



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 03:06 AM EDT

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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

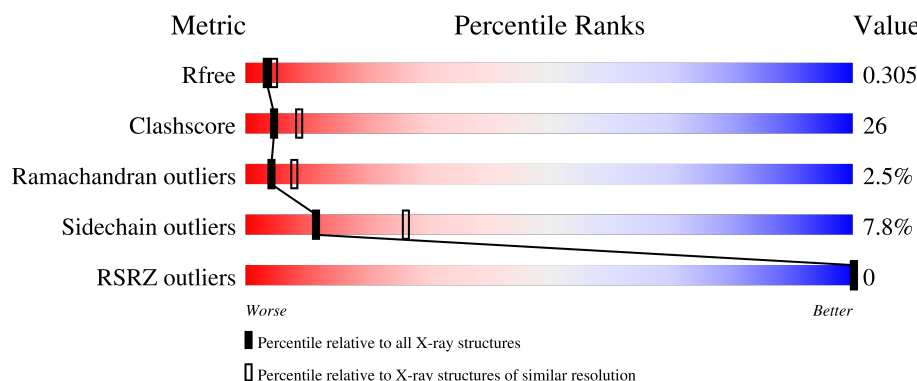
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



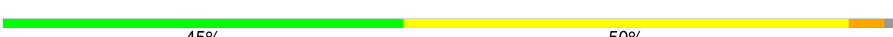
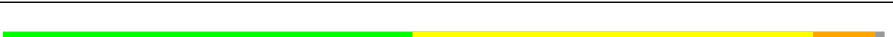
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	50% 40% 5% . .
1	C	266	43% 45% 8% . .
1	E	266	47% 44% 5% .
1	G	266	55% 39% . .
1	I	266	48% 43% 5% .

Continued on next page...

Continued from previous page...

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	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

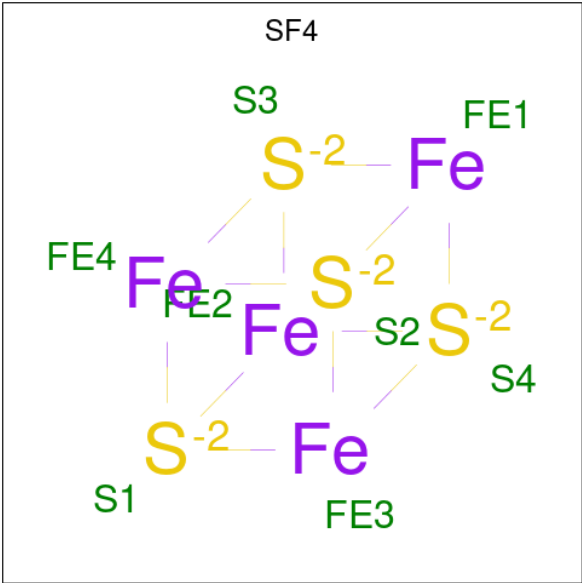
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	3	0
			3349	2158	559	617	15			
2	D	419	Total	C	N	O	S	0	1	0
			3332	2145	556	616	15			
2	F	419	Total	C	N	O	S	0	3	0
			3343	2153	557	618	15			
2	H	420	Total	C	N	O	S	0	0	0
			3330	2143	555	617	15			
2	J	419	Total	C	N	O	S	0	1	0
	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

Continued on next page...

Continued from previous page...

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).



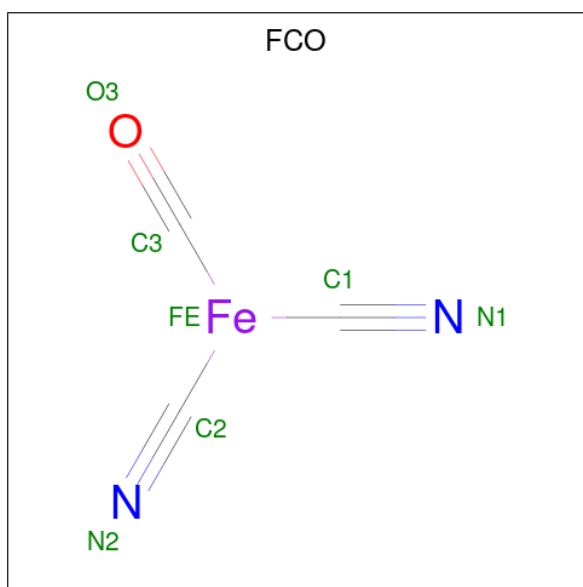
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3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

Continued on next page...

Continued from previous page...

