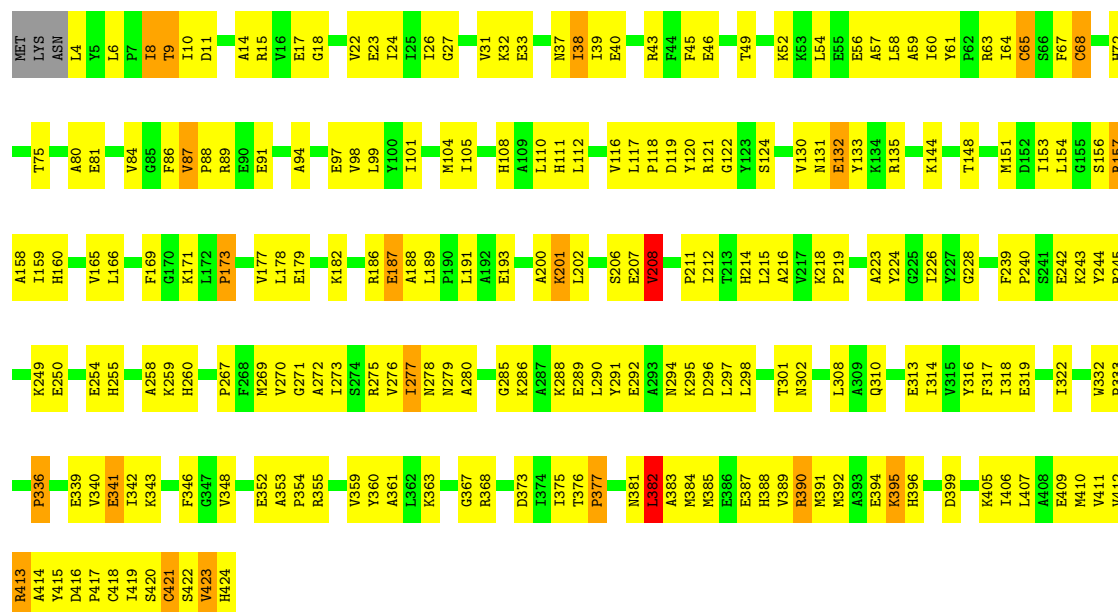
Chain J: 50% 45% 5% •





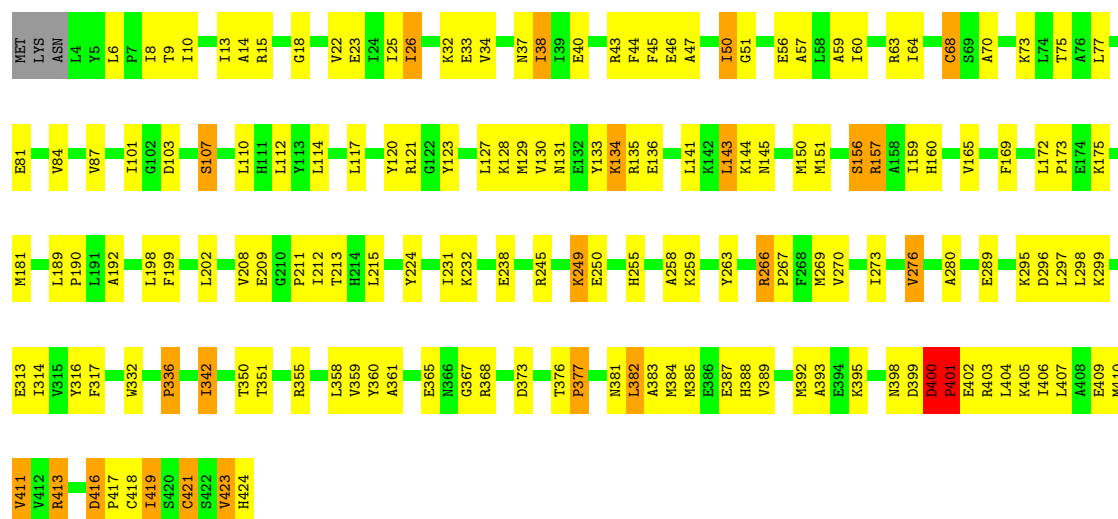
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain L: 47% 47% 5%



• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain N: 61% 33% 5%



• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain P:

46%

45%

7%

MET	L74	T75	A76	L77	E78	L6	E81	K82	F86	W87	A88	A14	R15	V16	E17	G18	K19	V22	E23	L24	G27	D28	D29	G30	V31	K32	L36	N37	E40	F44	F45	E46	A47	I48	T49	I50	K53	E56	A57	L58	A59	I60	Y61	F62	R63	T64	C65	S66	F67	C68	H72	K73
L74	T75	A76	L77	E78	L6	E81	K82	F86	W87	A88	A14	R15	V16	E17	G18	K19	V22	E23	L24	G27	D28	D29	G30	V31	K32	L36	N37	E40	F44	F45	E46	A47	I48	T49	I50	K53	E56	A57	L58	A59	I60	Y61	F62	R63	T64	C65	S66	F67	C68	H72	K73	
S156	R157	A158	I159	H160	Q161	E162	N163	A164	V165	L166	F169	L172	A173	V177	K182	L185	L189	P190	L191	Y194	T195	F196	E197	L198	F199	A200	Q204	V205	E209	G210	P211	H214	L215	A216	V217	K218	P219	R220	A223	Y227	G228	D229	Y230	T231	A232	K233	S234					
E237	E238	F239	P240	S241	E242	K243	Y244	R245	I248	K249	E250	F251	V252	V253	E254	H255	A258	K259	H260	S261	H262	Y263	K264	G265	R266	P267	F268	H269	V270	S274	R275	V276	Y284	G285	K286	A287	L290	L297	L298	T301	N302	F303	L308	A309	Q310	A311	L312	E313	I314	V315		
Y316	F317	I318	E319	R320	A321	I322	D323	L324	L325	A328	L329	I334	K335	P336	R337	V340	K343	F346	G347	V348	S349	T350	T351	E352	R355	G356	L358	V359	Y360	K363	N366	G367	R368	V369	S370	Y371	I375	T376	P377	T378	A379	F380	N381	K384	H385	E386	E387	H388				
V389	R390	N391	N392	A393	E394	K395	H396	Y397	N398	D399	D400	P401	E402	R403	L404	K405	L406	L407	A408	E409	N410	R413	A414	Y415	D416	P417	C418	L419	S420	C421	S422	V423	H424																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.23Å 111.15Å 141.09Å 90.06° 90.02° 90.00°	Depositor
Resolution (Å)	35.84 – 2.60 35.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.84-2.60) 90.2 (35.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.267 , 0.305 0.267 , 0.305	Depositor DCC
R_{free} test set	2007 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.417 for h,-k,-l 0.438 for -h,k,-l 0.407 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	43445	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 27.18 % 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 2.3037e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCO, NI, SF4, MG, PO4

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	0.88	7/2064 (0.3%)	1.14	11/2781 (0.4%)
1	C	0.61	1/2054 (0.0%)	0.97	8/2769 (0.3%)
1	E	0.56	0/2046	0.82	0/2758
1	G	0.51	0/2046	0.77	0/2758
1	I	0.46	0/2064	0.78	1/2780 (0.0%)
1	K	0.51	0/2046	0.76	1/2758 (0.0%)
1	M	0.48	0/2055	0.67	0/2769
1	O	0.46	0/2055	0.77	0/2769
2	B	0.52	0/3429	0.81	0/4628
2	D	0.55	0/3406	0.86	4/4599 (0.1%)
2	F	0.64	3/3423 (0.1%)	0.95	6/4621 (0.1%)
2	H	0.55	0/3400	0.82	2/4591 (0.0%)
2	J	0.53	0/3404	0.78	4/4595 (0.1%)
2	L	0.52	0/3416	0.85	3/4613 (0.1%)
2	N	0.71	8/3416 (0.2%)	1.02	17/4613 (0.4%)
2	P	0.51	0/3395	0.80	1/4584 (0.0%)
All	All	0.57	19/43719 (0.0%)	0.86	58/58986 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
2	D	0	1
2	H	0	1
2	N	0	1
All	All	0	6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	PRO	CB-CG	19.97	2.49	1.49
2	N	400	ASP	C-N	-17.92	1.10	1.33
1	A	196	PRO	N-CD	13.14	1.66	1.47
2	N	267	PRO	CB-CG	-11.84	0.90	1.49
2	F	240	PRO	CB-CG	10.37	2.01	1.49
2	N	416	ASP	C-O	-10.16	1.19	1.23
1	A	196	PRO	CA-CB	-9.96	1.39	1.53
2	F	240	PRO	CG-CD	9.38	1.82	1.50
1	A	196	PRO	N-CA	-9.31	1.35	1.47
2	N	267	PRO	CG-CD	-8.85	1.20	1.50
1	A	10	LEU	CA-C	-7.75	1.48	1.52
1	C	121	PRO	CG-CD	-6.93	1.27	1.50
2	F	255	HIS	CA-C	6.76	1.65	1.52
1	A	195	CYS	C-N	6.40	1.48	1.33
2	N	401	PRO	CG-CD	-6.12	1.29	1.50
2	N	401	PRO	CA-C	5.39	1.60	1.52
2	N	401	PRO	N-CA	5.23	1.54	1.47
2	N	266	ARG	C-O	-5.05	1.18	1.24
1	A	121	PRO	N-CD	5.04	1.54	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	401	PRO	N-CD-CG	-22.60	69.30	103.20
1	A	196	PRO	N-CD-CG	-20.87	71.90	103.20
1	A	196	PRO	CB-CG-CD	-19.80	42.75	106.10
2	N	267	PRO	CA-CB-CG	-19.58	67.30	104.50
2	N	267	PRO	N-CD-CG	-18.67	75.19	103.20
2	N	267	PRO	CB-CG-CD	18.03	163.78	106.10
1	A	196	PRO	N-CA-CB	-15.81	86.65	103.25
2	F	240	PRO	CA-N-CD	-15.43	90.40	112.00
2	F	240	PRO	CB-CG-CD	-14.63	59.27	106.10
2	N	401	PRO	CA-CB-CG	-14.15	77.61	104.50
1	A	121	PRO	N-CD-CG	-12.34	84.69	103.20
1	A	121	PRO	CA-CB-CG	-11.31	83.00	104.50
1	C	121	PRO	CA-CB-CG	-10.46	84.62	104.50
1	A	196	PRO	CA-N-CD	-8.57	100.00	112.00
2	L	173	PRO	N-CD-CG	-8.45	90.53	103.20
2	N	401	PRO	CA-N-CD	8.18	123.45	112.00
1	C	121	PRO	N-CD-CG	-7.80	91.50	103.20
1	A	121	PRO	CA-N-CD	-7.37	101.68	112.00
2	N	401	PRO	CB-CG-CD	7.35	129.63	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	240	PRO	N-CD-CG	-7.25	92.32	103.20
2	N	398	ASN	CA-C-N	7.22	134.09	122.10
2	N	398	ASN	C-N-CA	7.22	134.09	122.10
2	N	267	PRO	CA-N-CD	-7.12	102.03	112.00
2	N	401	PRO	CB-CA-C	6.89	122.96	112.21
1	A	196	PRO	CA-CB-CG	-6.89	91.41	104.50
1	C	121	PRO	CA-N-CD	-6.43	103.00	112.00
2	N	399	ASP	CA-C-N	6.22	129.72	120.83
2	N	399	ASP	C-N-CA	6.22	129.72	120.83
1	C	247	VAL	CA-CB-CG2	-6.14	99.95	110.40
2	D	334	ILE	CA-C-N	6.14	128.90	120.67
2	D	334	ILE	C-N-CA	6.14	128.90	120.67
2	L	173	PRO	CA-CB-CG	-5.96	93.17	104.50
2	H	86	PHE	CA-C-N	5.88	133.00	122.13
2	H	86	PHE	C-N-CA	5.88	133.00	122.13
2	L	187	GLU	CB-CG-CD	-5.85	102.66	112.60
2	J	53	LYS	CD-CE-NZ	5.66	130.02	111.90
2	F	240	PRO	CA-CB-CG	-5.54	93.98	104.50
1	C	237	MET	CG-SD-CE	5.52	113.05	100.90
1	C	247	VAL	N-CA-CB	-5.43	102.27	111.23
1	A	195	CYS	CA-C-N	-5.40	113.09	119.84
1	A	195	CYS	C-N-CA	-5.40	113.09	119.84
2	D	342	ILE	CG1-CB-CG2	-5.36	94.62	110.70
2	D	211	PRO	N-CA-C	5.35	123.48	112.47
2	N	400	ASP	CA-C-O	5.32	124.18	119.71
2	N	400	ASP	CA-C-N	5.27	125.08	119.28
2	N	400	ASP	C-N-CA	5.27	125.08	119.28
1	C	120	GLU	CA-C-N	5.26	125.18	119.76
1	C	120	GLU	C-N-CA	5.26	125.18	119.76
2	F	212	ILE	CB-CG1-CD1	-5.26	102.75	113.80
2	N	399	ASP	N-CA-C	-5.22	101.33	108.38
1	A	195	CYS	C-N-CD	5.22	146.39	125.00
2	P	142	LYS	N-CA-C	-5.21	106.05	112.72
2	J	174	GLU	CA-CB-CG	5.17	124.43	114.10
1	K	98	PRO	N-CD-CG	-5.16	95.46	103.20
1	I	58	GLY	N-CA-C	5.16	116.85	111.95
2	F	401	PRO	N-CA-C	5.08	122.94	112.47
2	J	305	ALA	CA-C-N	5.01	127.31	120.54
2	J	305	ALA	C-N-CA	5.01	127.31	120.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	MET	Peptide
1	C	120	GLU	Mainchain
1	C	121	PRO	Mainchain
2	D	15	ARG	Peptide
2	H	186	ARG	Peptide
2	N	401	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2015	0	2013	103	0
1	C	2008	0	2000	148	1
1	E	2003	0	1995	123	0
1	G	2003	0	1994	89	0
1	I	2018	0	2019	114	1
1	K	2003	0	1997	107	1
1	M	2009	0	2006	71	0
1	O	2009	0	2007	110	1
2	B	3349	0	3387	174	1
2	D	3332	0	3359	213	1
2	F	3343	0	3376	220	1
2	H	3330	0	3355	163	0
2	J	3331	0	3365	187	1
2	L	3342	0	3363	206	0
2	N	3342	0	3363	145	0
2	P	3325	0	3352	205	0
3	A	24	0	0	6	0
3	C	24	0	0	13	0
3	E	24	0	0	9	0
3	G	24	0	0	6	0
3	I	24	0	0	3	0
3	K	24	0	0	17	0
3	M	24	0	0	6	0
3	O	24	0	0	3	0
4	B	7	0	0	5	0
4	D	7	0	0	8	0
4	F	7	0	0	7	0
4	H	7	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	7	0	0	5	0
4	L	7	0	0	16	0
4	N	7	0	0	19	0
4	P	7	0	0	5	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	2	0
5	J	1	0	0	0	0
5	L	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	1	0
6	B	10	0	0	0	0
6	F	10	0	0	0	0
6	H	5	0	0	0	0
6	I	5	0	0	1	0
6	J	5	0	0	0	0
6	L	5	0	0	1	0
6	P	15	0	0	1	0
7	H	1	0	0	0	0
7	P	1	0	0	0	0
8	A	19	0	0	5	0
8	B	37	0	0	2	0
8	C	36	0	0	4	0
8	D	27	0	0	9	0
8	E	22	0	0	2	0
8	F	29	0	0	7	0
8	G	15	0	0	2	0
8	H	40	0	0	7	0
8	I	16	0	0	2	0
8	J	25	0	0	2	0
8	K	8	0	0	0	0
8	L	23	0	0	8	0
8	M	11	0	0	0	0
8	N	18	0	0	4	0
8	O	13	0	0	4	0
8	P	31	0	0	10	0
All	All	43445	0	42951	2217	4

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 26.