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).

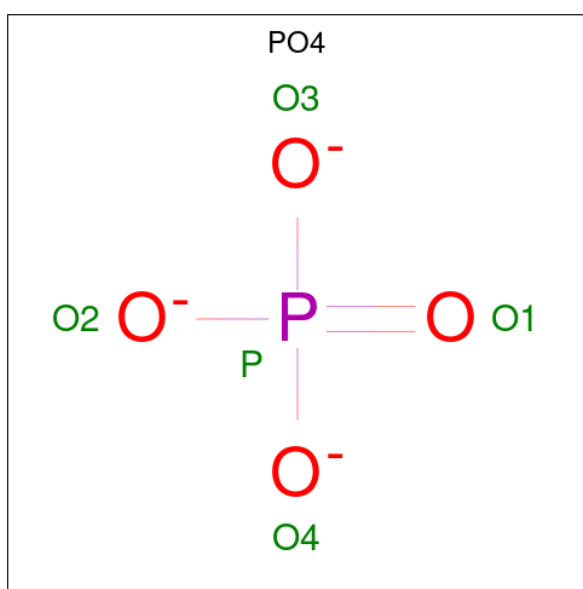
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		
5	F	1	Total	Ni	0	0
			1	1		
5	H	1	Total	Ni	0	0
			1	1		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

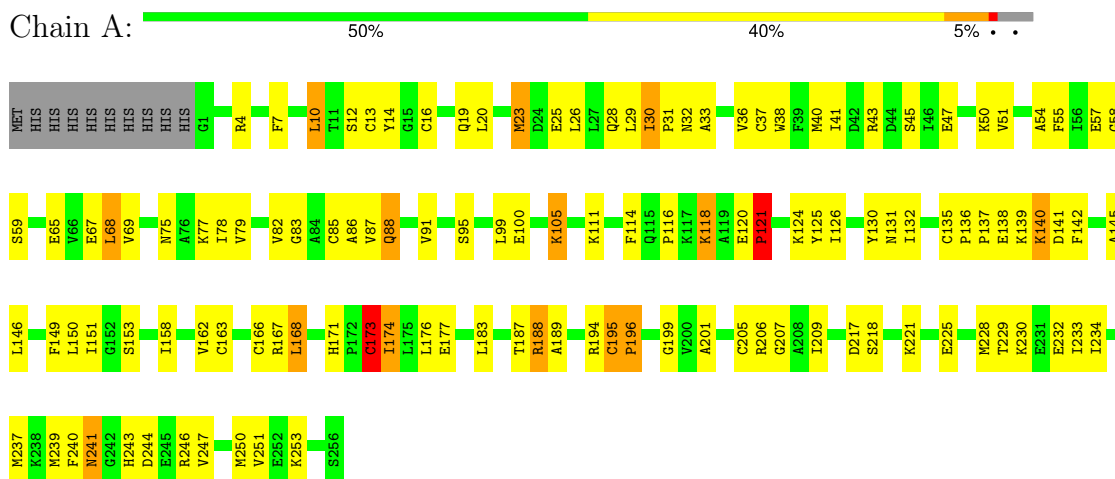
Continued from previous page...

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

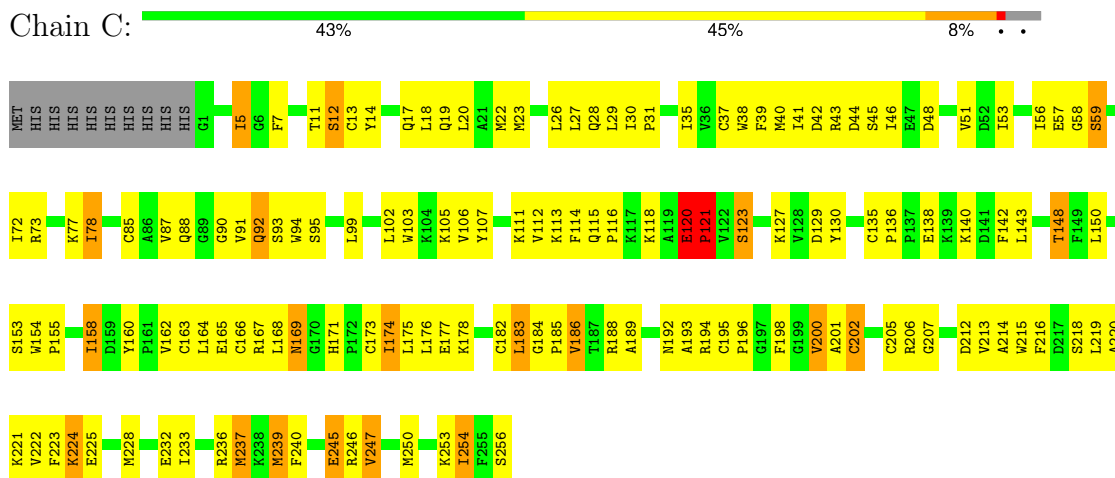
3 Residue-property plots

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

• Molecule 1: Sulfhydrogenase 1 subunit delta

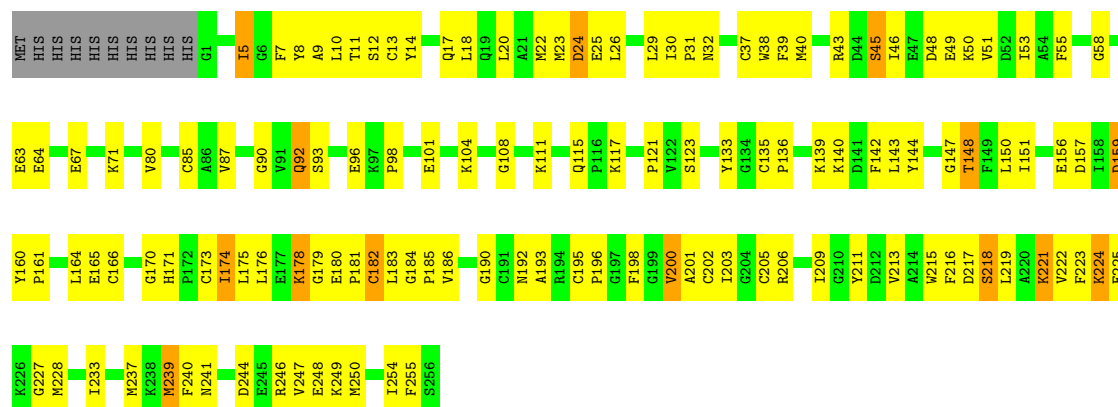


• Molecule 1: Sulfhydrogenase 1 subunit delta