All (2217) 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)
2:F:240:PRO:CG	2:F:240:PRO:CD	1.82	1.57
2:N:377:PRO:HD2	4:N:501:FCO:C1	1.25	1.56
2:L:377:PRO:HD2	4:L:501:FCO:C1	1.40	1.48
2:L:377:PRO:HD2	4:L:501:FCO:N1	1.24	1.45
2:N:377:PRO:CD	4:N:501:FCO:N1	1.78	1.42
2:F:240:PRO:CG	2:F:240:PRO:CB	2.01	1.39
2:N:377:PRO:CD	4:N:501:FCO:C1	2.03	1.33
2:N:377:PRO:HD2	4:N:501:FCO:N1	0.96	1.26
2:L:377:PRO:CD	4:L:501:FCO:N1	1.98	1.26
1:K:173:CYS:SG	3:K:503:SF4:S2	2.37	1.22
2:L:377:PRO:CD	4:L:501:FCO:C1	2.19	1.19
2:N:421:CYS:SG	4:N:501:FCO:C1	2.34	1.16
1:K:16:CYS:SG	3:K:501:SF4:FE4	1.42	1.11
2:H:68:CYS:SG	5:H:502:NI:NI	1.38	1.07
2:F:26:ILE:HG22	2:F:27:GLY:H	1.19	1.03
1:O:140:LYS:NZ	8:O:601:HOH:O	1.90	1.03
1:I:238:LYS:HD3	1:I:242:GLY:HA2	1.38	1.03
2:D:377:PRO:HD2	4:D:501:FCO:N1	1.74	1.03
2:L:68:CYS:SG	4:L:501:FCO:C3	2.47	1.02
2:P:286:LYS:NZ	2:P:290:LEU:HD21	1.75	1.02
2:P:81:GLU:OE2	8:P:601:HOH:O	1.78	1.01
2:D:377:PRO:HD2	4:D:501:FCO:C1	1.91	1.00
2:P:214:HIS:HD1	2:P:274:SER:HG	1.07	0.99
2:F:150:MET:HG2	2:F:181:MET:HE3	1.45	0.98
1:I:43:ARG:HH12	2:J:406:ILE:HG22	1.28	0.94
1:K:13:CYS:SG	3:K:501:SF4:FE2	1.60	0.93
2:L:68:CYS:SG	4:L:501:FCO:C2	2.57	0.93
2:F:240:PRO:HB2	2:F:243:LYS:HB2	1.49	0.93
2:L:68:CYS:SG	4:L:501:FCO:FE	1.60	0.92
1:K:16:CYS:HG	3:K:501:SF4:FE4	0.67	0.92
1:G:47:GLU:OE1	1:G:68:LEU:HD11	1.68	0.92
2:F:70:ALA:HB2	2:F:151:MET:HE3	1.49	0.92
2:L:269:MET:HE1	2:L:273:ILE:HG22	1.51	0.92
2:B:392:MET:HE3	2:B:407:LEU:HB3	1.53	0.91
2:P:68:CYS:SG	5:P:502:NI:NI	1.52	0.91
2:D:111:HIS:HA	2:D:115:LEU:HD12	1.50	0.91
1:E:186:VAL:HG11	1:E:237:MET:HE3	1.50	0.91
2:P:211:PRO:O	8:P:602:HOH:O	1.90	0.90
1:C:173:CYS:HG	3:C:503:SF4:FE1	0.78	0.89
1:E:173:CYS:HG	3:E:503:SF4:FE1	0.62	0.89
2:L:201:LYS:NZ	8:L:601:HOH:O	2.04	0.89
1:E:13:CYS:SG	3:E:501:SF4:S1	2.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:224:TYR:OH	2:H:313:GLU:OE2	1.91	0.88
2:H:377:PRO:HD2	4:H:501:FCO:C1	2.04	0.87
2:F:240:PRO:CG	2:F:240:PRO:N	2.37	0.87
1:K:163:CYS:SG	3:K:503:SF4:S1	2.72	0.87
2:P:209:GLU:HG3	2:P:302:ASN:HD22	1.39	0.87
2:F:70:ALA:HB2	2:F:151:MET:CE	2.05	0.87
1:A:195:CYS:CA	1:A:196:PRO:HG2	2.05	0.86
1:E:23:MET:HE1	1:E:142:PHE:HB2	1.57	0.86
2:H:62:PRO:HG3	2:H:73:LYS:HD2	1.56	0.86
2:F:350:THR:HG22	2:F:359:VAL:HG12	1.56	0.86
2:F:387:GLU:CD	2:F:390:ARG:HH21	1.83	0.86
1:I:136:PRO:HG3	2:J:159:ILE:HB	1.57	0.86
2:J:218:LYS:HB2	2:J:232:LYS:HG3	1.57	0.85
1:C:12:SER:HB3	1:C:58:GLY:HA2	1.55	0.85
2:N:377:PRO:CG	4:N:501:FCO:N1	2.39	0.85
2:D:403:ARG:HH11	2:D:403:ARG:HG3	1.42	0.85
2:P:286:LYS:HZ1	2:P:290:LEU:HD21	1.39	0.85
2:L:110:LEU:HD21	2:L:144:LYS:HG3	1.56	0.84
1:C:85:CYS:SG	3:C:501:SF4:FE3	1.68	0.84
2:H:377:PRO:HD2	4:H:501:FCO:N1	1.92	0.84
1:A:13:CYS:SG	3:A:501:SF4:FE2	1.69	0.84
2:N:38:ILE:HG13	2:N:382:LEU:HD11	1.59	0.84
2:F:346:PHE:HD1	2:F:363:LYS:HB2	1.43	0.83
2:H:110:LEU:HD21	2:H:144:LYS:HG3	1.61	0.83
1:E:195:CYS:HB3	1:E:200:VAL:HG22	1.61	0.83
2:H:53:LYS:HB2	2:H:56:GLU:HG3	1.61	0.83
2:J:390:ARG:HH21	2:J:391:MET:HA	1.42	0.83
1:K:138:GLU:HB3	1:K:140:LYS:HG3	1.59	0.82
2:H:175:LYS:HE3	2:H:329:LEU:HD22	1.61	0.82
1:A:239:MET:HG3	2:B:60:ILE:HD11	1.62	0.82
2:F:207:GLU:OE1	2:F:396:HIS:NE2	2.13	0.82
1:K:173:CYS:SG	3:K:503:SF4:FE1	1.72	0.82
1:E:22:MET:HE1	2:F:148:THR:OG1	1.79	0.82
2:F:170:GLY:O	8:F:601:HOH:O	1.97	0.82
2:N:250:GLU:HG2	2:N:259:LYS:HD2	1.61	0.82
1:G:10:LEU:HG	1:G:65:GLU:HG2	1.61	0.81
1:C:173:CYS:SG	3:C:503:SF4:FE1	1.71	0.81
2:F:26:ILE:HG22	2:F:27:GLY:N	1.90	0.81
1:I:229:THR:HG23	1:I:232:GLU:H	1.46	0.81
1:E:178:LYS:O	1:E:178:LYS:HD2	1.79	0.81
1:O:13:CYS:SG	3:O:501:SF4:S1	2.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:381:ASN:O	2:P:385:MET:HB2	1.81	0.81
1:E:211:TYR:OH	1:E:216:PHE:N	2.13	0.80
1:K:246:ARG:HA	1:K:249:LYS:HE2	1.63	0.80
2:L:250:GLU:HG2	2:L:259:LYS:HD2	1.63	0.80
2:N:68:CYS:SG	4:N:501:FCO:FE	1.74	0.80
2:F:388:HIS:HD1	2:F:415:TYR:HH	1.29	0.80
2:N:68:CYS:SG	4:N:501:FCO:C2	2.70	0.80
2:D:209:GLU:OE1	2:D:302:ASN:ND2	2.14	0.80
2:D:395:LYS:NZ	8:D:604:HOH:O	2.13	0.80
1:M:22:MET:HG2	2:N:144:LYS:HD2	1.62	0.80
1:A:195:CYS:N	1:A:196:PRO:HG2	1.97	0.79
2:L:38:ILE:HG13	2:L:382:LEU:HD11	1.64	0.79
2:L:387:GLU:OE2	2:L:390:ARG:NH2	2.14	0.79
2:P:237:GLU:OE1	2:P:263:TYR:OH	1.99	0.79
2:L:276:VAL:O	2:L:280:ALA:HB2	1.82	0.79
2:L:377:PRO:CG	4:L:501:FCO:N1	2.45	0.79
2:J:36:LEU:HD11	2:J:385:MET:HG2	1.64	0.79
2:D:8:ILE:H	2:D:24:ILE:HG22	1.49	0.79
1:E:211:TYR:HB2	1:E:254:ILE:HD11	1.65	0.78
2:P:108:HIS:HB2	2:P:314:ILE:HD11	1.65	0.78
1:E:43:ARG:HB2	2:F:15:ARG:HH21	1.48	0.78
2:L:211:PRO:O	2:L:212:ILE:HG13	1.84	0.78
1:C:164:LEU:HD21	1:C:215:TRP:CZ3	2.18	0.78
1:K:9:ALA:HB2	1:K:17:GLN:HE22	1.49	0.78
2:N:377:PRO:CG	4:N:501:FCO:C1	2.61	0.78
2:H:32:LYS:O	8:H:601:HOH:O	2.03	0.77
2:D:346:PHE:HD1	2:D:363:LYS:HB2	1.48	0.77
3:G:503:SF4:S2	8:G:606:HOH:O	2.41	0.77
2:L:382:LEU:HD21	8:L:610:HOH:O	1.84	0.77
1:C:43:ARG:HB3	2:D:124:SER:HB2	1.67	0.77
2:D:416:ASP:OD2	8:D:601:HOH:O	2.02	0.77
2:N:393:ALA:HA	2:N:404:LEU:HD11	1.67	0.77
1:C:22:MET:HE3	2:D:144:LYS:HD3	1.67	0.77
1:C:177:GLU:HG2	1:C:178:LYS:HD2	1.67	0.77
1:O:135:CYS:HB3	1:O:205:CYS:HB2	1.66	0.76
2:P:218:LYS:HG3	2:P:232:LYS:HD2	1.66	0.76
2:D:259:LYS:O	8:D:602:HOH:O	2.03	0.76
2:L:6:LEU:HG	2:L:26:ILE:HD11	1.66	0.76
2:P:286:LYS:HZ2	2:P:290:LEU:HD21	1.48	0.76
2:B:74:LEU:HD11	2:B:99:LEU:HD23	1.68	0.76
2:H:245:ARG:HH21	2:H:375:ILE:HD11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:289:GLU:OE1	2:N:289:GLU:N	2.19	0.76
2:F:240:PRO:CG	2:F:240:PRO:CA	2.64	0.76
2:D:388:HIS:ND1	2:D:415:TYR:OH	2.19	0.75
2:F:65:CYS:CB	2:F:68:CYS:SG	2.71	0.75
1:M:17:GLN:HE21	1:M:38:TRP:HE1	1.34	0.75
2:P:217:VAL:HG23	2:P:357:ILE:HG12	1.68	0.75
2:F:247:TYR:OH	8:F:602:HOH:O	2.03	0.75
2:H:222:ASP:OD2	8:H:602:HOH:O	2.03	0.75
1:M:166:CYS:SG	1:M:171:HIS:HB2	2.25	0.75
1:A:26:LEU:HA	1:A:29:LEU:HD12	1.68	0.75
2:D:9:THR:HG22	2:D:23:GLU:HG2	1.69	0.75
2:L:260:HIS:CE1	2:L:382:LEU:HD22	2.22	0.74
2:B:245:ARG:HH21	2:B:375:ILE:HD11	1.52	0.74
1:C:116:PRO:HG3	2:D:257:PHE:HE1	1.51	0.74
2:F:75:THR:HG22	2:F:360:TYR:HB2	1.70	0.74
2:L:377:PRO:CG	4:L:501:FCO:C1	2.65	0.74
2:P:139:ILE:HG23	2:P:191:LEU:HB3	1.67	0.74
2:F:74:LEU:HD22	2:F:96:ARG:HG2	1.68	0.74
1:I:47:GLU:OE1	1:I:47:GLU:N	2.21	0.74
2:L:4:LEU:N	8:L:604:HOH:O	2.20	0.74
2:N:361:ALA:HB3	2:N:373:ASP:HB3	1.68	0.74
1:O:39:PHE:HD1	2:P:14:ALA:HB2	1.53	0.74
2:J:121:ARG:HH12	2:J:198:LEU:HD11	1.52	0.73
2:J:355:ARG:N	4:J:501:FCO:N2	2.35	0.73
2:P:403:ARG:O	2:P:406:ILE:HG13	1.88	0.73
1:A:10:LEU:HD22	1:A:65:GLU:HG2	1.70	0.73
2:L:75:THR:HG22	2:L:360:TYR:HB2	1.71	0.73
2:P:50:ILE:O	8:P:605:HOH:O	2.06	0.73
1:C:85:CYS:HG	3:C:501:SF4:FE3	1.04	0.73
1:G:16:CYS:SG	3:G:501:SF4:FE4	1.78	0.73
1:I:174:ILE:HG22	1:I:178:LYS:HG3	1.70	0.73
1:I:224:LYS:O	1:I:226:LYS:N	2.22	0.73
2:F:123:TYR:OH	2:F:132:GLU:OE1	2.05	0.73
1:K:58:GLY:H	1:K:86:ALA:HB2	1.53	0.73
2:P:197:GLU:HA	2:P:200:ALA:HB3	1.70	0.73
1:E:13:CYS:SG	3:E:501:SF4:FE2	1.79	0.73
1:E:173:CYS:SG	3:E:503:SF4:FE1	1.78	0.73
2:F:281:ASP:OD2	8:F:603:HOH:O	2.06	0.73
1:C:223:PHE:HB3	1:C:228:MET:HB2	1.69	0.73
1:E:37:CYS:HG	1:E:45:SER:HG	1.37	0.73
1:O:18:LEU:HD11	2:P:110:LEU:HD21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:PRO:HG3	2:J:73:LYS:HB2	1.70	0.73
2:P:9:THR:OG1	8:P:606:HOH:O	2.07	0.73
2:P:248:ILE:O	8:P:603:HOH:O	2.06	0.73
2:L:289:GLU:OE1	2:L:289:GLU:N	2.17	0.72
2:N:232:LYS:HG2	2:N:238:GLU:HG2	1.70	0.72
2:P:387:GLU:OE2	8:P:604:HOH:O	2.06	0.72
2:B:35:LYS:HD3	2:B:255:HIS:CD2	2.24	0.72
2:J:230:TYR:HD1	2:J:240:PRO:HA	1.54	0.72
2:L:212:ILE:HG12	2:L:384:MET:HE2	1.71	0.72
2:H:242:GLU:OE1	8:H:603:HOH:O	2.07	0.72
2:H:166:LEU:HB3	2:H:340:VAL:HG21	1.70	0.72
1:K:98:PRO:HD2	1:K:101:GLU:HB2	1.71	0.72
1:K:166:CYS:SG	1:K:171:HIS:HB2	2.28	0.72
1:E:64:GLU:OE1	8:E:601:HOH:O	2.07	0.72
2:H:101:ILE:HG23	2:H:317:PHE:HB3	1.70	0.72
2:J:245:ARG:HA	2:J:245:ARG:HH11	1.54	0.72
2:P:409:GLU:HB3	2:P:413:ARG:NH2	2.05	0.72
2:B:34:VAL:HG11	2:B:390:ARG:HB2	1.72	0.72
2:H:276:VAL:O	2:H:280:ALA:HB2	1.90	0.72
1:C:136:PRO:HG3	2:D:159:ILE:HB	1.72	0.71
1:C:216:PHE:HB2	1:C:219:LEU:HB2	1.72	0.71
2:D:409:GLU:OE1	2:D:413:ARG:NH1	2.13	0.71
2:F:91:GLU:OE1	2:F:91:GLU:N	2.23	0.71
1:A:40:MET:HE3	2:B:67:PHE:HZ	1.55	0.71
2:D:355:ARG:HB2	4:D:501:FCO:N2	2.05	0.71
2:B:242:GLU:HA	2:B:348:VAL:HG11	1.71	0.71
1:E:17:GLN:HE21	1:E:38:TRP:HE1	1.37	0.71
2:F:387:GLU:OE2	2:F:390:ARG:NH2	2.22	0.71
1:A:4:ARG:HG3	1:A:36:VAL:HG11	1.72	0.71
2:H:14:ALA:O	2:H:413:ARG:NH1	2.23	0.71
2:J:388:HIS:ND1	2:J:415:TYR:OH	2.23	0.71
2:N:68:CYS:SG	4:N:501:FCO:C3	2.78	0.71
2:B:380:PHE:O	8:B:601:HOH:O	2.09	0.71
2:D:79:ALA:HB2	2:D:349:SER:HB2	1.73	0.71
2:N:14:ALA:O	2:N:413:ARG:NH1	2.24	0.70
2:H:265:GLY:O	2:P:131:ASN:ND2	2.23	0.70
2:B:385:MET:HE1	2:B:412:VAL:HG13	1.73	0.70
2:D:392:MET:SD	2:D:407:LEU:HB3	2.31	0.70
1:E:37:CYS:SG	1:E:45:SER:OG	2.49	0.70
1:I:167:ARG:HD3	1:K:28:GLN:HB3	1.71	0.70
1:I:39:PHE:O	2:J:14:ALA:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:113:TYR:OH	2:J:195:THR:OG1	2.10	0.70
1:C:116:PRO:HG3	2:D:257:PHE:CE1	2.26	0.70
1:E:40:MET:O	2:F:15:ARG:HA	1.91	0.70
1:C:37:CYS:SG	8:C:604:HOH:O	2.39	0.70
1:I:2:LYS:HB3	1:I:34:GLU:HG3	1.74	0.70
2:L:353:ALA:O	2:L:355:ARG:N	2.24	0.70
2:B:43:ARG:N	2:B:424:HIS:OXT	2.14	0.69
2:D:242:GLU:HA	2:D:348:VAL:HG11	1.74	0.69
1:K:163:CYS:SG	3:K:503:SF4:FE3	1.84	0.69
1:O:63:GLU:HB2	1:O:115:GLN:HB2	1.74	0.69
2:P:356:GLY:O	2:P:377:PRO:HG3	1.92	0.69
1:E:164:LEU:HD11	1:E:215:TRP:CZ3	2.27	0.69
1:O:43:ARG:HH12	2:P:406:ILE:HG22	1.57	0.69
2:P:368:ARG:HD3	6:P:504:PO4:O1	1.92	0.69
2:F:26:ILE:CG2	2:F:27:GLY:H	2.02	0.69
2:J:235:ASP:OD1	2:J:237:GLU:N	2.26	0.69
1:K:232:GLU:HG2	1:K:236:ARG:NH2	2.06	0.69
1:M:18:LEU:HG	1:M:22:MET:HE2	1.73	0.69
1:O:239:MET:HE3	2:P:60:ILE:HG12	1.74	0.69
1:O:247:VAL:HG13	1:O:248:GLU:HG2	1.73	0.69
2:F:157:ARG:O	2:F:161:GLN:HG3	1.93	0.69
1:K:232:GLU:HG2	1:K:236:ARG:HH21	1.57	0.69
2:B:275:ARG:HD3	2:B:352:GLU:CD	2.18	0.69
1:A:141:ASP:OD2	1:A:206:ARG:NH2	2.26	0.69
2:D:108:HIS:CE1	2:D:310:GLN:HG2	2.28	0.69
1:O:27:LEU:H	1:O:27:LEU:HD22	1.58	0.69
1:C:173:CYS:SG	3:C:503:SF4:S4	2.91	0.68
2:H:173:PRO:HG2	2:H:178:LEU:HD21	1.75	0.68
2:L:38:ILE:HG23	2:L:419:ILE:HG23	1.76	0.68
2:B:208:VAL:HB	2:B:303:PRO:HG2	1.75	0.68
2:F:381:ASN:O	2:F:383:ALA:N	2.26	0.68
1:I:159:ASP:OD1	1:I:188:ARG:NH1	2.26	0.68
1:I:182:CYS:HA	1:I:201:ALA:HB1	1.74	0.68
2:L:18:GLY:HA3	2:L:419:ILE:HB	1.75	0.68
1:A:244:ASP:OD2	1:A:246:ARG:NH2	2.26	0.68
3:C:502:SF4:S2	8:D:620:HOH:O	2.50	0.68
1:G:13:CYS:HB2	2:H:65:CYS:HA	1.73	0.68
1:O:167:ARG:HH12	1:O:215:TRP:HB3	1.58	0.68
1:C:120:GLU:HG3	1:C:121:PRO:HD2	1.75	0.68
2:N:169:PHE:O	2:N:336:PRO:HB2	1.94	0.68
2:B:10:ILE:HG13	2:B:405:LYS:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:57:ALA:O	2:N:60:ILE:HG22	1.94	0.68
1:O:118:LYS:O	8:O:602:HOH:O	2.12	0.68
2:P:114:LEU:HD23	2:P:126:PRO:HB2	1.75	0.68
2:D:356:GLY:HA3	2:D:377:PRO:HB3	1.76	0.68
2:F:416:ASP:OD2	8:F:604:HOH:O	2.11	0.68
1:O:229:THR:HG23	1:O:232:GLU:H	1.59	0.68
1:G:99:LEU:O	1:G:103:TRP:N	2.24	0.68
2:H:18:GLY:HA3	2:H:419:ILE:HB	1.74	0.68
1:K:59:SER:OG	1:K:92:GLN:NE2	2.26	0.67
2:B:32:LYS:O	8:B:602:HOH:O	2.11	0.67
2:N:395:LYS:HE2	2:N:395:LYS:HA	1.76	0.67
1:A:43:ARG:HH22	2:B:406:ILE:HG12	1.59	0.67
2:H:397:TYR:HA	2:H:404:LEU:HD22	1.77	0.67
2:L:406:ILE:O	2:L:410:MET:HG3	1.93	0.67
2:P:19:LYS:HG3	2:P:40:GLU:HG2	1.75	0.67
2:F:147:GLY:HA2	2:F:150:MET:HE2	1.76	0.67
1:G:43:ARG:NH2	2:H:406:ILE:HG12	2.08	0.67
2:H:205:TYR:O	2:H:302:ASN:ND2	2.22	0.67
2:H:316:TYR:OH	2:H:320:ARG:HD2	1.94	0.67
2:N:421:CYS:SG	4:N:501:FCO:FE	1.85	0.67
2:J:215:LEU:O	2:J:270:VAL:HG12	1.94	0.67
2:N:384:MET:HE2	2:N:388:HIS:CE1	2.29	0.67
1:O:40:MET:O	2:P:15:ARG:HA	1.95	0.67
2:B:208:VAL:HG23	2:B:302:ASN:OD1	1.93	0.67
2:F:26:ILE:HD13	2:F:31:VAL:HG22	1.76	0.67
1:M:138:GLU:HB3	1:M:140[B]:LYS:HG3	1.77	0.67
1:A:168:LEU:HD13	1:C:143:LEU:HD22	1.76	0.67
1:I:62:THR:CG2	1:I:64:GLU:HG3	2.25	0.67
2:F:392:MET:SD	2:F:407:LEU:HB3	2.35	0.67
2:H:395:LYS:NZ	1:M:225:GLU:O	2.28	0.67
1:K:43:ARG:NH2	2:L:409:GLU:OE2	2.27	0.67
2:B:224:TYR:OH	2:B:313:GLU:OE2	2.11	0.66
2:D:146:LEU:HG	2:D:150:MET:HE3	1.76	0.66
1:E:186:VAL:CG1	1:E:237:MET:HE3	2.23	0.66
1:O:136:PRO:HD2	2:P:157:ARG:CZ	2.24	0.66
1:A:253:LYS:O	8:A:601:HOH:O	2.12	0.66
1:I:12:SER:HB2	3:I:501:SF4:S1	2.35	0.66
2:D:224:TYR:HB3	2:D:316:TYR:CE2	2.31	0.66
2:N:421:CYS:CB	4:N:501:FCO:C1	2.72	0.66
2:B:321:ALA:HA	2:B:324:LEU:HB2	1.78	0.66
2:L:166:LEU:HB3	2:L:340:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:377:PRO:HG2	4:L:501:FCO:N1	2.10	0.66
2:N:355:ARG:HG2	2:N:416:ASP:HB3	1.77	0.66
1:C:53:ILE:HG13	1:C:78:ILE:HD12	1.78	0.66
2:F:287:ALA:HB2	2:F:316:TYR:HB2	1.77	0.66
1:I:136:PRO:HD2	2:J:157:ARG:CZ	2.25	0.66
2:P:169:PHE:O	2:P:337:ARG:HG2	1.96	0.66
2:P:209:GLU:O	2:P:391:MET:HE1	1.96	0.65
2:L:15:ARG:HB2	2:L:413:ARG:HD3	1.78	0.65
1:A:135:CYS:HB3	1:A:205:CYS:HB2	1.78	0.65
2:L:224:TYR:OH	2:L:313:GLU:OE2	2.13	0.65
2:P:398:ASN:OD1	2:P:399:ASP:N	2.28	0.65
1:E:136:PRO:HG3	2:F:159:ILE:HB	1.79	0.65
2:L:45:PHE:HE2	2:L:61:TYR:HA	1.61	0.65
1:M:176:LEU:HD21	1:M:216:PHE:HE2	1.60	0.65
2:N:156:SER:OG	2:N:157:ARG:HG3	1.95	0.65
2:P:242:GLU:HG3	2:P:348:VAL:HB	1.79	0.65
2:F:355:ARG:HB2	4:F:501:FCO:N2	2.11	0.65
1:I:224:LYS:NZ	8:I:603:HOH:O	2.29	0.65
2:N:215:LEU:O	2:N:270:VAL:HG12	1.97	0.65
1:G:167:ARG:HH12	1:G:215:TRP:HB3	1.61	0.65
2:P:196:PHE:HE1	2:P:312:LEU:HB2	1.61	0.65
1:E:22:MET:HG2	2:F:144:LYS:HD2	1.78	0.65
2:H:181:MET:O	2:H:184:GLU:N	2.30	0.65
1:K:25:GLU:HB3	1:K:28:GLN:HB2	1.79	0.65
2:L:94:ALA:O	2:L:98:VAL:HG23	1.97	0.65
2:P:385:MET:HG2	8:P:613:HOH:O	1.96	0.65
1:C:188:ARG:NH1	1:C:207:GLY:HA3	2.12	0.65
1:O:236:ARG:HH21	2:P:53:LYS:HZ2	1.45	0.65
2:P:346:PHE:CE1	2:P:363:LYS:HB2	2.32	0.65
1:C:135:CYS:HG	3:C:501:SF4:FE1	1.10	0.64
1:C:135:CYS:SG	3:C:501:SF4:FE1	1.89	0.64
1:G:180:GLU:HB3	1:G:201:ALA:HB2	1.77	0.64
1:M:139:LYS:HE3	1:M:140[B]:LYS:HG2	1.78	0.64
1:A:19:GLN:NE2	1:A:137:PRO:O	2.30	0.64
2:P:95:LEU:HD13	2:P:172:LEU:HD22	1.78	0.64
1:A:23:MET:HB2	1:A:26:LEU:HD13	1.78	0.64
1:C:245:GLU:N	1:C:245:GLU:OE1	2.28	0.64
2:J:230:TYR:CD1	2:J:240:PRO:HA	2.32	0.64
2:L:260:HIS:HE1	2:L:382:LEU:HD22	1.60	0.64
1:E:216:PHE:HB2	1:E:219:LEU:HB2	1.80	0.64
2:F:406:ILE:O	2:F:410:MET:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:MET:HE1	2:D:185:LEU:HD21	1.80	0.64
2:D:57:ALA:O	2:D:60:ILE:HG22	1.98	0.64
1:E:136:PRO:O	2:F:157:ARG:NH2	2.29	0.64
1:E:244:ASP:HB3	1:E:247:VAL:HG23	1.78	0.64
1:G:138:GLU:HB3	1:G:140:LYS:HG3	1.80	0.64
1:I:26:LEU:HA	1:I:29:LEU:HB2	1.79	0.64
1:I:43:ARG:HB2	2:J:15:ARG:HH21	1.61	0.64
2:L:421:CYS:CB	4:L:501:FCO:C1	2.75	0.64
1:A:43:ARG:NH2	2:B:406:ILE:HG12	2.13	0.64
2:L:342:ILE:HG22	2:L:342:ILE:O	1.96	0.64
2:P:346:PHE:HE1	2:P:363:LYS:HB2	1.63	0.64
1:A:50:LYS:HA	1:A:75:ASN:HB3	1.80	0.63
2:D:215:LEU:O	2:D:270:VAL:HG12	1.98	0.63
2:N:276:VAL:O	2:N:280:ALA:HB2	1.98	0.63
1:I:239:MET:SD	2:J:60:ILE:HD11	2.38	0.63
2:F:421:CYS:CB	4:F:501:FCO:C1	2.75	0.63
2:H:19:LYS:HB2	2:H:40:GLU:HG2	1.79	0.63
1:I:230[A]:LYS:O	1:I:234:ILE:HG13	1.98	0.63
2:N:224:TYR:HB3	2:N:316:TYR:CE2	2.33	0.63
1:O:98:PRO:HG2	1:O:101:GLU:HB2	1.80	0.63
1:E:17:GLN:HE21	1:E:38:TRP:NE1	1.96	0.63
1:E:166:CYS:SG	1:E:171:HIS:HB2	2.38	0.63
1:G:47:GLU:CD	1:G:68:LEU:HD11	2.24	0.63
2:H:117:LEU:HG	2:H:121:ARG:HG3	1.80	0.63
2:J:78:GLU:OE1	2:J:82:LYS:NZ	2.32	0.63
2:J:239:PHE:HZ	2:J:248:ILE:HD11	1.64	0.63
1:A:195:CYS:H	1:A:196:PRO:HG2	1.63	0.63
1:O:27:LEU:HD21	2:P:127:LEU:HD22	1.80	0.63
8:O:608:HOH:O	2:P:60:ILE:HG21	1.97	0.63
1:C:20:LEU:HD23	1:C:38:TRP:CH2	2.34	0.63
1:I:88:GLN:NE2	1:I:240:PHE:O	2.32	0.63
2:J:415:TYR:HB3	8:J:615:HOH:O	1.98	0.63
2:F:364:VAL:HG23	2:F:368:ARG:O	1.98	0.63
1:I:5:ILE:HD13	1:I:33:ALA:HB1	1.80	0.63
1:K:98:PRO:HB2	1:K:100:GLU:HG2	1.80	0.63
2:L:296:ASP:N	8:L:608:HOH:O	2.30	0.63
2:N:258:ALA:HB2	2:N:423:VAL:HG22	1.79	0.63
1:A:218:SER:HB3	1:A:221:LYS:HB3	1.81	0.63
1:E:182:CYS:SG	1:E:183:LEU:N	2.71	0.63
2:D:355:ARG:HG2	2:D:416:ASP:HB3	1.80	0.63
2:L:224:TYR:HB3	2:L:316:TYR:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:GLU:HG3	1:E:71:LYS:NZ	2.14	0.62
2:J:15:ARG:HD3	2:J:126:PRO:HD3	1.81	0.62
1:K:246:ARG:HA	1:K:249:LYS:CE	2.29	0.62
1:C:37:CYS:SG	1:C:45:SER:OG	2.57	0.62
1:M:162:VAL:HG23	1:M:187:THR:O	1.99	0.62
2:H:245:ARG:NH2	2:H:375:ILE:HD11	2.13	0.62
1:I:18:LEU:HD11	2:J:110:LEU:HD21	1.81	0.62
2:L:214:HIS:O	2:L:278:ASN:ND2	2.31	0.62
1:O:10:LEU:HD22	1:O:65:GLU:HG2	1.80	0.62
2:D:365:GLU:O	2:D:366:ASN:HB3	1.99	0.62
2:F:10:ILE:HB	2:F:22:VAL:HB	1.80	0.62
1:A:234:ILE:HD11	1:A:251:VAL:HG21	1.81	0.62
1:C:91:VAL:C	1:C:93:SER:H	2.06	0.62
1:C:120:GLU:HG3	1:C:121:PRO:CD	2.28	0.62
1:C:166:CYS:SG	1:C:171:HIS:HB2	2.39	0.62
2:D:157:ARG:O	2:D:161:GLN:HG3	1.99	0.62
2:N:350:THR:HG22	2:N:359:VAL:HB	1.81	0.62
1:O:9:ALA:O	2:P:19:LYS:HD3	1.99	0.62
1:A:28:GLN:HB3	1:C:167:ARG:HD3	1.80	0.62
1:A:78:ILE:HD13	1:A:149:PHE:CE1	2.35	0.62
1:E:67:GLU:HG3	1:E:71:LYS:HZ1	1.65	0.62
2:F:283:LEU:HD22	2:F:287:ALA:HB1	1.80	0.62
2:F:224:TYR:OH	2:F:275:ARG:HB3	2.00	0.62
1:I:43:ARG:NH1	2:J:406:ILE:HG22	2.08	0.62
1:K:63:GLU:HB2	1:K:115:GLN:HB2	1.81	0.62
1:G:158:ILE:O	1:G:188:ARG:NH1	2.33	0.62
1:I:229:THR:HG23	1:I:232:GLU:N	2.13	0.62
1:K:41:ILE:HG13	1:K:42:ASP:N	2.14	0.62
1:O:43:ARG:NH1	2:P:406:ILE:HG22	2.14	0.62
1:I:40:MET:O	2:J:15:ARG:HA	2.00	0.62
1:O:236:ARG:HH21	2:P:53:LYS:NZ	1.98	0.62
1:C:246:ARG:HH21	1:C:250:MET:HE1	1.65	0.61
2:F:195:THR:HG22	2:F:311:ALA:HB1	1.80	0.61
1:G:16:CYS:HB2	1:G:57:GLU:HG3	1.81	0.61
1:K:96:GLU:OE1	1:K:96:GLU:N	2.24	0.61
1:O:182:CYS:HA	1:O:201:ALA:HB1	1.82	0.61
1:A:162:VAL:HG23	1:A:187:THR:O	2.00	0.61
1:E:185:PRO:HD3	3:E:503:SF4:S4	2.41	0.61
2:H:44:PHE:O	2:H:48:ILE:HG23	2.00	0.61
2:L:33:GLU:OE2	2:L:390:ARG:HD3	2.01	0.61
1:C:224:LYS:HG2	1:C:225:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ARG:NH2	1:C:250:MET:HE1	2.16	0.61
2:D:46:GLU:HB3	2:D:372:ALA:O	2.00	0.61
1:E:63:GLU:HG3	1:E:115:GLN:HB3	1.83	0.61
2:J:74:LEU:HD22	2:J:96:ARG:HG2	1.81	0.61
2:L:156:SER:OG	2:L:157:ARG:HG3	2.00	0.61
2:D:68:CYS:HA	2:D:103:ASP:OD2	2.01	0.61
2:D:100:TYR:CD1	2:D:226:ILE:HD13	2.35	0.61
1:O:26:LEU:HA	1:O:29:LEU:HG	1.80	0.61
1:O:195:CYS:HB3	1:O:200:VAL:HG23	1.82	0.61
2:B:31:VAL:HG21	2:B:394:GLU:HG2	1.83	0.61
2:H:34:VAL:HG21	2:H:389:VAL:HG23	1.81	0.61
2:L:65:CYS:HB3	2:L:68:CYS:H	1.66	0.61
2:B:377:PRO:HD2	4:B:501:FCO:C1	2.30	0.61
1:E:246:ARG:HB2	1:E:250:MET:HE3	1.83	0.61
1:G:43:ARG:HH22	2:H:406:ILE:HG12	1.65	0.61
2:N:377:PRO:HG2	4:N:501:FCO:N1	2.14	0.61
1:C:160:TYR:HB2	1:C:164:LEU:HD12	1.83	0.61
1:E:246:ARG:O	1:E:250:MET:HG3	2.00	0.61
2:F:344:ASP:HA	2:F:364:VAL:CG1	2.31	0.61
2:F:125:SER:HB3	2:F:128:LYS:HG3	1.83	0.61
2:H:250:GLU:OE2	2:H:261:SER:OG	2.18	0.61
1:M:220:ALA:HB2	1:M:254:ILE:O	2.00	0.61
1:C:163:CYS:SG	1:C:185:PRO:HD3	2.40	0.60
2:D:241:SER:O	2:D:244:TYR:HB3	2.01	0.60
1:G:25:GLU:O	1:G:28:GLN:N	2.33	0.60
1:C:182:CYS:SG	1:C:183:LEU:N	2.72	0.60
2:D:337:ARG:NH1	8:D:605:HOH:O	2.34	0.60
1:I:12:SER:HB3	1:I:58:GLY:HA2	1.83	0.60
2:J:396:HIS:HD2	2:J:403:ARG:HH22	1.49	0.60
1:K:246:ARG:O	1:K:250:MET:HG3	2.00	0.60
1:C:90:GLY:O	1:C:93:SER:HB2	2.00	0.60
2:L:110:LEU:H	2:L:110:LEU:HD22	1.67	0.60
1:G:141:ASP:OD2	1:G:206:ARG:NH2	2.33	0.60
2:L:117:LEU:O	2:L:119:ASP:N	2.34	0.60
2:N:407:LEU:HA	2:N:410:MET:HE3	1.82	0.60
2:H:68:CYS:HG	5:H:502:NI:NI	0.25	0.60
1:K:220:ALA:HB2	1:K:254:ILE:HG22	1.84	0.60
2:B:181:MET:O	2:B:184:GLU:N	2.32	0.60
2:D:409:GLU:HB3	2:D:413:ARG:CZ	2.32	0.60
1:E:182:CYS:HA	1:E:201:ALA:HB1	1.84	0.60
1:O:134:GLY:HA2	1:O:206:ARG:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:OE1	1:A:68:LEU:HD11	2.01	0.60
1:A:221:LYS:HD2	1:A:225:GLU:OE2	2.02	0.60
2:H:34:VAL:HG21	2:H:389:VAL:CG2	2.32	0.60
1:K:40:MET:HE3	2:L:67:PHE:HZ	1.66	0.60
2:L:26:ILE:HG22	2:L:31:VAL:HG22	1.84	0.60
2:H:296:ASP:HA	2:H:299:LYS:HE3	1.84	0.60
2:L:81:GLU:HA	2:L:84:VAL:HG22	1.81	0.60
2:L:273:ILE:HD13	2:L:298:LEU:HD22	1.82	0.60
2:N:381:ASN:O	2:N:383:ALA:N	2.30	0.60
2:P:123:TYR:CD1	2:P:129:MET:HG2	2.35	0.60
2:P:153:ILE:HD12	2:P:177:VAL:HG11	1.84	0.60
1:E:247:VAL:HA	1:E:250:MET:SD	2.42	0.60
1:C:39:PHE:O	2:D:15:ARG:N	2.22	0.60
2:H:45:PHE:CD2	2:H:64:ILE:HG12	2.37	0.60
2:P:215:LEU:O	2:P:270:VAL:HG12	2.02	0.60
1:K:174:ILE:HB	1:K:180:GLU:OE2	2.02	0.59
2:D:270:VAL:N	2:D:381:ASN:OD1	2.34	0.59
2:F:248:ILE:HG22	2:F:250:GLU:OE2	2.02	0.59
1:I:22:MET:HE1	2:J:106:GLU:CD	2.27	0.59
2:L:219:PRO:HD3	2:L:279:ASN:ND2	2.17	0.59
2:P:77:LEU:HD13	2:P:96:ARG:HH21	1.67	0.59
2:F:377:PRO:HD2	4:F:501:FCO:C1	2.32	0.59
2:J:217:VAL:HB	2:J:352:GLU:HG2	1.83	0.59
2:P:395:LYS:NZ	8:P:609:HOH:O	2.35	0.59
2:H:255:HIS:NE2	2:H:386:GLU:OE2	2.35	0.59
1:O:94:TRP:HH2	2:P:56:GLU:HB2	1.67	0.59
2:P:78:GLU:OE1	2:P:349:SER:OG	2.15	0.59
2:F:99:LEU:HD12	2:F:151:MET:HG2	1.84	0.59
1:G:25:GLU:HB3	1:G:28:GLN:HB2	1.84	0.59
2:H:111:HIS:HA	2:H:115:LEU:HB2	1.84	0.59
1:C:11:THR:O	1:C:59:SER:N	2.34	0.59
2:F:388:HIS:ND1	2:F:415:TYR:OH	2.20	0.59
2:D:288:LYS:O	2:D:292:GLU:HG2	2.03	0.59
1:E:26:LEU:O	1:E:30:ILE:HG12	2.02	0.59
2:L:110:LEU:HD11	2:L:144:LYS:HD3	1.85	0.59
2:B:220:ARG:HB3	2:B:228:GLY:HA2	1.85	0.59
1:C:87:VAL:HG12	1:C:88:GLN:HG3	1.83	0.59
2:F:355:ARG:HG2	2:F:416:ASP:HB3	1.84	0.59
2:L:121:ARG:O	8:L:602:HOH:O	2.16	0.59
2:L:269:MET:HE1	2:L:273:ILE:CG2	2.30	0.59
2:N:377:PRO:HD3	4:N:501:FCO:C3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:375:ILE:HG21	2:P:380:PHE:CE1	2.38	0.59
2:F:46:GLU:HB3	2:F:372:ALA:O	2.02	0.59
2:F:104:MET:HE3	2:F:317:PHE:CE2	2.38	0.59
2:H:403:ARG:O	2:H:407:LEU:HD12	2.03	0.59
2:P:242:GLU:H	2:P:242:GLU:CD	2.11	0.59
2:D:39:ILE:HD11	8:D:616:HOH:O	2.03	0.58
1:E:29:LEU:C	1:E:31:PRO:HD3	2.28	0.58
1:E:63:GLU:HG3	1:E:115:GLN:CB	2.32	0.58
1:I:230[B]:LYS:O	1:I:234:ILE:HG13	2.03	0.58
2:J:396:HIS:HD2	2:J:403:ARG:NH2	2.00	0.58
2:B:355:ARG:HB2	4:B:501:FCO:N2	2.18	0.58
1:G:85:CYS:HA	1:G:90:GLY:HA2	1.85	0.58
2:N:103:ASP:O	2:N:107:SER:HB2	2.03	0.58
1:G:145:ALA:O	1:G:149:PHE:HB2	2.04	0.58
1:K:223:PHE:CD1	1:K:228:MET:HE2	2.37	0.58
2:L:417:PRO:HB2	2:L:419:ILE:HD11	1.85	0.58
2:N:75:THR:OG1	2:N:351:THR:OG1	2.21	0.58
1:O:106:VAL:HG21	2:P:44:PHE:HD1	1.65	0.58
2:D:138:GLU:O	2:D:142:LYS:HG3	2.03	0.58
1:I:173:CYS:HB3	1:I:176:LEU:HB2	1.83	0.58
1:K:222:VAL:HA	1:K:225:GLU:HB2	1.85	0.58
2:L:91:GLU:OE1	2:L:91:GLU:N	2.26	0.58
2:N:421:CYS:HB3	4:N:501:FCO:C1	2.34	0.58
2:P:182:LYS:HB3	2:P:322:ILE:HG23	1.84	0.58
2:P:363:LYS:HB3	2:P:371:TYR:H	1.69	0.58
2:P:384:MET:HE3	2:P:388:HIS:CE1	2.38	0.58
1:A:13:CYS:HG	3:A:501:SF4:FE2	1.19	0.58
2:B:54:LEU:HD21	2:B:80:ALA:HB1	1.84	0.58
1:G:4:ARG:NH1	1:G:49:GLU:OE2	2.36	0.58
1:O:173:CYS:SG	1:O:176:LEU:HD12	2.43	0.58
2:F:150:MET:HG2	2:F:181:MET:CE	2.29	0.58
2:L:250:GLU:HG3	2:L:260:HIS:O	2.04	0.58
1:G:5:ILE:HD13	1:G:53:ILE:HB	1.84	0.58
1:K:237:MET:HE2	1:K:247:VAL:HG22	1.85	0.58
1:A:4:ARG:HB3	1:A:51:VAL:HA	1.86	0.58
2:F:275:ARG:HD3	2:F:352:GLU:HG3	1.86	0.58
1:I:62:THR:HG22	1:I:64:GLU:HG3	1.85	0.58
1:M:160:TYR:HB2	1:M:164:LEU:HD22	1.84	0.58
1:O:229:THR:OG1	1:O:230:LYS:N	2.37	0.58
1:K:164:LEU:HD21	1:K:215:TRP:CZ3	2.39	0.58
2:N:208:VAL:HG11	2:N:411:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:29:LEU:HD13	1:O:143:LEU:HD23	1.84	0.58
2:P:378:THR:HA	2:P:381:ASN:HB2	1.85	0.58
1:E:98:PRO:HB2	1:E:101:GLU:HG3	1.86	0.58
2:L:63:ARG:HA	2:L:160:HIS:CE1	2.38	0.58
1:O:91:VAL:HG11	2:P:63:ARG:HD3	1.86	0.58
2:B:271:GLY:HA2	2:B:355:ARG:C	2.29	0.57
1:I:91:VAL:HA	1:I:239:MET:O	2.04	0.57
1:M:138:GLU:HB3	1:M:140[A]:LYS:HG3	1.85	0.57
2:N:213:THR:OG1	2:N:266:ARG:NH1	2.37	0.57
1:O:167:ARG:NH2	1:O:215:TRP:O	2.37	0.57
1:C:59:SER:HB2	1:C:92:GLN:HE21	1.69	0.57
1:E:32:ASN:HB3	1:E:150:LEU:HD13	1.85	0.57
1:E:143:LEU:HD22	1:G:168:LEU:HD22	1.86	0.57
1:E:193:ALA:HB1	1:E:196:PRO:HG2	1.85	0.57
2:F:13:ILE:HD13	2:F:412:VAL:HG11	1.86	0.57
2:J:49:THR:HG21	2:J:61:TYR:CE1	2.39	0.57
2:J:108:HIS:CE1	2:J:310:GLN:HG2	2.39	0.57
1:K:41:ILE:HG13	1:K:42:ASP:H	1.69	0.57
1:O:136:PRO:HG3	2:P:159:ILE:HB	1.85	0.57
2:P:28:ASP:OD1	2:P:28:ASP:N	2.37	0.57
2:F:43:ARG:NH2	2:F:63:ARG:O	2.37	0.57
2:H:15:ARG:HH12	2:H:119:ASP:CG	2.13	0.57
2:L:37:ASN:O	2:L:39:ILE:HG23	2.05	0.57
2:N:75:THR:HG22	2:N:360:TYR:HB2	1.86	0.57
2:N:342:ILE:HG21	2:N:367:GLY:HA2	1.86	0.57
1:O:12:SER:HB3	1:O:58:GLY:HA2	1.86	0.57
2:B:275:ARG:NH1	2:B:352:GLU:OE1	2.32	0.57
1:E:239:MET:HE1	2:F:56:GLU:HB3	1.85	0.57
2:F:326:ASP:HA	2:F:329:LEU:HB2	1.85	0.57
1:I:224:LYS:C	1:I:226:LYS:H	2.11	0.57
1:K:160:TYR:CD1	1:K:164:LEU:HD12	2.39	0.57
2:L:101:ILE:HG22	2:L:105:ILE:HD11	1.87	0.57
2:N:172:LEU:HD12	2:N:336:PRO:HA	1.87	0.57
2:D:344:ASP:HA	2:D:364:VAL:HG13	1.86	0.57
1:E:176:LEU:HD21	1:E:216:PHE:HE2	1.70	0.57
2:F:153:ILE:HG22	2:F:154:LEU:HD22	1.87	0.57
1:O:229:THR:HG23	1:O:232:GLU:N	2.19	0.57
2:B:19:LYS:HB2	2:B:40:GLU:HG2	1.86	0.57
1:E:178:LYS:HB3	1:E:180:GLU:HG2	1.85	0.57
2:L:49:THR:HG21	2:L:61:TYR:CE1	2.40	0.57
2:L:135:ARG:HG3	8:L:618:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:VAL:HG13	2:D:392:MET:HB2	1.87	0.57
2:D:357:ILE:HB	2:D:380:PHE:CE2	2.39	0.57
2:F:92:ILE:O	2:F:96:ARG:HB2	2.04	0.57
1:G:24:ASP:C	1:G:26:LEU:H	2.12	0.57
2:H:352:GLU:OE2	2:H:357:ILE:HG12	2.05	0.57
2:J:355:ARG:HB2	4:J:501:FCO:N2	2.19	0.57
2:N:273:ILE:HD13	2:N:298:LEU:HD22	1.86	0.57
2:N:402:GLU:O	2:N:406:ILE:HG13	2.05	0.57
2:P:239:PHE:CZ	2:P:248:ILE:HD11	2.39	0.57
2:P:325:LEU:O	2:P:329:LEU:HB2	2.05	0.57
1:C:176:LEU:HD21	1:C:216:PHE:HE2	1.69	0.57
2:D:240:PRO:HB2	2:D:243:LYS:HB2	1.87	0.57
2:D:421:CYS:CB	4:D:501:FCO:C1	2.82	0.57
2:F:207:GLU:HG2	2:F:395:LYS:NZ	2.19	0.57
1:K:12:SER:HB2	3:K:501:SF4:S1	2.45	0.57
2:L:177:VAL:C	2:L:179:GLU:H	2.12	0.57
1:O:38:TRP:HB3	1:O:41:ILE:HD11	1.86	0.57
2:P:146:LEU:O	2:P:150:MET:HG3	2.04	0.57
2:B:292:GLU:HA	2:B:295:LYS:HD3	1.87	0.57
1:G:60:VAL:HG13	1:G:65:GLU:HB3	1.86	0.57
2:H:262:HIS:HE1	2:P:131:ASN:O	1.88	0.57
1:M:203:ILE:HD11	2:N:63:ARG:HH22	1.69	0.57
2:N:403:ARG:HH11	2:N:403:ARG:HG3	1.69	0.57
2:D:275:ARG:HH21	2:D:313:GLU:CD	2.13	0.57
1:G:13:CYS:HB2	2:H:65:CYS:CA	2.35	0.57
1:G:130:TYR:HE2	1:G:132:ILE:HG12	1.70	0.57
1:I:194:ARG:O	1:I:198:PHE:HD1	1.88	0.57
2:J:113:TYR:HH	2:J:195:THR:HG1	1.43	0.57
2:J:196:PHE:CD2	2:J:290:LEU:HD22	2.39	0.57
1:O:55:PHE:HB3	1:O:82:VAL:HG21	1.87	0.57
2:B:89:ARG:NH2	2:B:338:ASP:OD1	2.38	0.56
2:D:381:ASN:O	2:D:383:ALA:N	2.37	0.56
2:H:376:THR:OG1	2:H:421:CYS:O	2.17	0.56
2:L:91:GLU:H	2:L:91:GLU:CD	2.13	0.56
1:O:138:GLU:CD	1:O:194:ARG:HH22	2.13	0.56
2:B:215:LEU:HD13	2:B:268:PHE:CD2	2.40	0.56
1:C:28:GLN:HG3	1:C:28:GLN:O	2.05	0.56
2:F:58:LEU:HD13	2:F:77:LEU:HD23	1.87	0.56
1:O:39:PHE:O	2:P:14:ALA:HA	2.04	0.56
1:O:92:GLN:HA	2:P:48:ILE:HD13	1.87	0.56
1:A:16:CYS:HB2	1:A:57:GLU:HG3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:ASN:HB3	2:B:282:LEU:HD12	1.87	0.56
2:D:358:LEU:HG	4:D:501:FCO:O3	2.04	0.56
1:E:11:THR:HG22	2:F:43:ARG:HD2	1.87	0.56
2:F:209:GLU:HG3	2:F:301:THR:CG2	2.35	0.56
1:K:246:ARG:HE	1:K:250:MET:CE	2.18	0.56
2:L:169:PHE:O	2:L:336:PRO:HB2	2.05	0.56
2:L:376:THR:OG1	2:L:421:CYS:O	2.15	0.56
2:L:417:PRO:HB2	2:L:419:ILE:CD1	2.35	0.56
2:L:421:CYS:HB3	4:L:501:FCO:C1	2.34	0.56
1:M:12:SER:HB2	3:M:501:SF4:S1	2.45	0.56
1:C:73:ARG:NH2	1:C:77:LYS:O	2.37	0.56
2:F:173:PRO:HG2	2:F:178:LEU:HD21	1.87	0.56
2:H:275:ARG:HD3	2:H:352:GLU:CG	2.35	0.56
1:I:164:LEU:HB3	1:K:143:LEU:HD21	1.88	0.56
2:J:355:ARG:HG2	2:J:416:ASP:HB3	1.88	0.56
2:L:97:GLU:O	2:L:101:ILE:HD12	2.06	0.56
1:O:173:CYS:HB3	1:O:176:LEU:HB2	1.88	0.56
2:D:44:PHE:O	2:D:48:ILE:HG12	2.05	0.56
1:E:18:LEU:HD23	2:F:159:ILE:HD11	1.88	0.56
1:G:239:MET:HE2	2:H:60:ILE:HD11	1.87	0.56
2:J:377:PRO:HB2	4:J:501:FCO:N1	2.21	0.56
2:B:175:LYS:HG2	2:B:179:GLU:OE2	2.06	0.56
2:D:214:HIS:HD2	2:D:277:ILE:HG13	1.70	0.56
2:D:376:THR:OG1	2:D:422:SER:HA	2.04	0.56
2:L:117:LEU:C	2:L:119:ASP:H	2.14	0.56
1:M:149:PHE:HE1	1:M:154:TRP:CZ3	2.23	0.56
2:D:357:ILE:HB	2:D:380:PHE:HE2	1.71	0.56
1:E:37:CYS:HA	1:E:45:SER:HB2	1.88	0.56
3:I:501:SF4:S4	2:J:63:ARG:HG2	2.45	0.56
2:N:199:PHE:CD1	2:N:202:LEU:HD12	2.40	0.56
1:G:87:VAL:HG12	1:G:88:GLN:HG3	1.87	0.56
1:G:116:PRO:HG3	2:H:257:PHE:CZ	2.41	0.56
1:M:91:VAL:C	1:M:93:SER:H	2.14	0.56
2:N:134:LYS:HG3	2:N:135:ARG:N	2.21	0.56
2:P:68:CYS:HB3	4:P:501:FCO:C2	2.36	0.56
2:P:350:THR:HG22	2:P:359:VAL:HG12	1.86	0.56
2:F:104:MET:O	2:F:108:HIS:HB2	2.05	0.56
1:G:14:TYR:O	1:G:18:LEU:HB2	2.06	0.56
2:H:102:GLY:O	2:H:151:MET:HE2	2.06	0.56
1:K:174:ILE:HD12	1:K:180:GLU:HB2	1.88	0.56
2:P:266:ARG:HE	2:P:267:PRO:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ILE:HD12	1:E:175:LEU:N	2.21	0.55
1:E:203:ILE:HD12	1:E:240:PHE:HE2	1.71	0.55
2:H:275:ARG:HD3	2:H:352:GLU:HG3	1.87	0.55
1:M:206:ARG:HG3	3:M:502:SF4:S3	2.46	0.55
1:A:23:MET:O	1:A:26:LEU:HB2	2.06	0.55
1:C:173:CYS:HA	3:C:503:SF4:S3	2.46	0.55
2:F:94:ALA:O	2:F:98:VAL:HG23	2.06	0.55
2:H:364:VAL:HA	2:H:368:ARG:O	2.06	0.55
1:I:183:LEU:HB2	1:I:202:CYS:O	2.06	0.55
2:J:212:ILE:HG21	2:J:388:HIS:CE1	2.41	0.55
2:J:379:ALA:HA	2:J:382:LEU:HD12	1.88	0.55
2:J:232:LYS:HA	2:J:238:GLU:HA	1.88	0.55
2:P:19:LYS:H	2:P:40:GLU:HG3	1.71	0.55
2:P:258:ALA:HB1	2:P:422:SER:HB2	1.88	0.55
2:B:220:ARG:HE	2:B:228:GLY:HA2	1.70	0.55
2:D:356:GLY:CA	2:D:377:PRO:HB3	2.35	0.55
2:F:150:MET:CG	2:F:181:MET:HE3	2.28	0.55
2:F:359:VAL:CG2	2:F:375:ILE:HB	2.37	0.55
1:G:25:GLU:O	1:G:26:LEU:C	2.50	0.55
1:I:140:LYS:HA	1:I:143:LEU:HB3	1.87	0.55
2:J:358:LEU:HD21	2:J:360:TYR:HE2	1.72	0.55
2:L:15:ARG:HH12	2:L:119:ASP:HB2	1.71	0.55
2:L:148:THR:HG23	2:L:158:ALA:HB2	1.89	0.55
2:L:245:ARG:NH1	6:L:503:PO4:O3	2.40	0.55
2:P:88:PRO:HG2	2:P:93:GLN:HG3	1.88	0.55
1:A:124:LYS:HD2	1:A:125:TYR:CE1	2.42	0.55
2:B:408:ALA:O	2:B:411:VAL:HB	2.05	0.55
1:C:14:TYR:HA	1:C:57:GLU:OE1	2.06	0.55
2:F:91:GLU:CD	2:F:91:GLU:H	2.14	0.55
1:I:239:MET:SD	2:J:60:ILE:CD1	2.95	0.55
2:N:13:ILE:CD1	2:N:409:GLU:HG2	2.37	0.55
2:B:276:VAL:O	2:B:280:ALA:HB2	2.07	0.55
2:F:80:ALA:O	2:F:84:VAL:HG22	2.06	0.55
2:J:104:MET:O	2:J:108:HIS:HB2	2.07	0.55
2:L:267:PRO:HB3	2:L:383:ALA:HB3	1.88	0.55
1:O:41:ILE:HA	2:P:15:ARG:HG2	1.89	0.55
2:B:86:PHE:CD1	2:B:340:VAL:HG12	2.42	0.55
2:P:358:LEU:HD21	2:P:360:TYR:HE2	1.70	0.55
2:H:10:ILE:CG1	2:H:405:LYS:HG2	2.37	0.55
2:J:363:LYS:HB3	2:J:371:TYR:H	1.70	0.55
2:J:421:CYS:CB	4:J:501:FCO:C1	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:65:GLU:HA	1:M:68:LEU:HB2	1.88	0.55
2:P:239:PHE:HZ	2:P:248:ILE:HD11	1.72	0.55
2:P:253:VAL:HA	8:P:625:HOH:O	2.07	0.55
1:C:138:GLU:OE2	1:C:194:ARG:NH1	2.39	0.55
2:D:342:ILE:HG22	2:D:342:ILE:O	2.06	0.55
1:G:130:TYR:CE2	1:G:132:ILE:HG12	2.41	0.55
1:G:141:ASP:CG	1:G:206:ARG:HH22	2.15	0.55
2:L:385:MET:HE1	2:L:417:PRO:HG3	1.88	0.55
2:L:385:MET:HE1	2:L:417:PRO:HB3	1.87	0.55
1:C:232:GLU:O	1:C:236:ARG:HG3	2.07	0.55
2:D:114:LEU:HA	2:D:126:PRO:HB3	1.89	0.55
1:E:174:ILE:HD12	1:E:175:LEU:H	1.72	0.55
2:J:191:LEU:O	2:J:194:TYR:HB3	2.06	0.55
2:N:117:LEU:HD23	2:N:129:MET:HE1	1.88	0.55
1:O:14:TYR:CD2	1:O:40:MET:HE2	2.42	0.55
2:D:195:THR:HG22	2:D:311:ALA:HB1	1.89	0.54
1:E:55:PHE:CD1	1:E:80:VAL:HB	2.43	0.54
2:F:68:CYS:HA	2:F:103:ASP:OD2	2.06	0.54
2:H:90:GLU:OE1	2:H:90:GLU:N	2.29	0.54
2:H:385:MET:HG2	2:H:415:TYR:CD1	2.41	0.54
1:K:139:LYS:HG3	1:K:140:LYS:H	1.72	0.54
2:N:211:PRO:O	2:N:212:ILE:HG13	2.07	0.54
2:P:86:PHE:CD1	2:P:340:VAL:HG12	2.42	0.54
1:A:20:LEU:N	8:A:602:HOH:O	2.40	0.54
2:D:310:GLN:O	2:D:314:ILE:HG13	2.07	0.54
2:F:100:TYR:CD1	2:F:226:ILE:HD13	2.43	0.54
2:H:64:ILE:HD13	2:H:424:HIS:HB3	1.89	0.54
1:I:3:VAL:O	1:I:33:ALA:HA	2.08	0.54
2:L:250:GLU:CG	2:L:259:LYS:HB3	2.38	0.54
1:M:165:GLU:CD	1:M:189:ALA:HB1	2.33	0.54
2:L:270:VAL:N	2:L:381:ASN:OD1	2.32	0.54
1:O:41:ILE:HD12	1:O:42:ASP:N	2.22	0.54
2:P:400:ASP:OD1	2:P:401:PRO:HD2	2.08	0.54
2:B:226:ILE:HA	2:B:352:GLU:HB2	1.90	0.54
2:F:93:GLN:HA	2:F:96:ARG:HB2	1.89	0.54
1:G:220:ALA:O	1:G:224:LYS:N	2.39	0.54
2:H:130:VAL:O	2:H:134:LYS:HE3	2.07	0.54
2:H:139:ILE:HD13	2:H:194:TYR:CD2	2.42	0.54