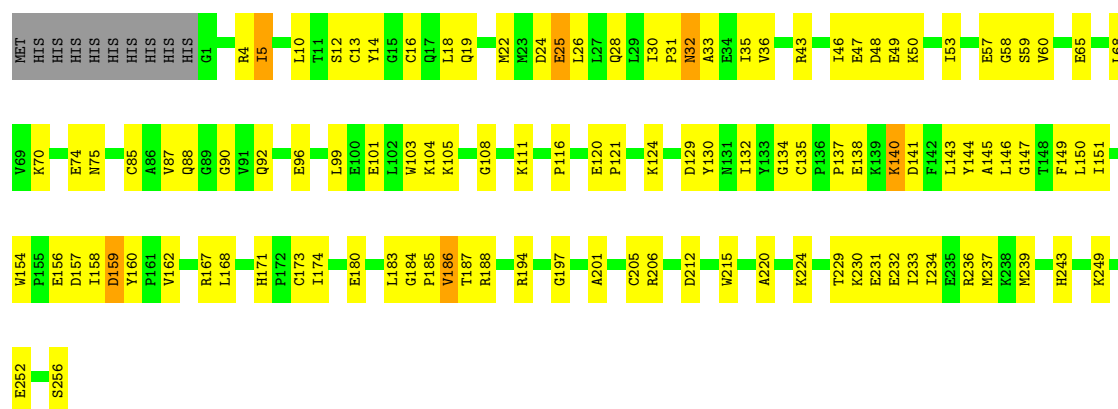


• Molecule 1: Sulfhydrogenase 1 subunit delta

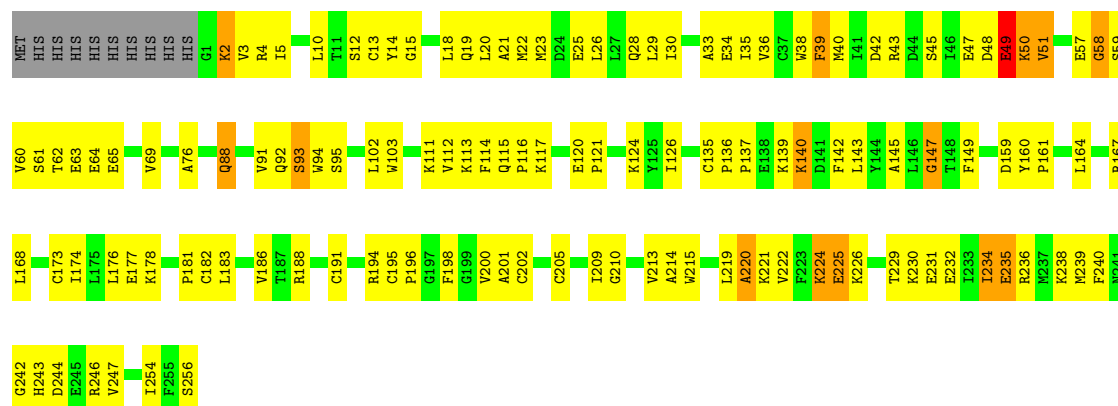




- Molecule 1: Sulfhydrogenase 1 subunit delta

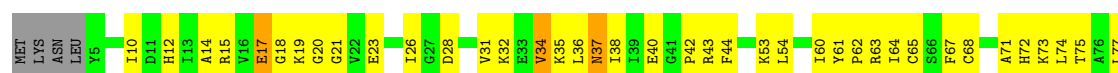


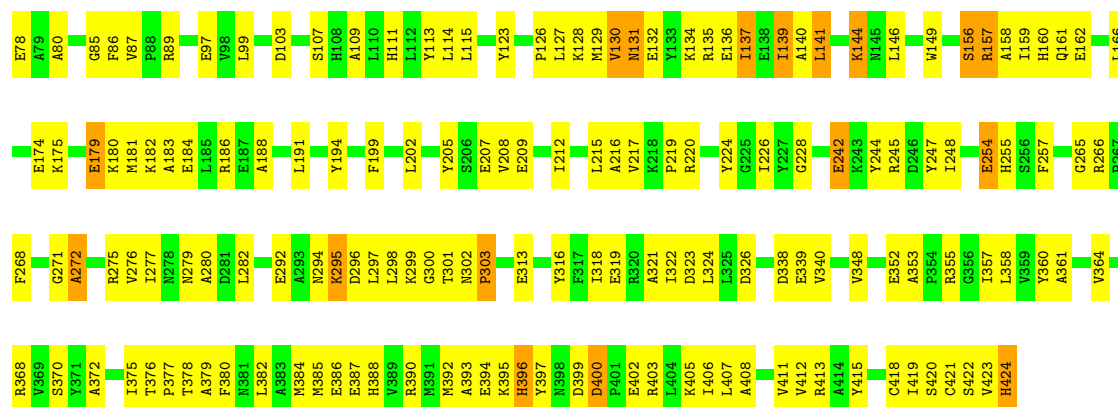
- Molecule 1: Sulphydrogenase 1 subunit delta



- Molecule 1: Sulphydrogenase 1 subunit delta

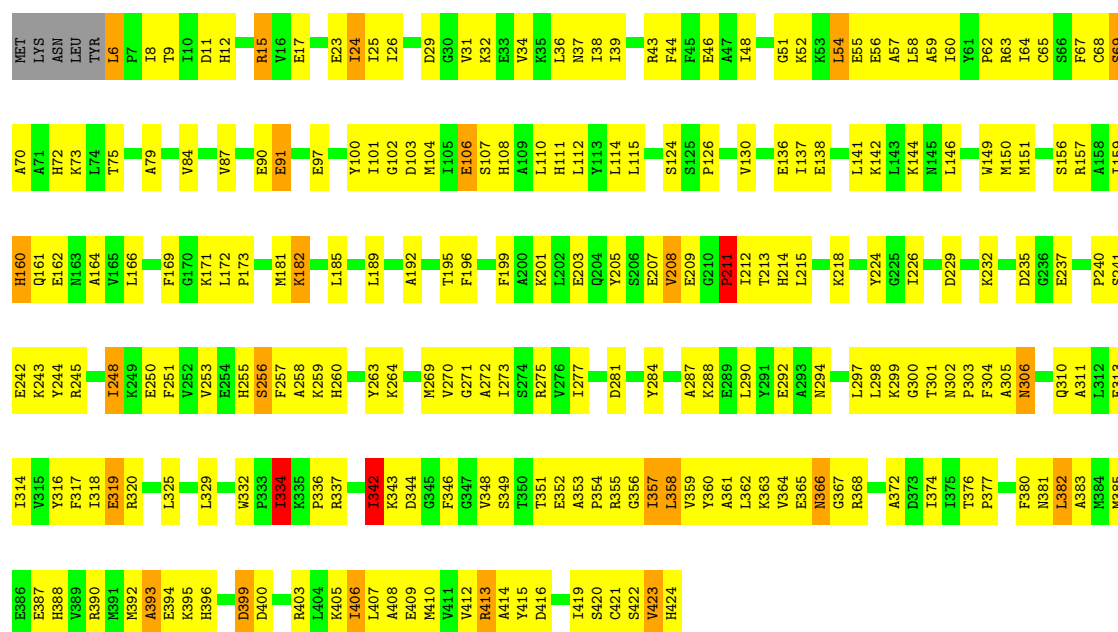






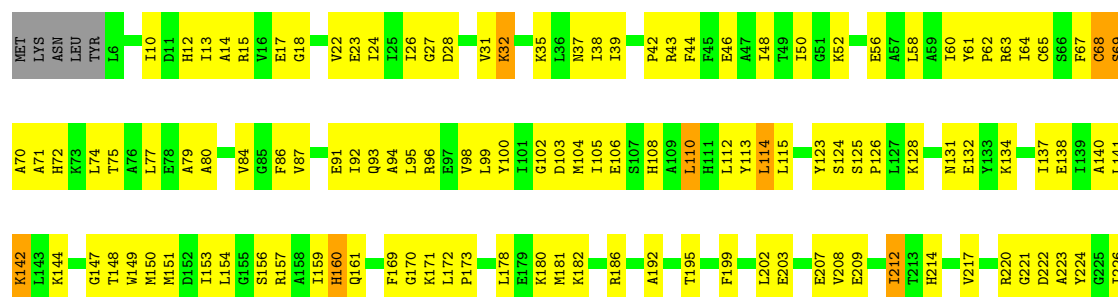
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain D: 44% 48% 5% ..



• Molecule 2: Sulfhydrogenase 1 subunit alpha

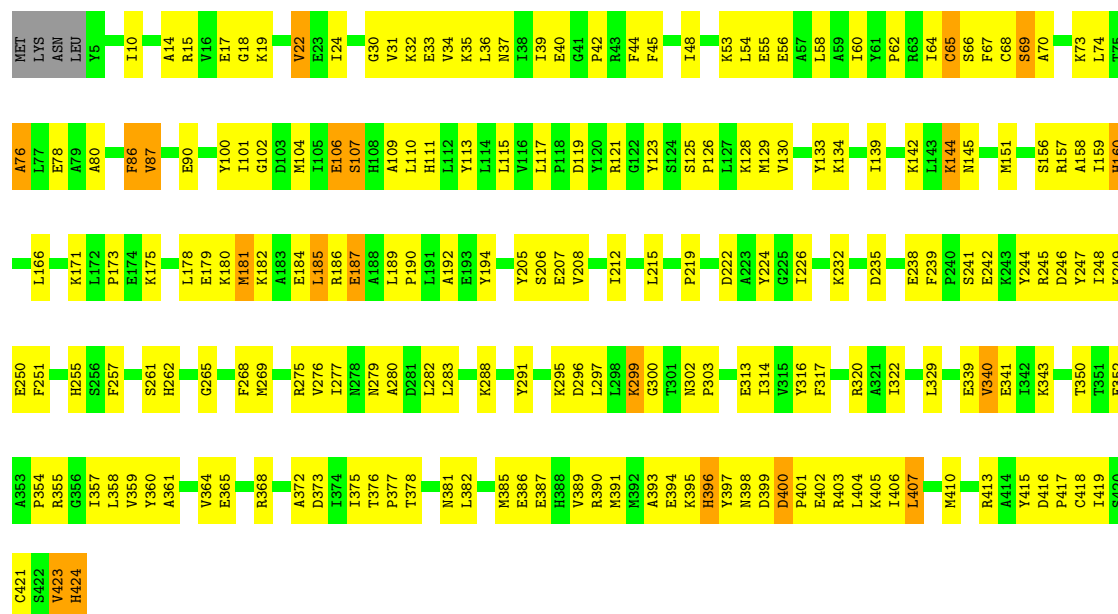
Chain F: 45% 50% ..