2:P:287:ALA:CB	2:P:316:TYR:HB2	2.38	0.54
2:D:192:ALA:HB2	2:D:318:ILE:HD12	1.89	0.54
2:F:37:ASN:HA	2:F:255:HIS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:CYS:O	2:F:69:SER:C	2.50	0.54
1:O:203:ILE:HD12	1:O:239:MET:HE2	1.89	0.54
1:A:54:ALA:HB3	1:A:79:VAL:HA	1.89	0.54
2:F:70:ALA:HB2	2:F:151:MET:HE1	1.89	0.54
2:F:212:ILE:HD11	2:F:388:HIS:CE1	2.42	0.54
2:F:224:TYR:HB3	2:F:316:TYR:CE2	2.43	0.54
2:J:86:PHE:CE2	2:J:167:GLY:HA2	2.43	0.54
1:K:91:VAL:C	1:K:93:SER:H	2.15	0.54
2:D:348:VAL:HG13	8:D:618:HOH:O	2.07	0.54
1:E:98:PRO:HD2	1:E:101:GLU:OE1	2.07	0.54
2:H:31:VAL:CG2	2:H:394:GLU:HG2	2.37	0.54
2:H:358:LEU:HD13	2:H:376:THR:HG22	1.89	0.54
2:L:108:HIS:HB2	2:L:314:ILE:HD11	1.90	0.54
2:N:133:TYR:OH	8:N:601:HOH:O	2.17	0.54
1:A:195:CYS:CB	1:A:196:PRO:HG2	2.37	0.54
3:E:502:SF4:S1	2:F:157:ARG:NH1	2.81	0.54
2:H:54:LEU:HD21	2:H:80:ALA:HB1	1.90	0.54
1:I:62:THR:HG22	1:I:64:GLU:H	1.73	0.54
2:J:375:ILE:HG21	2:J:380:PHE:CE1	2.43	0.54
2:L:104:MET:HE3	2:L:226:ILE:HG12	1.89	0.54
2:L:193:GLU:OE2	2:L:286:LYS:NZ	2.40	0.54
2:P:196:PHE:CE1	2:P:312:LEU:HB2	2.41	0.54
2:B:126:PRO:C	2:B:128:LYS:H	2.16	0.54
2:B:226:ILE:HG23	2:B:352:GLU:O	2.07	0.54
2:D:269:MET:HA	2:D:381:ASN:OD1	2.07	0.54
2:F:10:ILE:N	2:F:22:VAL:O	2.35	0.54
2:J:65:CYS:HB2	2:J:421:CYS:SG	2.47	0.54
2:L:392:MET:SD	2:L:407:LEU:HB3	2.48	0.54
2:B:364:VAL:HG23	2:B:368:ARG:O	2.08	0.53
1:E:87:VAL:HG11	1:E:133:TYR:CE1	2.43	0.53
2:F:221:GLY:C	2:F:223:ALA:H	2.16	0.53
2:F:253:VAL:HG23	2:F:256:SER:HB3	1.90	0.53
2:L:272:ALA:O	2:L:276:VAL:HG23	2.08	0.53
2:N:38:ILE:HG23	2:N:419:ILE:HG23	1.91	0.53
2:P:74:LEU:HD21	2:P:99:LEU:HD23	1.90	0.53
2:P:328:ALA:O	2:P:334:ILE:HD11	2.08	0.53
1:G:149:PHE:HE1	1:G:154:TRP:CZ3	2.25	0.53
2:H:393:ALA:HA	2:H:404:LEU:HD11	1.90	0.53
2:J:65:CYS:CB	2:J:68:CYS:SG	2.94	0.53
2:L:108:HIS:O	2:L:112:LEU:N	2.27	0.53
1:M:247:VAL:O	1:M:251:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:501:SF4:S3	2:P:160:HIS:NE2	2.81	0.53
2:P:189:LEU:HD21	2:P:319:GLU:HG3	1.90	0.53
2:H:22:VAL:HG13	2:H:36:LEU:HD22	1.90	0.53
1:K:4:ARG:O	1:K:52:ASP:N	2.38	0.53
2:F:356:GLY:CA	2:F:377:PRO:HB3	2.38	0.53
2:L:45:PHE:CE2	2:L:60:ILE:HG12	2.43	0.53
1:M:246:ARG:O	1:M:250:MET:HG3	2.08	0.53
2:N:209:GLU:O	8:N:602:HOH:O	2.18	0.53
2:N:384:MET:HE3	2:N:387:GLU:HB3	1.91	0.53
2:D:211:PRO:O	2:D:212:ILE:HD13	2.08	0.53
2:F:381:ASN:C	2:F:383:ALA:H	2.17	0.53
2:F:385:MET:HG2	2:F:415:TYR:CG	2.43	0.53
2:H:157:ARG:HD3	2:H:159:ILE:O	2.08	0.53
1:I:94:TRP:HB3	1:I:238:LYS:O	2.08	0.53
1:O:28:GLN:OE1	1:O:28:GLN:N	2.40	0.53
1:O:124:LYS:HD2	1:O:124:LYS:O	2.08	0.53
2:B:14:ALA:O	2:B:413:ARG:NH1	2.37	0.53
1:E:219:LEU:O	1:E:222:VAL:HG12	2.08	0.53
1:I:116:PRO:HG3	2:J:257:PHE:HE1	1.74	0.53
1:M:37:CYS:SG	1:M:39:PHE:HE1	2.31	0.53
2:N:120:TYR:CD2	2:N:202:LEU:HD13	2.44	0.53
2:B:137:ILE:O	2:B:141:LEU:HG	2.09	0.53
2:D:342:ILE:CG2	2:D:367:GLY:HA2	2.39	0.53
2:H:130:VAL:O	2:H:134:LYS:HG2	2.08	0.53
2:N:418:CYS:SG	2:N:421:CYS:HB2	2.48	0.53
2:B:136:GLU:O	2:B:140:ALA:N	2.36	0.53
1:C:30:ILE:CD1	1:C:35:ILE:HD11	2.39	0.53
1:I:5:ILE:O	1:I:35:ILE:HA	2.09	0.53
1:I:182:CYS:CA	1:I:201:ALA:HB1	2.39	0.53
2:D:37:ASN:O	2:D:39:ILE:HG23	2.09	0.53
2:F:275:ARG:HH21	2:F:313:GLU:CD	2.17	0.53
2:H:361:ALA:O	2:H:372:ALA:HA	2.08	0.53
2:H:402:GLU:O	2:H:406:ILE:HG13	2.09	0.53
1:I:135:CYS:HB3	1:I:205:CYS:HB2	1.91	0.53
2:J:196:PHE:CE1	2:J:312:LEU:HB2	2.43	0.53
2:J:226:ILE:HD11	2:J:317:PHE:CE1	2.44	0.53
2:B:247:TYR:O	2:B:248:ILE:HG13	2.08	0.53
1:E:161:PRO:HG2	1:E:164:LEU:HD13	1.91	0.53
1:E:164:LEU:HD11	1:E:215:TRP:CH2	2.44	0.53
2:F:212:ILE:HD11	2:F:388:HIS:HE1	1.73	0.53
2:H:239:PHE:HE2	2:H:244:TYR:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:207:GLU:HG2	2:J:396:HIS:HE1	1.74	0.53
2:J:224:TYR:OH	2:J:275:ARG:HB2	2.09	0.53
2:J:235:ASP:OD1	2:J:236:GLY:N	2.42	0.53
1:K:246:ARG:HE	1:K:250:MET:HE3	1.74	0.53
2:P:223:ALA:HB1	2:P:316:TYR:OH	2.09	0.53
1:A:174:ILE:HD11	1:A:201:ALA:HA	1.90	0.52
2:B:275:ARG:HD3	2:B:352:GLU:OE1	2.08	0.52
1:C:95:SER:HB3	2:D:48:ILE:HG22	1.90	0.52
2:D:101:ILE:HA	2:D:104:MET:HB2	1.92	0.52
2:J:25:ILE:HG13	2:J:33:GLU:HB3	1.91	0.52
2:J:245:ARG:NH2	2:J:373:ASP:OD2	2.42	0.52
1:K:16:CYS:SG	3:K:501:SF4:S2	3.07	0.52
2:L:40:GLU:O	2:L:423:VAL:HG11	2.09	0.52
1:M:174:ILE:HD13	1:M:180:GLU:OE1	2.07	0.52
1:A:138:GLU:HB3	1:A:140:LYS:HG3	1.90	0.52
1:I:116:PRO:HB3	2:J:42:PRO:HG3	1.91	0.52
2:N:101:ILE:HG23	2:N:317:PHE:HB3	1.91	0.52
1:O:65:GLU:O	1:O:69:VAL:HG13	2.09	0.52
2:B:34:VAL:CG1	2:B:390:ARG:HB2	2.39	0.52
2:B:89:ARG:NE	2:B:338:ASP:OD2	2.40	0.52
2:B:141:LEU:HD23	2:B:144:LYS:NZ	2.24	0.52
2:B:219:PRO:HG2	2:B:282:LEU:HD13	1.91	0.52
1:C:12:SER:HB3	1:C:58:GLY:CA	2.33	0.52
1:C:216:PHE:CB	1:C:219:LEU:HB2	2.39	0.52
2:F:37:ASN:OD1	2:F:255:HIS:HB2	2.10	0.52
2:H:219:PRO:HG2	2:H:282:LEU:HD12	1.91	0.52
1:K:175:LEU:HA	1:K:180:GLU:H	1.74	0.52
2:N:6:LEU:HG	2:N:26:ILE:HD11	1.92	0.52
2:B:418:CYS:O	2:B:421:CYS:HB2	2.09	0.52
2:F:239:PHE:CD1	2:F:239:PHE:C	2.88	0.52
2:J:245:ARG:HH22	2:J:375:ILE:HD11	1.75	0.52
1:O:195:CYS:HB2	1:O:196:PRO:HD3	1.90	0.52
2:P:217:VAL:HB	2:P:352:GLU:HG2	1.91	0.52
1:A:38:TRP:CG	1:A:41:ILE:HG12	2.45	0.52
1:C:7:PHE:HE1	1:C:57:GLU:HB2	1.73	0.52
1:C:106:VAL:O	2:D:259:LYS:NZ	2.39	0.52
2:D:17:GLU:OE2	2:D:420:SER:HB2	2.09	0.52
2:F:37:ASN:O	2:F:39:ILE:HG23	2.09	0.52
2:F:269:MET:HA	2:F:381:ASN:OD1	2.09	0.52
1:G:158:ILE:HG23	1:G:160:TYR:CE2	2.45	0.52
2:P:209:GLU:HA	2:P:301:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ILE:HG23	2:B:384:MET:HE2	1.90	0.52
2:B:403:ARG:O	2:B:407:LEU:HD13	2.09	0.52
1:C:165:GLU:CD	1:C:189:ALA:HB1	2.34	0.52
2:F:14:ALA:O	2:F:413:ARG:NH1	2.42	0.52
2:J:91:GLU:HG3	2:J:334:ILE:HG23	1.91	0.52
1:K:85:CYS:HA	1:K:90:GLY:CA	2.40	0.52
2:L:159:ILE:HG22	2:L:160:HIS:CG	2.44	0.52
2:L:267:PRO:HB3	2:L:383:ALA:CB	2.39	0.52
2:B:123:TYR:OH	2:B:132:GLU:OE1	2.14	0.52
2:D:360:TYR:CE2	2:D:374:ILE:HG12	2.45	0.52
2:F:113:TYR:CD1	2:F:140:ALA:HB2	2.45	0.52
2:F:232:LYS:HG3	2:F:238:GLU:HG3	1.91	0.52
2:J:111:HIS:HA	2:J:115:LEU:HB2	1.92	0.52
1:K:146:LEU:O	1:K:150:LEU:HG	2.09	0.52
2:N:212:ILE:HD11	2:N:388:HIS:CE1	2.43	0.52
2:P:146:LEU:HD21	2:P:185:LEU:HD23	1.91	0.52
1:C:5:ILE:HG22	1:C:35:ILE:HG23	1.92	0.52
1:C:224:LYS:HG2	1:C:225:GLU:H	1.73	0.52
2:D:300:GLY:O	2:D:302:ASN:N	2.43	0.52
2:B:199:PHE:HA	2:B:202:LEU:HD12	1.91	0.52
1:C:40:MET:O	2:D:15:ARG:HA	2.10	0.52
2:D:69:SER:O	2:D:72:HIS:HB2	2.10	0.52
2:D:75:THR:HG23	2:D:351:THR:HG23	1.92	0.52
2:D:385:MET:HG3	2:D:415:TYR:CD2	2.45	0.52
1:E:90:GLY:O	1:E:93:SER:HB2	2.09	0.52
2:H:245:ARG:HD3	8:H:618:HOH:O	2.10	0.52
1:I:213:VAL:HG12	1:I:214:ALA:H	1.74	0.52
2:J:363:LYS:HB2	2:J:371:TYR:HB3	1.90	0.52
1:M:59:SER:OG	1:M:92:GLN:NE2	2.37	0.52
1:O:91:VAL:HA	1:O:239:MET:O	2.10	0.52
2:B:128:LYS:C	2:B:130:VAL:H	2.18	0.52
1:C:23:MET:HE1	1:C:142:PHE:HB2	1.92	0.52
2:D:242:GLU:HA	2:D:348:VAL:CG1	2.39	0.52
1:E:7:PHE:CE2	1:E:17:GLN:HA	2.44	0.52
1:E:147:GLY:O	1:E:151:ILE:HG12	2.10	0.52
1:E:182:CYS:CA	1:E:201:ALA:HB1	2.40	0.52
2:F:376:THR:HB	2:F:421:CYS:HB3	1.92	0.52
2:H:58:LEU:HD23	2:H:76:ALA:HB1	1.90	0.52
2:J:224:TYR:HB3	2:J:316:TYR:CE2	2.45	0.52
2:J:397:TYR:HA	2:J:404:LEU:HD22	1.92	0.52
2:L:385:MET:HE2	2:L:415:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:CYS:O	1:A:177:GLU:HG2	2.10	0.51
1:C:219:LEU:O	1:C:222:VAL:HB	2.11	0.51
2:D:393:ALA:O	2:D:396:HIS:N	2.39	0.51
1:E:23:MET:HE2	1:E:139:LYS:HA	1.92	0.51
1:E:92:GLN:HB3	2:F:43:ARG:HG2	1.92	0.51
1:E:135:CYS:HB3	1:E:205:CYS:HB2	1.92	0.51
1:I:39:PHE:HD1	2:J:14:ALA:HB2	1.75	0.51
1:K:22:MET:SD	2:L:144:LYS:HD2	2.50	0.51
2:L:54:LEU:HD21	2:L:80:ALA:HB1	1.92	0.51
1:M:219:LEU:O	1:M:222:VAL:HG22	2.10	0.51
2:P:119:ASP:HB3	2:P:410:MET:HE2	1.92	0.51
2:P:189:LEU:CD2	2:P:319:GLU:HG3	2.40	0.51
2:P:298:LEU:HD21	2:P:308:LEU:HG	1.91	0.51
1:A:121:PRO:HD3	1:A:243:HIS:CD2	2.44	0.51
2:B:109:ALA:O	2:B:113:TYR:HB2	2.10	0.51
1:C:202:CYS:HB2	3:C:502:SF4:S4	2.50	0.51
1:C:213:VAL:O	1:C:215:TRP:N	2.42	0.51
2:D:64:ILE:HD13	2:D:424:HIS:HB2	1.92	0.51
2:D:381:ASN:C	2:D:383:ALA:H	2.18	0.51
1:E:24:ASP:OD1	2:F:141:LEU:HD21	2.10	0.51
1:E:223:PHE:HB3	1:E:228:MET:HB2	1.92	0.51
2:L:86:PHE:HB2	2:L:340:VAL:HG23	1.91	0.51
2:L:240:PRO:HB2	2:L:243:LYS:HB2	1.92	0.51
2:L:273:ILE:HG13	2:L:277:ILE:HD13	1.93	0.51
2:N:295:LYS:HE3	2:N:296:ASP:CG	2.34	0.51
2:B:296:ASP:C	2:B:299:LYS:HE3	2.35	0.51
1:C:91:VAL:C	1:C:93:SER:N	2.68	0.51
2:H:144:LYS:NZ	2:H:145:ASN:OD1	2.35	0.51
2:H:359:VAL:HG22	2:H:375:ILE:HB	1.92	0.51
2:N:10:ILE:HD11	2:N:405:LYS:HG2	1.92	0.51
2:P:49:THR:HG21	2:P:61:TYR:CE1	2.45	0.51
1:A:195:CYS:N	1:A:196:PRO:CG	2.72	0.51
2:D:37:ASN:HA	2:D:255:HIS:O	2.10	0.51
2:F:10:ILE:HD11	2:F:405:LYS:HB3	1.92	0.51
2:H:377:PRO:CD	4:H:501:FCO:N1	2.70	0.51
2:H:421:CYS:CB	4:H:501:FCO:C1	2.87	0.51
1:I:220:ALA:HB2	1:I:254:ILE:O	2.10	0.51
2:L:131:ASN:O	2:L:132:GLU:HG3	2.09	0.51
2:P:220:ARG:HG2	2:P:227:TYR:O	2.11	0.51
2:B:10:ILE:CG1	2:B:405:LYS:HD3	2.39	0.51
2:B:62:PRO:HG3	2:B:73:LYS:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ASP:HB3	1:E:247:VAL:CG2	2.40	0.51
2:F:105:ILE:HD12	2:F:150:MET:HE1	1.93	0.51
2:J:95:LEU:HB3	2:J:154:LEU:HD11	1.93	0.51
2:L:242:GLU:HA	2:L:348:VAL:HG11	1.91	0.51
2:L:341:GLU:OE2	2:L:343:LYS:HD2	2.11	0.51
1:A:4:ARG:HG3	1:A:36:VAL:CG1	2.39	0.51
1:A:20:LEU:HB3	1:A:38:TRP:CH2	2.45	0.51
1:A:139:LYS:HB3	1:C:168:LEU:HD11	1.93	0.51
1:A:145:ALA:O	1:A:149:PHE:HB2	2.10	0.51
2:B:157:ARG:HD3	2:B:159:ILE:O	2.10	0.51
2:B:296:ASP:O	2:B:297:LEU:HD13	2.10	0.51
1:C:218:SER:HB3	1:C:221:LYS:HD3	1.93	0.51
1:G:58:GLY:HA2	1:G:85:CYS:HB3	1.91	0.51
2:J:134:LYS:O	2:J:137:ILE:HG13	2.10	0.51
1:K:63:GLU:HG2	1:K:117:LYS:HD3	1.93	0.51
1:K:90:GLY:O	1:K:93:SER:HB2	2.10	0.51
2:L:37:ASN:O	2:L:39:ILE:N	2.44	0.51
2:N:358:LEU:HD22	4:N:501:FCO:O3	2.10	0.51
1:A:25:GLU:O	1:A:28:GLN:N	2.41	0.51
1:C:212:ASP:OD1	1:C:253:LYS:NZ	2.40	0.51
2:D:159:ILE:O	2:D:160:HIS:HB2	2.11	0.51
1:G:174:ILE:HD11	1:G:201:ALA:HA	1.91	0.51
2:H:171:LYS:NZ	8:H:607:HOH:O	2.44	0.51
1:I:120:GLU:HG2	1:I:124:LYS:CB	2.41	0.51
1:I:236:ARG:HG2	2:J:56:GLU:OE2	2.10	0.51
2:P:108:HIS:CB	2:P:314:ILE:HD11	2.40	0.51
1:C:102:LEU:HD22	2:D:44:PHE:HB3	1.93	0.51
2:H:17:GLU:HG3	2:H:67:PHE:CD1	2.45	0.51
2:H:262:HIS:CE1	2:P:131:ASN:O	2.64	0.51
2:H:378:THR:OG1	2:H:418:CYS:N	2.32	0.51
2:J:65:CYS:HB3	2:J:68:CYS:SG	2.50	0.51
1:O:69:VAL:O	1:O:126:ILE:HG21	2.11	0.51
2:P:237:GLU:CD	2:P:264:LYS:HZ1	2.19	0.51
2:B:255:HIS:ND1	2:B:255:HIS:O	2.42	0.51
2:F:108:HIS:CE1	2:F:310:GLN:HG2	2.46	0.51
2:F:242:GLU:HB3	2:F:348:VAL:HB	1.93	0.51
2:H:151:MET:HB3	2:H:158:ALA:HA	1.93	0.51
2:J:54:LEU:HD21	2:J:80:ALA:HB1	1.92	0.51
1:K:193:ALA:HB1	1:K:196:PRO:HG2	1.93	0.51
2:L:49:THR:HG21	2:L:61:TYR:HE1	1.75	0.51
1:M:164:LEU:HD11	1:M:215:TRP:CZ3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:MET:O	1:A:241:ASN:ND2	2.37	0.51
1:E:156:GLU:CB	1:G:156:GLU:HG3	2.41	0.51
2:F:394:GLU:HA	2:F:397:TYR:HD2	1.76	0.51
2:H:341:GLU:OE1	2:H:343:LYS:HD3	2.11	0.51
2:J:24:ILE:CD1	2:J:34:VAL:HG12	2.40	0.51
2:J:220:ARG:HG3	2:J:227:TYR:O	2.11	0.51
1:K:85:CYS:HA	1:K:90:GLY:HA2	1.93	0.51
1:K:104:LYS:NZ	1:K:109:ASP:OD2	2.34	0.51
2:N:269:MET:HE2	2:N:273:ILE:HG22	1.93	0.51
2:P:403:ARG:O	2:P:407:LEU:HD12	2.11	0.51
1:A:38:TRP:CD2	1:A:41:ILE:HG12	2.46	0.50
2:B:358:LEU:HD21	2:B:360:TYR:HE1	1.76	0.50
2:F:138:GLU:O	2:F:142:LYS:HD3	2.11	0.50
1:G:167:ARG:HG3	8:G:606:HOH:O	2.10	0.50
2:H:400:ASP:OD2	2:H:402:GLU:HG2	2.11	0.50
2:J:91:GLU:HG3	2:J:334:ILE:CG2	2.41	0.50
1:K:17:GLN:O	1:K:18:LEU:C	2.54	0.50
2:L:130:VAL:HG23	2:L:131:ASN:N	2.26	0.50
2:L:250:GLU:HG2	2:L:259:LYS:HB3	1.92	0.50
1:O:16:CYS:HB2	1:O:57:GLU:HG3	1.93	0.50
1:O:93:SER:OG	1:O:243:HIS:CD2	2.64	0.50
1:G:33:ALA:HB2	1:G:150:LEU:HD21	1.94	0.50
2:H:246:ASP:C	2:H:247:TYR:HD1	2.19	0.50
2:J:151:MET:HB3	2:J:161:GLN:HE21	1.76	0.50
2:L:101:ILE:HG12	2:L:317:PHE:HB3	1.93	0.50
2:B:61:TYR:N	2:B:62:PRO:HD2	2.27	0.50
2:B:245:ARG:NH2	2:B:375:ILE:HD11	2.25	0.50
1:C:223:PHE:HE2	1:C:254:ILE:HG21	1.75	0.50
2:D:387:GLU:CD	2:D:390:ARG:HH21	2.19	0.50
1:E:12:SER:HB3	1:E:58:GLY:HA3	1.93	0.50
1:E:160:TYR:CE1	1:G:143:LEU:HD21	2.46	0.50
1:G:47:GLU:OE1	1:G:68:LEU:CD1	2.51	0.50
1:G:171:HIS:CE1	1:G:197:GLY:HA2	2.47	0.50
1:I:12:SER:OG	1:I:57:GLU:OE1	2.28	0.50
2:N:421:CYS:HB3	4:N:501:FCO:N1	2.26	0.50
2:P:29:ASP:OD1	2:P:30:GLY:N	2.43	0.50
2:P:37:ASN:HA	2:P:255:HIS:O	2.12	0.50
2:B:64:ILE:HB	2:B:72:HIS:CD2	2.46	0.50
1:C:94:TRP:HZ3	2:D:56:GLU:OE1	1.93	0.50
1:E:175:LEU:O	1:E:179:GLY:HA2	2.12	0.50
2:F:26:ILE:CD1	2:F:397:TYR:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:44:PHE:O	2:F:48:ILE:HG12	2.11	0.50
2:H:109:ALA:O	2:H:113:TYR:HB2	2.11	0.50
1:O:198:PHE:CZ	2:P:156:SER:HA	2.47	0.50
1:G:85:CYS:HA	1:G:90:GLY:CA	2.41	0.50
2:H:364:VAL:HG13	2:H:368:ARG:O	2.11	0.50
2:N:421:CYS:SG	4:N:501:FCO:C3	2.99	0.50
2:P:18:GLY:HA3	2:P:419:ILE:HB	1.94	0.50
1:A:195:CYS:HB2	1:A:196:PRO:HG2	1.94	0.50
2:B:43:ARG:NH1	2:B:63:ARG:O	2.45	0.50
2:D:258:ALA:HB2	2:D:423:VAL:CG2	2.42	0.50
2:D:421:CYS:HB3	4:D:501:FCO:C1	2.41	0.50
1:E:43:ARG:HB2	2:F:15:ARG:NH2	2.22	0.50
2:H:189:LEU:HB3	2:H:190:PRO:HD3	1.93	0.50
1:K:25:GLU:O	1:K:29:LEU:HG	2.11	0.50
1:K:223:PHE:HD1	1:K:228:MET:HE2	1.77	0.50
2:L:10:ILE:HD12	2:L:22:VAL:HB	1.93	0.50
2:N:406:ILE:HG22	2:N:410:MET:HE2	1.93	0.50
1:O:18:LEU:HD23	2:P:159:ILE:HD11	1.93	0.50
2:P:27:GLY:HA3	2:P:32:LYS:HE3	1.94	0.50
2:B:111:HIS:O	2:B:115:LEU:HB2	2.12	0.50
2:D:424:HIS:HD1	2:D:424:HIS:H	1.58	0.50
1:E:160:TYR:CD1	1:E:164:LEU:HD22	2.47	0.50
1:G:230:LYS:HG3	1:G:231:GLU:HG3	1.92	0.50
1:I:39:PHE:O	8:I:601:HOH:O	2.20	0.50
1:C:17:GLN:HG2	1:C:38:TRP:HE1	1.77	0.50
1:C:19:GLN:OE1	2:D:159:ILE:HD12	2.11	0.50
2:F:26:ILE:HD12	2:F:397:TYR:HB2	1.93	0.50
2:F:284:TYR:OH	2:F:320:ARG:HD2	2.12	0.50
1:K:27:LEU:HA	1:K:30:ILE:HG12	1.93	0.50
1:M:228:MET:HB3	1:M:233:ILE:HD11	1.93	0.50
1:O:69:VAL:HG23	1:O:126:ILE:HG23	1.93	0.50
2:P:209:GLU:HG3	2:P:302:ASN:ND2	2.19	0.50
2:B:146:LEU:HD13	2:B:184:GLU:HB3	1.93	0.50
2:F:61:TYR:O	2:F:64:ILE:HD12	2.12	0.50
2:H:355:ARG:HG2	2:H:416:ASP:HB3	1.92	0.50
1:I:91:VAL:HG11	2:J:60:ILE:HG13	1.93	0.50
2:J:77:LEU:HD13	2:J:96:ARG:HH21	1.77	0.50
2:J:352:GLU:OE2	2:J:357:ILE:HG12	2.12	0.50
1:K:94:TRP:CH2	2:L:56:GLU:HB3	2.47	0.50
2:L:275:ARG:HD3	2:L:352:GLU:OE1	2.12	0.50
2:L:294:ASN:HB3	2:L:297:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:ARG:HB2	1:M:126:ILE:HD13	1.94	0.50
2:B:72:HIS:ND1	2:B:358:LEU:HD21	2.27	0.49
2:B:387:GLU:CD	2:B:390:ARG:HH21	2.20	0.49
2:D:151:MET:HE2	2:D:161:GLN:HE21	1.77	0.49
1:E:173:CYS:SG	3:E:503:SF4:S4	3.10	0.49
1:G:31:PRO:C	1:G:33:ALA:H	2.19	0.49
1:G:59:SER:OG	1:G:92:GLN:NE2	2.45	0.49
2:B:123:TYR:CZ	2:B:132:GLU:OE1	2.65	0.49
2:B:212:ILE:HD12	2:B:300:GLY:O	2.12	0.49
2:J:67:PHE:HD2	2:J:355:ARG:NH2	2.09	0.49
2:L:319:GLU:HA	2:L:322:ILE:HD12	1.93	0.49
2:L:377:PRO:HD3	4:L:501:FCO:C3	2.42	0.49
2:D:112:LEU:HB3	2:D:199:PHE:CZ	2.47	0.49
2:D:273:ILE:HG22	2:D:306:ASN:OD1	2.12	0.49
1:E:121:PRO:C	1:E:123:SER:H	2.20	0.49
2:H:70:ALA:O	2:H:74:LEU:N	2.27	0.49
2:H:396:HIS:C	2:H:404:LEU:HD13	2.37	0.49
2:J:54:LEU:HD23	2:J:166:LEU:HD21	1.93	0.49
2:J:219:PRO:HG2	2:J:282:LEU:HD12	1.95	0.49
1:K:87:VAL:HG12	1:K:88:GLN:HG3	1.93	0.49
2:L:314:ILE:O	2:L:318:ILE:HB	2.13	0.49
2:N:110:LEU:HD21	2:N:144:LYS:CG	2.42	0.49
2:P:393:ALA:C	2:P:395:LYS:H	2.20	0.49
1:A:114:PHE:O	1:A:116:PRO:HD3	2.12	0.49
1:C:246:ARG:HB2	1:C:250:MET:HE3	1.93	0.49
2:D:207:GLU:HB2	2:D:392:MET:HE2	1.93	0.49
2:D:235:ASP:OD2	2:D:263:TYR:CE2	2.66	0.49
1:E:190:GLY:HA3	1:E:206:ARG:NH2	2.27	0.49
2:J:214:HIS:HA	2:J:269:MET:O	2.11	0.49
2:P:241:SER:O	2:P:244:TYR:HB3	2.13	0.49
2:P:251:PHE:CZ	2:P:262:HIS:ND1	2.81	0.49
1:A:195:CYS:H	1:A:196:PRO:CG	2.25	0.49
1:A:206:ARG:HG3	3:A:502:SF4:S3	2.52	0.49
2:B:149:TRP:HZ3	2:B:181:MET:HG3	1.76	0.49
1:C:12:SER:CB	1:C:58:GLY:HA2	2.34	0.49
1:C:26:LEU:O	1:C:30:ILE:HG12	2.13	0.49
1:C:150:LEU:HD12	8:C:620:HOH:O	2.11	0.49
1:C:205:CYS:SG	1:C:206:ARG:HG3	2.52	0.49
1:E:18:LEU:HD11	2:F:110:LEU:HD11	1.94	0.49
1:E:104:LYS:HG3	1:E:108:GLY:O	2.13	0.49
1:E:205:CYS:HA	1:E:240:PHE:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:272:ALA:HA	2:F:275:ARG:NH2	2.27	0.49
1:G:31:PRO:O	1:G:33:ALA:N	2.45	0.49
2:J:419:ILE:O	2:J:422:SER:N	2.46	0.49
2:L:43:ARG:NH2	2:L:64:ILE:HA	2.27	0.49
2:L:177:VAL:C	2:L:179:GLU:N	2.70	0.49
2:L:405:LYS:O	2:L:409:GLU:HG3	2.13	0.49
2:N:165:VAL:HG12	8:N:605:HOH:O	2.12	0.49
2:B:399:ASP:OD2	2:B:403:ARG:NH1	2.46	0.49
2:D:46:GLU:HG2	2:D:374:ILE:HD12	1.93	0.49
2:D:423:VAL:O	2:D:423:VAL:HG12	2.13	0.49
2:F:419:ILE:O	2:F:422:SER:OG	2.21	0.49
2:H:30:GLY:HA2	2:H:397:TYR:CE2	2.47	0.49
1:I:112:VAL:HG22	2:J:254:GLU:HA	1.95	0.49
2:J:126:PRO:C	2:J:128:LYS:H	2.20	0.49
2:J:237:GLU:CD	2:J:264:LYS:HZ1	2.21	0.49
2:L:275:ARG:HD3	2:L:352:GLU:CD	2.38	0.49
2:N:224:TYR:HB3	2:N:316:TYR:CZ	2.47	0.49
1:A:14:TYR:HB2	2:B:17:GLU:OE1	2.12	0.49
2:D:251:PHE:CE1	2:D:260:HIS:HB2	2.48	0.49
2:B:19:LYS:H	2:B:40:GLU:HG3	1.78	0.49
2:B:188:ALA:O	2:B:191:LEU:N	2.45	0.49
2:B:384:MET:HE3	2:B:388:HIS:CE1	2.48	0.49
2:D:342:ILE:HG22	2:D:367:GLY:HA2	1.93	0.49
2:F:271:GLY:HA2	2:F:356:GLY:HA2	1.93	0.49
2:F:390:ARG:HD3	8:F:627:HOH:O	2.12	0.49
2:F:421:CYS:O	2:F:422:SER:C	2.56	0.49
1:G:233:ILE:O	1:G:237:MET:HB2	2.13	0.49
2:J:17:GLU:HB3	2:J:418:CYS:HA	1.94	0.49
1:K:40:MET:HE3	2:L:67:PHE:CZ	2.48	0.49
2:N:376:THR:OG1	2:N:421:CYS:O	2.22	0.49
2:F:169:PHE:O	2:F:337:ARG:HB3	2.13	0.49
1:G:12:SER:HB2	3:G:501:SF4:S1	2.53	0.49
1:G:120:GLU:CD	1:G:124:LYS:HE2	2.38	0.49
2:D:68:CYS:O	2:D:69:SER:C	2.54	0.49
2:H:206:SER:C	2:H:208:VAL:H	2.21	0.49
1:I:13:CYS:HB2	1:I:15:GLY:H	1.78	0.49
1:I:232:GLU:O	1:I:236:ARG:HG3	2.13	0.49
2:J:121:ARG:HH12	2:J:198:LEU:CD1	2.24	0.49
1:O:247:VAL:HG13	1:O:248:GLU:CG	2.43	0.49
2:B:387:GLU:OE2	2:B:390:ARG:NH2	2.44	0.48
1:C:43:ARG:NH2	8:C:607:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:99:LEU:CD1	2:F:151:MET:HG2	2.42	0.48
1:G:5:ILE:O	1:G:36:VAL:HG22	2.13	0.48
1:K:113:LYS:HB2	2:L:254:GLU:HG3	1.95	0.48
2:L:101:ILE:HG22	2:L:105:ILE:CD1	2.43	0.48
1:M:174:ILE:HB	1:M:180:GLU:CD	2.38	0.48
2:B:17:GLU:OE2	2:B:420:SER:OG	2.31	0.48
1:C:195:CYS:HB3	1:C:200:VAL:HG22	1.94	0.48
1:G:135:CYS:HB3	1:G:205:CYS:HB2	1.95	0.48
2:H:418:CYS:O	2:H:421:CYS:HB2	2.13	0.48
1:I:63:GLU:HG2	1:I:117:LYS:HD2	1.93	0.48
2:J:163:ASN:O	2:J:169:PHE:HA	2.13	0.48
2:L:310:GLN:O	2:L:314:ILE:HG13	2.13	0.48
1:M:176:LEU:HD21	1:M:216:PHE:CE2	2.44	0.48
2:N:392:MET:SD	2:N:407:LEU:HB3	2.53	0.48
2:P:355:ARG:HD3	2:P:418:CYS:HB2	1.95	0.48
2:P:395:LYS:C	2:P:396:HIS:CG	2.91	0.48
1:A:228:MET:HB3	1:A:233:ILE:HD11	1.94	0.48
2:D:412:VAL:O	2:D:414:ALA:N	2.46	0.48
2:F:65:CYS:HB3	2:F:68:CYS:SG	2.44	0.48
2:F:192:ALA:HB1	2:F:315:VAL:HG22	1.94	0.48
2:F:332:TRP:CE3	2:F:334:ILE:HG13	2.48	0.48
2:J:235:ASP:OD2	2:J:263:TYR:OH	2.31	0.48
1:M:87:VAL:HG12	1:M:88:GLN:HG3	1.95	0.48
1:M:105:LYS:NZ	2:N:50:ILE:HG12	2.28	0.48
2:P:27:GLY:N	2:P:30:GLY:O	2.44	0.48
2:P:421:CYS:CB	4:P:501:FCO:C1	2.91	0.48
1:C:228:MET:HG2	1:C:232:GLU:OE1	2.13	0.48
2:D:108:HIS:HB3	2:D:314:ILE:HD11	1.96	0.48
2:D:332:TRP:CE3	2:D:334:ILE:HG13	2.48	0.48
2:F:46:GLU:O	2:F:50:ILE:HG12	2.13	0.48
1:G:30:ILE:HG21	1:G:146:LEU:HD22	1.95	0.48
2:H:291:TYR:O	2:H:295:LYS:HG3	2.14	0.48
2:J:376:THR:HG21	2:J:421:CYS:HB3	1.95	0.48
1:K:218:SER:HB3	1:K:221:LYS:HB3	1.95	0.48
2:N:123:TYR:CG	2:N:129:MET:HG2	2.49	0.48
1:A:31:PRO:C	1:A:33:ALA:H	2.21	0.48
1:A:146:LEU:HA	1:A:146:LEU:HD23	1.69	0.48
2:B:175:LYS:HE3	2:B:179:GLU:OE2	2.13	0.48
1:E:39:PHE:CE1	1:E:45:SER:HB3	2.49	0.48
2:F:359:VAL:CG2	2:F:375:ILE:HD13	2.43	0.48
1:I:63:GLU:HB2	1:I:115:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:SER:HG	1:I:243:HIS:CD2	2.31	0.48
1:I:209:ILE:HG13	1:I:210:GLY:N	2.29	0.48
1:K:163:CYS:O	1:K:167:ARG:HG3	2.13	0.48
1:M:203:ILE:HG12	3:M:502:SF4:S2	2.53	0.48
2:N:401:PRO:HG2	2:N:402:GLU:N	2.28	0.48
2:P:355:ARG:HB2	4:P:501:FCO:N2	2.28	0.48
2:P:387:GLU:CG	2:P:390:ARG:HH22	2.26	0.48
1:A:163:CYS:O	1:A:167:ARG:HG3	2.13	0.48
2:B:141:LEU:HD23	2:B:144:LYS:HZ3	1.79	0.48
1:C:103:TRP:CZ2	1:C:111:LYS:HA	2.48	0.48
2:D:235:ASP:OD1	2:D:237:GLU:HB2	2.14	0.48
2:D:297:LEU:HD12	2:D:297:LEU:HA	1.64	0.48
1:E:246:ARG:HH21	1:E:250:MET:HE1	1.78	0.48
2:F:68:CYS:O	2:F:70:ALA:N	2.47	0.48
2:F:359:VAL:HG22	2:F:375:ILE:HB	1.94	0.48
2:H:275:ARG:HD3	2:H:352:GLU:CD	2.39	0.48
2:H:355:ARG:HB2	4:H:501:FCO:N2	2.28	0.48
1:I:69:VAL:O	1:I:126:ILE:HG21	2.13	0.48
2:J:355:ARG:C	2:J:377:PRO:HB3	2.38	0.48
1:K:94:TRP:HH2	2:L:56:GLU:HB3	1.78	0.48
2:L:182:LYS:O	2:L:186:ARG:HG3	2.13	0.48
2:P:396:HIS:HA	2:P:399:ASP:HB2	1.95	0.48
2:D:104:MET:O	2:D:108:HIS:HB2	2.14	0.48
1:E:43:ARG:HB3	2:F:124:SER:HB2	1.95	0.48
2:F:69:SER:O	2:F:72:HIS:HB2	2.14	0.48
2:F:240:PRO:HB2	2:F:240:PRO:HD2	1.17	0.48
2:F:355:ARG:N	4:F:501:FCO:N2	2.60	0.48
2:H:232:LYS:HG3	2:H:238:GLU:HG3	1.94	0.48
2:J:196:PHE:HE1	2:J:312:LEU:HB2	1.79	0.48
2:J:223:ALA:HB1	2:J:316:TYR:OH	2.13	0.48
1:M:148:THR:O	1:M:151:ILE:HG12	2.13	0.48
1:O:3:VAL:HG23	1:O:32:ASN:O	2.14	0.48
2:B:19:LYS:H	2:B:40:GLU:CG	2.27	0.48
1:C:29:LEU:HD12	1:C:30:ILE:HG23	1.95	0.48
1:C:42:ASP:CG	1:C:44:ASP:H	2.21	0.48
1:C:59:SER:CB	1:C:92:GLN:HE21	2.27	0.48
2:H:192:ALA:HB2	2:H:314:ILE:CG2	2.44	0.48
2:J:138:GLU:HG3	2:J:142:LYS:HE3	1.96	0.48
2:L:65:CYS:CB	2:L:68:CYS:SG	3.01	0.48
2:D:284:TYR:OH	2:D:320:ARG:HD2	2.14	0.48
1:E:174:ILE:HD11	1:E:182:CYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:214:HIS:HB3	2:F:274:SER:HA	1.95	0.48
1:I:103:TRP:HE3	2:J:44:PHE:HZ	1.62	0.48
1:K:13:CYS:SG	3:K:501:SF4:S4	3.06	0.48
2:L:385:MET:CE	2:L:415:TYR:HB2	2.44	0.48
1:M:140[B]:LYS:HB2	1:M:140[B]:LYS:HE2	1.65	0.48
2:N:263:TYR:O	2:N:266:ARG:HG2	2.13	0.48
2:P:63:ARG:NH2	2:P:162:GLU:OE2	2.41	0.48
2:D:102:GLY:O	2:D:106:GLU:HB3	2.14	0.48
2:F:393:ALA:O	2:F:396:HIS:N	2.46	0.48
1:I:51:VAL:HG23	1:I:76:ALA:HB2	1.95	0.48
2:J:117:LEU:HD21	2:J:136:GLU:OE1	2.14	0.48
2:J:218:LYS:HB2	2:J:232:LYS:CG	2.35	0.48
2:P:346:PHE:HZ	2:P:371:TYR:CD2	2.31	0.48
1:A:111:LYS:O	2:B:254:GLU:HG2	2.14	0.47
2:B:378:THR:HG21	2:B:419:ILE:HD12	1.95	0.47
1:C:103:TRP:CD1	1:C:107:TYR:HD2	2.31	0.47
2:D:101:ILE:HG23	2:D:317:PHE:HB3	1.95	0.47
2:D:403:ARG:HG3	2:D:403:ARG:NH1	2.19	0.47
2:H:249:LYS:HE2	8:H:625:HOH:O	2.14	0.47
1:I:168:LEU:HD13	1:K:143:LEU:HD12	1.96	0.47
1:I:173:CYS:SG	1:I:176:LEU:HD12	2.54	0.47
1:K:9:ALA:HB2	1:K:17:GLN:NE2	2.25	0.47
1:K:237:MET:O	1:K:241:ASN:HB2	2.14	0.47
2:L:258:ALA:HB2	2:L:423:VAL:HG22	1.95	0.47
2:N:133:TYR:HB3	2:N:136:GLU:HG3	1.96	0.47
2:P:8:ILE:HB	2:P:24:ILE:H	1.79	0.47
1:A:20:LEU:HB2	8:A:602:HOH:O	2.13	0.47
1:A:243:HIS:CE1	8:A:607:HOH:O	2.67	0.47
1:G:50:LYS:HA	1:G:75:ASN:HB3	1.95	0.47
2:H:142:LYS:HD2	2:H:187:GLU:OE2	2.15	0.47
2:P:101:ILE:HG21	2:P:321:ALA:HB2	1.95	0.47
2:P:388:HIS:ND1	2:P:415:TYR:OH	2.35	0.47
1:E:9:ALA:HB1	1:E:14:TYR:CE1	2.48	0.47
2:F:365:GLU:O	2:F:366:ASN:HB3	2.14	0.47
2:H:62:PRO:HB3	2:H:73:LYS:HB2	1.94	0.47
2:H:246:ASP:C	2:H:247:TYR:CD1	2.92	0.47
2:H:399:ASP:CG	2:H:403:ARG:HH11	2.22	0.47
2:J:64:ILE:HD13	2:J:424:HIS:HB3	1.96	0.47
2:J:225:GLY:C	2:J:226:ILE:HD12	2.38	0.47
2:L:361:ALA:HB3	2:L:373:ASP:HB3	1.95	0.47
1:M:24:ASP:OD1	2:N:141:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:224:TYR:OH	2:N:313:GLU:OE2	2.26	0.47
1:O:216:PHE:CD2	1:O:219:LEU:HD13	2.49	0.47
1:A:130:TYR:CE2	1:A:132:ILE:HG12	2.49	0.47
2:B:34:VAL:HG11	2:B:386:GLU:O	2.14	0.47
2:B:114:LEU:O	2:B:115:LEU:HD23	2.15	0.47
2:B:224:TYR:HB3	2:B:316:TYR:CE2	2.50	0.47
1:E:20:LEU:HA	1:E:23:MET:HE3	1.97	0.47
2:F:346:PHE:CD1	2:F:363:LYS:HB2	2.35	0.47
1:I:244:ASP:C	1:I:246:ARG:H	2.22	0.47
2:J:34:VAL:HG21	2:J:386:GLU:O	2.15	0.47
2:P:65:CYS:SG	2:P:66:SER:N	2.87	0.47
2:F:17:GLU:O	2:F:419:ILE:HG13	2.14	0.47
1:G:146:LEU:O	1:G:150:LEU:HB2	2.15	0.47
2:H:104:MET:SD	2:H:354:PRO:HA	2.53	0.47
2:L:43:ARG:NH1	2:L:63:ARG:O	2.45	0.47
1:O:21:ALA:HB2	1:O:38:TRP:CZ2	2.49	0.47
1:O:91:VAL:HG11	2:P:60:ILE:HD12	1.96	0.47
1:A:194:ARG:HD3	2:B:156:SER:OG	2.15	0.47
1:C:220:ALA:HB2	1:C:254:ILE:O	2.15	0.47
2:D:56:GLU:O	2:D:59:ALA:HB3	2.14	0.47
2:D:64:ILE:HD13	2:D:424:HIS:CB	2.45	0.47
2:H:111:HIS:O	2:H:115:LEU:HB2	2.15	0.47
2:H:187:GLU:O	2:H:190:PRO:HD2	2.14	0.47
2:J:226:ILE:HD12	2:J:226:ILE:N	2.30	0.47
1:K:216:PHE:HB2	1:K:219:LEU:HB2	1.96	0.47
2:L:33:GLU:OE1	8:L:603:HOH:O	2.20	0.47
1:M:105:LYS:HZ1	2:N:50:ILE:HG12	1.80	0.47
1:M:213:VAL:HG22	1:O:32:ASN:OD1	2.14	0.47
2:N:121:ARG:HD3	2:N:121:ARG:HA	1.70	0.47
2:B:74:LEU:HD23	2:B:77:LEU:HD12	1.96	0.47
2:B:396:HIS:O	2:B:399:ASP:HB2	2.14	0.47
1:C:186:VAL:HG11	1:C:237:MET:HE3	1.97	0.47
1:C:223:PHE:CD1	1:C:228:MET:SD	3.07	0.47
2:D:169:PHE:N	2:D:336:PRO:O	2.41	0.47
2:F:172:LEU:HA	2:F:172:LEU:HD23	1.73	0.47
2:F:207:GLU:HG2	2:F:395:LYS:HZ2	1.79	0.47
2:F:214:HIS:H	2:F:234:SER:HB3	1.80	0.47
2:H:269:MET:HG3	2:H:415:TYR:HE2	1.80	0.47
2:H:316:TYR:CZ	2:H:320:ARG:HD2	2.50	0.47
2:J:286:LYS:HB3	2:J:286:LYS:HE3	1.69	0.47
2:L:101:ILE:HG23	2:L:317:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:332:TRP:CG	2:L:333:PRO:HA	2.49	0.47
1:M:27:LEU:HD11	2:N:127:LEU:HB3	1.95	0.47
2:N:45:PHE:CE2	2:N:60:ILE:HG12	2.50	0.47
2:P:123:TYR:CG	2:P:129:MET:HG2	2.49	0.47
2:P:258:ALA:CB	2:P:422:SER:HB2	2.44	0.47
2:B:175:LYS:O	2:B:179:GLU:HG2	2.15	0.47
2:B:224:TYR:HB3	2:B:316:TYR:CZ	2.50	0.47
2:D:69:SER:O	2:D:72:HIS:N	2.48	0.47
2:D:205:TYR:HB3	2:D:207:GLU:OE1	2.14	0.47
2:F:15:ARG:HD2	2:F:115:LEU:HA	1.96	0.47
2:J:385:MET:HE2	2:J:385:MET:HB2	1.76	0.47
1:M:203:ILE:HD11	2:N:63:ARG:NH2	2.30	0.47
1:O:5:ILE:HD13	1:O:33:ALA:HB1	1.97	0.47
2:P:65:CYS:CB	2:P:68:CYS:SG	2.95	0.47
2:B:34:VAL:HG22	2:B:386:GLU:HG2	1.96	0.47
2:B:377:PRO:HD2	4:B:501:FCO:N1	2.29	0.47
1:C:183:LEU:HD21	1:C:237:MET:HG3	1.97	0.47
1:G:140:LYS:HB2	1:G:140:LYS:HE3	1.47	0.47
2:H:34:VAL:HG11	2:H:386:GLU:O	2.14	0.47
2:J:91:GLU:HG2	2:J:92:ILE:HG12	1.97	0.47
2:L:117:LEU:C	2:L:119:ASP:N	2.73	0.47
2:N:63:ARG:HA	2:N:160:HIS:CE1	2.50	0.47
2:P:377:PRO:HB2	4:P:501:FCO:N1	2.29	0.47
2:B:385:MET:HG2	2:B:415:TYR:CD1	2.50	0.47
1:C:92:GLN:HB3	2:D:43:ARG:HB3	1.97	0.47
1:C:136:PRO:HD3	2:D:159:ILE:O	2.15	0.47
1:C:225:GLU:HB2	8:C:621:HOH:O	2.14	0.47
2:D:54:LEU:HG	2:D:58:LEU:HD12	1.97	0.47
2:D:303:PRO:C	2:D:305:ALA:H	2.23	0.47
2:D:353:ALA:HB3	2:D:377:PRO:HG2	1.97	0.47
2:F:42:PRO:HD3	2:F:257:PHE:CE2	2.50	0.47
1:G:58:GLY:HA2	1:G:85:CYS:CB	2.44	0.47
1:G:149:PHE:HE1	1:G:154:TRP:CE3	2.33	0.47
1:I:20:LEU:HD23	1:I:38:TRP:CZ2	2.50	0.47
1:I:234:ILE:HG23	1:I:247:VAL:HG22	1.96	0.47
2:J:385:MET:HE2	2:J:415:TYR:CG	2.50	0.47
2:L:99:LEU:HB2	2:L:154:LEU:HB3	1.96	0.47
2:N:400:ASP:HB3	2:N:403:ARG:H	1.80	0.47
2:P:82:LYS:HB3	2:P:347:GLY:HA3	1.96	0.47
2:P:237:GLU:OE1	2:P:264:LYS:NZ	2.48	0.47
1:A:174:ILE:HG21	1:A:199:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:ILE:HD11	2:D:393:ALA:HB1	1.96	0.46
2:D:25:ILE:O	2:D:31:VAL:HA	2.14	0.46
2:D:406:ILE:O	2:D:410:MET:HG3	2.14	0.46
1:E:98:PRO:HD2	1:E:101:GLU:CD	2.41	0.46
2:J:124:SER:OG	2:J:125:SER:N	2.48	0.46
1:K:39:PHE:HE1	1:K:47:GLU:HG3	1.79	0.46
1:K:73:ARG:NH2	1:K:129:ASP:OD2	2.47	0.46
2:L:27:GLY:C	8:L:604:HOH:O	2.57	0.46
1:O:112:VAL:HA	2:P:254:GLU:HG3	1.96	0.46
2:B:31:VAL:CG2	2:B:394:GLU:HG2	2.43	0.46
1:C:129:ASP:HB3	1:C:154:TRP:HH2	1.80	0.46
2:D:235:ASP:OD1	2:D:235:ASP:C	2.59	0.46
2:D:256:SER:OG	2:D:258:ALA:O	2.34	0.46
1:G:18:LEU:HG	1:G:22:MET:HE2	1.97	0.46
1:G:70:LYS:O	1:G:74:GLU:HG3	2.15	0.46
2:H:381:ASN:O	2:H:382:LEU:C	2.58	0.46
2:J:154:LEU:HD12	2:J:169:PHE:CE2	2.50	0.46
1:K:139:LYS:HE3	1:K:140:LYS:HG2	1.97	0.46
2:L:37:ASN:HA	2:L:255:HIS:O	2.14	0.46
2:L:421:CYS:HB3	4:L:501:FCO:N1	2.29	0.46
1:M:216:PHE:HB2	1:M:219:LEU:HB2	1.96	0.46
2:N:134:LYS:HG3	2:N:135:ARG:H	1.79	0.46
2:N:387:GLU:OE1	2:N:387:GLU:HA	2.15	0.46
2:B:21:GLY:O	2:B:36:LEU:HD23	2.14	0.46
2:D:38:ILE:HG23	2:D:419:ILE:CG2	2.45	0.46
2:F:75:THR:HG23	2:F:351:THR:HG23	1.98	0.46
2:H:126:PRO:C	2:H:128:LYS:H	2.23	0.46
1:K:162:VAL:HG23	1:K:187:THR:O	2.15	0.46
1:C:165:GLU:O	1:C:169:ASN:HB2	2.15	0.46
2:D:54:LEU:HG	2:D:58:LEU:CD1	2.46	0.46
2:D:255:HIS:HE1	8:D:622:HOH:O	1.97	0.46
2:D:271:GLY:HA2	2:D:356:GLY:HA2	1.97	0.46
2:H:320:ARG:HH11	2:H:320:ARG:HG3	1.81	0.46
1:I:23:MET:HE3	1:K:168:LEU:HD12	1.97	0.46
2:J:86:PHE:CG	2:J:340:VAL:HG12	2.50	0.46
1:M:127:LYS:HD3	1:M:128:VAL:H	1.81	0.46
1:O:38:TRP:CE3	1:O:41:ILE:HD11	2.51	0.46
2:P:22:VAL:HG12	2:P:23:GLU:H	1.81	0.46
2:P:346:PHE:HZ	2:P:371:TYR:CE2	2.34	0.46
1:A:207:GLY:C	8:A:604:HOH:O	2.57	0.46
2:B:36:LEU:HD12	2:B:386:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:MET:HG2	2:B:415:TYR:CE1	2.50	0.46
2:D:298:LEU:HA	2:D:298:LEU:HD23	1.72	0.46
2:F:32:LYS:HE2	2:F:32:LYS:HB2	1.67	0.46
2:F:52:LYS:NZ	8:F:607:HOH:O	2.38	0.46
2:F:359:VAL:HG23	2:F:375:ILE:CD1	2.45	0.46
1:I:18:LEU:HD23	2:J:159:ILE:CD1	2.44	0.46
2:J:215:LEU:C	2:J:270:VAL:HG12	2.40	0.46
1:K:144:TYR:HE2	1:K:156:GLU:H	1.64	0.46
2:L:59:ALA:O	2:L:63:ARG:NH1	2.48	0.46
2:L:208:VAL:HG23	2:L:302:ASN:OD1	2.15	0.46
1:M:37:CYS:SG	1:M:39:PHE:CE1	3.08	0.46
1:M:173:CYS:HA	3:M:503:SF4:S3	2.56	0.46
1:M:186:VAL:HG11	1:M:237:MET:HE3	1.98	0.46
2:N:342:ILE:HG22	2:N:342:ILE:O	2.16	0.46
2:P:220:ARG:HB3	2:P:228:GLY:HA2	1.98	0.46
1:A:239:MET:CG	2:B:60:ILE:HD11	2.39	0.46
1:C:205:CYS:HA	1:C:240:PHE:CD2	2.50	0.46
2:D:358:LEU:HD23	2:D:358:LEU:HA	1.68	0.46
2:D:377:PRO:O	2:D:380:PHE:HB2	2.16	0.46
2:H:24:ILE:HD13	2:H:393:ALA:HB2	1.98	0.46
2:H:123:TYR:CE2	2:H:129:MET:HB3	2.51	0.46
2:H:123:TYR:CD2	2:H:129:MET:HB3	2.51	0.46
1:I:92:GLN:H	1:I:92:GLN:HG2	1.48	0.46
1:I:221:LYS:O	1:I:225:GLU:HB3	2.15	0.46
2:J:29:ASP:HB3	2:J:32[B]:LYS:HG2	1.97	0.46
2:N:6:LEU:HD12	2:N:6:LEU:O	2.16	0.46
2:N:175:LYS:HB2	2:N:332:TRP:CZ2	2.51	0.46
1:O:154:TRP:CD1	1:O:155:PRO:HD2	2.50	0.46
1:A:58:GLY:H	1:A:86:ALA:HB2	1.79	0.46
2:D:275:ARG:HD3	2:D:352:GLU:CD	2.41	0.46
1:E:165:GLU:HG2	1:E:192:ASN:HA	1.97	0.46
1:E:186:VAL:HG11	1:E:237:MET:CE	2.34	0.46
2:F:38:ILE:HG21	2:F:258:ALA:HB2	1.98	0.46
2:J:108:HIS:HB3	2:J:314:ILE:HD11	1.97	0.46
1:K:163:CYS:SG	3:K:503:SF4:S4	3.13	0.46
2:L:289:GLU:HA	2:L:292:GLU:HB3	1.98	0.46
1:M:167:ARG:HB3	1:O:25:GLU:OE1	2.15	0.46
2:P:169:PHE:CD2	2:P:172:LEU:HD21	2.51	0.46
2:D:410:MET:HE3	2:D:410:MET:HB3	1.75	0.46
1:E:198:PHE:C	2:F:171:LYS:HG3	2.41	0.46
1:E:218:SER:O	1:E:221:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:ARG:HG3	2:F:322:ILE:HD13	1.97	0.46
2:L:64:ILE:HB	2:L:72:HIS:CD2	2.50	0.46
1:M:185:PRO:HD3	3:M:503:SF4:S4	2.55	0.46
2:N:385:MET:HE1	2:N:417:PRO:HG3	1.97	0.46
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.75	0.46
2:B:68:CYS:HA	2:B:103:ASP:OD2	2.15	0.46
2:B:131:ASN:HA	2:B:134:LYS:HZ2	1.81	0.46
2:B:319:GLU:O	2:B:322:ILE:HB	2.15	0.46
2:B:421:CYS:CB	4:B:501:FCO:C1	2.94	0.46
1:C:73:ARG:NH1	1:C:129:ASP:OD2	2.41	0.46
2:D:235:ASP:OD2	2:D:263:TYR:HE2	1.98	0.46
2:D:362:LEU:HD23	2:D:372:ALA:HA	1.98	0.46
2:D:422:SER:O	2:D:424:HIS:ND1	2.48	0.46
1:I:26:LEU:O	1:I:30:ILE:HG12	2.15	0.46
2:J:239:PHE:CZ	2:J:248:ILE:HD11	2.49	0.46
2:L:45:PHE:CE2	2:L:61:TYR:HA	2.47	0.46
2:B:73:LYS:O	2:B:77:LEU:HG	2.16	0.46
2:F:366:ASN:O	2:F:367:GLY:C	2.59	0.46
1:I:219:LEU:C	1:I:221:LYS:H	2.24	0.46
2:J:181:MET:SD	2:J:325:LEU:HD11	2.56	0.46
1:K:161:PRO:HG2	1:K:215:TRP:NE1	2.30	0.46
2:N:110:LEU:HD21	2:N:144:LYS:CD	2.46	0.46
2:N:245:ARG:HH21	2:N:249:LYS:HE2	1.81	0.46
1:A:83:GLY:O	1:A:87:VAL:HG23	2.16	0.45
1:A:174:ILE:HG13	3:A:503:SF4:S3	2.56	0.45
1:A:196:PRO:CG	1:A:196:PRO:CB	2.49	0.45
2:B:209:GLU:HA	2:B:301:THR:O	2.15	0.45
2:B:265:GLY:O	2:B:266:ARG:HG2	2.15	0.45
1:C:38:TRP:CE2	1:C:41:ILE:CD1	2.99	0.45
1:C:42:ASP:OD1	2:D:124:SER:OG	2.31	0.45
1:C:182:CYS:HA	1:C:201:ALA:HB1	1.98	0.45
2:D:90:GLU:HG3	2:D:91:GLU:HG3	1.98	0.45
2:D:104:MET:HE3	2:D:317:PHE:CE2	2.51	0.45
1:E:184:GLY:N	1:E:185:PRO:HD2	2.31	0.45
1:E:223:PHE:HE2	1:E:254:ILE:HG21	1.80	0.45
2:F:68:CYS:O	2:F:71:ALA:N	2.49	0.45
2:F:217:VAL:HB	2:F:352:GLU:HG2	1.98	0.45
1:G:183:LEU:HD11	1:G:236:ARG:HB3	1.98	0.45
2:H:389:VAL:O	2:H:393:ALA:N	2.45	0.45