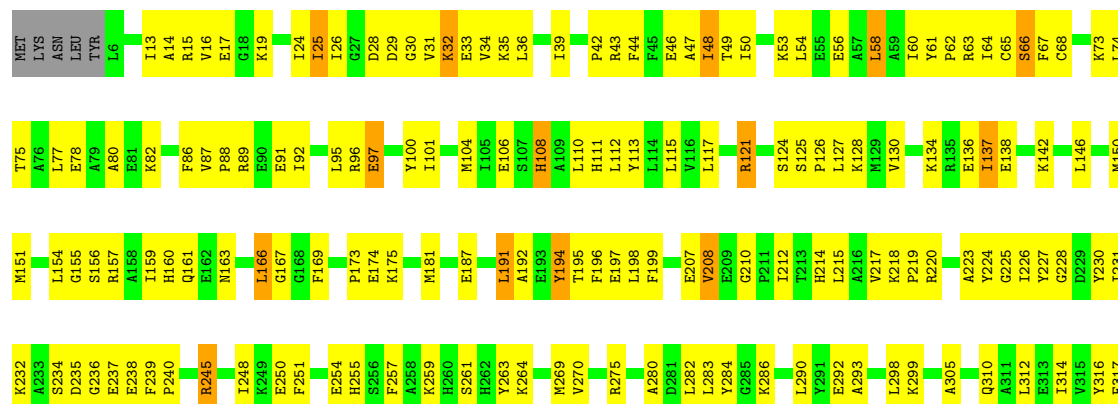
• Molecule 2: Sulfhydrogenase 1 subunit alpha

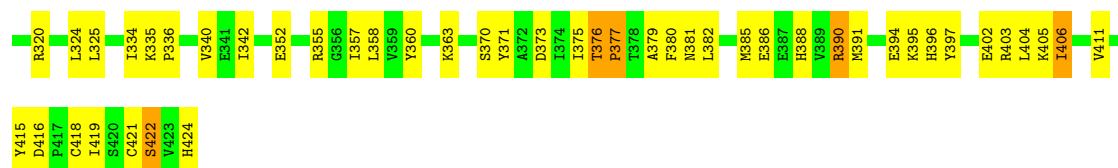
Chain H: 51% 43% 5%



• Molecule 2: Sulfhydrogenase 1 subunit alpha

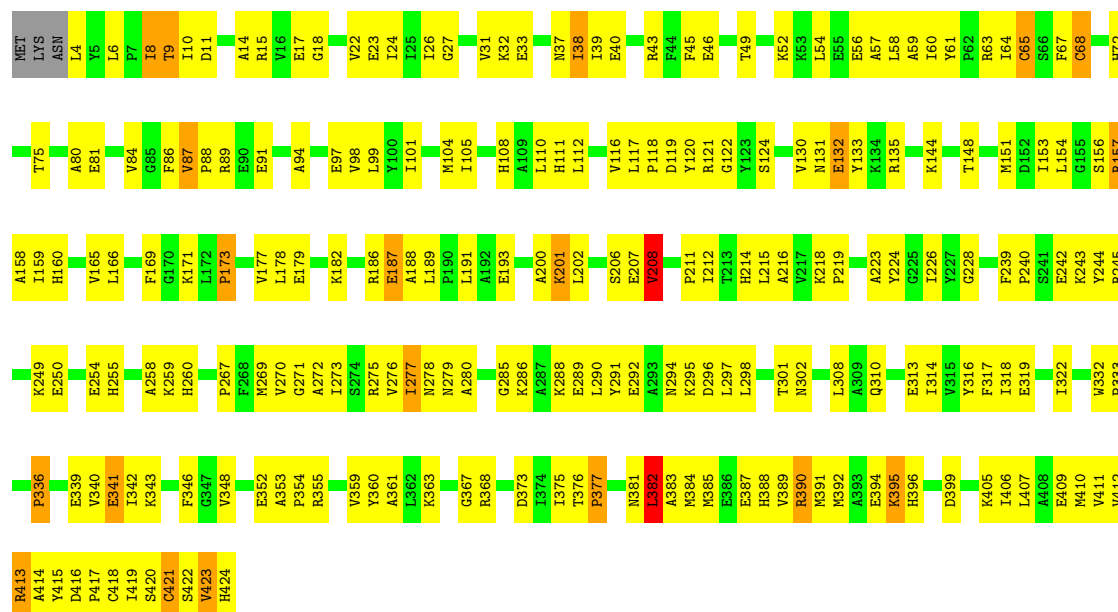
Chain J: 50% 45% 5%





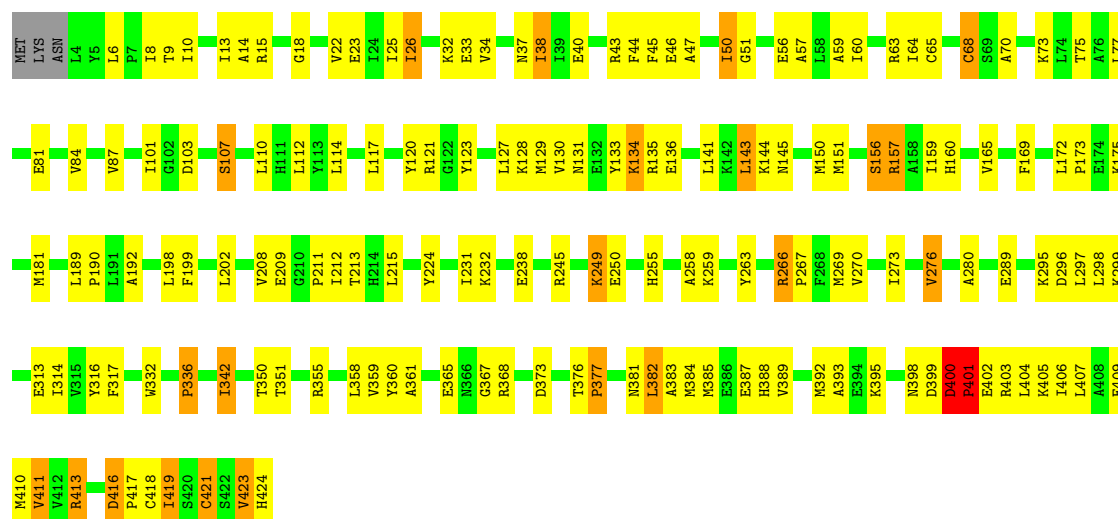
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain L: 47% 47% 5% •



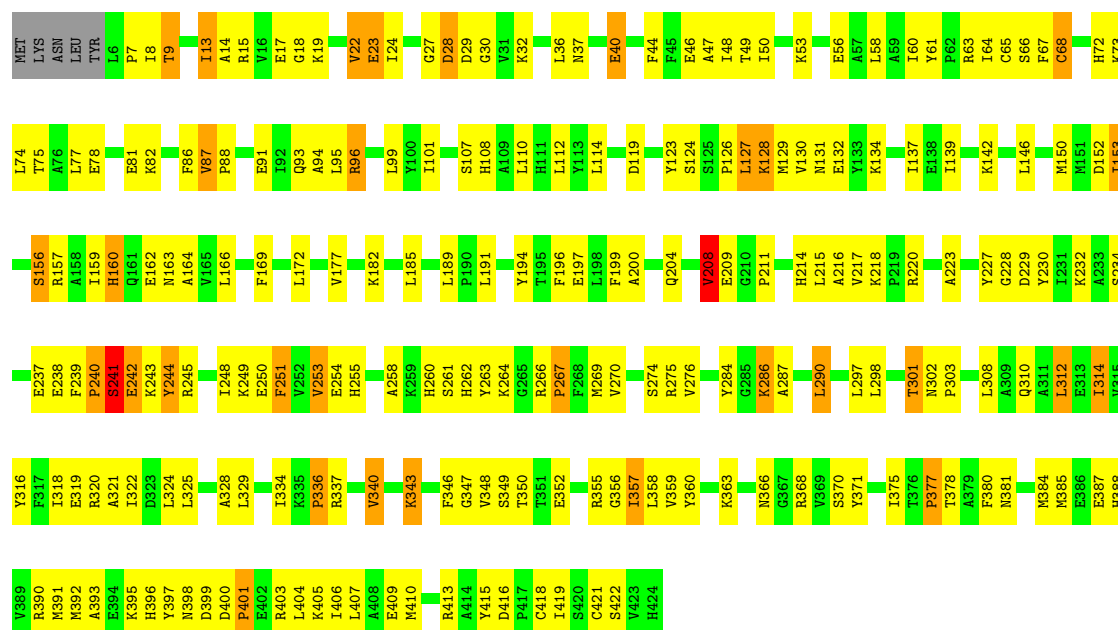
• Molecule 2: Sulfhydrogenase 1 subunit alpha

Chain N: 61% 33% 5% •



• Molecule 2: Sulfhydrogenase 1 subunit alpha

Category	Percentage
Very bad	46%
Bad	45%
Good	7%



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: SF4, PO4, FCO, NI, MG

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

Continued on next page...

Continued from previous page...

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	147	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	106	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	207	0
2	N	3342	0	3363	145	0
2	P	3325	0	3352	206	0
3	A	24	0	0	6	0
3	C	24	0	0	12	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	16	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

Continued on next page...

Continued from previous page...