1:I:39:PHE:CE1	1:I:45:SER:HB2	2.51	0.45
2:J:26:ILE:HA	2:J:30:GLY:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:136:GLU:OE2	2:J:198:LEU:HD22	2.15	0.45
2:J:217:VAL:HG23	2:J:357:ILE:HG23	1.98	0.45
1:K:174:ILE:HB	1:K:180:GLU:CD	2.41	0.45
1:K:191:CYS:HB3	1:K:206:ARG:HD2	1.97	0.45
2:L:218:LYS:HA	2:L:279:ASN:ND2	2.31	0.45
2:L:288:LYS:O	2:L:292:GLU:HB2	2.16	0.45
2:L:394:GLU:HA	2:L:394:GLU:OE1	2.16	0.45
2:N:46:GLU:OE2	2:N:424:HIS:NE2	2.49	0.45
1:A:58:GLY:HA2	1:A:85:CYS:HB2	1.97	0.45
2:B:361:ALA:O	2:B:372:ALA:HA	2.17	0.45
2:F:377:PRO:HD2	4:F:501:FCO:N1	2.30	0.45
2:L:46:GLU:OE2	2:L:424:HIS:CD2	2.69	0.45
1:M:139:LYS:HE3	1:M:140[A]:LYS:HG2	1.98	0.45
2:N:9:THR:HG22	2:N:23:GLU:HG3	1.98	0.45
2:N:401:PRO:O	2:N:402:GLU:C	2.58	0.45
2:P:67:PHE:HD1	2:P:67:PHE:H	1.63	0.45
1:C:221:LYS:O	1:C:225:GLU:HG3	2.16	0.45
2:J:75:THR:HG22	2:J:360:TYR:HB2	1.97	0.45
2:J:269:MET:HA	2:J:381:ASN:OD1	2.16	0.45
2:J:299:LYS:HE3	2:J:299:LYS:HB3	1.54	0.45
2:L:153:ILE:HD12	2:L:177:VAL:HG11	1.98	0.45
2:L:216:ALA:HB1	2:L:275:ARG:HG2	1.98	0.45
2:P:230:TYR:CD2	2:P:240:PRO:HA	2.51	0.45
2:P:346:PHE:CZ	2:P:371:TYR:HD2	2.34	0.45
1:A:7:PHE:HD1	1:A:55:PHE:O	1.98	0.45
1:A:12:SER:HB2	3:A:501:SF4:S1	2.55	0.45
2:B:135:ARG:HA	2:B:135:ARG:HD3	1.64	0.45
2:B:158:ALA:O	2:B:161:GLN:NE2	2.50	0.45
1:C:130:TYR:CZ	1:C:155:PRO:HB2	2.51	0.45
2:D:37:ASN:OD1	2:D:255:HIS:HB2	2.16	0.45
2:D:46:GLU:O	2:D:372:ALA:HB3	2.16	0.45
2:D:149:TRP:CZ3	2:D:181:MET:HG3	2.52	0.45
2:F:149:TRP:CH2	2:F:180:LYS:HD2	2.51	0.45
1:G:121:PRO:HD3	1:G:243:HIS:CD2	2.51	0.45
2:H:42:PRO:HA	2:H:423:VAL:HG12	1.98	0.45
1:I:120:GLU:OE2	1:I:243:HIS:CE1	2.70	0.45
2:L:289:GLU:H	2:L:289:GLU:CD	2.18	0.45
2:L:346:PHE:HD1	2:L:363:LYS:HB2	1.81	0.45
2:N:13:ILE:HD12	2:N:409:GLU:HG2	1.97	0.45
1:O:73:ARG:NH1	1:O:79:VAL:HB	2.32	0.45
2:P:208:VAL:HB	2:P:303:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:TRP:CZ3	2:B:181:MET:HG3	2.50	0.45
2:D:325:LEU:O	2:D:329:LEU:HB2	2.17	0.45
2:F:248:ILE:HG21	2:F:380:PHE:HE1	1.81	0.45
2:H:269:MET:HE3	2:H:415:TYR:CE2	2.51	0.45
1:I:23:MET:HG2	1:I:139:LYS:HE3	1.98	0.45
2:J:220:ARG:CG	2:J:228:GLY:HA2	2.46	0.45
2:J:358:LEU:HD21	2:J:360:TYR:CE2	2.52	0.45
2:L:187:GLU:HG2	2:L:187:GLU:O	2.16	0.45
1:O:73:ARG:NH1	1:O:127:LYS:O	2.46	0.45
1:O:156:GLU:OE1	1:O:156:GLU:HA	2.17	0.45
1:O:198:PHE:CE2	2:P:156:SER:HA	2.52	0.45
2:P:346:PHE:CZ	2:P:371:TYR:CD2	3.04	0.45
1:A:58:GLY:N	1:A:86:ALA:HB2	2.31	0.45
1:A:135:CYS:O	2:B:63:ARG:NH1	2.48	0.45
1:A:137:PRO:HB2	1:A:142:PHE:CE2	2.51	0.45
1:A:247:VAL:O	1:A:251:VAL:HG22	2.16	0.45
2:B:35:LYS:HA	2:B:386:GLU:OE2	2.17	0.45
2:D:248:ILE:HG22	2:D:250:GLU:OE2	2.16	0.45
1:E:224:LYS:NZ	1:E:255:PHE:HD2	2.15	0.45
2:F:366:ASN:O	2:F:366:ASN:CG	2.59	0.45
2:H:277:ILE:HD13	2:H:277:ILE:HA	1.71	0.45
2:J:77:LEU:HD13	2:J:96:ARG:NH2	2.32	0.45
2:L:154:LEU:HD13	2:L:154:LEU:HA	1.81	0.45
2:L:215:LEU:O	2:L:270:VAL:HG12	2.16	0.45
2:N:385:MET:HE1	2:N:417:PRO:HB3	1.98	0.45
2:P:13:ILE:HG23	2:P:409:GLU:HG2	1.98	0.45
1:A:250:MET:HE3	1:A:250:MET:HB3	1.83	0.45
2:B:38:ILE:HD13	2:B:419:ILE:HG13	1.98	0.45
2:B:244:TYR:CE1	2:B:245:ARG:HG2	2.51	0.45
2:D:406:ILE:HG22	2:D:407:LEU:N	2.32	0.45
1:E:111:LYS:HB2	1:E:111:LYS:NZ	2.31	0.45
3:E:501:SF4:S3	2:F:160:HIS:NE2	2.90	0.45
2:J:250:GLU:C	2:J:251:PHE:CD1	2.95	0.45
2:L:200:ALA:HB1	2:L:297:LEU:HD23	1.99	0.45
2:L:208:VAL:HA	2:L:391:MET:HE2	1.98	0.45
1:O:68:LEU:O	1:O:72:ILE:HD12	2.17	0.45
2:P:74:LEU:HD22	2:P:96:ARG:HG2	1.99	0.45
2:P:250:GLU:OE2	8:P:603:HOH:O	2.21	0.45
1:A:173:CYS:HB3	1:A:176:LEU:HB2	1.98	0.45
1:C:121:PRO:C	1:C:123:SER:N	2.72	0.45
2:D:70:ALA:HB2	2:D:151:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:GLY:HA3	2:F:419:ILE:HB	1.98	0.45
2:J:46:GLU:HG3	2:J:424:HIS:HD2	1.82	0.45
2:J:237:GLU:OE1	2:J:263:TYR:OH	2.25	0.45
2:L:80:ALA:O	2:L:84:VAL:HG22	2.17	0.45
2:L:291:TYR:CZ	2:L:295:LYS:HG3	2.51	0.45
2:N:34:VAL:HG11	2:N:389:VAL:CG1	2.46	0.45
2:N:297:LEU:HD23	2:N:297:LEU:HA	1.84	0.45
1:O:68:LEU:O	1:O:71:LYS:N	2.41	0.45
1:O:112:VAL:HG12	1:O:114:PHE:H	1.81	0.45
2:P:72:HIS:ND1	2:P:358:LEU:HD21	2.31	0.45
2:P:73:LYS:HE3	2:P:164:ALA:O	2.16	0.45
2:B:183:ALA:HA	2:B:186:ARG:HE	1.81	0.45
1:C:30:ILE:HD12	1:C:35:ILE:HD11	1.99	0.45
2:D:201:LYS:NZ	8:D:603:HOH:O	2.05	0.45
1:E:173:CYS:HA	3:E:503:SF4:S3	2.57	0.45
2:H:192:ALA:HB2	2:H:314:ILE:HG22	1.99	0.45
1:I:94:TRP:HZ3	1:I:235:GLU:HG2	1.81	0.45
2:J:67:PHE:N	2:J:67:PHE:CD1	2.84	0.45
2:N:159:ILE:HG22	2:N:160:HIS:CD2	2.51	0.45
1:O:183:LEU:HD21	1:O:237:MET:HG3	1.99	0.45
2:B:302:ASN:HA	2:B:303:PRO:HD2	1.79	0.45
1:C:18:LEU:HD23	2:D:159:ILE:HD11	1.99	0.45
2:D:302:ASN:OD1	2:D:304:PHE:HB2	2.16	0.45
2:F:102:GLY:HA2	2:F:150:MET:HE3	1.98	0.45
1:G:174:ILE:HG13	3:G:503:SF4:S3	2.57	0.45
1:I:195:CYS:HB2	1:I:196:PRO:HD3	1.98	0.45
2:J:355:ARG:HB2	4:J:501:FCO:C2	2.47	0.45
1:K:13:CYS:SG	3:K:501:SF4:S3	3.15	0.45
1:K:16:CYS:HB2	1:K:57:GLU:HG3	1.98	0.45
2:L:377:PRO:CD	4:L:501:FCO:C3	2.95	0.45
1:M:17:GLN:NE2	1:M:38:TRP:HE1	2.10	0.45
1:O:106:VAL:HG13	2:P:46:GLU:OE2	2.17	0.45
2:P:94:ALA:HA	2:P:324:LEU:HD22	1.98	0.45
2:P:284:TYR:OH	2:P:320:ARG:NH1	2.44	0.45
2:B:17:GLU:HG2	2:B:418:CYS:SG	2.57	0.44
2:B:72:HIS:HE1	2:B:376:THR:HG22	1.82	0.44
2:H:358:LEU:HD21	2:H:360:TYR:CE1	2.51	0.44
2:L:188:ALA:O	2:L:191:LEU:N	2.50	0.44
2:L:211:PRO:C	2:L:212:ILE:HG13	2.40	0.44
2:L:218:LYS:O	2:L:228:GLY:HA3	2.17	0.44
2:N:15:ARG:HB2	2:N:413:ARG:NH1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:192:ALA:HB2	2:N:314:ILE:HG22	1.98	0.44
2:N:400:ASP:HA	2:N:401:PRO:HD2	1.25	0.44
1:O:14:TYR:CE2	2:P:18:GLY:N	2.78	0.44
1:C:224:LYS:O	1:C:225:GLU:C	2.60	0.44
2:F:199:PHE:HA	2:F:202:LEU:HD12	1.99	0.44
2:H:34:VAL:CG1	2:H:390:ARG:HB2	2.47	0.44
1:I:173:CYS:O	1:I:177:GLU:HB3	2.17	0.44
2:J:231:ILE:O	2:J:239:PHE:N	2.48	0.44
2:J:335:LYS:HG3	2:J:336:PRO:HD2	1.98	0.44
1:K:220:ALA:HA	1:K:223:PHE:HB2	2.00	0.44
2:N:130:VAL:HG23	2:N:131:ASN:N	2.31	0.44
2:N:417:PRO:HB2	2:N:419:ILE:CD1	2.48	0.44
1:C:169:ASN:HD21	1:C:192:ASN:HD21	1.65	0.44
2:D:196:PHE:CD2	2:D:290:LEU:HD22	2.52	0.44
2:F:35:LYS:HE3	2:F:255:HIS:ND1	2.33	0.44
2:H:255:HIS:CD2	2:H:255:HIS:O	2.71	0.44
1:I:13:CYS:O	2:J:66:SER:OG	2.26	0.44
2:J:44:PHE:O	2:J:48:ILE:HG23	2.18	0.44
2:J:97:GLU:HG2	2:J:324:LEU:HD11	1.99	0.44
2:L:98:VAL:HA	2:L:101:ILE:HD12	1.98	0.44
2:N:250:GLU:CG	2:N:259:LYS:HB3	2.47	0.44
1:O:244:ASP:O	1:O:247:VAL:HG12	2.17	0.44
2:P:44:PHE:O	2:P:48:ILE:HG23	2.17	0.44
1:C:5:ILE:CG2	1:C:35:ILE:HG12	2.46	0.44
2:D:141:LEU:HD22	2:D:144:LYS:NZ	2.32	0.44
2:D:346:PHE:CE2	2:D:348:VAL:HG23	2.52	0.44
2:F:421:CYS:HB3	4:F:501:FCO:C1	2.42	0.44
1:I:116:PRO:HG3	2:J:257:PHE:CE1	2.51	0.44
2:J:245:ARG:NH2	2:J:375:ILE:HD11	2.32	0.44
2:L:120:TYR:CD2	2:L:202:LEU:HD22	2.52	0.44
1:O:173:CYS:O	1:O:177:GLU:N	2.35	0.44
2:B:38:ILE:HD12	2:B:382:LEU:HD11	2.00	0.44
1:C:43:ARG:HH22	2:D:405:LYS:HB3	1.82	0.44
1:C:94:TRP:CZ3	1:C:239:MET:HE3	2.53	0.44
1:C:94:TRP:CZ2	2:D:52:LYS:HG3	2.53	0.44
1:C:216:PHE:CD2	1:C:222:VAL:HG21	2.52	0.44
2:D:348:VAL:HG22	2:D:361:ALA:HB2	1.99	0.44
2:F:99:LEU:HD12	2:F:99:LEU:O	2.18	0.44
2:F:134:LYS:HA	2:F:137:ILE:HG22	1.99	0.44
2:F:209:GLU:HG3	2:F:301:THR:HG22	1.98	0.44
2:F:356:GLY:HA3	2:F:377:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:MET:HG3	2:H:415:TYR:CE2	2.52	0.44
1:I:145:ALA:C	1:I:147:GLY:H	2.25	0.44
2:J:67:PHE:N	2:J:67:PHE:HD1	2.15	0.44
2:J:155:GLY:O	2:J:161:GLN:HA	2.17	0.44
1:K:246:ARG:O	1:K:250:MET:N	2.46	0.44
2:L:89:ARG:NH1	2:L:91:GLU:OE2	2.50	0.44
2:L:289:GLU:N	2:L:289:GLU:CD	2.76	0.44
2:P:358:LEU:HD21	2:P:360:TYR:CE2	2.51	0.44
1:A:13:CYS:SG	3:A:501:SF4:S3	3.15	0.44
1:A:36:VAL:HG21	1:A:51:VAL:HG12	1.99	0.44
1:A:69:VAL:O	1:A:126:ILE:HG21	2.18	0.44
1:E:248:GLU:H	1:E:248:GLU:CD	2.26	0.44
2:F:242:GLU:OE1	2:F:242:GLU:N	2.46	0.44
2:H:19:LYS:HA	8:H:604:HOH:O	2.17	0.44
1:K:148:THR:O	1:K:151:ILE:HG12	2.18	0.44
1:M:163:CYS:HA	3:M:503:SF4:S1	2.57	0.44
2:P:134:LYS:HE3	2:P:134:LYS:HB2	1.82	0.44
1:A:7:PHE:CD1	1:A:55:PHE:O	2.71	0.44
1:A:124:LYS:HD2	1:A:125:TYR:CD1	2.52	0.44
2:B:37:ASN:HA	2:B:255:HIS:O	2.17	0.44
2:B:141:LEU:HG	2:B:141:LEU:H	1.67	0.44
2:B:382:LEU:HD23	2:B:382:LEU:HA	1.55	0.44
2:D:25:ILE:HG21	2:D:32:LYS:HD3	1.99	0.44
2:H:33:GLU:HB3	2:H:35:LYS:HE3	2.00	0.44
1:I:10:LEU:HB3	1:I:59:SER:O	2.17	0.44
1:I:191:CYS:HB2	1:I:194:ARG:NH1	2.32	0.44
2:J:101:ILE:HA	2:J:104:MET:HB2	2.00	0.44
1:K:89:GLY:O	1:K:93:SER:OG	2.33	0.44
2:L:239:PHE:CE1	2:L:244:TYR:HA	2.52	0.44
2:L:269:MET:HA	2:L:381:ASN:OD1	2.18	0.44
2:N:157:ARG:HD3	2:N:159:ILE:O	2.18	0.44
2:N:401:PRO:HG2	2:N:402:GLU:H	1.82	0.44
2:P:58:LEU:HD21	2:P:77:LEU:HG	2.00	0.44
2:P:169:PHE:O	2:P:336:PRO:HB2	2.18	0.44
2:P:355:ARG:C	2:P:377:PRO:HB3	2.43	0.44
2:P:363:LYS:HB3	2:P:371:TYR:N	2.31	0.44
2:B:35:LYS:HD3	2:B:255:HIS:CG	2.53	0.44
2:B:77:LEU:HD23	2:B:77:LEU:HA	1.79	0.44
2:B:323:ASP:O	2:B:326:ASP:HB2	2.18	0.44
1:C:103:TRP:HZ2	1:C:111:LYS:HA	1.83	0.44
1:C:246:ARG:HB2	1:C:246:ARG:HE	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:HA	1:C:256:SER:HB3	2.00	0.44
2:D:303:PRO:HG3	2:D:388:HIS:ND1	2.33	0.44
2:D:414:ALA:C	2:D:416:ASP:H	2.26	0.44
2:H:212:ILE:HD12	2:H:300:GLY:O	2.18	0.44
2:H:358:LEU:HD21	2:H:360:TYR:HE1	1.83	0.44
1:I:18:LEU:HD23	2:J:159:ILE:HD12	2.00	0.44
2:J:24:ILE:HG22	2:J:26:ILE:HG13	2.00	0.44
2:J:284:TYR:OH	2:J:320:ARG:NH1	2.47	0.44
2:L:110:LEU:HD11	2:L:144:LYS:CD	2.46	0.44
2:L:355:ARG:HG2	2:L:416:ASP:HB3	2.00	0.44
2:L:377:PRO:HG2	4:L:501:FCO:C1	2.44	0.44
1:O:145:ALA:O	1:O:149:PHE:HB2	2.18	0.44
1:O:163:CYS:O	1:O:167:ARG:HD2	2.17	0.44
2:P:387:GLU:HG2	2:P:390:ARG:NH2	2.32	0.44
2:P:397:TYR:HA	2:P:404:LEU:HD22	2.00	0.44
1:A:118:LYS:HB3	1:A:118:LYS:HE3	1.42	0.44
2:D:6:LEU:O	2:D:26:ILE:HD11	2.18	0.44
1:E:144:TYR:O	1:E:148:THR:OG1	2.31	0.44
2:F:46:GLU:O	2:F:372:ALA:HB3	2.17	0.44
2:F:207:GLU:HB3	2:F:395:LYS:HD3	1.99	0.44
2:F:349:SER:N	2:F:360:TYR:O	2.44	0.44
1:G:158:ILE:HG23	1:G:160:TYR:CD2	2.53	0.44
2:H:208:VAL:HA	2:H:391:MET:HE2	1.99	0.44
2:J:128:LYS:C	2:J:130:VAL:H	2.25	0.44
2:L:104:MET:SD	2:L:317:PHE:CE2	3.11	0.44
2:L:207:GLU:HG3	2:L:395:LYS:NZ	2.33	0.44
1:O:105:LYS:HA	1:O:105:LYS:HD3	1.93	0.44
1:O:158:ILE:HG23	1:O:160:TYR:CE2	2.53	0.44
1:O:182:CYS:CA	1:O:201:ALA:HB1	2.47	0.44
1:C:112:VAL:HG22	2:D:253:VAL:O	2.18	0.43
2:F:84:VAL:HG12	2:F:343:LYS:O	2.18	0.43
2:H:31:VAL:HG21	2:H:394:GLU:HG2	1.98	0.43
1:K:206:ARG:HG3	3:K:502:SF4:S3	2.57	0.43
1:A:187:THR:HG22	1:A:188:ARG:O	2.18	0.43
2:D:182:LYS:HE3	2:D:182:LYS:HB2	1.43	0.43
1:I:213:VAL:HG12	1:I:214:ALA:N	2.33	0.43
1:K:221:LYS:O	1:K:225:GLU:HB2	2.17	0.43
2:L:121:ARG:HA	2:L:121:ARG:HD3	1.61	0.43
2:L:200:ALA:C	2:L:202:LEU:H	2.26	0.43
2:L:200:ALA:N	2:L:308:LEU:HD13	2.33	0.43
1:M:16:CYS:HB2	1:M:57:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:160:TYR:HB2	1:O:164:LEU:HD22	1.99	0.43
1:O:249:LYS:HA	1:O:249:LYS:HD3	1.70	0.43
2:P:284:TYR:OH	2:P:320:ARG:HD2	2.18	0.43
2:P:387:GLU:HG3	2:P:390:ARG:HH22	1.83	0.43
1:A:10:LEU:HB3	1:A:59:SER:O	2.18	0.43
1:A:136:PRO:HG3	2:B:159:ILE:HB	2.01	0.43
2:B:54:LEU:HD23	2:B:166:LEU:HD11	2.01	0.43
2:B:63:ARG:HD3	2:B:160:HIS:CD2	2.53	0.43
2:D:290:LEU:O	2:D:294:ASN:HB2	2.18	0.43
1:E:9:ALA:O	1:E:10:LEU:HD23	2.18	0.43
1:E:29:LEU:HD12	1:E:30:ILE:HG23	1.99	0.43
1:G:229:THR:O	1:G:233:ILE:HG12	2.19	0.43
2:J:29:ASP:HB3	2:J:32[A]:LYS:HG2	1.99	0.43
2:J:86:PHE:CD1	2:J:340:VAL:HG12	2.52	0.43
2:J:101:ILE:HG23	2:J:317:PHE:HB3	2.01	0.43
2:L:385:MET:O	2:L:389:VAL:HG23	2.18	0.43
1:M:183:LEU:HD23	1:M:237:MET:HG2	2.01	0.43
2:N:117:LEU:HD11	2:N:198:LEU:HD21	2.00	0.43
2:P:169:PHE:CG	2:P:172:LEU:HD21	2.53	0.43
2:P:218:LYS:HB2	2:P:232:LYS:HG3	2.00	0.43
2:B:53[B]:LYS:HA	2:B:368:ARG:HA	2.00	0.43
2:B:393:ALA:O	2:B:397:TYR:HB3	2.18	0.43
1:C:193:ALA:HB1	1:C:196:PRO:HG2	2.00	0.43
2:D:60:ILE:HD13	2:D:60:ILE:HG21	1.61	0.43
2:F:316:TYR:OH	2:F:320:ARG:HD3	2.17	0.43
2:H:19:LYS:HB3	2:H:19:LYS:HE3	1.68	0.43
1:I:42:ASP:OD1	2:J:125:SER:HB2	2.19	0.43
1:I:213:VAL:HB	1:I:215:TRP:CE2	2.53	0.43
2:J:259:LYS:HB2	2:J:259:LYS:HE2	1.52	0.43
1:K:16:CYS:SG	3:K:501:SF4:S3	3.14	0.43
2:N:40:GLU:O	2:N:423:VAL:HG11	2.18	0.43
2:N:45:PHE:CE2	2:N:64:ILE:HG13	2.53	0.43
2:B:64:ILE:HG21	2:B:72:HIS:HE2	1.84	0.43
2:B:295:LYS:C	2:B:297:LEU:H	2.25	0.43
2:B:353:ALA:O	2:B:355:ARG:N	2.52	0.43
2:B:392:MET:CE	2:B:407:LEU:HB3	2.36	0.43
1:C:26:LEU:HA	1:C:29:LEU:HG	2.01	0.43
2:D:272:ALA:H	2:D:306:ASN:HD21	1.66	0.43
1:E:85:CYS:HA	1:E:90:GLY:CA	2.48	0.43
1:E:244:ASP:OD2	1:E:247:VAL:HG23	2.17	0.43
2:H:100:TYR:CZ	2:H:226:ILE:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:283:LEU:O	2:H:288:LYS:HD2	2.19	0.43
1:I:94:TRP:CZ3	1:I:235:GLU:HG2	2.53	0.43
1:I:254:ILE:C	1:I:256:SER:H	2.26	0.43
2:J:97:GLU:HB3	2:J:324:LEU:HD13	2.01	0.43
1:K:163:CYS:HA	3:K:503:SF4:S1	2.58	0.43
1:O:99:LEU:HD11	1:O:117:LYS:CA	2.48	0.43
1:O:232:GLU:OE2	2:P:53:LYS:NZ	2.50	0.43
2:P:166:LEU:HA	2:P:166:LEU:HD23	1.62	0.43
2:P:216:ALA:HB1	2:P:275:ARG:HG2	2.00	0.43
2:P:355:ARG:HG2	2:P:416:ASP:O	2.18	0.43
1:A:12:SER:O	2:B:420:SER:OG	2.32	0.43
1:A:88:GLN:NE2	1:A:240:PHE:O	2.52	0.43
2:D:151:MET:HE2	2:D:161:GLN:NE2	2.34	0.43
1:E:186:VAL:O	1:E:209:ILE:HG22	2.18	0.43
2:H:215:LEU:HD13	2:H:268:PHE:CD2	2.54	0.43
2:J:47:ALA:HA	2:J:50:ILE:HG12	2.01	0.43
2:L:271:GLY:O	2:L:275:ARG:HG3	2.19	0.43
2:N:34:VAL:HG11	2:N:389:VAL:HG11	2.00	0.43
2:N:110:LEU:O	2:N:114:LEU:HB2	2.19	0.43
2:N:295:LYS:HD2	2:N:295:LYS:C	2.43	0.43
2:N:377:PRO:CD	4:N:501:FCO:C3	2.97	0.43
1:O:2:LYS:HD2	1:O:34:GLU:HG3	2.01	0.43
2:P:232:LYS:HA	2:P:238:GLU:HA	2.00	0.43
1:A:13:CYS:HB2	2:B:65:CYS:HA	2.01	0.43
1:C:26:LEU:C	1:C:28:GLN:H	2.27	0.43
1:C:188:ARG:HH12	1:C:207:GLY:HA3	1.82	0.43
2:D:349:SER:N	2:D:360:TYR:O	2.52	0.43
2:D:396:HIS:ND1	2:D:399:ASP:OD2	2.49	0.43
1:E:12:SER:HB3	1:E:58:GLY:CA	2.48	0.43
2:F:108:HIS:O	2:F:112:LEU:HD12	2.18	0.43
2:F:192:ALA:O	2:F:195:THR:HB	2.19	0.43
2:F:217:VAL:HG23	2:F:357:ILE:HG12	1.99	0.43
1:I:120:GLU:HG3	1:I:121:PRO:HD2	1.99	0.43
2:J:19:LYS:HE3	2:J:39:ILE:HD11	2.01	0.43
1:K:23:MET:HE2	1:K:139:LYS:HA	2.01	0.43
2:P:128:LYS:C	2:P:130:VAL:H	2.27	0.43
2:P:139:ILE:HD13	2:P:194:TYR:CG	2.54	0.43
1:A:91:VAL:HA	1:A:239:MET:O	2.19	0.43
2:B:19:LYS:CB	2:B:40:GLU:HG2	2.48	0.43
2:B:353:ALA:C	2:B:355:ARG:H	2.27	0.43
2:D:218:LYS:HG3	2:D:232:LYS:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:THR:HG21	2:D:421:CYS:C	2.43	0.43
2:F:91:GLU:HA	2:F:94:ALA:HB3	2.01	0.43
2:F:251:PHE:HE1	2:F:262:HIS:CD2	2.37	0.43
2:H:245:ARG:CZ	2:H:373:ASP:OD2	2.66	0.43
2:J:24:ILE:HD12	2:J:34:VAL:HG12	2.01	0.43
2:L:17:GLU:OE1	2:L:420:SER:HB2	2.19	0.43
2:L:117:LEU:HD22	2:L:121:ARG:HG2	2.01	0.43
1:M:246:ARG:C	1:M:250:MET:HG3	2.44	0.43
2:N:403:ARG:HH11	2:N:403:ARG:CG	2.32	0.43
1:O:42:ASP:O	1:O:45:SER:OG	2.32	0.43
1:O:60:VAL:HG11	1:O:125:TYR:CE2	2.54	0.43
2:P:316:TYR:OH	2:P:320:ARG:HD3	2.18	0.43
1:C:87:VAL:CG1	1:C:88:GLN:HE21	2.31	0.43
1:C:165:GLU:HG2	1:C:192:ASN:HA	2.01	0.43
1:C:186:VAL:HG21	1:C:237:MET:CE	2.49	0.43
2:D:15:ARG:NH1	2:D:115:LEU:O	2.51	0.43
2:D:67:PHE:CD1	2:D:67:PHE:N	2.87	0.43
2:D:287:ALA:CB	2:D:316:TYR:HB2	2.49	0.43
2:D:412:VAL:C	2:D:414:ALA:H	2.26	0.43
1:G:101:GLU:O	1:G:105:LYS:HB2	2.18	0.43
2:H:166:LEU:HD23	2:H:166:LEU:HA	1.71	0.43
2:L:422:SER:OG	2:L:423:VAL:N	2.51	0.43
1:M:94:TRP:HH2	2:N:56:GLU:HB3	1.83	0.43
2:P:392:MET:HE2	2:P:392:MET:HB2	1.86	0.43
1:C:120:GLU:CG	1:C:121:PRO:HD2	2.46	0.43
2:D:103:ASP:O	2:D:107:SER:HB3	2.19	0.43
2:F:344:ASP:HA	2:F:364:VAL:HG12	2.00	0.43
2:H:185:LEU:CB	2:H:322:ILE:HD11	2.48	0.43
2:H:215:LEU:CD2	2:H:248:ILE:HD11	2.48	0.43
2:J:207:GLU:O	2:J:208:VAL:HG13	2.18	0.43
2:L:40:GLU:HB2	2:L:419:ILE:HG22	2.01	0.43
1:M:37:CYS:HB2	1:M:46:ILE:O	2.19	0.43
1:M:91:VAL:C	1:M:93:SER:N	2.77	0.43
2:P:22:VAL:HG13	2:P:36:LEU:HD23	2.01	0.43
2:P:287:ALA:HB2	2:P:316:TYR:HB2	2.01	0.43
1:A:30:ILE:HG22	1:A:150:LEU:HD12	1.99	0.42
1:A:183:LEU:HD13	1:A:237:MET:HG3	2.01	0.42
2:B:42:PRO:HB2	2:B:44:PHE:CE1	2.53	0.42
1:C:115:GLN:HA	1:C:116:PRO:HD3	1.85	0.42
1:C:121:PRO:O	1:C:121:PRO:HG2	2.17	0.42
2:D:303:PRO:HD3	2:D:388:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:LEU:O	2:F:329:LEU:N	2.47	0.42
2:H:299:LYS:HE2	2:H:299:LYS:HB3	1.71	0.42
2:H:302:ASN:HA	2:H:303:PRO:HD2	1.79	0.42
2:J:146:LEU:O	2:J:150:MET:HG3	2.19	0.42
1:O:18:LEU:HD23	2:P:159:ILE:CD1	2.48	0.42
1:O:233:ILE:HD13	1:O:233:ILE:HA	1.81	0.42
2:P:358:LEU:HD12	2:P:358:LEU:HA	1.73	0.42
2:B:64:ILE:O	2:B:420:SER:HB3	2.19	0.42
2:B:71:ALA:O	2:B:75:THR:OG1	2.23	0.42
1:C:22:MET:HG2	2:D:144:LYS:HD3	2.00	0.42
1:C:245:GLU:N	1:C:245:GLU:CD	2.77	0.42
2:F:159:ILE:O	2:F:160:HIS:HB2	2.19	0.42
2:F:172:LEU:HA	2:F:173:PRO:HD2	1.87	0.42
1:G:185:PRO:HD3	3:G:503:SF4:S4	2.59	0.42
2:H:387:GLU:O	2:H:391:MET:HG3	2.20	0.42
1:I:25:GLU:OE2	1:K:170:GLY:HA2	2.19	0.42
1:I:198:PHE:CZ	2:J:156:SER:HA	2.54	0.42
2:J:210:GLY:O	8:J:601:HOH:O	2.22	0.42
1:K:96:GLU:H	1:K:96:GLU:CD	2.22	0.42
2:L:8:ILE:HD12	2:L:24:ILE:HB	2.01	0.42
2:L:58:LEU:HD12	2:L:166:LEU:HD11	2.01	0.42
2:L:86:PHE:O	2:L:87:VAL:HB	2.19	0.42
1:M:246:ARG:HE	1:M:246:ARG:HB2	1.51	0.42
2:N:10:ILE:HB	2:N:22:VAL:HG23	2.01	0.42
2:P:363:LYS:HG2	2:P:370:SER:OG	2.18	0.42
2:B:15:ARG:CA	2:B:115:LEU:HD22	2.48	0.42
2:B:18:GLY:HA3	2:B:419:ILE:HB	2.01	0.42
2:B:139:ILE:HD13	2:B:194:TYR:CD2	2.54	0.42
1:C:121:PRO:C	1:C:123:SER:H	2.27	0.42
2:H:17:GLU:HB3	2:H:418:CYS:HA	2.00	0.42
2:H:86:PHE:O	2:H:87:VAL:HG23	2.19	0.42
2:J:19:LYS:HE3	2:J:39:ILE:CD1	2.49	0.42
2:J:403:ARG:O	2:J:406:ILE:HG13	2.20	0.42
2:N:32:LYS:O	2:N:33:GLU:HG3	2.19	0.42
2:N:231:ILE:HD11	2:N:350:THR:HG21	2.00	0.42
2:B:63:ARG:NH2	2:B:162:GLU:OE2	2.53	0.42
1:C:41:ILE:HG23	2:D:126:PRO:HD2	2.01	0.42
1:C:160:TYR:HB2	1:C:164:LEU:CD1	2.49	0.42
1:C:184:GLY:HA3	3:C:503:SF4:S1	2.60	0.42
2:D:34:VAL:HG12	2:D:390:ARG:HB2	2.01	0.42
2:D:65:CYS:HB3	2:D:68:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:SER:OG	2:D:355:ARG:NH1	2.42	0.42
2:D:258:ALA:HB2	2:D:423:VAL:HG22	2.02	0.42
1:E:143:LEU:HD22	1:G:168:LEU:HD13	2.02	0.42
2:J:212:ILE:HG21	2:J:388:HIS:HE1	1.85	0.42
2:J:280:ALA:O	2:J:283:LEU:HB2	2.19	0.42
1:K:6:GLY:O	1:K:55:PHE:N	2.53	0.42
1:K:10:LEU:HB2	1:K:58:GLY:HA3	2.02	0.42
1:K:93:SER:O	1:K:242:GLY:HA3	2.20	0.42
1:K:112:VAL:HG13	2:L:254:GLU:O	2.19	0.42
2:L:319:GLU:O	2:L:322:ILE:HB	2.19	0.42
1:O:181:PRO:HG3	1:O:236:ARG:CZ	2.50	0.42
1:A:37:CYS:HA	1:A:45:SER:OG	2.19	0.42
1:C:198:PHE:HA	2:D:171:LYS:HB2	2.02	0.42
2:D:58:LEU:HD13	2:D:166:LEU:HD13	2.01	0.42
1:E:25:GLU:CD	1:G:167:ARG:HG2	2.44	0.42
2:F:355:ARG:HB2	4:F:501:FCO:C2	2.48	0.42
2:F:400:ASP:HA	2:F:401:PRO:HD2	1.77	0.42
1:G:104:LYS:HA	1:G:108:GLY:O	2.19	0.42
2:H:65:CYS:SG	2:H:68:CYS:SG	3.17	0.42
1:I:28:GLN:NE2	6:I:504:PO4:O3	2.51	0.42
2:J:187:GLU:O	2:J:187:GLU:HG2	2.19	0.42
1:M:91:VAL:HB	2:N:60:ILE:HG13	2.01	0.42
2:N:43:ARG:NH1	2:N:63:ARG:O	2.51	0.42
2:N:59:ALA:O	2:N:63:ARG:NH1	2.50	0.42
2:N:73:LYS:O	2:N:77:LEU:HG	2.20	0.42
1:O:195:CYS:O	1:O:198:PHE:N	2.42	0.42
3:O:501:SF4:S4	2:P:63:ARG:HG2	2.59	0.42
2:P:86:PHE:O	2:P:87:VAL:HB	2.20	0.42
2:P:310:GLN:O	2:P:314:ILE:HG12	2.20	0.42
1:A:188:ARG:HG3	1:A:189:ALA:N	2.33	0.42
2:B:53[A]:LYS:HA	2:B:368:ARG:HA	2.00	0.42
2:D:36:LEU:HD23	2:D:36:LEU:HA	1.77	0.42
2:D:172:LEU:HD23	2:D:172:LEU:HA	1.82	0.42
2:D:226:ILE:HA	2:D:352:GLU:HB2	2.00	0.42
1:I:195:CYS:HB2	3:I:502:SF4:S4	2.59	0.42
1:K:187:THR:HG23	1:K:207:GLY:O	2.19	0.42
2:L:212:ILE:CG1	2:L:384:MET:HE2	2.45	0.42
1:M:211:TYR:CE1	1:M:215:TRP:HD1	2.37	0.42
2:N:51:GLY:HA2	2:N:368:ARG:NE	2.35	0.42
2:N:141:LEU:O	2:N:145:ASN:ND2	2.53	0.42
2:P:94:ALA:HB3	2:P:328:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:189:LEU:HD13	2:P:318:ILE:HB	2.00	0.42
2:B:12[A]:HIS:HA	2:B:20:GLY:O	2.20	0.42
1:C:7:PHE:CE1	1:C:57:GLU:HB2	2.53	0.42
1:E:151:ILE:HD12	1:G:159:ASP:HB3	2.02	0.42
2:F:38:ILE:HD11	2:F:382:LEU:HD21	2.02	0.42
2:F:251:PHE:CE1	2:F:262:HIS:CD2	3.08	0.42
2:F:410:MET:HE3	2:F:410:MET:HB3	1.72	0.42
1:G:184:GLY:C	1:G:186:VAL:H	2.28	0.42
1:G:194:ARG:HD3	2:H:156:SER:HB2	2.02	0.42
2:H:55:GLU:HG2	2:H:56:GLU:H	1.85	0.42
2:J:36:LEU:HG	2:J:386:GLU:HG3	2.01	0.42
1:K:83:GLY:O	1:K:87:VAL:HB	2.20	0.42
2:L:130:VAL:CG2	2:L:131:ASN:H	2.33	0.42
2:L:359:VAL:HG11	2:L:375:ILE:HD12	2.00	0.42
1:M:94:TRP:CH2	2:N:56:GLU:HB3	2.55	0.42
1:M:198:PHE:CZ	2:N:156:SER:HA	2.55	0.42
2:N:44:PHE:HB3	2:N:47:ALA:HB3	2.02	0.42
2:B:216:ALA:HA	2:B:357:ILE:HD11	2.02	0.42
2:B:385:MET:HE3	2:B:412:VAL:HA	2.02	0.42
2:B:400:ASP:OD1	2:B:402:GLU:HG2	2.19	0.42
2:D:38:ILE:HG23	2:D:419:ILE:HG23	2.01	0.42
2:D:51:GLY:O	2:D:368:ARG:HD3	2.19	0.42
2:D:354:PRO:HD2	4:D:501:FCO:N2	2.35	0.42
1:E:183:LEU:HD13	1:E:203:ILE:HA	2.01	0.42
2:F:26:ILE:CG2	2:F:27:GLY:N	2.64	0.42
2:F:58:LEU:HD13	2:F:77:LEU:CD2	2.50	0.42
1:G:134:GLY:HA2	1:G:206:ARG:HA	2.02	0.42
2:J:78:GLU:OE2	2:J:227:TYR:CD1	2.72	0.42
1:M:93:SER:O	1:M:242:GLY:HA3	2.20	0.42
1:M:186:VAL:HG11	1:M:237:MET:CE	2.50	0.42
2:B:205:TYR:HB3	2:B:207:GLU:OE1	2.20	0.42
2:B:277:ILE:HD13	2:B:277:ILE:HA	1.85	0.42
2:J:125:SER:HB3	2:J:128:LYS:HG3	2.01	0.42
2:J:231:ILE:O	2:J:238:GLU:HA	2.20	0.42
2:J:355:ARG:O	2:J:377:PRO:HB3	2.19	0.42
2:L:57:ALA:O	2:L:60:ILE:HG22	2.20	0.42
2:L:297:LEU:HA	2:L:297:LEU:HD12	1.68	0.42
2:N:8:ILE:HD13	2:N:404:LEU:HD23	2.02	0.42
2:B:23:GLU:N	2:B:35:LYS:O	2.38	0.42
2:B:137:ILE:HA	2:B:140:ALA:HB3	2.01	0.42
1:C:56:ILE:HD11	1:C:72:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:ILE:HG13	1:G:47:GLU:N	2.34	0.42
2:H:296:ASP:O	2:H:299:LYS:HD2	2.20	0.42
2:J:100:TYR:CZ	2:J:226:ILE:HG21	2.55	0.42
2:J:196:PHE:CE2	2:J:290:LEU:HB3	2.55	0.42
1:K:23:MET:HE1	1:K:142:PHE:HD2	1.85	0.42
2:L:52:LYS:HA	2:L:52:LYS:HD3	1.74	0.42
1:M:173:CYS:SG	1:M:176:LEU:HG	2.60	0.42
2:N:81:GLU:HA	2:N:84:VAL:HG22	2.02	0.42
2:B:166:LEU:HD23	2:B:166:LEU:HA	1.89	0.41
2:D:64:ILE:HG23	2:D:424:HIS:HB3	2.02	0.41
2:D:253:VAL:HG21	2:D:260:HIS:CE1	2.54	0.41
1:E:143:LEU:HD12	1:E:143:LEU:HA	1.77	0.41
2:F:86:PHE:HB2	2:F:340:VAL:HG13	2.02	0.41
2:H:178:LEU:HA	2:H:181:MET:HE3	2.02	0.41
1:I:181:PRO:HG3	1:I:236:ARG:CZ	2.50	0.41
2:L:130:VAL:CG2	2:L:131:ASN:N	2.83	0.41
1:O:29:LEU:HD12	1:O:30:ILE:HG23	2.02	0.41
1:A:166:CYS:O	1:A:171:HIS:HB2	2.20	0.41
1:C:174:ILE:HD12	1:C:175:LEU:N	2.35	0.41
2:D:100:TYR:CE2	2:D:226:ILE:HG21	2.55	0.41
1:E:5:ILE:HD11	1:E:53:ILE:HD12	2.01	0.41
2:F:79:ALA:HB2	2:F:349:SER:HB3	2.01	0.41
2:F:208:VAL:HG13	2:F:392:MET:HB2	2.02	0.41
1:G:147:GLY:O	1:G:151:ILE:HG23	2.19	0.41
1:G:252:GLU:O	1:G:256:SER:HB2	2.19	0.41
2:J:78:GLU:OE2	2:J:227:TYR:HD1	2.03	0.41
2:L:101:ILE:O	2:L:105:ILE:HG13	2.19	0.41
2:L:189:LEU:HG	2:L:193:GLU:OE2	2.20	0.41
1:M:58:GLY:H	1:M:86:ALA:HB2	1.85	0.41
2:N:70:ALA:HB2	2:N:151:MET:HE3	2.01	0.41
1:O:55:PHE:CD1	1:O:80:VAL:HB	2.55	0.41
1:O:238:LYS:HD3	1:O:242:GLY:HA2	2.00	0.41
2:P:163:ASN:O	2:P:169:PHE:HA	2.20	0.41
1:C:175:LEU:HD21	1:C:219:LEU:HD11	2.01	0.41
2:D:408:ALA:O	2:D:412:VAL:HG23	2.20	0.41
1:E:249:LYS:H	1:E:249:LYS:HD2	1.85	0.41
2:F:110:LEU:O	2:F:114:LEU:HB2	2.21	0.41
2:F:212:ILE:CD1	2:F:388:HIS:HE1	2.33	0.41
2:F:283:LEU:HD22	2:F:287:ALA:CB	2.49	0.41
2:F:405:LYS:O	2:F:406:ILE:C	2.64	0.41
2:H:378:THR:OG1	2:H:417:PRO:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:ARG:C	1:I:5:ILE:HD12	2.45	0.41
1:I:48:ASP:O	1:I:49:GLU:C	2.64	0.41
2:J:50:ILE:HD13	2:J:50:ILE:HA	1.90	0.41
1:M:62:THR:OG1	1:M:64:GLU:HG2	2.21	0.41
1:M:237:MET:HE2	1:M:247:VAL:HG22	2.01	0.41
2:N:110:LEU:HD21	2:N:144:LYS:HG3	2.03	0.41
1:O:237:MET:O	1:O:241:ASN:HB2	2.20	0.41
1:A:230:LYS:O	1:A:234:ILE:HG13	2.21	0.41
2:B:131:ASN:HB3	2:B:134:LYS:NZ	2.35	0.41
2:D:34:VAL:CG1	2:D:390:ARG:HB2	2.49	0.41
2:D:353:ALA:N	2:D:356:GLY:O	2.53	0.41
1:E:17:GLN:HE21	1:E:38:TRP:CD1	2.38	0.41
1:E:46:ILE:HG22	1:E:49:GLU:HB2	2.03	0.41
1:E:223:PHE:O	1:E:227:GLY:N	2.52	0.41
2:F:195:THR:O	2:F:199:PHE:HD1	2.03	0.41
1:G:19:GLN:NE2	1:G:137:PRO:O	2.53	0.41
1:I:160:TYR:HB2	1:I:161:PRO:HD2	2.01	0.41
2:L:111:HIS:O	2:L:116:VAL:HG23	2.20	0.41
2:L:342:ILE:HG21	2:L:367:GLY:HA2	2.02	0.41
2:P:75:THR:HG22	2:P:360:TYR:HB2	2.03	0.41
2:P:88:PRO:HG2	2:P:93:GLN:CG	2.50	0.41
1:C:11:THR:HG22	2:D:43:ARG:HD3	2.01	0.41
1:C:43:ARG:NH1	2:D:409:GLU:OE2	2.54	0.41
1:C:232:GLU:OE2	1:C:236:ARG:HD2	2.20	0.41
2:D:343:LYS:HB3	2:D:343:LYS:HE3	1.75	0.41
2:F:114:LEU:HA	2:F:126:PRO:HB3	2.02	0.41
2:H:242:GLU:H	2:H:242:GLU:HG3	1.38	0.41
2:J:207:GLU:HG2	2:J:396:HIS:CE1	2.56	0.41
1:K:174:ILE:HD13	1:K:180:GLU:OE1	2.20	0.41
1:K:205:CYS:HB3	3:K:502:SF4:S2	2.59	0.41
2:L:17:GLU:OE1	2:L:418:CYS:SG	2.79	0.41
2:L:381:ASN:O	2:L:383:ALA:N	2.54	0.41
2:N:18:GLY:HA3	2:N:419:ILE:HB	2.02	0.41
2:N:143:LEU:HD12	2:N:143:LEU:HA	1.91	0.41
2:N:189:LEU:HB3	2:N:190:PRO:HD3	2.02	0.41
1:O:27:LEU:HD11	2:P:127:LEU:HD13	2.03	0.41
1:A:158:ILE:O	1:A:188:ARG:NH1	2.49	0.41
2:B:126:PRO:C	2:B:128:LYS:N	2.78	0.41
2:B:271:GLY:O	2:B:272:ALA:CB	2.67	0.41
2:B:421:CYS:HB3	4:B:501:FCO:C1	2.50	0.41
1:C:176:LEU:HD23	1:C:222:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:ASP:N	2:D:11:ASP:OD1	2.51	0.41
2:F:38:ILE:N	2:F:38:ILE:HD12	2.36	0.41
2:F:275:ARG:NE	2:F:313:GLU:OE2	2.52	0.41
2:F:287:ALA:CB	2:F:316:TYR:HB2	2.47	0.41
2:F:385:MET:HG2	2:F:415:TYR:CD2	2.56	0.41
1:G:16:CYS:HG	3:G:501:SF4:FE4	1.35	0.41
2:H:19:LYS:O	2:H:39:ILE:HG13	2.20	0.41
2:H:119:ASP:HB3	2:H:410:MET:SD	2.60	0.41
2:H:185:LEU:HB2	2:H:322:ILE:HD11	2.02	0.41
1:I:21:ALA:HB2	1:I:38:TRP:CH2	2.55	0.41
2:N:150:MET:HG2	2:N:181:MET:SD	2.61	0.41
2:N:211:PRO:C	2:N:212:ILE:HG13	2.46	0.41
1:O:106:VAL:HG21	2:P:44:PHE:CD1	2.52	0.41
2:P:67:PHE:N	2:P:67:PHE:CD1	2.88	0.41
1:C:135:CYS:SG	3:C:501:SF4:S4	3.18	0.41
2:D:58:LEU:O	2:D:73:LYS:HE3	2.20	0.41
2:D:189:LEU:HD13	2:D:319:GLU:HG3	2.03	0.41
1:E:7:PHE:HD1	1:E:8:TYR:H	1.69	0.41
1:E:225:GLU:O	8:E:602:HOH:O	2.22	0.41
2:F:318:ILE:HD13	2:F:318:ILE:HG21	1.85	0.41
1:G:230:LYS:C	1:G:232:GLU:H	2.29	0.41
2:H:34:VAL:HG11	2:H:390:ARG:HB2	2.02	0.41
1:I:13:CYS:O	1:I:14:TYR:HB2	2.21	0.41
2:J:112:LEU:HB3	2:J:199:PHE:CZ	2.55	0.41
2:J:235:ASP:OD2	2:J:263:TYR:CE2	2.74	0.41
1:K:149:PHE:HE1	1:K:154:TRP:CZ3	2.39	0.41
2:L:101:ILE:CG2	2:L:105:ILE:HD11	2.51	0.41
2:L:218:LYS:HA	2:L:219:PRO:HD3	1.87	0.41
2:N:37:ASN:HA	2:N:255:HIS:O	2.21	0.41
2:P:64:ILE:HB	2:P:72:HIS:CD2	2.55	0.41
2:B:379:ALA:HB2	2:B:422:SER:HA	2.03	0.41
2:D:75:THR:HG21	2:D:358:LEU:HB3	2.02	0.41
2:F:24:ILE:HD13	2:F:24:ILE:HG21	1.86	0.41
2:F:38:ILE:HD12	2:F:38:ILE:H	1.85	0.41
2:F:67:PHE:HD2	2:F:355:ARG:NH2	2.18	0.41
1:G:232:GLU:C	1:G:234:ILE:N	2.79	0.41
2:H:399:ASP:CG	2:H:403:ARG:NH1	2.79	0.41
1:I:50:LYS:H	1:I:50:LYS:HD2	1.86	0.41
1:I:92:GLN:OE1	2:J:43:ARG:HG2	2.20	0.41
2:J:24:ILE:HD13	2:J:34:VAL:HG12	2.03	0.41
2:J:58:LEU:HD11	2:J:166:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ILE:CG2	1:K:146:LEU:HD13	2.50	0.41
2:L:9:THR:HG23	2:L:23:GLU:HG3	2.02	0.41
2:L:388:HIS:HA	2:L:391:MET:HB2	2.01	0.41
1:M:117:LYS:HB3	1:M:117:LYS:HE3	1.72	0.41
1:O:175:LEU:HG	1:O:222:VAL:HG21	2.02	0.41
2:P:17:GLU:OE1	2:P:419:ILE:N	2.54	0.41
1:A:253:LYS:HD2	1:A:253:LYS:HA	1.95	0.41
2:B:12[B]:HIS:HA	2:B:20:GLY:O	2.20	0.41
2:B:224:TYR:O	2:B:316:TYR:OH	2.34	0.41
2:B:294:ASN:O	2:B:297:LEU:HB2	2.20	0.41
1:C:173:CYS:SG	3:C:503:SF4:S2	3.18	0.41
1:C:200:VAL:HG23	1:C:201:ALA:O	2.21	0.41
2:D:38:ILE:HD11	2:D:382:LEU:HD21	2.03	0.41
2:D:400:ASP:O	2:D:403:ARG:HB3	2.20	0.41
1:E:186:VAL:O	1:E:209:ILE:N	2.49	0.41
2:F:38:ILE:HG23	2:F:419:ILE:CG2	2.51	0.41
2:F:375:ILE:HG21	2:F:380:PHE:CE1	2.56	0.41
2:H:69:SER:CB	2:H:160:HIS:H	2.34	0.41
2:H:123:TYR:HH	2:H:133:TYR:HE1	1.68	0.41
2:H:241:SER:HB3	2:H:350:THR:CG2	2.50	0.41
2:H:251:PHE:HB3	2:P:132:GLU:HB3	2.02	0.41
1:I:136:PRO:HD2	2:J:157:ARG:NE	2.35	0.41
1:I:177:GLU:O	1:I:177:GLU:HG3	2.21	0.41
2:J:126:PRO:O	2:J:128:LYS:N	2.54	0.41
1:K:147:GLY:O	1:K:150:LEU:N	2.54	0.41
1:K:244:ASP:HB3	1:K:247:VAL:HG23	2.02	0.41
2:L:223:ALA:HB1	2:L:316:TYR:OH	2.20	0.41
2:L:285:GLY:O	2:L:289:GLU:OE1	2.39	0.41
1:M:78:ILE:HG12	1:M:154:TRP:CH2	2.56	0.41
2:N:159:ILE:HG22	2:N:160:HIS:CG	2.56	0.41
1:O:224:LYS:HE3	8:O:610:HOH:O	2.21	0.41
2:P:91:GLU:HG3	2:P:334:ILE:HG23	2.02	0.41
2:P:112:LEU:HB3	2:P:199:PHE:CZ	2.55	0.41
2:P:355:ARG:HD2	4:P:501:FCO:C2	2.51	0.41
1:A:105:LYS:HE2	1:A:105:LYS:HB2	1.97	0.41
1:A:114:PHE:HB2	2:B:257:PHE:CE2	2.55	0.41
1:C:29:LEU:C	1:C:31:PRO:HD3	2.46	0.41
1:C:186:VAL:HG11	1:C:237:MET:SD	2.61	0.41
2:D:15:ARG:HD2	2:D:115:LEU:HA	2.02	0.41
2:D:377:PRO:CD	4:D:501:FCO:N1	2.64	0.41
1:E:175:LEU:HA	1:E:180:GLU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:297:LEU:HD13	2:F:297:LEU:HA	1.89	0.41
1:G:43:ARG:HH21	2:H:406:ILE:HA	1.86	0.41
2:J:192:ALA:CB	2:J:314:ILE:HG22	2.51	0.41
2:L:14:ALA:O	2:L:413:ARG:NH1	2.48	0.41
2:L:412:VAL:C	2:L:414:ALA:N	2.79	0.41
1:M:246:ARG:O	1:M:247:VAL:C	2.64	0.41
1:O:103:TRP:HE3	2:P:44:PHE:HZ	1.68	0.41
2:P:56:GLU:H	2:P:56:GLU:HG3	1.63	0.41
2:P:243:LYS:O	2:P:245:ARG:N	2.54	0.41
2:P:401:PRO:C	2:P:403:ARG:N	2.78	0.41
2:B:217:VAL:CG2	2:B:357:ILE:HG23	2.51	0.40
1:C:162:VAL:HB	1:C:184:GLY:CA	2.51	0.40
2:D:242:GLU:HG2	2:D:243:LYS:N	2.36	0.40
1:E:63:GLU:HG2	1:E:117:LYS:HG3	2.02	0.40
1:E:183:LEU:HD13	1:E:202:CYS:O	2.21	0.40
1:E:213:VAL:HG13	1:G:32:ASN:OD1	2.21	0.40
2:F:74:LEU:CD2	2:F:96:ARG:HG2	2.45	0.40
2:F:104:MET:HE3	2:F:317:PHE:HE2	1.86	0.40
2:F:259:LYS:HB3	8:F:609:HOH:O	2.20	0.40
1:G:162:VAL:HG23	1:G:187:THR:O	2.21	0.40
1:I:221:LYS:HD2	1:I:222:VAL:N	2.35	0.40
2:J:35:LYS:HD3	2:J:255:HIS:CB	2.51	0.40
2:L:63:ARG:HG3	2:L:160:HIS:NE2	2.36	0.40
1:O:91:VAL:CG1	2:P:60:ILE:HD12	2.50	0.40
1:O:111[B]:LYS:HE3	1:O:111[B]:LYS:HB2	1.37	0.40
1:O:237:MET:HE1	1:O:251:VAL:CG2	2.51	0.40
1:A:130:TYR:CG	1:A:131:ASN:N	2.90	0.40
1:C:148:THR:HG22	1:C:153:SER:HB3	2.02	0.40
2:D:137:ILE:HD12	2:D:137:ILE:HA	1.99	0.40
2:F:62:PRO:HG2	2:F:63:ARG:HH11	1.86	0.40
2:F:105:ILE:CD1	2:F:150:MET:HE1	2.51	0.40
1:G:35:ILE:HD12	1:G:35:ILE:O	2.21	0.40
1:G:129:ASP:HB3	1:G:154:TRP:HZ2	1.86	0.40
2:H:232:LYS:HE3	2:H:238:GLU:OE1	2.21	0.40
1:I:114:PHE:HE2	2:J:255:HIS:C	2.29	0.40
2:J:298:LEU:HA	2:J:298:LEU:HD23	1.91	0.40
1:K:10:LEU:HG	1:K:56:ILE:HG22	2.02	0.40
2:B:219:PRO:CG	2:B:282:LEU:HD13	2.51	0.40
1:C:41:ILE:CG2	2:D:126:PRO:HD2	2.51	0.40
2:D:144:LYS:HE2	2:D:144:LYS:HB3	1.97	0.40
2:F:10:ILE:HD11	2:F:405:LYS:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:GLU:HG3	2:F:148:THR:OG1	2.21	0.40
2:F:240:PRO:O	2:F:241:SER:C	2.64	0.40
2:F:358:LEU:HA	2:F:358:LEU:HD12	1.74	0.40
1:G:144:TYR:HE2	1:G:156:GLU:H	1.69	0.40
2:H:106:GLU:O	2:H:107:SER:C	2.65	0.40
1:I:137:PRO:HB2	1:I:142:PHE:CE2	2.57	0.40
1:I:167:ARG:HH12	1:I:215:TRP:HB3	1.86	0.40
2:J:404:LEU:O	2:J:405:LYS:C	2.64	0.40
1:K:140:LYS:HE2	1:K:140:LYS:HB2	1.94	0.40
1:K:175:LEU:HD23	3:K:503:SF4:S4	2.62	0.40
2:L:151:MET:HB3	2:L:158:ALA:HA	2.02	0.40
1:O:99:LEU:O	1:O:102:LEU:N	2.54	0.40
2:P:114:LEU:HA	2:P:126:PRO:HB3	2.03	0.40
2:B:15:ARG:HA	2:B:115:LEU:HD22	2.04	0.40
2:B:376:THR:OG1	2:B:421:CYS:O	2.29	0.40
1:C:42:ASP:HA	2:D:124:SER:O	2.21	0.40
1:E:121:PRO:C	1:E:123:SER:N	2.79	0.40
2:F:15:ARG:HD2	2:F:15:ARG:HH11	1.77	0.40
2:H:65:CYS:SG	2:H:66:SER:N	2.92	0.40
1:I:61:SER:N	1:I:65:GLU:OE1	2.45	0.40
1:I:230[B]:LYS:HG3	1:I:231:GLU:OE1	2.22	0.40
2:J:26:ILE:HG12	2:J:31:VAL:HG22	2.04	0.40
2:J:394:GLU:O	2:J:394:GLU:HG3	2.18	0.40
2:P:214:HIS:HA	2:P:269:MET:O	2.22	0.40
2:P:262:HIS:NE2	2:P:267:PRO:HD3	2.36	0.40
1:A:4:ARG:CG	1:A:36:VAL:HG11	2.45	0.40
1:A:229:THR:O	1:A:232:GLU:N	2.54	0.40
1:C:158:ILE:H	1:C:158:ILE:HG13	1.39	0.40
2:D:62:PRO:HB2	2:D:63:ARG:HH11	1.86	0.40
2:D:366:ASN:CG	2:D:366:ASN:O	2.65	0.40
1:E:159:ASP:O	1:G:151:ILE:HD12	2.21	0.40
1:E:166:CYS:O	1:E:170:GLY:N	2.53	0.40
2:F:418:CYS:HB3	2:F:421:CYS:HB2	2.04	0.40
2:H:382:LEU:HD23	2:H:382:LEU:HA	1.83	0.40
2:H:400:ASP:HA	2:H:401:PRO:HD2	1.86	0.40
2:L:45:PHE:CD2	2:L:64:ILE:HD11	2.56	0.40
2:L:412:VAL:C	2:L:414:ALA:H	2.29	0.40
2:N:112:LEU:HD23	2:N:112:LEU:HA	1.77	0.40
2:N:209:GLU:N	8:N:602:HOH:O	2.54	0.40
1:O:15:GLY:CA	2:P:66:SER:HB3	2.52	0.40
2:P:204:GLN:HE22	2:P:297:LEU:CA	2.35	0.40

All (4) 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)
2:D:390:ARG:NH1	1:I:225:GLU:OE2[1_455]	2.07	0.13
2:F:387:GLU:OE2	1:O:221:LYS:NZ[1_656]	2.11	0.09
2:B:395:LYS:NZ	1:K:225:GLU:O[1_556]	2.12	0.08
1:C:225:GLU:OE1	2:J:390:ARG:NH1[1_456]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/266 (96%)	228 (89%)	25 (10%)	3 (1%)	10	23
1	C	255/266 (96%)	224 (88%)	24 (9%)	7 (3%)	4	7
1	E	254/266 (96%)	226 (89%)	23 (9%)	5 (2%)	6	12
1	G	254/266 (96%)	218 (86%)	34 (13%)	2 (1%)	16	34
1	I	256/266 (96%)	224 (88%)	26 (10%)	6 (2%)	5	9
1	K	254/266 (96%)	215 (85%)	32 (13%)	7 (3%)	4	6
1	M	255/266 (96%)	239 (94%)	14 (6%)	2 (1%)	16	34
1	O	255/266 (96%)	230 (90%)	21 (8%)	4 (2%)	7	16
2	B	421/424 (99%)	358 (85%)	54 (13%)	9 (2%)	5	11
2	D	418/424 (99%)	362 (87%)	34 (8%)	22 (5%)	1	1
2	F	420/424 (99%)	366 (87%)	44 (10%)	10 (2%)	4	9
2	H	418/424 (99%)	371 (89%)	38 (9%)	9 (2%)	5	10
2	J	418/424 (99%)	360 (86%)	48 (12%)	10 (2%)	4	9
2	L	420/424 (99%)	356 (85%)	49 (12%)	15 (4%)	2	4
2	N	420/424 (99%)	384 (91%)	28 (7%)	8 (2%)	6	13
2	P	417/424 (98%)	354 (85%)	45 (11%)	18 (4%)	2	2
All	All	5391/5520 (98%)	4715 (88%)	539 (10%)	137 (2%)	4	8