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	18	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:P:65:CYS:SG	2:P:68:CYS:SG	2.38	1.21
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:L:65:CYS:SG	2:L:68:CYS:SG	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N:65:CYS:SG	2:N:68:CYS:SG	2.86	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:166:LEU:HB3	2:L:340:VAL:HG11	1.77	0.66
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: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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	O	501	2,1	0,12,12	-	-	-		
6	PO4	F	504	-	4,4,4	0.86	0	6,6,6	0.43	0
6	PO4	I	504	-	4,4,4	0.98	0	6,6,6	0.89	0
6	PO4	L	503	-	4,4,4	0.81	0	6,6,6	0.67	0
6	PO4	B	504	-	4,4,4	0.68	0	6,6,6	0.58	0
3	SF4	C	503	1	0,12,12	-	-	-		
6	PO4	B	503	-	4,4,4	0.68	0	6,6,6	1.11	0
6	PO4	P	505	-	4,4,4	0.67	0	6,6,6	0.75	0
6	PO4	P	503	-	4,4,4	0.83	0	6,6,6	0.86	0
3	SF4	K	501	1	0,12,12	-	-	-		
4	FCO	J	501	2	3,6,6	0.87	0	-		
3	SF4	G	502	1	0,12,12	-	-	-		
6	PO4	P	504	-	4,4,4	0.82	0	6,6,6	1.02	0
4	FCO	H	501	2	3,6,6	0.86	0	-		
3	SF4	E	502	1	0,12,12	-	-	-		
3	SF4	G	501	1	0,12,12	-	-	-		
3	SF4	I	502	1	0,12,12	-	-	-		
3	SF4	M	503	1	0,12,12	-	-	-		
4	FCO	F	501	2	3,6,6	0.87	0	-		
3	SF4	A	502	1	0,12,12	-	-	-		
3	SF4	E	501	2,1	0,12,12	-	-	-		
3	SF4	A	501	1	0,12,12	-	-	-		
3	SF4	C	502	1	0,12,12	-	-	-		
3	SF4	I	501	1	0,12,12	-	-	-		
4	FCO	N	501	2	3,6,6	0.88	0	-		
4	FCO	B	501	2	3,6,6	0.79	0	-		
3	SF4	C	501	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FCO	D	501	2	3,6,6	0.84	0	-		
6	PO4	F	503	-	4,4,4	0.86	0	6,6,6	0.62	0
3	SF4	M	502	1	0,12,12	-	-	-		
3	SF4	O	503	1	0,12,12	-	-	-		
3	SF4	O	502	1	0,12,12	-	-	-		
3	SF4	E	503	1	0,12,12	-	-	-		
3	SF4	M	501	1	0,12,12	-	-	-		
3	SF4	K	503	1	0,12,12	-	-	-		
4	FCO	L	501	2	3,6,6	0.86	0	-		
3	SF4	A	503	1	0,12,12	-	-	-		
3	SF4	I	503	1	0,12,12	-	-	-		
4	FCO	P	501	2	3,6,6	0.83	0	-		
6	PO4	J	503	-	4,4,4	0.92	0	6,6,6	0.79	0
3	SF4	G	503	1	0,12,12	-	-	-		
6	PO4	H	503	-	4,4,4	1.05	0	6,6,6	1.01	0
3	SF4	K	502	1	0,12,12	-	-	-		

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	503	1	-	-	0/6/5/5
3	SF4	I	503	1	-	-	0/6/5/5
3	SF4	G	503	1	-	-	0/6/5/5
3	SF4	K	502	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 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	501	SF4	3	0
6	I	504	PO4	1	0
6	L	503	PO4	1	0
3	C	503	SF4	6	0
3	K	501	SF4	8	0
4	J	501	FCO	5	0
6	P	504	PO4	1	0
4	H	501	FCO	5	0
3	E	502	SF4	1	0
3	G	501	SF4	3	0
3	I	502	SF4	1	0
3	M	503	SF4	3	0
4	F	501	FCO	7	0
3	A	502	SF4	1	0
3	E	501	SF4	3	0
3	A	501	SF4	4	0
3	C	502	SF4	2	0
3	I	501	SF4	2	0
4	N	501	FCO	18	0
4	B	501	FCO	5	0
3	C	501	SF4	4	0
4	D	501	FCO	8	0
3	M	502	SF4	2	0
3	E	503	SF4	5	0
3	M	501	SF4	1	0
3	K	503	SF4	6	0
4	L	501	FCO	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	SF4	1	0
4	P	501	FCO	5	0
3	G	503	SF4	3	0
3	K	502	SF4	2	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	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.