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	214	ALA
2	D	382	LEU
2	F	69	SER
2	F	382	LEU
2	F	401	PRO
1	G	32	ASN
2	H	87	VAL
1	I	224	LYS
1	I	225	GLU
1	K	113	LYS
2	L	354	PRO
2	N	382	LEU
2	P	153	ILE
2	P	240	PRO
1	A	32	ASN
1	A	173	CYS
2	B	85	GLY
2	B	182	LYS
2	B	272	ALA
2	B	303	PRO
1	C	92	GLN
1	C	224	LYS
1	C	245	GLU
2	D	29	ASP
2	D	54	LEU
2	D	55	GLU
2	D	160	HIS
2	D	164	ALA
2	D	366	ASN
2	D	413	ARG
1	E	92	GLN
2	F	160	HIS
2	H	398	ASN
1	K	147	GLY
2	L	38	ILE
2	L	118	PRO
2	L	382	LEU
1	M	92	GLN
2	N	413	ARG
2	P	244	TYR
2	P	357	ILE
2	P	366	ASN

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Mol	Chain	Res	Type
2	B	129	MET
1	C	12	SER
1	C	239	MET
2	D	211	PRO
2	F	222	ASP
1	I	49	GLU
2	J	127	LEU
2	J	208	VAL
2	J	293	ALA
1	K	92	GLN
2	L	133	TYR
2	L	173	PRO
2	L	178	LEU
1	M	176	LEU
1	O	39	PHE
1	O	49	GLU
2	P	127	LEU
2	P	160	HIS
2	P	336	PRO
2	B	127	LEU
2	B	396	HIS
2	D	87	VAL
2	D	156	SER
2	D	301	THR
2	D	399	ASP
1	E	239	MET
2	F	87	VAL
2	F	156	SER
2	F	366	ASN
1	G	25	GLU
2	H	182	LYS
2	H	396	HIS
1	I	39	PHE
1	I	220	ALA
2	J	377	PRO
2	J	422	SER
1	K	21	ALA
1	K	177	GLU
1	K	188	ARG
2	L	87	VAL
2	L	396	HIS
2	L	399	ASP

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Mol	Chain	Res	Type
2	N	87	VAL
1	O	38	TRP
1	O	224	LYS
2	P	47	ALA
2	P	156	SER
2	P	241	SER
2	P	267	PRO
2	B	87	VAL
2	B	157	ARG
2	D	69	SER
2	D	173	PRO
2	D	264	LYS
2	D	393	ALA
2	D	394	GLU
1	E	182	CYS
2	H	76	ALA
2	H	181	MET
2	H	207	GLU
2	J	160	HIS
2	L	413	ARG
2	N	156	SER
2	P	87	VAL
2	P	343	LYS
2	D	342	ILE
1	E	217	ASP
2	H	160	HIS
2	H	185	LEU
2	J	194	TYR
2	N	173	PRO
2	P	7	PRO
2	P	377	PRO
1	C	247	VAL
2	D	406	ILE
2	D	423	VAL
2	F	416	ASP
1	I	147	GLY
2	J	87	VAL
2	D	84	VAL
2	J	88	PRO
2	L	208	VAL
2	N	342	ILE
2	P	208	VAL

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Mol	Chain	Res	Type
1	A	121	PRO
2	F	417	PRO
1	K	31	PRO
2	L	88	PRO
2	L	122	GLY
2	L	336	PRO
2	J	173	PRO
2	N	38	ILE
1	E	181	PRO
2	N	336	PRO
2	P	401	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/227 (96%)	193 (89%)	24 (11%)	6	12
1	C	216/227 (95%)	189 (88%)	27 (12%)	4	9
1	E	215/227 (95%)	196 (91%)	19 (9%)	9	21
1	G	215/227 (95%)	204 (95%)	11 (5%)	21	45
1	I	217/227 (96%)	197 (91%)	20 (9%)	8	19
1	K	215/227 (95%)	199 (93%)	16 (7%)	13	29
1	M	216/227 (95%)	207 (96%)	9 (4%)	26	52
1	O	216/227 (95%)	198 (92%)	18 (8%)	10	23
2	B	353/355 (99%)	324 (92%)	29 (8%)	10	24
2	D	351/355 (99%)	324 (92%)	27 (8%)	12	27
2	F	353/355 (99%)	324 (92%)	29 (8%)	10	24
2	H	350/355 (99%)	327 (93%)	23 (7%)	15	34
2	J	351/355 (99%)	321 (92%)	30 (8%)	10	22
2	L	351/355 (99%)	323 (92%)	28 (8%)	11	25
2	N	351/355 (99%)	332 (95%)	19 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	350/355 (99%)	318 (91%)	32 (9%)	9	19
All	All	4537/4656 (97%)	4176 (92%)	361 (8%)	11	25

All (361) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	67	GLU
1	A	68	LEU
1	A	77[A]	LYS
1	A	77[B]	LYS
1	A	82	VAL
1	A	88	GLN
1	A	95	SER
1	A	99	LEU
1	A	100	GLU
1	A	105	LYS
1	A	118	LYS
1	A	120	GLU
1	A	121	PRO
1	A	140	LYS
1	A	151	ILE
1	A	153	SER
1	A	168	LEU
1	A	173	CYS
1	A	174	ILE
1	A	188	ARG
1	A	209	ILE
1	A	217	ASP
1	A	241	ASN
2	B	17	GLU
2	B	26	ILE
2	B	28	ASP
2	B	34	VAL
2	B	37	ASN
2	B	78	GLU
2	B	97	GLU
2	B	107	SER
2	B	130	VAL
2	B	131	ASN
2	B	137	ILE
2	B	139	ILE

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Mol	Chain	Res	Type
2	B	141	LEU
2	B	144	LYS
2	B	156	SER
2	B	174	GLU
2	B	179	GLU
2	B	180[A]	LYS
2	B	180[B]	LYS
2	B	242	GLU
2	B	254	GLU
2	B	295	LYS
2	B	298	LEU
2	B	318	ILE
2	B	339	GLU
2	B	370	SER
2	B	400	ASP
2	B	423	VAL
2	B	424	HIS
1	C	5	ILE
1	C	13	CYS
1	C	27	LEU
1	C	46	ILE
1	C	48	ASP
1	C	51	VAL
1	C	59	SER
1	C	78	ILE
1	C	99	LEU
1	C	105	LYS
1	C	113	LYS
1	C	114	PHE
1	C	118	LYS
1	C	120	GLU
1	C	123	SER
1	C	127	LYS
1	C	140	LYS
1	C	148	THR
1	C	158	ILE
1	C	169	ASN
1	C	174	ILE
1	C	183	LEU
1	C	186	VAL
1	C	200	VAL
1	C	202	CYS

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Mol	Chain	Res	Type
1	C	233	ILE
1	C	254	ILE
2	D	6	LEU
2	D	12[A]	HIS
2	D	12[B]	HIS
2	D	24	ILE
2	D	91	GLU
2	D	97	GLU
2	D	106	GLU
2	D	110	LEU
2	D	130	VAL
2	D	136	GLU
2	D	162	GLU
2	D	182	LYS
2	D	203	GLU
2	D	208	VAL
2	D	213	THR
2	D	229	ASP
2	D	245	ARG
2	D	248	ILE
2	D	256	SER
2	D	281	ASP
2	D	299	LYS
2	D	306	ASN
2	D	319	GLU
2	D	334	ILE
2	D	357	ILE
2	D	358	LEU
2	D	359	VAL
1	E	5	ILE
1	E	24	ASP
1	E	45	SER
1	E	48	ASP
1	E	50	LYS
1	E	51	VAL
1	E	96	GLU
1	E	140	LYS
1	E	148	THR
1	E	157	ASP
1	E	159	ASP
1	E	174	ILE
1	E	178	LYS

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Mol	Chain	Res	Type
1	E	200	VAL
1	E	218	SER
1	E	221	LYS
1	E	224	LYS
1	E	233	ILE
1	E	241	ASN
2	F	12[A]	HIS
2	F	12[B]	HIS
2	F	23	GLU
2	F	28	ASP
2	F	32	LYS
2	F	60	ILE
2	F	68	CYS
2	F	95	LEU
2	F	110	LEU
2	F	114	LEU
2	F	131	ASN
2	F	142	LYS
2	F	182	LYS
2	F	203	GLU
2	F	220	ARG
2	F	229	ASP
2	F	231	ILE
2	F	235[A]	ASP
2	F	235[B]	ASP
2	F	239	PHE
2	F	242	GLU
2	F	245	ARG
2	F	273	ILE
2	F	301	THR
2	F	319	GLU
2	F	334	ILE
2	F	335	LYS
2	F	339	GLU
2	F	341	GLU
1	G	5	ILE
1	G	48	ASP
1	G	96	GLU
1	G	111	LYS
1	G	140	LYS
1	G	157	ASP
1	G	159	ASP

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Mol	Chain	Res	Type
1	G	173	CYS
1	G	186	VAL
1	G	212	ASP
1	G	249	LYS
2	H	22	VAL
2	H	37	ASN
2	H	65	CYS
2	H	69	SER
2	H	78	GLU
2	H	106	GLU
2	H	107	SER
2	H	125	SER
2	H	144	LYS
2	H	179	GLU
2	H	180	LYS
2	H	187	GLU
2	H	235	ASP
2	H	279	ASN
2	H	297	LEU
2	H	299	LYS
2	H	339	GLU
2	H	340	VAL
2	H	365	GLU
2	H	400	ASP
2	H	407	LEU
2	H	423	VAL
2	H	424	HIS
1	I	2	LYS
1	I	19	GLN
1	I	36	VAL
1	I	49	GLU
1	I	50	LYS
1	I	51	VAL
1	I	60	VAL
1	I	88	GLN
1	I	93	SER
1	I	95	SER
1	I	102	LEU
1	I	111[A]	LYS
1	I	111[B]	LYS
1	I	113	LYS
1	I	140	LYS

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Mol	Chain	Res	Type
1	I	149	PHE
1	I	186	VAL
1	I	200	VAL
1	I	234	ILE
1	I	235	GLU
2	J	13	ILE
2	J	16	VAL
2	J	25	ILE
2	J	28	ASP
2	J	32[A]	LYS
2	J	32[B]	LYS
2	J	48	ILE
2	J	58	LEU
2	J	66	SER
2	J	89	ARG
2	J	97	GLU
2	J	108	HIS
2	J	121	ARG
2	J	137	ILE
2	J	166	LEU
2	J	175	LYS
2	J	191	LEU
2	J	197	GLU
2	J	234	SER
2	J	245	ARG
2	J	261	SER
2	J	292	GLU
2	J	342	ILE
2	J	370	SER
2	J	376	THR
2	J	390	ARG
2	J	395	LYS
2	J	402	GLU
2	J	406	ILE
2	J	411	VAL
1	K	29	LEU
1	K	49	GLU
1	K	70	LYS
1	K	109	ASP
1	K	114	PHE
1	K	126	ILE
1	K	127	LYS

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Mol	Chain	Res	Type
1	K	140	LYS
1	K	169	ASN
1	K	173	CYS
1	K	174	ILE
1	K	178	LYS
1	K	192	ASN
1	K	200	VAL
1	K	225	GLU
1	K	229	THR
2	L	8	ILE
2	L	9	THR
2	L	11	ASP
2	L	32	LYS
2	L	65	CYS
2	L	68	CYS
2	L	124	SER
2	L	132	GLU
2	L	157	ARG
2	L	165	VAL
2	L	171	LYS
2	L	201	LYS
2	L	206	SER
2	L	208	VAL
2	L	249	LYS
2	L	277	ILE
2	L	290	LEU
2	L	301	THR
2	L	339	GLU
2	L	341	GLU
2	L	368	ARG
2	L	377	PRO
2	L	382	LEU
2	L	390	ARG
2	L	395	LYS
2	L	411	VAL
2	L	421	CYS
2	L	423	VAL
1	M	41	ILE
1	M	46	ILE
1	M	51	VAL
1	M	95	SER
1	M	140[A]	LYS

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Mol	Chain	Res	Type
1	M	140[B]	LYS
1	M	157	ASP
1	M	209	ILE
1	M	231	GLU
2	N	25	ILE
2	N	26	ILE
2	N	50	ILE
2	N	68	CYS
2	N	107	SER
2	N	128	LYS
2	N	134	LYS
2	N	143	LEU
2	N	157	ARG
2	N	249	LYS
2	N	276	VAL
2	N	299	LYS
2	N	365	GLU
2	N	377	PRO
2	N	400	ASP
2	N	411	VAL
2	N	419	ILE
2	N	421	CYS
2	N	423	VAL
1	O	3	VAL
1	O	13	CYS
1	O	19	GLN
1	O	35	ILE
1	O	36	VAL
1	O	51	VAL
1	O	67	GLU
1	O	93	SER
1	O	94	TRP
1	O	95	SER
1	O	111[A]	LYS
1	O	111[B]	LYS
1	O	149	PHE
1	O	183	LEU
1	O	218	SER
1	O	230	LYS
1	O	245	GLU
1	O	246	ARG
2	P	9	THR

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Mol	Chain	Res	Type
2	P	13	ILE
2	P	22	VAL
2	P	23	GLU
2	P	28	ASP
2	P	40	GLU
2	P	68	CYS
2	P	96	ARG
2	P	107	SER
2	P	124	SER
2	P	128	LYS
2	P	137	ILE
2	P	152	ASP
2	P	208	VAL
2	P	229	ASP
2	P	234	SER
2	P	241	SER
2	P	242	GLU
2	P	249	LYS
2	P	251	PHE
2	P	253	VAL
2	P	260	HIS
2	P	261	SER
2	P	276	VAL
2	P	286	LYS
2	P	290	LEU
2	P	301	THR
2	P	312	LEU
2	P	314	ILE
2	P	340	VAL
2	P	343	LYS
2	P	405	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	115	GLN
1	A	171	HIS
2	B	306	ASN
1	C	28	GLN
1	C	88	GLN
1	C	169	ASN

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Mol	Chain	Res	Type
2	D	145	ASN
2	D	214	HIS
1	E	17	GLN
1	E	169	ASN
2	F	111	HIS
2	F	161	GLN
2	F	204	GLN
2	F	366	ASN
1	G	75	ASN
1	G	88	GLN
2	H	163	ASN
2	H	262	HIS
2	H	278	ASN
1	I	17	GLN
1	I	19	GLN
2	J	93	GLN
2	J	161	GLN
2	J	278	ASN
2	J	307	ASN
2	J	366	ASN
2	J	396	HIS
1	K	75	ASN
2	L	72	HIS
2	L	424	HIS
1	M	17	GLN
1	M	19	GLN
1	M	169	ASN
2	N	145	ASN
2	N	278	ASN
2	P	37	ASN
2	P	204	GLN
2	P	255	HIS
2	P	279	ASN
2	P	302	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 53 ligands modelled in this entry, 10 are monoatomic - leaving 43 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SF4	G	503	1	0,12,12	-	-	-		
3	SF4	K	501	1	0,12,12	-	-	-		
6	PO4	P	503	-	4,4,4	0.83	0	6,6,6	0.86	0
3	SF4	K	502	1	0,12,12	-	-	-		
3	SF4	O	503	1	0,12,12	-	-	-		
6	PO4	J	503	-	4,4,4	0.92	0	6,6,6	0.79	0
3	SF4	I	502	1	0,12,12	-	-	-		
4	FCO	F	501	2	0,6,6	-	-	-		
4	FCO	H	501	2	0,6,6	-	-	-		
4	FCO	N	501	-	0,6,6	-	-	-		
3	SF4	O	502	1	0,12,12	-	-	-		
3	SF4	E	503	1	0,12,12	-	-	-		
3	SF4	C	501	1	0,12,12	-	-	-		
3	SF4	M	503	1	0,12,12	-	-	-		
4	FCO	J	501	2	0,6,6	-	-	-		
4	FCO	B	501	2	0,6,6	-	-	-		
3	SF4	O	501	1,2	0,12,12	-	-	-		
6	PO4	P	505	-	4,4,4	0.67	0	6,6,6	0.75	0
3	SF4	C	502	1	0,12,12	-	-	-		
3	SF4	G	501	1	0,12,12	-	-	-		
3	SF4	M	502	1	0,12,12	-	-	-		
6	PO4	I	504	-	4,4,4	0.98	0	6,6,6	0.89	0
4	FCO	L	501	2	0,6,6	-	-	-		
3	SF4	E	501	1,2	0,12,12	-	-	-		
3	SF4	M	501	1	0,12,12	-	-	-		
3	SF4	A	503	1	0,12,12	-	-	-		
3	SF4	I	503	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SF4	K	503	1	0,12,12	-	-	-		
3	SF4	A	501	1	0,12,12	-	-	-		
6	PO4	F	504	-	4,4,4	0.86	0	6,6,6	0.43	0
6	PO4	L	503	-	4,4,4	0.81	0	6,6,6	0.67	0
3	SF4	A	502	1	0,12,12	-	-	-		
4	FCO	D	501	2	0,6,6	-	-	-		
6	PO4	B	504	-	4,4,4	0.68	0	6,6,6	0.58	0
4	FCO	P	501	2	0,6,6	-	-	-		
3	SF4	C	503	1	0,12,12	-	-	-		
6	PO4	B	503	-	4,4,4	0.68	0	6,6,6	1.11	0
3	SF4	G	502	1	0,12,12	-	-	-		
3	SF4	E	502	1	0,12,12	-	-	-		
3	SF4	I	501	1	0,12,12	-	-	-		
6	PO4	H	503	-	4,4,4	1.05	0	6,6,6	1.01	0
6	PO4	F	503	-	4,4,4	0.86	0	6,6,6	0.62	0
6	PO4	P	504	-	4,4,4	0.82	0	6,6,6	1.02	0

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	SF4	G	503	1	-	-	0/6/5/5
3	SF4	K	501	1	-	-	0/6/5/5
3	SF4	K	502	1	-	-	0/6/5/5
3	SF4	O	503	1	-	-	0/6/5/5
3	SF4	I	502	1	-	-	0/6/5/5
3	SF4	O	502	1	-	-	0/6/5/5
3	SF4	E	503	1	-	-	0/6/5/5
3	SF4	C	501	1	-	-	0/6/5/5
3	SF4	M	503	1	-	-	0/6/5/5
3	SF4	O	501	1,2	-	-	0/6/5/5
3	SF4	C	502	1	-	-	0/6/5/5
3	SF4	G	501	1	-	-	0/6/5/5
3	SF4	M	502	1	-	-	0/6/5/5
3	SF4	E	501	1,2	-	-	0/6/5/5
3	SF4	M	501	1	-	-	0/6/5/5
3	SF4	A	503	1	-	-	0/6/5/5
3	SF4	I	503	1	-	-	0/6/5/5
3	SF4	K	503	1	-	-	0/6/5/5
3	SF4	A	501	1	-	-	0/6/5/5
3	SF4	A	502	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	C	503	1	-	-	0/6/5/5
3	SF4	G	502	1	-	-	0/6/5/5
3	SF4	E	502	1	-	-	0/6/5/5
3	SF4	I	501	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

31 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	503	SF4	3	0
3	K	501	SF4	8	0
3	K	502	SF4	2	0
3	I	502	SF4	1	0
4	F	501	FCO	7	0
4	H	501	FCO	5	0
4	N	501	FCO	19	0
3	E	503	SF4	5	0
3	C	501	SF4	5	0
3	M	503	SF4	3	0
4	J	501	FCO	5	0
4	B	501	FCO	5	0
3	O	501	SF4	3	0
3	C	502	SF4	2	0
3	G	501	SF4	3	0
3	M	502	SF4	2	0
6	I	504	PO4	1	0
4	L	501	FCO	16	0
3	E	501	SF4	3	0
3	M	501	SF4	1	0
3	A	503	SF4	1	0
3	K	503	SF4	7	0
3	A	501	SF4	4	0
6	L	503	PO4	1	0
3	A	502	SF4	1	0
4	D	501	FCO	8	0
4	P	501	FCO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	SF4	6	0
3	E	502	SF4	1	0
3	I	501	SF4	2	0
6	P	504	PO4	1	0

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
2	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	400:ASP	C	401:PRO	N	1.11

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	256/266 (96%)	-1.32	0 100 100	31, 46, 60, 68	2 (0%)
1	C	256/266 (96%)	-1.26	0 100 100	30, 48, 58, 69	1 (0%)
1	E	256/266 (96%)	-1.33	0 100 100	31, 46, 57, 63	0
1	G	256/266 (96%)	-1.36	0 100 100	28, 46, 58, 68	0
1	I	256/266 (96%)	-1.27	0 100 100	25, 51, 65, 78	2 (0%)
1	K	256/266 (96%)	-1.31	0 100 100	24, 50, 65, 80	0
1	M	256/266 (96%)	-1.30	0 100 100	25, 50, 63, 75	1 (0%)
1	O	256/266 (96%)	-1.29	0 100 100	30, 50, 63, 73	1 (0%)
2	B	420/424 (99%)	-1.34	0 100 100	24, 44, 56, 64	3 (0%)
2	D	419/424 (98%)	-1.35	0 100 100	29, 45, 58, 73	1 (0%)
2	F	419/424 (98%)	-1.33	0 100 100	27, 44, 58, 68	3 (0%)
2	H	420/424 (99%)	-1.35	0 100 100	29, 43, 57, 76	0
2	J	419/424 (98%)	-1.31	0 100 100	33, 47, 61, 72	1 (0%)
2	L	421/424 (99%)	-1.31	0 100 100	28, 46, 61, 78	1 (0%)
2	N	421/424 (99%)	-1.33	0 100 100	29, 46, 60, 75	1 (0%)
2	P	419/424 (98%)	-1.32	0 100 100	32, 47, 61, 71	0
All	All	5406/5520 (97%)	-1.32	0 100 100	24, 46, 61, 80	17 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	F	503	5/5	0.95	0.08	52,56,63,76	0
6	PO4	H	503	5/5	0.96	0.08	30,40,52,61	0
6	PO4	B	503	5/5	0.97	0.06	39,49,57,64	0
6	PO4	F	504	5/5	0.97	0.07	59,68,84,86	0
6	PO4	B	504	5/5	0.97	0.06	41,51,65,71	0
6	PO4	I	504	5/5	0.97	0.08	36,47,57,60	0
6	PO4	J	503	5/5	0.97	0.07	50,55,67,71	0
6	PO4	L	503	5/5	0.97	0.05	55,65,71,75	0
6	PO4	P	503	5/5	0.97	0.05	45,51,58,63	0
6	PO4	P	504	5/5	0.97	0.07	37,48,59,61	0
6	PO4	P	505	5/5	0.97	0.06	51,58,66,78	0
7	MG	H	504	1/1	0.97	0.03	18,18,18,18	0
3	SF4	M	502	8/8	0.99	0.03	33,43,47,62	0
3	SF4	O	501	8/8	0.99	0.03	24,37,41,55	0
5	NI	J	502	1/1	0.99	0.04	76,76,76,76	0
5	NI	P	502	1/1	0.99	0.02	72,72,72,72	0
3	SF4	C	501	8/8	0.99	0.02	18,28,39,41	0
3	SF4	C	502	8/8	0.99	0.04	33,45,59,70	0
3	SF4	E	502	8/8	0.99	0.03	31,42,54,59	0
3	SF4	I	501	8/8	0.99	0.02	23,30,35,35	0
7	MG	P	506	1/1	0.99	0.02	26,26,26,26	0
3	SF4	C	503	8/8	1.00	0.02	56,59,68,69	0
3	SF4	O	502	8/8	1.00	0.02	31,52,60,63	0
3	SF4	O	503	8/8	1.00	0.02	36,43,48,56	0
4	FCO	B	501	7/7	1.00	0.03	37,42,53,57	0
4	FCO	D	501	7/7	1.00	0.04	49,51,59,60	0
4	FCO	F	501	7/7	1.00	0.04	43,45,48,53	0
4	FCO	H	501	7/7	1.00	0.04	45,46,53,63	0
4	FCO	J	501	7/7	1.00	0.04	39,43,62,67	0
4	FCO	L	501	7/7	1.00	0.03	40,45,57,88	0
4	FCO	N	501	7/7	1.00	0.03	43,50,65,149	0
4	FCO	P	501	7/7	1.00	0.05	44,47,49,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NI	B	502	1/1	1.00	0.03	71,71,71,71	0
5	NI	D	502	1/1	1.00	0.01	69,69,69,69	0
5	NI	F	502	1/1	1.00	0.02	51,51,51,51	0
5	NI	H	502	1/1	1.00	0.02	83,83,83,83	0
3	SF4	E	501	8/8	1.00	0.02	24,29,39,41	0
5	NI	L	502	1/1	1.00	0.01	87,87,87,87	0
5	NI	N	502	1/1	1.00	0.01	69,69,69,69	0
3	SF4	A	503	8/8	1.00	0.03	36,41,47,61	0
3	SF4	E	503	8/8	1.00	0.02	41,55,57,58	0
3	SF4	G	501	8/8	1.00	0.02	26,35,42,44	0
3	SF4	G	502	8/8	1.00	0.02	24,31,41,46	0
3	SF4	G	503	8/8	1.00	0.03	30,43,52,54	0
3	SF4	A	501	8/8	1.00	0.01	34,39,46,46	0
3	SF4	I	502	8/8	1.00	0.02	40,50,57,65	0
3	SF4	I	503	8/8	1.00	0.03	30,43,48,54	0
3	SF4	K	501	8/8	1.00	0.02	26,43,46,62	0
3	SF4	K	502	8/8	1.00	0.02	34,40,49,52	0
3	SF4	K	503	8/8	1.00	0.02	35,58,66,80	0
3	SF4	M	501	8/8	1.00	0.02	28,36,41,43	0
3	SF4	A	502	8/8	1.00	0.02	31,40,46,47	0
3	SF4	M	503	8/8	1.00	0.02	45,55,71,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.